

Supporting Information  
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# Investigation on Enantioselective Synthesis of 2,3-Dihydroquinazolinones Using Sc(III)-*inda*-pybox

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## Supporting Information

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**General remarks:** Amino alcohols required for the synthesise of ligands, Anthranilamide and aldehydes were purchased from Aldrich chemicals. *N*-Ph-anthranilamide is purchased from Alfa Aesar. All reactions were carried out in a flame dried flask. Solvents used for reactions and column chromatography were commercial grade and distilled prior to use. Toluene and THF were dried over sodium/ benzophenone, whereas CH<sub>2</sub>Cl<sub>2</sub> and CHCl<sub>3</sub> were dried over CaH<sub>2</sub>. Solvents for HPLC analysis were bought as analytical grade and used without further purification. TLC was performed on pre-coated Merck silica gel aluminium plates with 60F254 indicator, visualised by irradiation with UV light. Column chromatography was performed using silica gel Merck 60-100 mesh. Melting points were determined by open glass capillary method and uncorrected. <sup>1</sup>H-NMR and <sup>13</sup>C-NMR were recorded on a Bruker AV 500 MHz using DMSO-*d*<sub>6</sub> or CDCl<sub>3</sub> as solvent and multiplicity indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), dt (doublet of triplet) bs (broad singlet). Coupling constants *J* are reported in Hz. High resolution mass spectra were obtained by ESI using Waters/Micromass Q-TOF mass spectrometer. IR spectra were recorded on a Perkin Elmer FT/IR-420 spectrometer and are reported in terms of frequency of absorption (cm<sup>-1</sup>). The enantiomeric excesses were obtained by HPLC analysis on a chiral stationary phase column (CHIRALPAK AD-H; AS-H, and CHIRAL CEL OD-H). Optical rotation was recorded on a Jasco DIP polarimeter at a wavelength of 589 nm.

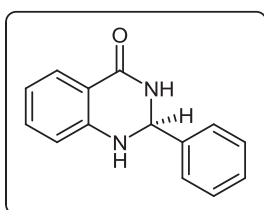
**General procedure for the enantioselective synthesis of 2-alkyl and 2-aryl-2,3-dihydroquinazolinones.**

In an oven dried flask pybox ligand **10** (7.5 μmol) and Sc(OTf)<sub>3</sub> (3 μmol) were taken in 1 mL of anhydrous dichloromethane. 50mg of 4Å molecular sieves was added to the solution and the resulting mixture was stirred further. After 3 h, Anthranilamide (**1a**) (300 μmol) solubilized in 1 mL of dichloromethane was added at the indicated temperature, followed by aldehyde (360 μmol) and stirred until the reaction was completed. Completion of the reaction was ascertained by TLC, and the product was purified by using a small pad of silica gel 60-100 mesh with an eluent of (PE\EA, 1:1) to afford dihydroquinazolinones as colourless solids.

**General procedure for the enantioselective synthesis of *N*-Ph-2-aryl-2,3-dihydroquinazolinones.**

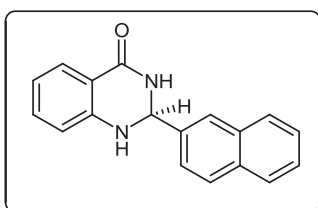
In an oven dried flask pybox ligand **10** (30  $\mu\text{mol}$ ) and  $\text{Sc}(\text{OTf})_3$  (15  $\mu\text{mol}$ ) were taken in 1 mL of anhydrous dichloromethane. 50mg of 4Å molecular sieves was added to the solution and the resulting mixture was stirred further. After 3 h, *N*-Ph-anthranilamide (**1c**) (300  $\mu\text{mol}$ ) solubilized in 1 mL of dichloromethane was added at the indicated temperature, followed by aldehyde (360  $\mu\text{mol}$ ) and stirred until the reaction was completed. Completion of the reaction was ascertained by TLC, and the product was purified by using a small pad of silica gel 60-100 mesh with an eluent of (PE\EA, 3:1) to afford corresponding 2,3-diaryl-2,3-dihydroquinazolinones as colourless solids.

**(S)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3a)**<sup>1</sup>



Colorless solid, **Isolated yield (63mg, 94%), Mp:** 218 °C,  $R_f = 0.4$  (PE/EA, 1:1); **<sup>1</sup>H NMR** (500 MHz, DMSO- $d_6$ ):  $\delta = 8.29$  (bs, 1H), 7.63 (dd,  $J = 7.8$  and 1.5 Hz, 1H), 7.51 – 7.40 (m, 2H), 7.44 – 7.30 (m, 3H), 7.28 – 7.17 (m, 1H), 7.11 (bs, 1H), 6.77 (d,  $J = 8$  Hz, 1H), 6.68 (m, 1H), 5.75 (t,  $J = 1.5$  Hz, 1H); **<sup>13</sup>C NMR** (125 MHz, DMSO- $d_6$ ):  $\delta = 164.04, 148.32, 142.10, 133.79, 128.90, 128.79, 127.82, 127.31, 117.59, 115.41, 114.87, 67.03$ ; **FTIR** (KBr): 3303, 3186, 3062, 1652, 1613, 1511, 1391, 1300, 1148, 809, 748, 699  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +214.1^\circ$  ( $c = 1.0$  in THF, e.r. 99 : 1); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_R = 15.27$  min, major enantiomer:  $t_R = 12.40$  min.

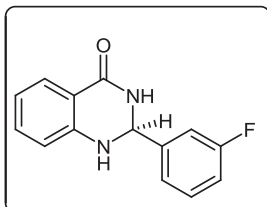
**(S)-2-(naphthalen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (3b)**<sup>1</sup>



Colorless solid, **Isolated yield (75mg, 92%), Mp:** 216 °C,  $R_f = 0.45$  (PE/EA, 1:1); **<sup>1</sup>H NMR** (500 MHz, DMSO- $d_6$ ):  $\delta = 8.37$  (bs, 1H), 7.96 – 7.92 (m, 4H), 7.70 (d,  $J = 7.5$  Hz, 1H), 7.64 (d,  $J = 7.5$  Hz, 1H), 7.55 – 7.53 (m, 2H), 7.25 (t,  $J = 8$  Hz, 1H), 7.19 (bs, 1H), 6.73 (d,  $J = 8$  Hz, 1H), 6.69 (t,  $J = 7.5$  Hz, 1H), 5.96 (bs, 1H); **<sup>13</sup>C NMR** (125 MHz, DMSO- $d_6$ ):  $\delta = 164.05, 148.35, 139.34, 133.81, 133.47, 132.94, 128.58, 128.44,$

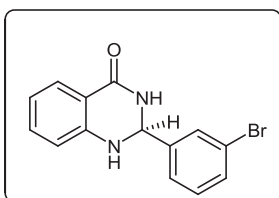
128.04, 127.84, 126.89, 126.84, 126.32, 125.31, 117.64, 115.42, 114.488, 67.30; **FTIR** (KBr): 3447, 3281, 3187, 3052, 1660, 1610, 1513, 1387, 1297, 1157, 809, 744, 689  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +193.0^{\circ}$  ( $c = 0.75$  in THF, e.r. 99 : 1); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 21.46$  min, major enantiomer:  $t_{\text{R}} = 19.14$  min.

**(S)-2-(3-fluorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3c)<sup>1</sup>**



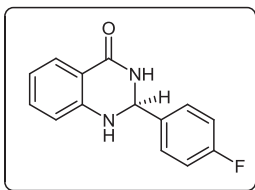
Colorless solid, **Isolated yield (66mg, 91%), Mp:** 174 °C,  $R_f = 0.4$  (PE/EA, 1:1); **<sup>1</sup>H NMR** (500 MHz, DMSO- $d_6$ ):  $\delta = 8.40$  (bs, 1H), 7.63-7.61 (dd,  $J = 7.5, 1.5$  Hz, 1H), 7.46 – 7.41 (m, 1H), 7.34 (d,  $J = 8$ Hz, 1H), 7.31 (dt,  $J = 10, 2.5$ Hz, 1H), 7.26 (m, 1H), 6.78 (d,  $J = 8$ Hz, 1H), 6.70 – 6.67 (m, 1H), 5.79 (bs, 1H); **<sup>13</sup>C NMR** (125 MHz, DMSO- $d_6$ ):  $\delta = 163.91, 162.52$  (d,  $J = 242.37$  Hz), 148.01, 145.29 (d,  $J = 6.25$  Hz), 133.89, 130.25 (d,  $J = 8$  Hz), 127.82, 123.24 (d,  $J = 2.5$ Hz), 117.16, 115.12, 114.84, 114.34, 114.04 (d,  $J = 21.87$  Hz), 66.08 (d,  $J = 1.12$ Hz); **FTIR** (KBr): 3421, 3212, 3075, 2629, 1676, 1607, 1523, 1424, 1208, 1121, 837, 799, 744, 720, 598;  $[\alpha]_{\text{D}}^{25} = +173.4^{\circ}$  ( $c = 1.0$  in THF, e.r. 99 : 1); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 19.00$  min, major enantiomer:  $t_{\text{R}} = 13.19$  min.

**(S)-2-(3-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3d)<sup>1</sup>**



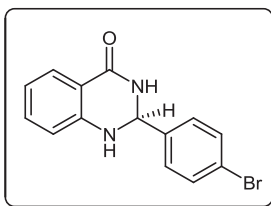
Colorless solid, **Isolated yield (84mg, 94%), Mp:** 187 °C,  $R_f = 0.5$  (PE/EA, 1:1); **<sup>1</sup>H NMR** (500 MHz, DMSO- $d_6$ ):  $\delta = 8.40$  (bs, 1H), 7.68 (t,  $J = 1.8$  Hz, 1H), 7.62-7.60 (dd,  $J = 7.5$  and 1.5 Hz, 1H), 7.55-7.53 (m, 1H), 7.50-7.48 (m, 1H), 7.36 (t,  $J = 7.5$ Hz), 7.28-7.24 (m, 1H), 7.22 (bs, 1H), 6.76 (d,  $J = 7.5$  Hz, 1H), 6.70 – 6.67 (m, 1H), 5.79 (t,  $J = 2$ Hz, 1H); **<sup>13</sup>C NMR** (125 MHz, DMSO- $d_6$ ):  $\delta = 163.87, 147.95, 145.01, 133.93, 131.63, 131.05, 130.11, 127.83, 126.25, 122.06, 117.79, 115.36, 114.94, 65.99$ ; **FTIR** (KBr): 3289, 3198, 3062, 1645, 1613, 1515, 1429, 1299, 1157, 865, 791, 757, 698  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +115.3^{\circ}$  ( $c = 1.0$  in THF, e.r. 90 : 10); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 21.12$  min, major enantiomer:  $t_{\text{R}} = 17.82$  min.

**(S)-2-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3e)<sup>1</sup>**



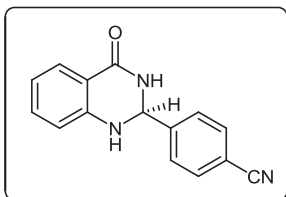
Colorless solid, **Isolated yield (67mg, 92%), Mp:** 201 °C,  $R_f$  = 0.4 (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta$  = 8.30 (s, 1 H), 7.61 (d,  $J$  = 7.2 Hz, 1 H), 7.54 (dd,  $J$  = 5.6, 8.4 Hz, 2 H), 7.21 – 7.27 (m, 3 H), 7.11 (s, 1 H), 6.75 (d,  $J$  = 8.0 Hz, 1 H), 6.68 (t,  $J$  = 7.2 Hz, 1 H), 5.78 (s, 1 H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta$  = 164.04, 162.58 (d,  $J$  = 243.75 Hz), 148.27, 138.27, 133.83, 129.5 (d,  $J$  = 8.75 Hz), 127.83, 117.72, 115.53 (d,  $J$  = 21.25 Hz), 115.42, 115.17, 66.41; **FTIR** (KBr): 3414, 3300, 3184, 3067, 2935, 1651, 1614, 1486, 1389, 1232, 1157, 841, 757, 673  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25}$  = +158.7° (c = 1.0 in THF, e.r. 95 : 5); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_R$  = 17.57 min, major enantiomer:  $t_R$  = 12.30 min.

**(S)-2-(4-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3f)<sup>1</sup>**



Colorless solid, **Isolated yield (81mg, 90%), Mp:** 207 °C,  $R_f$  = 0.5 (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta$  = 8.32 (s, 1 H), 7.61 – 7.59 (m, 3 H), 7.51 (d,  $J$  = 8.4 Hz, 2 H), 7.23 – 7.27 (m, 1 H), 7.16 (s, 1 H), 6.74 (d,  $J$  = 8.4 Hz, 1 H), 6.68 (t,  $J$  = 7.6 Hz, 1 H), 5.76 (s, 1H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta$  = 163.93, 148.07, 141.58, 133.86, 131.69, 129.53, 127.83, 122.02, 117.76, 115.41, 114.49, 62.27; **FTIR** (KBr): 3446, 3308, 3190, 3064, 2936, 1654, 1608, 1484, 1384, 1152, 834, 795, 752, 678  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25}$  = +146.9° (c = 0.5 in THF, e.r. 97 : 3); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_R$  = 17.80 min, major enantiomer:  $t_R$  = 12.21 min.

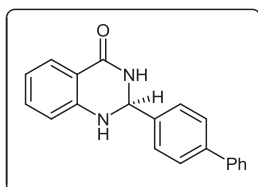
**(S)-4-(4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzonitrile (3g)<sup>1</sup>**



Colorless solid, **Isolated yield (66mg, 88%), Mp:** 254 °C,  $R_f$  = 0.35 (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta$  = 8.47 (s, 1H), 7.75 (d,  $J$  = 8 Hz, 2H), 7.66 (d,  $J$  = 8 Hz, 2H), 7.60 (d,  $J$  = 7.5 Hz, 1H), 7.29-7.24

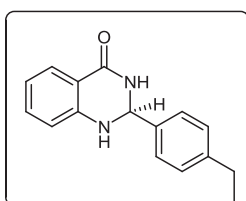
(m, 2H), 6.76 (d,  $J = 7$  Hz, 1H), 6.69 (t,  $J = 7.5$  Hz, 1H), 5.85 (s, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ):  $\delta = 163.77, 147.83, 147.78, 134.00, 133.00, 132.87, 128.14, 127.85, 119.11, 117.88, 115.36, 114.97, 111.51, 65.97$ ; FTIR (KBr): 3452, 3353, 3335, 2227, 1666, 1611, 1486, 1374, 1150, 838, 799, 772, 617  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +174.08^\circ$  ( $c = 0.5$  in THF, e.r. 97 : 3); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_R = 18.52$  min, major enantiomer:  $t_R = 14.77$  min.

**(S)-2-(Biphenyl-4-yl)-2,3-dihydroquinazolin-4(1H)-one (3h)<sup>1</sup>**



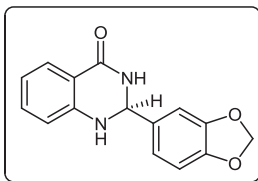
Colorless solid, **Isolated yield (85mg, 95%), Mp:** 225 °C,  $R_f = 0.5$  (PE/EA, 1:1);  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ):  $\delta = 8.35$  (bs, 1H), 7.70 – 7.58 (m, 7H), 7.48 – 7.45 (m, 2H), 7.39 – 7.36 (m, 1H), 7.28 – 7.25 (m, 1H), 7.18 (bs, 1H), 6.78 (d,  $J = 8$  Hz, 1H), 6.71 – 6.68 (m, 1H), 5.81 (bs, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ):  $\delta = 164.10, 148.30, 141.32, 140.81, 140.19, 133.83, 129.43, 128.04, 127.92, 127.87, 127.17, 127.12, 117.63, 115.46, 114.92, 66.69$ ; FTIR (KBr): 3290, 3183, 3057, 1652, 1611, 1508, 1386, 1297, 1153, 750, 689  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +158.0^\circ$  ( $c = 1.0$  in THF, e.r. 98 : 2); HPLC conditions: AS-H column, *n*-hexane/2-propanol = 70/30, flow rate = 0.6  $\text{mL min}^{-1}$ , minor enantiomer:  $t_R = 33.58$  min, major enantiomer:  $t_R = 43.41$  min.

**(S)-2-(4-ethylphenyl)-2,3-dihydroquinazolin-4(1H)-one (3i)<sup>1</sup>**



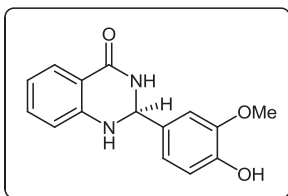
Colorless solid, **Isolated yield (68mg, 91%), Mp:** 197 °C,  $R_f = 0.45$  (PE/EA, 1:1);  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ):  $\delta = 8.26$  (s, 1H), 7.61 (d,  $J = 8$  Hz, 1H), 7.40 (d,  $J = 8$  Hz, 2H), 7.24 – 7.22 (m, 3H), 7.056 (bs, 1H), 6.74 (d,  $J = 8.0$  Hz, 1H), 6.66 (t,  $J = 8\text{Hz}$ , 1H), 5.72 (s, 1H), 2.06 (q,  $J = 7.5$  Hz, 2H), 1.16 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ):  $\delta = 164.19, 148.36, 144.68, 139.51, 133.83, 128.35, 127.74, 127.29, 117.57, 115.33, 114.84, 67.11, 28.37, 16.12$ ; FTIR (KBr): 3446, 3302, 3192, 3060, 1655, 1612, 1512, 1388, 1297, 1157, 809, 744, 689  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +185.4^\circ$  ( $c = 1.0$  in THF, e.r. 93 : 7); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_R = 14.23$  min, major enantiomer:  $t_R = 12.02$  min.

**(S)-2-(Benzo[d][1,3]dioxol-5-yl)-2,3-dihydroquinazolin-4(1H)-one (3j)<sup>1</sup>**



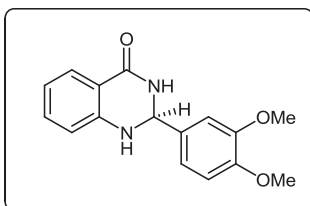
Colorless solid, **Isolated yield (77mg, 95%), Mp:** 204 °C,  $R_f = 0.35$  (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta = 8.24$  (bs, 1H), 7.52 (d,  $J = 7.5$  Hz, 1H), 7.25 (t,  $J = 7.3$  Hz, 1H), 7.11 – 7.03 (m, 2H), 7.01 – 6.87 (m, 2H), 6.81 – 6.61 (m, 2H), 6.02 (bs, 2H), 5.68 (bs, 1H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta = 163.55$ , 147.80, 147.27, 147.19, 135.55, 133.27, 127.31, 120.40, 117.12, 114.94, 114.40, 107.84, 107.15, 101.09, 66.25; **FTIR** (KBr): 3282, 3186, 3127, 2903, 1653, 1611, 1486, 1445, 1383, 1248, 1036, 755  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +170.2^\circ$  (c = 1.0 in THF, e.r. 95 : 5); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 70/30, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_R = 16.66$  min, major enantiomer:  $t_R = 15.05$  min.

**(S)-2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3k)<sup>1</sup>**



Colorless solid, **Isolated yield (73mg, 90%), Mp:** 217 °C,  $R_f = 0.25$  (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta = 9.15$  (bs, 1H), 8.09 (bs, 1H), 7.62 3 (d,  $J = 7.5$  Hz, 1H), 7.24 (t,  $J = 7.5$  Hz, 1H), 7.09 (bs, 1H), 6.95 (s, 1H), 6.89 (d,  $J = 7.5$  Hz, 1H), 6.77 – 6.74 (m, 2H), 6.82 (t,  $J = 7.5$  Hz, 1H), 5.66 (bs, 1H), 3.77 (s, 3H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta = 164.23$ , 148.64, 147.87, 147.62, 133.57, 132.36, 127.87, 120.16, 117.55, 115.53, 115.37, 114.69, 111.47, 67.37, 55.93; **FTIR** (KBr): 3388, 3354, 3058, 2969, 2935, 2841, 1646, 1610, 1499, 1427, 1357, 1270, 1125, 1021, 766  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +159.2^\circ$  (c = 1.0 in THF, e.r. 95 : 5); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_R = 21.58$  min, major enantiomer:  $t_R = 26.49$  min.

**(S)-2-(3,4-Dimethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3l)<sup>1</sup>**

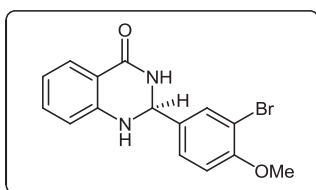


Colorless solid, **Isolated yield (81mg, 95%), Mp:** 214 °C,  $R_f = 0.35$  (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta = 8.17$  (bs, 1H), 7.62 (dd,  $J = 7.8$  and 1.5 Hz, 1H), 7.30 – 7.19 (m, 1H), 7.13 (d,  $J = 1.8$



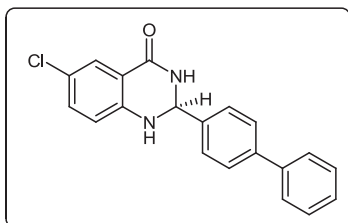
Hz, 1H), 7.06 – 6.89 (m, 3H), 6.76 (d,  $J = 7.8$  Hz, 1H), 6.72 – 6.63 (m, 1H), 5.70 (bs, 1H), 3.80 – 3.71 (2 x s, 6H);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 164.19, 149.48, 149.07, 148.51, 134.10, 133.69, 127.80, 119.67, 117.60, 114.90, 114.90, 111.80, 111.13, 66.98, 56.07, 55.96$ ; FTIR (KBr): 3356, 3332, 2967, 2835, 1669, 1609, 1496, 1414, 1364, 1270, 1227, 1144, 1014, 769  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +151.2^\circ$  ( $c = 1.0$  in THF, e.r. 95 : 5); HPLC conditions: AS-H column, *n*-hexane/2-propanol = 50/50, flow rate = 0.6 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 20.79$  min, major enantiomer:  $t_{\text{R}} = 34.54$  min.

**(S)-2-(3-Bromo-4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3m)<sup>1</sup>**



Colorless solid, **Isolated yield (93mg, 93%), Mp:** 226 °C,  $R_f = 0.45$  (PE/EA, 1:1);  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 8.29$  (bs, 1H), 7.69 (d,  $J = 2.0$  Hz, 1H), 7.61 (dd,  $J = 7.8$  and 1.5 Hz, 1H), 7.42 (dd,  $J = 8.5$  and 2.3 Hz, 1H), 7.32 – 7.20 (m, 1H), 7.18 – 7.04 (m, 2H), 6.82 – 6.58 (m, 2H), 5.73 (bs, 1H), 3.84 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 163.40, 155.27, 147.54, 135.25, 133.23, 131.26, 127.30, 127.22, 117.13, 114.85, 114.35, 112.25, 110.20, 65.21, 56.21$ ; FTIR (KBr): 3281, 3180, 2836, 1644, 1612, 1496, 1438, 1386, 1298, 1266, 1158, 1054, 890, 808, 747, 675, 623  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +136.41^\circ$  ( $c = 0.75$  in THF, e.r. 96 : 4); HPLC conditions: AS-H column, *n*-hexane/2-propanol = 50/50, flow rate = 0.6 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 27.45$  min, major enantiomer:  $t_{\text{R}} = 20.60$  min.

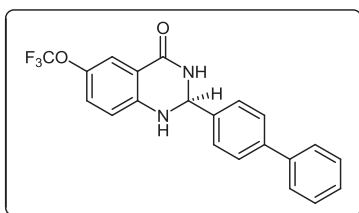
**(S)-2-(biphenyl-4-yl)-6-chloro-2,3-dihydroquinazolin-4(1H)-one (3n)<sup>1</sup>**



Colorless solid, **Isolated yield (104mg, 95%), Mp:** 245 °C,  $R_f = 0.5$  (PE/EA, 1:1);  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 8.6$  (bs, 1H), 7.71 – 7.65 (m, 4H), 7.58 – 7.57 (m, 3H), 7.48 – 7.45 (m, 2H), 7.41 (bs, 1H), 7.39–7.36 (m, 1H), 7.31–7.29 (dd,  $J = 7.5$  and 2.5 Hz, 1H), 6.81 (d,  $J = 9$  Hz, 1H), 5.85 (bs, 1H);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 162.91, 147.02, 140.95, 140.92, 140.14, 133.60, 129.43, 128.07, 127.88, 127.19, 127.18, 126.92, 121.25, 116.93, 116.55, 66.55$ ; FTIR (KBr): 3435, 3272, 3177, 3057, 1647, 1611, 1513, 1388, 1299, 1153, 805, 755, 664  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +168.6^\circ$  ( $c = 1.0$  in THF, e.r. 98 : 2); HPLC conditions: AD-H column, *n*-hexane/2-

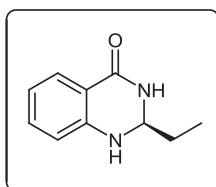
propanol = 80/20, flow rate = 0.8 mL min<sup>-1</sup>, minor enantiomer: t<sub>R</sub> = 11.41 min, major enantiomer: t<sub>R</sub> = 12.91 min.

**(S)-2-(biphenyl-4-yl)-6-(trifluoromethoxy)-2,3-dihydroquinazolin-4(1H)-one (3o)**<sup>1</sup>



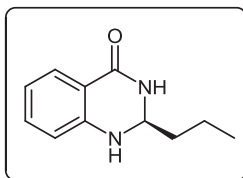
Colorless solid, **Isolated yield (90mg, 95%), Mp:** 209 °C, *R<sub>f</sub>* = 0.5 (PE/EA, 1:1); <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ = 8.6 (bs, 1H), 7.72 – 7.70 (d, *J* = 8.5 Hz 2H), 7.68 – 7.66 (d, *J* = 7.5 Hz 2H), 7.59 – 7.58 (d, *J* = 8 Hz 2H), 7.52 (s, 1H), 7.49-7.45 (m, 3H), 7.39 – 7.36 (t, *J* = 7.5 Hz, 1H), 7.30 - 7.28 (dd, *J* = 7.5 and 2.5 Hz, 1H), 6.88 – 6.86 (d, *J* = 9 Hz 1H), 5.89 (bs, 1H); <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>): δ = 162.92, 147.33, 141.00, 140.82, 140.13, 139.72, 129.43, 128.08, 127.91, 127.40, 127.21, 127.18, 123.81, 121.78, 120.01, 119.76, 116.41, 115.55, 66.60; **FTIR** (KBr): 3547, 3468, 3414, 3187, 3120, 3087, 1672, 1601, 1553, 1485, 1348, 1264, 1175, 842, 733, 693 cm<sup>-1</sup>; [α]<sub>D</sub><sup>25</sup> = +196.04° (c = 1.0 in THF, e.r. 97 : 3); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL min<sup>-1</sup>, minor enantiomer: t<sub>R</sub> = 8.02 min, major enantiomer: t<sub>R</sub> = 9.57 min.

**(S)-2-ethyl-2,3-dihydroquinazolin-4(1H)-one (13a)**



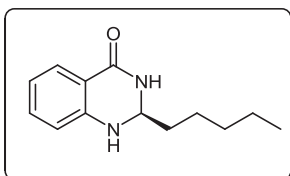
Colorless solid, **Isolated yield (42mg, 80%), Mp:** 148 °C, *R<sub>f</sub>* = 0.3 (PE/EA, 1:1); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.89 (dd, *J* = 8 Hz, 1.5 Hz, 1H), 7.34 – 7.30 (m, 1H), 6.88-6.85 (m, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 6.43 (bs, 1H), 4.88-4.85 (m, 1H), 1.86 – 1.81 (m, 2H), 1.08 (t, *J* = 7.5 Hz, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ = 165.43, 147.44, 133.85, 128.57, 119.34, 115.86, 114.69, 66.43, 28.59, 8.28; HRMS (ESI): *m/z* calculated for C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O [M<sup>+</sup>+Na] 199.0847, found: 119.0845; **FTIR** (KBr): 3294, 3081, 2958, 1654, 1613, 1506, 1385, 1264, 1153, 755, 699 cm<sup>-1</sup>; [α]<sub>D</sub><sup>25</sup> = + 75.2° (c = 1.0 in THF, e.r. 89 : 11); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL min<sup>-1</sup>, minor enantiomer: t<sub>R</sub> = 11.32 min, major enantiomer: t<sub>R</sub> = 9.77 min.

**(S)-2-propyl-2,3-dihydroquinazolin-4(1H)-one (13b)**<sup>1</sup>



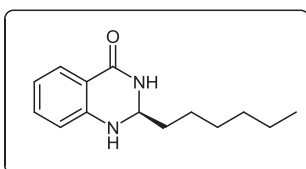
Colorless solid, **Isolated yield (47mg, 82%), Mp:** 151 °C,  $R_f = 0.3$  (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.91 – 7.89 (m, 1H), 7.33 – 7.28 (m, 1H), 6.86 (t,  $J = 7.5$  Hz, 1H), 6.67 (d,  $J = 8.0$  Hz, 1H), 6.56 (bs, 1H), 4.90 (t,  $J = 5.5$  Hz, 1H), 4.26 (bs, 1H), 1.74 – 1.79 (m, 2H), 1.44 – 1.54 (m, 2H), 1.01 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ):  $\delta = 165.39, 147.48, 133.75, 128.55, 119.30, 116.06, 114.73, 65.15, 37.67, 17.40, 13.82$ ; **FTIR** (KBr): 3326, 3165, 3041, 2965, 1642, 1621, 1502, 1384, 1252, 1146, 756, 687  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +84.22^\circ$  ( $c = 1.0$  in THF, e.r. 93 : 7); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 11.14$  min, major enantiomer:  $t_{\text{R}} = 9.47$  min.

**(S)-2-pentyl-2,3-dihydroquinazolin-4(1H)-one (13c)**



Colorless solid, **Isolated yield (52mg, 79%), Mp:** 154 °C,  $R_f = 0.35$  (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.91 (d,  $J = 1.5$ , 1H), 7.35 – 7.28 (m, 1H), 6.90-6.87 (m, 1H), 6.69 (d,  $J = 8.0$  Hz, 1H), 6.16 (bs, 1H), 4.91 (t,  $J = 6$  Hz, 1H), 1.80 – 1.77 (m, 2H), 1.38-1.36 (m, 5H), 0.95-0.92 (m, 4H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ):  $\delta = 165.37, 147.42, 133.89, 128.63, 119.46, 115.91, 114.74, 65.38, 35.59, 31.45, 23.72, 22.49, 13.91$ ; HRMS (ESI):  $m/z$  calculated for  $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}$  [ $\text{M}^+ + \text{Na}$ ] 241.1317, found: 241.1311; **FTIR** (KBr): 3329, 3206, 3069, 2953, 1643, 1614, 1507, 1387, 1261, 1152, 752, 690  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +79.7^\circ$  ( $c = 1.0$  in THF, e.r. 88 : 12); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 90/10, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 23.45$  min, major enantiomer:  $t_{\text{R}} = 20.66$  min.

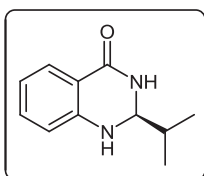
**(S)-2-hexyl-2,3-dihydroquinazolin-4(1H)-one (13d)<sup>1</sup>**



Colorless solid, **Isolated yield (59mg, 84%), Mp:** 158 °C,  $R_f = 0.35$  (PE/EA, 1:1);  $[\alpha]_{\text{D}}^{25}$   $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.91 – 7.89 (dd,  $J = 1.0, 8$  Hz, 1H) 7.34 – 7.31 (m, 1H), 6.89-6.86 (t,  $J = 7.5$  Hz, 1H), 6.69 (d,  $J = 8.0$

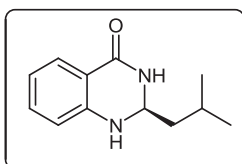
Hz, 1H), 6.22 (bs, 1H), 4.88 (t,  $J = 5.5$  Hz, 1H), 1.81 – 1.77 (m, 2H), 1.49 – 1.45 (m, 2H), 1.37-1.3 (m, 7H), 0.92 (t,  $J = 7$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta = 165.37, 147.42, 133.89, 128.63, 119.48, 115.91, 114.74, 65.38, 35.59, 31.45, 23.72, 22.49, 13.91$ ; FTIR (KBr): 3326, 3215, 3072, 2953, 1644, 1616, 1509, 1388, 1259, 1153, 754, 699  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = + 91.7^\circ$  ( $c = 1.0$  in THF, e.r. 96 : 4); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 90/10, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 15.45$  min, major enantiomer:  $t_{\text{R}} = 13.40$  min.

**(S)-2-isopropyl-2,3-dihydroquinazolin-4(1H)-one (13e)<sup>2</sup>**



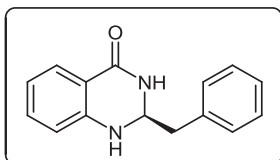
Colorless solid, **Isolated yield (44mg, 78%), Mp:** 170 °C,  $R_f = 0.3$  (PE/EA, 1:1);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.88 (d,  $J = 7.8$  Hz, 1H), 7.30 (t,  $J = 7.7$  Hz, 1H), 6.83 (t,  $J = 7.7$  Hz, 1H), 6.66 (d,  $J = 8.1$  Hz, 1H), 6.01 (s, 1H), 4.70 (d,  $J = 4.8$  Hz, 1H), 1.92-2.01 (m, 1H), 1.06 (t,  $J = 6.8$  Hz, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  165.2, 147.4, 133.9, 128.5, 119.1, 115.5, 114.5, 70.2, 32.8, 17.0, 16.9; FTIR (KBr): 3366, 3171, 3056, 2923, 2851, 1646, 1505, 1396, 1314, 752  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = + 59.2^\circ$  ( $c = 1.0$  in THF, e.r. 82: 18); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 11.53$  min, major enantiomer:  $t_{\text{R}} = 9.30$  min.

**(S)-2-isobutyl-2,3-dihydroquinazolin-4(1H)-one (13f)<sup>2</sup>**



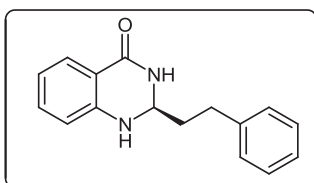
Colorless solid, **Isolated yield (49mg, 81%), Mp:** 176 °C,  $R_f = 0.3$  (PE/EA, 1:1);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.89 (d,  $J = 1.5$  Hz, 1H), 7.33-29 (m, 1H), 6.88-6.85 (t,  $J = 7.5$  Hz, 1H), 6.69 (d,  $J = 8.1$  Hz, 1H), 6.66 (s, 1H), 4.95-4.93 (m, 1H), 1.84-1.81 (m, 1H), 1.67-1.71 (m, 2H), 0.99 (d,  $J = 6.5$  Hz, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  165.51, 147.49, 133.76, 128.56, 119.38, 116.24, 114.88, 63.66, 44.41, 23.86, 22.64, 22.62; FTIR (KBr): 3366, 3171, 3056, 2923, 2851, 1644, 1505, 1396, 1314, 752  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = + 64.22^\circ$  ( $c = 1.0$  in THF, e.r. 83 : 17); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 11.49$  min, major enantiomer:  $t_{\text{R}} = 7.96$  min.

**(S)-2-benzyl-2,3-dihydroquinazolin-4(1H)-one (13g)<sup>4</sup>**



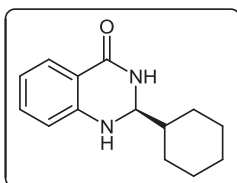
Colorless solid, **Isolated yield (55mg, 77%), Mp:** 189 °C,  $R_f$  = 0.4 (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.38 (t,  $J$  = 7.5 Hz, 2H), 7.29-7.33 (m, 2H), 7.22 (d,  $J$  = 7.1 Hz, 2H), 6.86 (t,  $J$  = 7.5 Hz, 1H), 6.61 (d,  $J$  = 8.0 Hz, 1H), 6.18 (s, 1H), 5.04 (t,  $J$  = 7.0 Hz, 1H), 3.02-3.12 (m, 2H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.8, 17.4, 37.7, 65.1, 114.7, 116.0, 119.4, 128.6, 133.8, 147.4, 165.3; **FTIR** (KBr): 3290, 3162, 3048, 2953, 1657, 1606, 1513, 1390, 1255, 1153, 778, 700  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25}$  = +69.22° (c = 1.0 in THF, e.r. 82 : 18); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_{\text{R}}$  = 28.29 min, major enantiomer:  $t_{\text{R}}$  = 22.34 min.

**(S)-2-phenethyl-2,3-dihydroquinazolin-4(1H)-one (13h)<sup>1</sup>**



Colorless solid, **Isolated yield (66mg, 87%), Mp:** 204 °C,  $R_f$  = 0.4 (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.92 – 7.90 (dd,  $J$  = 7.5 and 1.5 Hz, 1H), 7.35 – 7.24 (m, 6H), 6.87 (t,  $J$  = 7.5 Hz, 1H), 6.60 (d,  $J$  = 7.5 Hz, 1H), 4.94 (t,  $J$  = 5.5 Hz, 1H), 4.18 (bs, 1H), 2.87 – 2.78 (m, 2H), 2.19 – 2.12 (m, 2H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.86, 146.89, 134.66, 134.19, 129.23, 128.40, 127.66, 119.76, 115.99, 114.81, 42.31; **FTIR** (KBr): 3296, 3169, 3052, 2950, 1654, 1609, 1519, 1391, 1256, 1155, 780, 700  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25}$  = +98.03° (c = 1.0 in THF, e.r. 93 : 7); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate = 0.8 mL  $\text{min}^{-1}$ , minor enantiomer:  $t_{\text{R}}$  = 10.99 min, major enantiomer:  $t_{\text{R}}$  = 9.69 min.

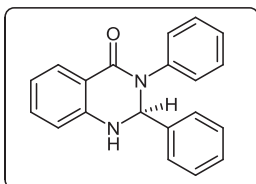
**(S)-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (13i)<sup>3</sup>**



Colorless solid, **Isolated yield (54mg, 79%), Mp:** 177 °C,  $R_f$  = 0.35 (PE/EA, 1:1);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.87-7.85 (dd,  $J$  = 7.8, 1.4 Hz, 1H), 7.30-7.268 (m, 1H), 6.83-6.80 (m, 1H), 6.66-6.65 (d,  $J$  = 7.5 Hz, 1H), 6.61 (s, br., 1H), 4.64 (dd,  $J$  = 5, 1.5 Hz, 1H), 4.30 (, bs, 1H), 1.86-1.80 (m, 4H), 1.77-1.61 (m, 2H), 1.26-1.23 (m, 2H), 1.17-1.08 (m, 3H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.35, 147.48, 133.81, 128.44, 118.91,

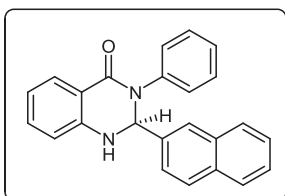
115.64, 114.50, 69.60, 42.69, 27.51, 26.19, 25.79, 25.78; **FTIR** (KBr): 3366, 3171, 3056, 2923, 2851, 1644, 1505, 1396, 1314, 752  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +79.22^\circ$  ( $c = 1.0$  in THF, e.r. 82 : 18); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate =  $0.8 \text{ mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 14.17 \text{ min}$ , major enantiomer:  $t_{\text{R}} = 11.17 \text{ min}$ .

**(S)-2,3-diphenylquinazolin-4(1H)-one (15a)**<sup>5</sup>



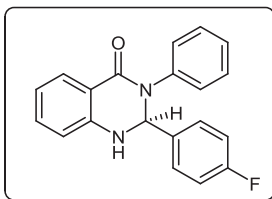
Colorless solid, **Isolated yield (65mg, 74%)**, **Mp:** 207 °C,  $R_f = 0.4$  (PE/EA, 3:1); **<sup>1</sup>H NMR** (500 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 8.03 (d, 1H,  $J = 7.9 \text{ Hz}$ ), 7.58–7.50 (m, 2H), 7.45–7.35 (m, 6H), 7.29–7.25 (m, 3H), 6.91–6.88 (m, 1H), 6.65 (d, 1H,  $J = 8.0 \text{ Hz}$ ), 6.10 (s, 1H), 4.95 (s, 1H); **<sup>13</sup>C NMR** (125 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 74.64, 114.8, 116.89, 119.55, 126.78, 126.84, 126.99, 127.02, 127.04, 128.71, 128.91, 128.96, 129.03, 133.87, 139.89, 140.61, 145.38, 163.15; **FTIR** (KBr): 3427, 3294, 3061, 2932, 1633, 1511, 1392, 1332, 1257, 1158, 1025, 754  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +121.04^\circ$  ( $c = 1.0$  in THF, e.r. 90 : 10); HPLC conditions: OD-H column, *n*-hexane/2-propanol = 80/20, flow rate =  $0.8 \text{ mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 29.57 \text{ min}$ , major enantiomer:  $t_{\text{R}} = 20.43 \text{ min}$ .

**(S)-2-(naphthalene-2-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15b)**<sup>6</sup>



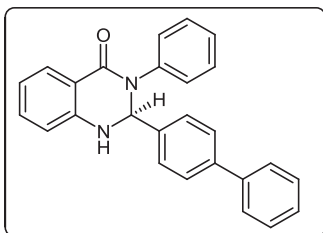
Colorless solid, **Isolated yield (81mg, 78%)**, **Mp:** 243 °C,  $R_f = 0.45$  (PE/EA, 3:1); **<sup>1</sup>H NMR** (500 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 7.87 – 7.92 (m, 4H), 7.73 (s, 1H), 7.70 (d,  $J = 7.5 \text{ Hz}$ , 1H), 7.64 (d,  $J = 7.5 \text{ Hz}$ , 1H), 7.51–7.54 (m, 2H), 7.25–7.35 (m, 5H), 7.15–7.18 (t,  $J = 7.5 \text{ Hz}$ , 1H), 6.46 (bs, 1H), 6.69 (t,  $J = 7.5 \text{ Hz}$ , 1H), 6.73 (d,  $J = 8 \text{ Hz}$ , 1H); **<sup>13</sup>C NMR** (125 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 162.83, 147.02, 147.31, 138.52, 134.24, 133.18, 132.74, 129.09, 128.78, 128.47, 128.42, 127.96, 126.86, 126.54, 126.09, 125.0, 118.04, 115.85, 115.25, 73.36; **FTIR** (KBr): 3447, 3291, 2932, 1640, 1513, 1387, 1297, 1158, 847, 754, 689  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +114.27^\circ$  ( $c = 1.0$  in THF, e.r. 87 : 13); HPLC conditions: AD-H column, *n*-hexane/2-propanol = 80/20, flow rate =  $0.8 \text{ mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}} = 32.19 \text{ min}$ , major enantiomer:  $t_{\text{R}} = 27.60 \text{ min}$ .

**(S)-2-(4-fluoro-phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15c)**<sup>7</sup>



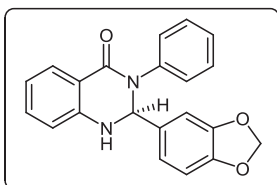
Colorless solid, **Isolated yield (66mg, 70%), Mp:** 237 °C,  $R_f = 0.4$  (PE/EA, 3:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 7.74 (d,  $J = 7.5$  Hz, 1H), 7.43 (m, 1H), 7.6 (s, 1H), 7.18–7.38 (m, 5H), 7.13 (t,  $J = 8$  Hz, 2H), 6.78 (d,  $J = 8$  Hz, 2H), 6.73 (t,  $J = 8$  Hz, 2H), 6.32 (s, 1H), 4.79 (s, 1H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 162.7, 162.52 (d,  $J = 246.7$  Hz), 147.02, 141.11, 134.28, 129.33, 129.27, 129.11, 128.46 (d,  $J = 8.25$  Hz), 126.92, 118.11, 115.73, 115.56 (d,  $J = 21.5$  Hz), 115.26, 115.29, 72.51; **FTIR** (KBr): 3411, 2962, 1641, 1616, 1508, 1448, 1390, 1247, 1068, 985, 871, 619  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +104.12^\circ$  ( $c = 1.0$  in THF, e.r. 81 : 19); HPLC conditions: OD-H column,  $n$ -hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_R = 28.19$  min, major enantiomer:  $t_R = 22.81$  min.

**(S)-2-(biphenyl-4-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15d)<sup>1</sup>**



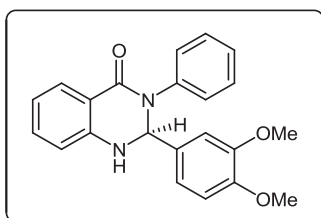
Colorless solid, **Isolated yield (101mg, 92%), Mp:** 241 °C,  $R_f = 0.45$  (PE/EA, 3:1);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta = 8.05 - 8.03$  (dd,  $J = 8$  and 1.5 Hz, 1H), 7.52 – 7.47 (m, 4H), 7.42 – 7.39 (m, 4H), 7.34 – 7.29 (m, 4H), 7.24 – 7.22 (m, 2H), 7.20-7.18 (m, 1H), 6.90 – 6.87 (td,  $J = 4$  and 1Hz, 1H), 6.65 – 6.63 (d,  $J = 7.5$ , 1H), 6.12 (s, 1H), 4.92 (s, 1H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ):  $\delta = 163.09, 145.29, 141.75, 140.69, 140.16, 138.91, 133.90, 129.07, 128.98, 128.85, 127.61, 127.39, 127.21, 127.01, 126.88, 126.80, 119.65, 117.02, 115.00, 74.36$ ; **FTIR** (KBr): 3415, 3300, 2933, 1637, 1586, 1397, 1262, 1155, 844, 736, 696  $\text{cm}^{-1}$ ;  $[\alpha]_D^{25} = +139.7^\circ$  ( $c = 1.0$  in THF, e.r. 92 : 8); HPLC conditions: AD-H column,  $n$ -hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_R = 26.57$  min, major enantiomer:  $t_R = 21.51$  min.

**(S)-2-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15e)**



Colorless solid, **Isolated yield (71mg, 70%), Mp:** 239 °C,  $R_f$  = 0.3 (PE/EA, 3:1);  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ ):  $\delta$  (ppm)  $\delta$  = 7.72 (d,  $J$  = 7.5 Hz, 1H), 7.75 (m, 1H) 7.34 (t,  $J$  = 8 Hz, 2H), 7.30 – 7.25 (m, 3H), 7.20 (t,  $J$  = 7.5 Hz, 1H), 6.93 (s, 1H), 6.81 (s, 2H), 6.67-6.71(m, 2H), 6.20 (d,  $J$  = 2.5 Hz, 1H), 5.97 (d,  $J$  = 4.5 Hz, 1H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 162.73, 147.82, 147.66, 147.02, 141.2, 135.07, 134.23, 129.06, 128.40, 126.72, 126.28, 120.74, 118.00, 115.76, 115.26, 108.26, 107.30, 101.64, 72.85; HRMS (ESI):  $m/z$  calculated for  $\text{C}_{21}\text{H}_{16}\text{N}_2\text{O}_3$  [ $\text{M}^+\text{+H}$ ] 345.1239, found: 345.1233; **FTIR** (KBr): 3297, 3039, 2928, 1639, 1614, 1500, 1450, 1393, 1244, 1035, 937, 856, 697  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +97.1^\circ$  ( $c$  = 1.0 in THF, e.r. 79 : 21); HPLC conditions: OD-H column,  $n$ -hexane/2-propanol = 80/20, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}}$  = 32.35 min, major enantiomer:  $t_{\text{R}}$  = 22.42 min.

**(S)-2-(3,4-dimethoxy-phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15f)<sup>5</sup>**



Colorless solid, **Isolated yield (78mg, 73%), Mp:** 246 °C,  $R_f$  = 0.3 (PE/EA, 3:1);  $^1\text{H NMR}$  (DMSO- $d_6$ ):  $\delta$  (ppm) 8.01 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 7.25–7.32 (m, 3H), 7.15–7.18 (m, 3H), 6.84–6.89 (m, 3H), 6.69 (d,  $J$  = 8.0 Hz, 1H), 6.64 (d,  $J$  = 8.0 Hz, 1H), 6.05 (s, 1H), 4.78 (s, 1H), 3.81 (s, 3H), 3.71 (s, 3H);  $^{13}\text{C NMR}$  (125 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) 163.33, 152.51, 145.5, 145.32, 141.39, 133.72, 133.6, 128.87, 126.34, 125.5, 123.9, 119.21, 119.14, 116.51, 114.82, 112.93, 112.18, 69.99, 60.8, 55.7; **FTIR** (KBr): 3411, 2932, 1635, 1616, 1508, 1390, 1267, 1236, 1029, 997, 952, 862, 694, 617  $\text{cm}^{-1}$ ;  $[\alpha]_{\text{D}}^{25} = +88.22^\circ$  ( $c$  = 1.0 in THF, e.r. 76 : 24); HPLC conditions: AD-H column,  $n$ -hexane/2-propanol = 70/30, flow rate = 0.8  $\text{mL min}^{-1}$ , minor enantiomer:  $t_{\text{R}}$  = 22.9 min, major enantiomer:  $t_{\text{R}}$  = 15.23 min.

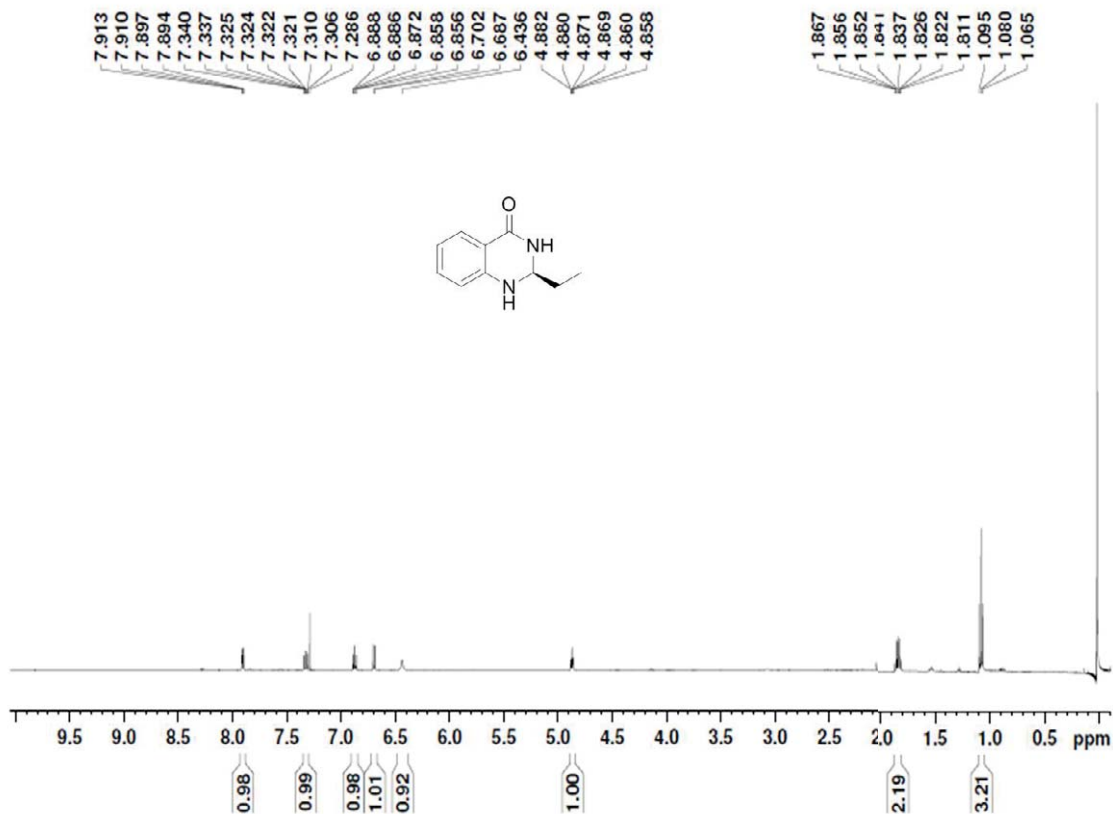
**References:**

- (1) Prakash, M and Kesavan, V. *Org.Lett.* **2012**, *14*, 1896.
- (2) Xu, C.; Sreekumar, V.; Richard, G.; Benjamin, L. *J. Am. Chem. Soc.* **2008**, *130*, 15786.
- (3) Rueping, M.; Antonchick, A. P.; Sugiono, E.; Grenader, K. *Angew. Chem. Int. Ed.* **2009**, *48*, 908.
- (4) Cheng, D.-J.; Tian, Y.; Tian, S.-K. *Adv. Synth. Catal.* **2012**, *354*, 995.
- (5) Zhang, Z-H; Lu, H-Y; Yang, S-H; Gao, J-W. *J. Comb. Chem.* **2010**, *12*, 643.
- (6) Ghorbani-Choghamarani, A and Taghipour T. *Lett. Org. Chem.* **2011**, *8*, 470.
- (7) Niknam, K; Mohammadzadeh, M. R and Mirzaee, S. *Chin. J. Chem.*, **2011**, *29*, 1417.

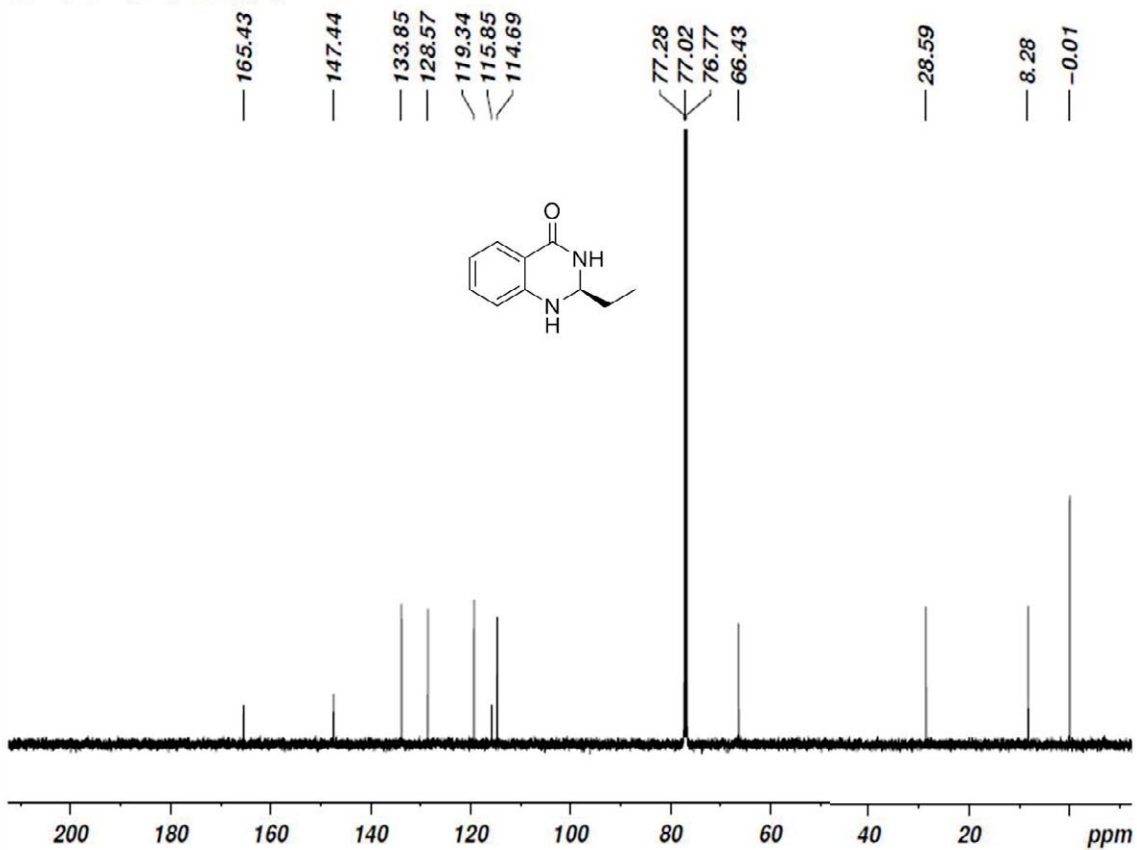


# $^1\text{H}$ , $^{13}\text{C}$ NMR Spectrum of 2-ethyl-2,3-dihydroquinazolin-4(1H)-one (13a)

MP-07-Pro-DHQ.....Prakash.



MP-07-Pro-DHQ.....Prakash.



# HRMS of 2-ethyl-2,3-dihydroquinazolin-4(1H)-one (13a)

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

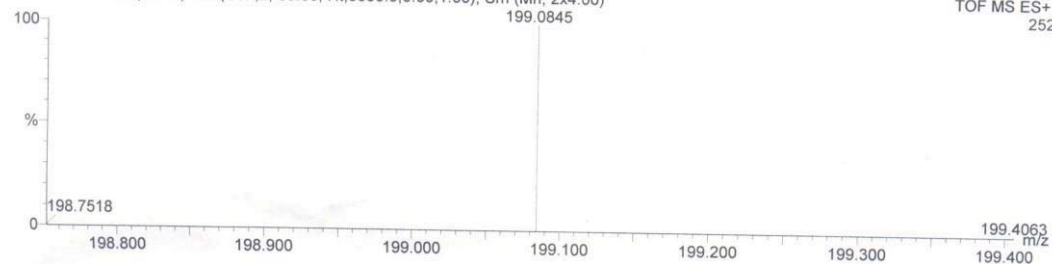
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

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

QTOF MICRO DEPARTMENT OF CHEMISTRY IITM  
RD-KSP-INI-II 32 (0.541) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

13-Feb-2013 15:49:23  
TOF MS ES+  
252



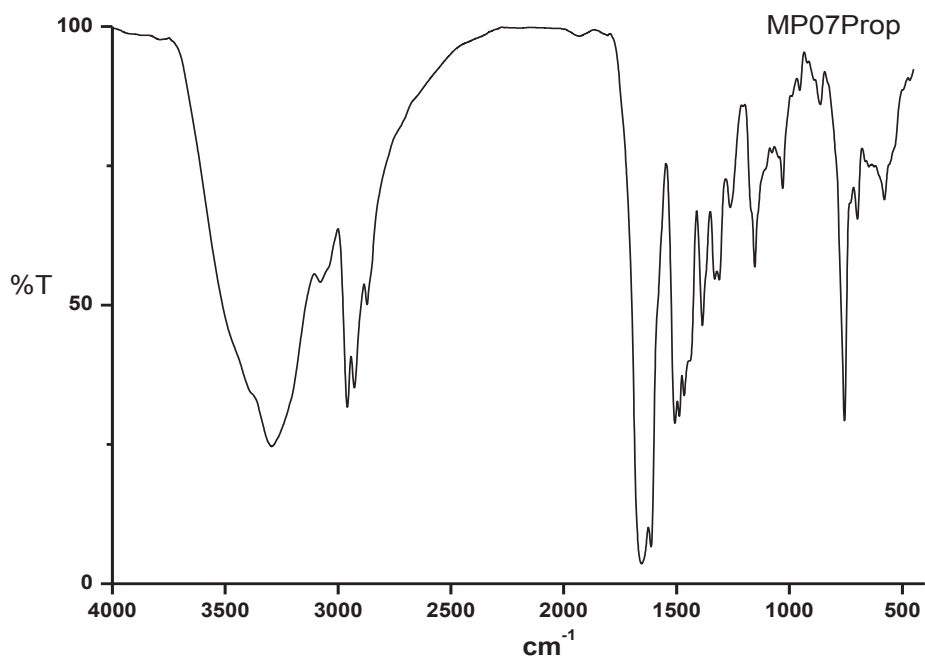
Minimum:  
Maximum:

200.0 5.0 -1.5

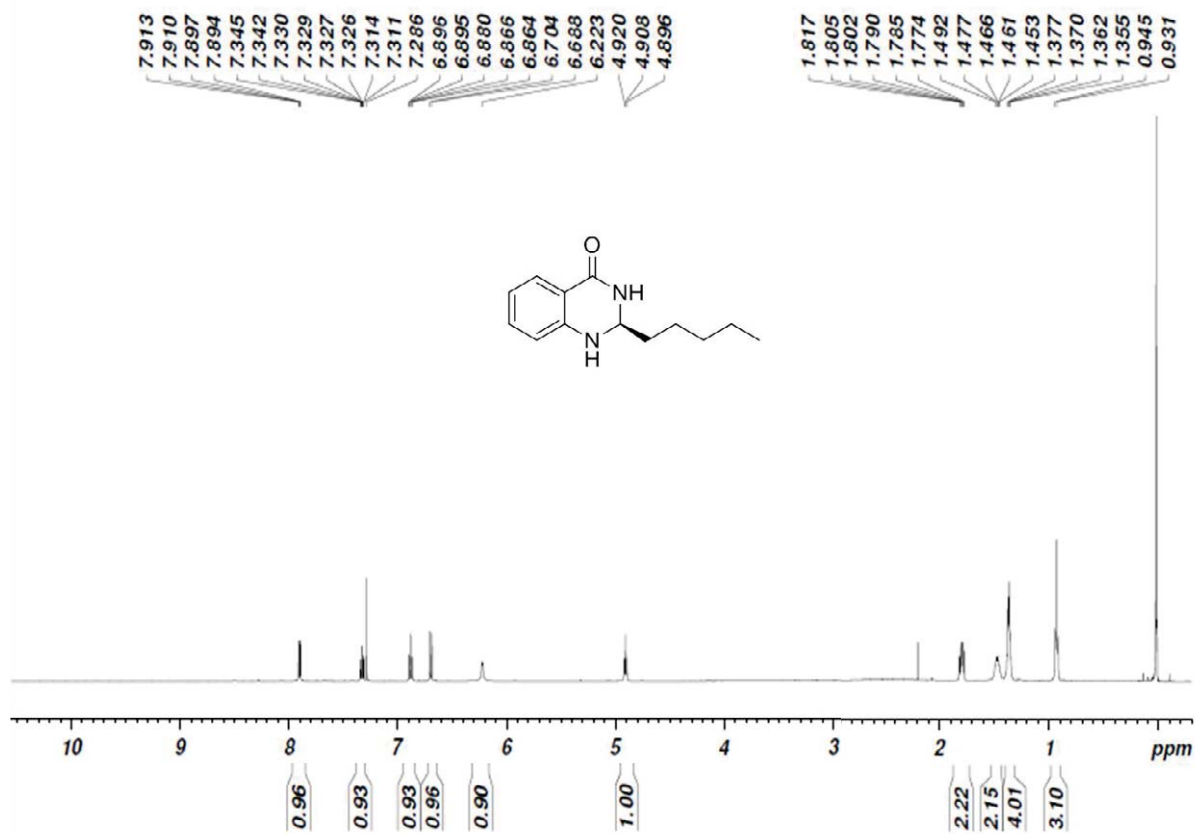
50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
199.0845	199.0847	-0.3	-1.4	5.5	1	C10 H12 N2 O Na

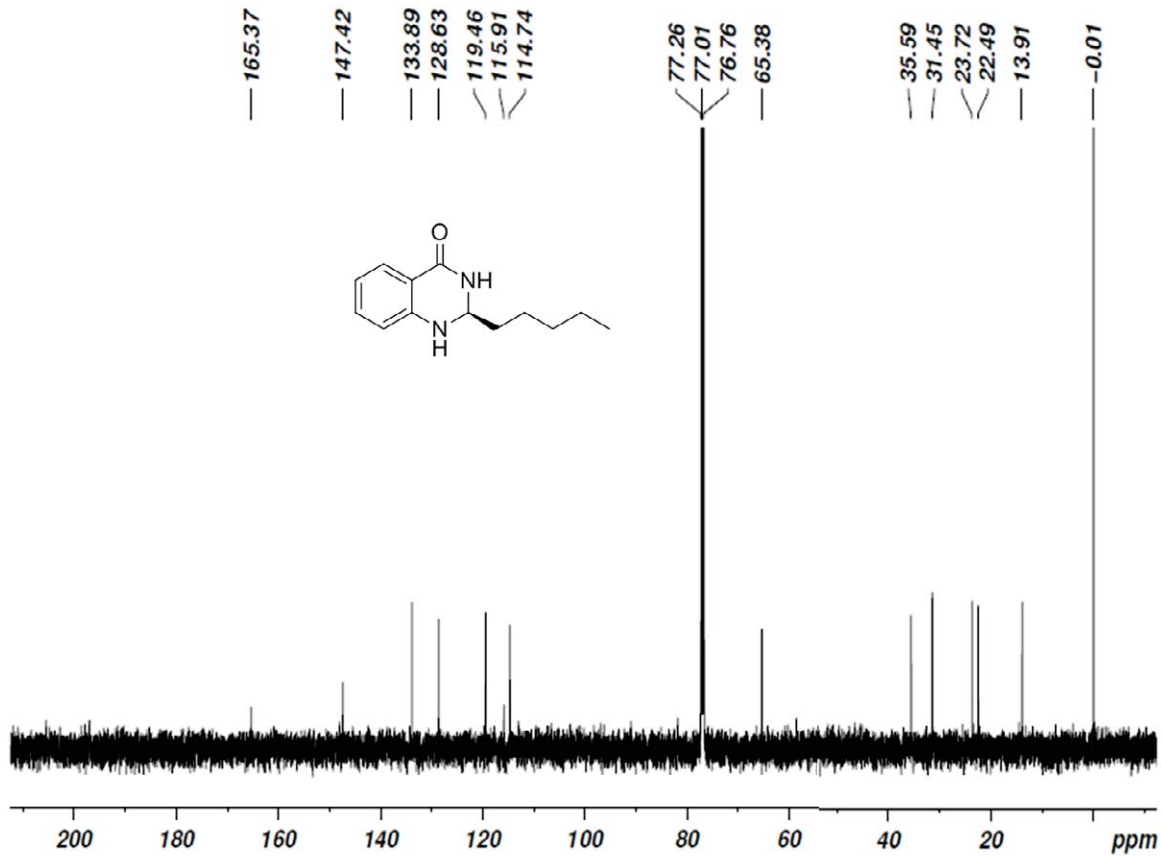
## IR Spectra of 2-ethyl-2,3-dihydroquinazolin-4(1H)-one (13a)



$^1\text{H}$ ,  $^{13}\text{C}$  NMR Spectrum of 2-pentyl-2,3-dihydroquinazolin-4(1H)-one (13c)



MP-07-Hex-DHQ.....Prakash.



# HRMS of 2-pentyl-2,3-dihydroquinazolin-4(1H)-one (13c)

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

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

QTOF MICRO

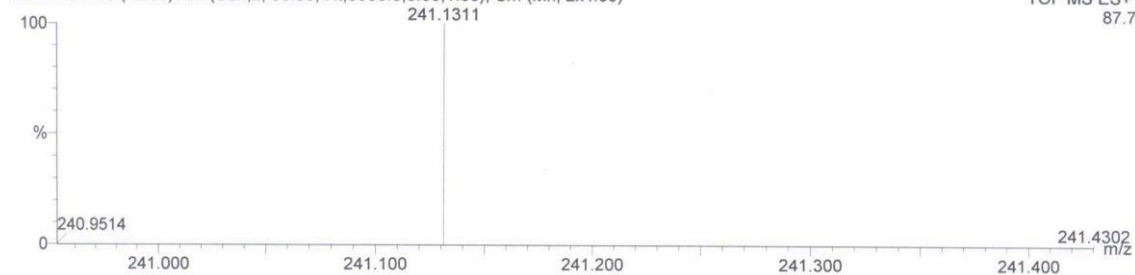
RD-KPS-2 69 (1.293) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

DEPARTMENT OF CHEMISTRY IITM

07-Feb-2013 15:16:18

TOF MS ES+

87.7

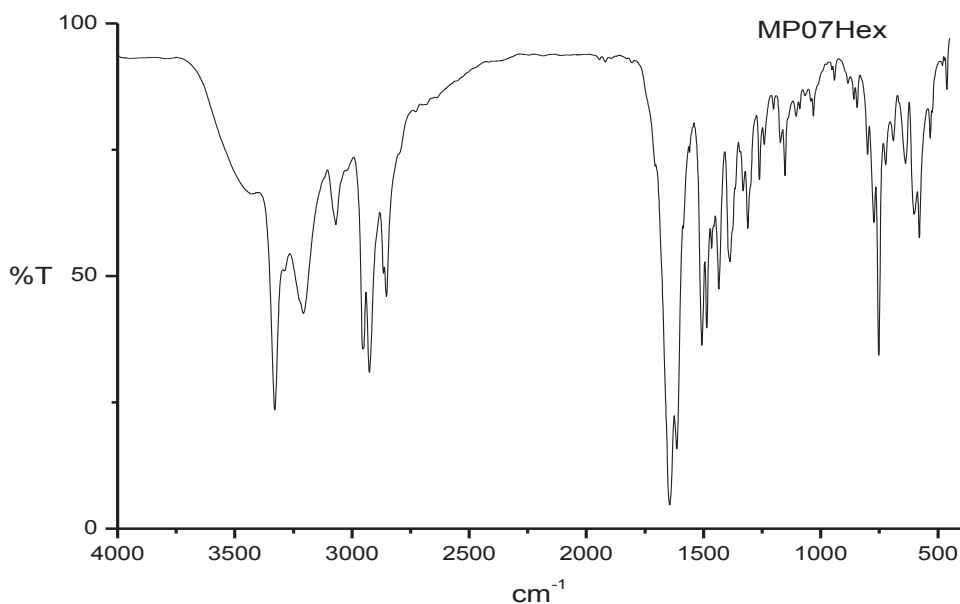


Minimum:

Maximum: 200.0 5.0 -1.5

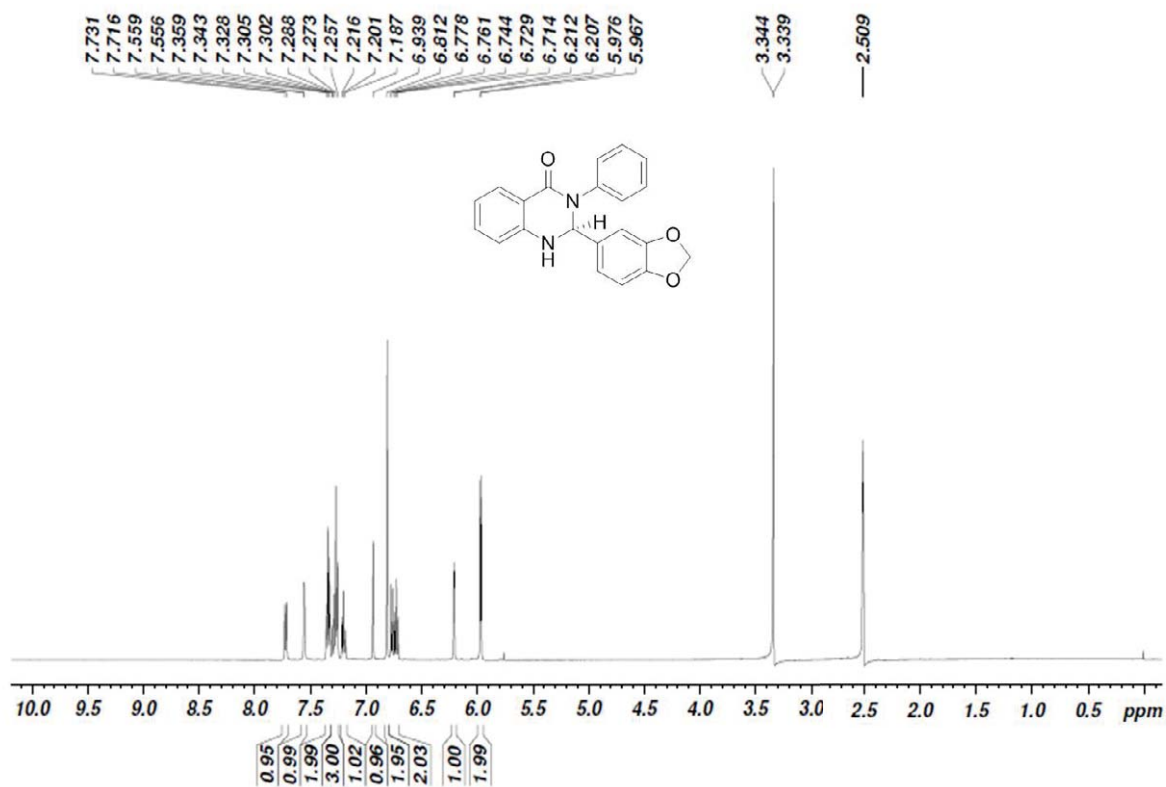
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
241.1311	241.1317	-0.6	-2.5	5.5	1	C13 H18 N2 O Na

## IR Spectra of 2-pentyl-2,3-dihydroquinazolin-4(1H)-one (13c)

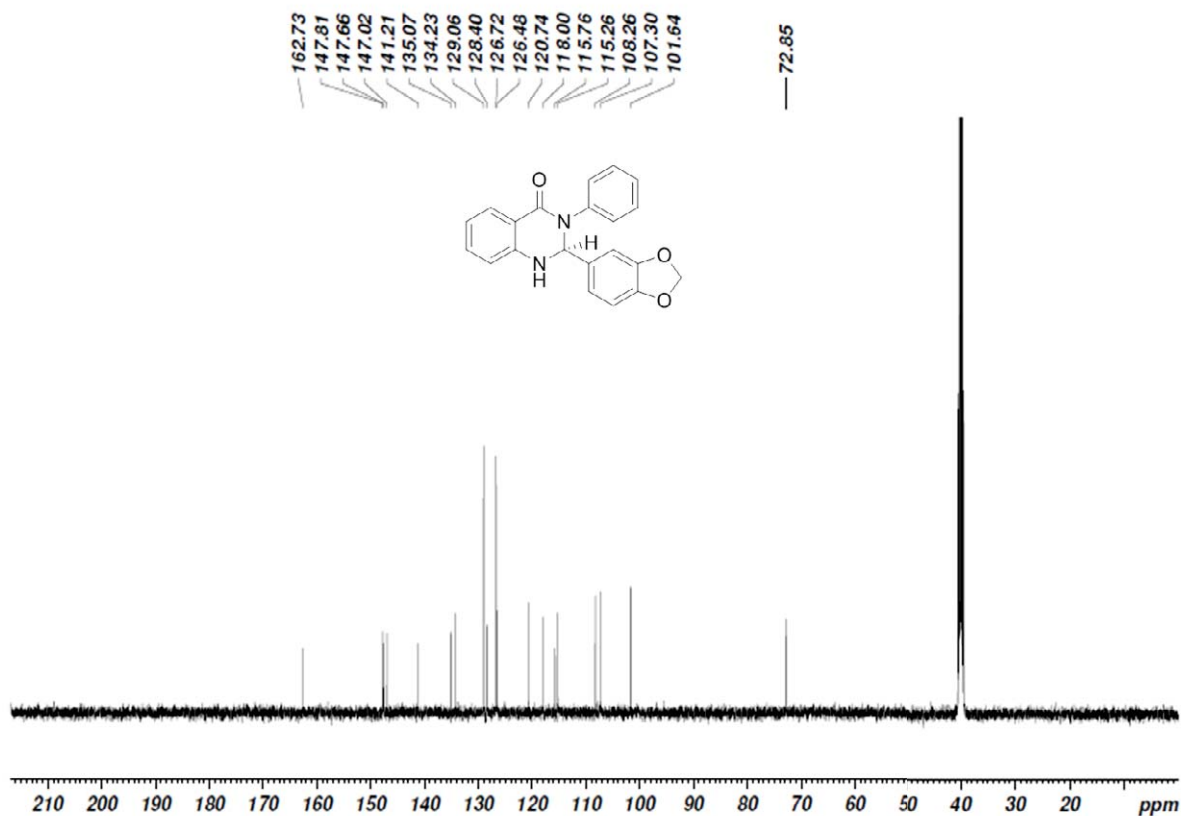


<sup>1</sup>H, <sup>13</sup>C NMR Spectrum of 2-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15e)

MP-07-N-Ph-PiP.....Prakash,



MP-07-N-Ph-PiP.....Prakash,



## HRMS of 2-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15e)

### Single Mass Analysis

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

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

QTOF MICRO

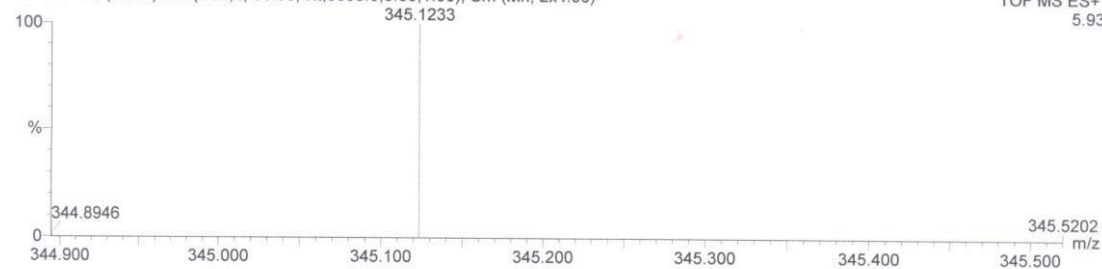
RD-KPS-1 8 (0.149) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

DEPARTMENT OF CHEMISTRY IITM

07-Feb-2013 15:13:06

TOF MS ES+

5.93



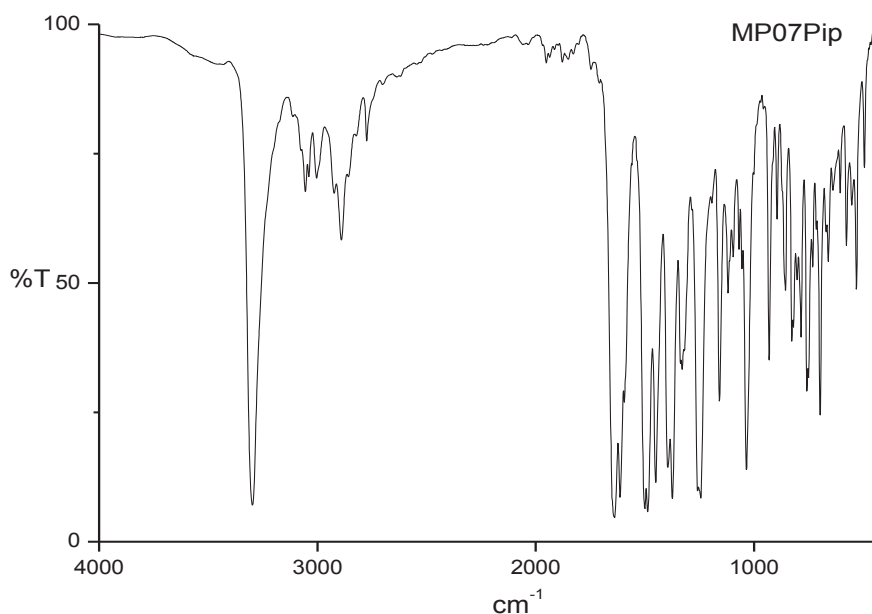
Minimum:

Maximum: 200.0 5.0 -1.5

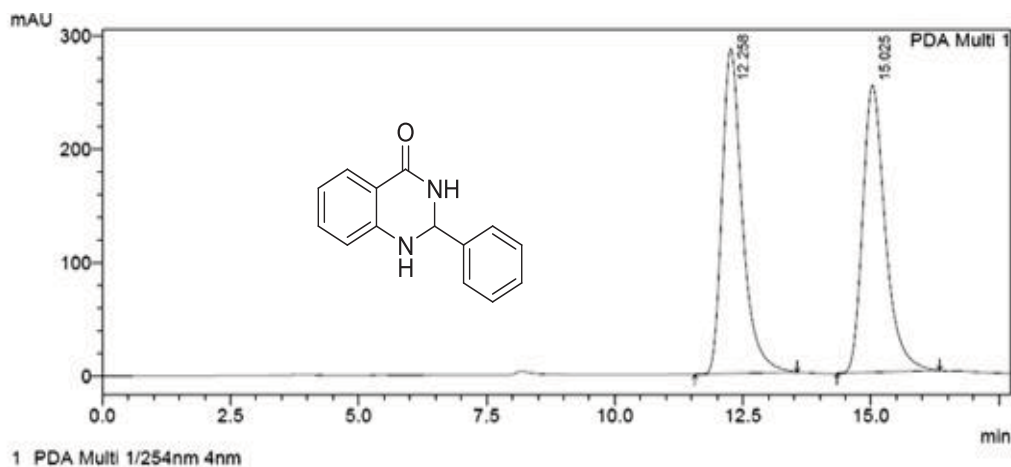
Mass Calc. Mass mDa PPM DBE Score Formula

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
345.1233	345.1239	-0.7	-1.9	14.5	1	C21 H17 N2 O3

## IR Spectra of 2-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15e)

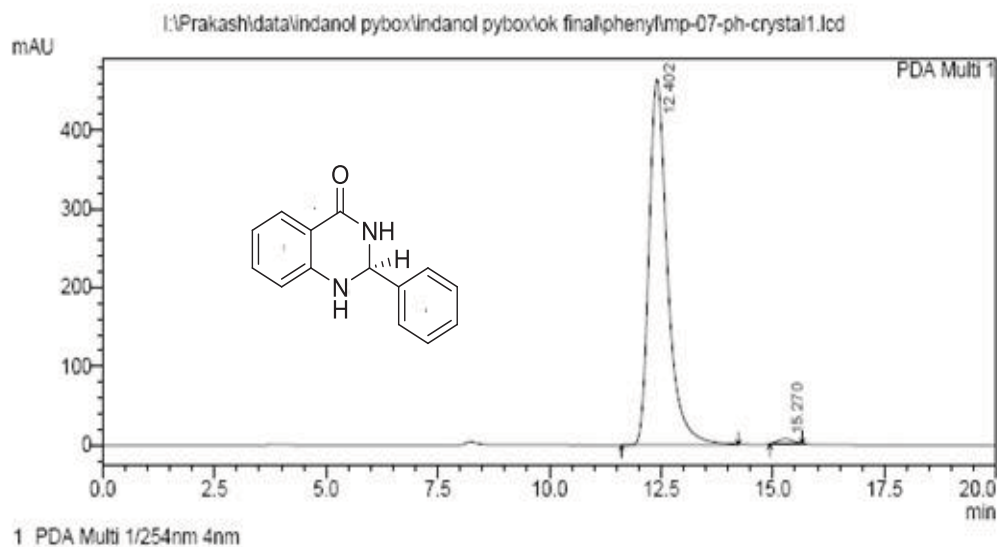


**Table 5**  
**HPLC Chromatogram of 2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3a)**



PeakTable

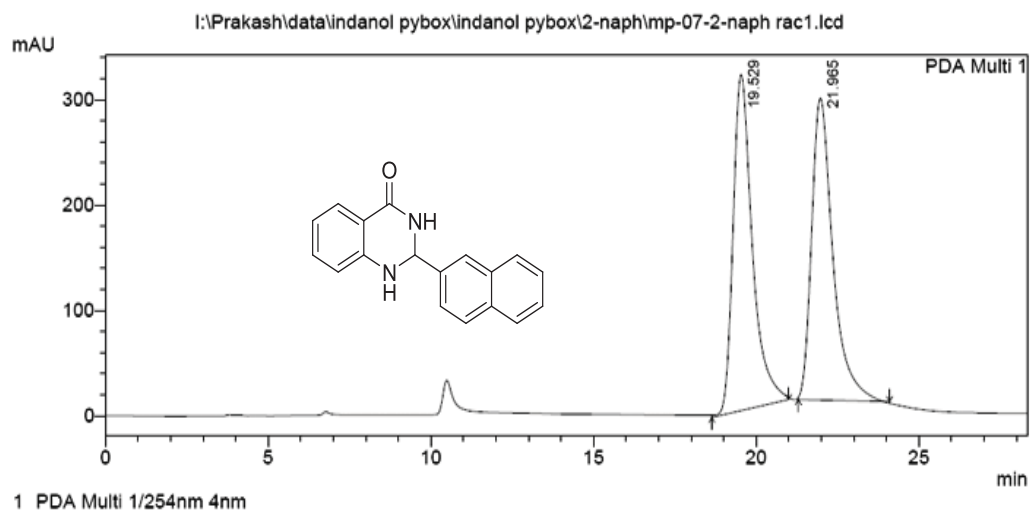
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.258	7887327	286543	50.401	53.098
2	15.025	7761719	253110	49.599	46.902
Total		15649046	539653	100.000	100.000



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.402	13440387	464856	98.913	98.712
2	15.270	147707	6065	1.087	1.288
Total		13588093	470921	100.000	100.000

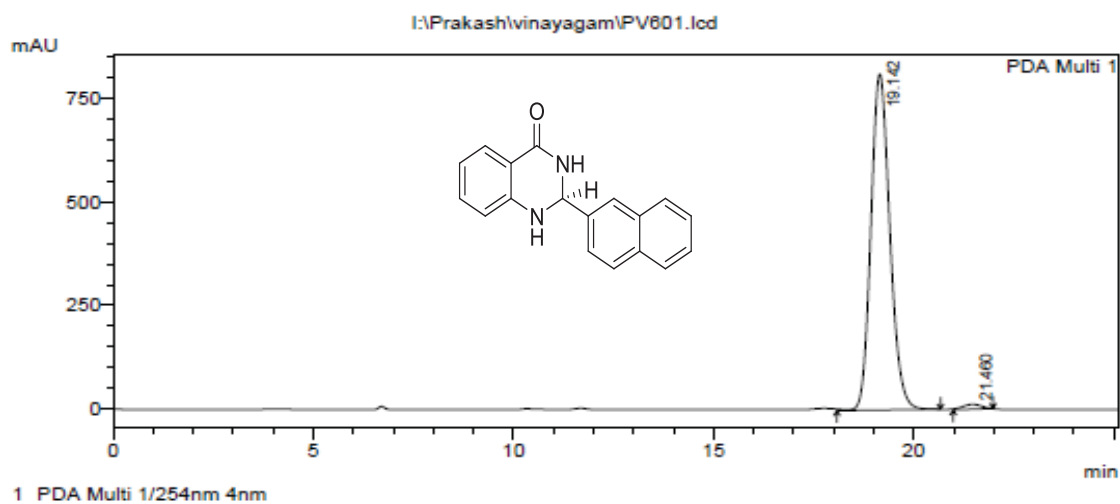
### HPLC Chromatogram of 2-(naphthalen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (3b).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.529	13158241	318981	50.294	52.674
2	21.965	13004462	286599	49.706	47.326
Total		26162702	605580	100.000	100.000



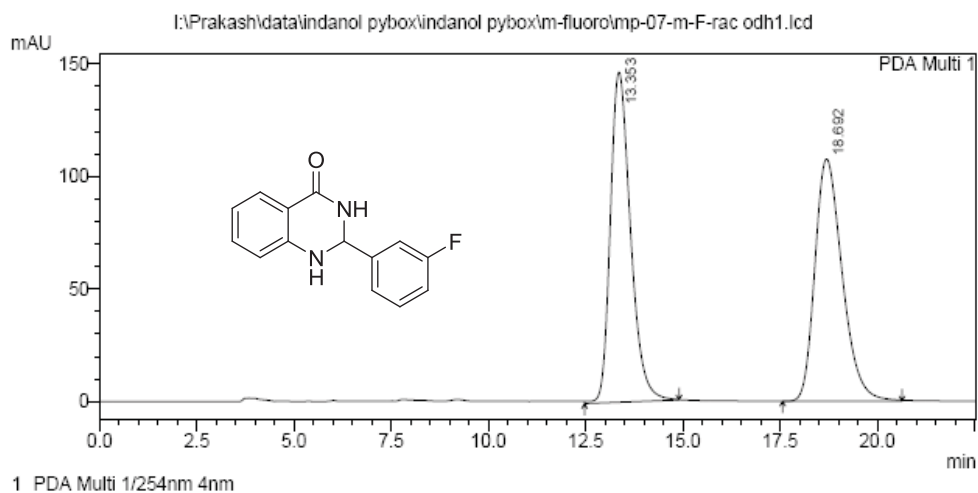
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.142	26727681	808695	98.601	98.577
2	21.460	379187	11677	1.399	1.423
Total		27106867	820372	100.000	100.000



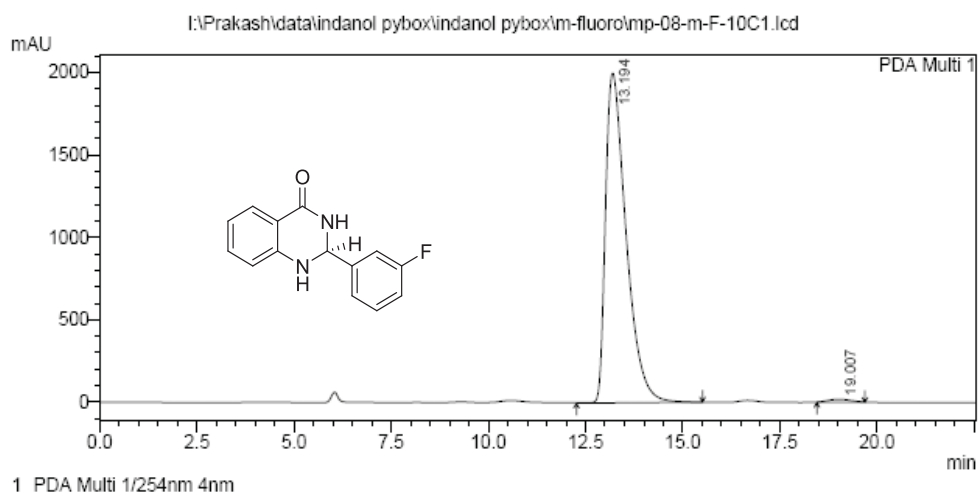
## HPLC Chromatogram of 2-(3-fluorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3c).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.353	5299826	146752	50.143	57.687
2	18.692	5269647	107643	49.857	42.313
Total		10569473	254396	100.000	100.000

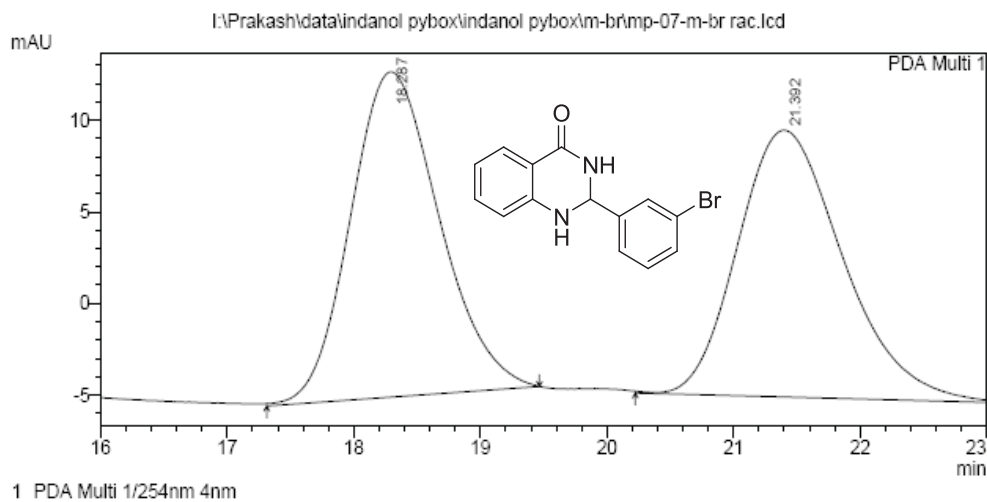


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.194	73668553	1999344	98.902	99.083
2	19.007	817735	18500	1.098	0.917
Total		74486288	2017844	100.000	100.000

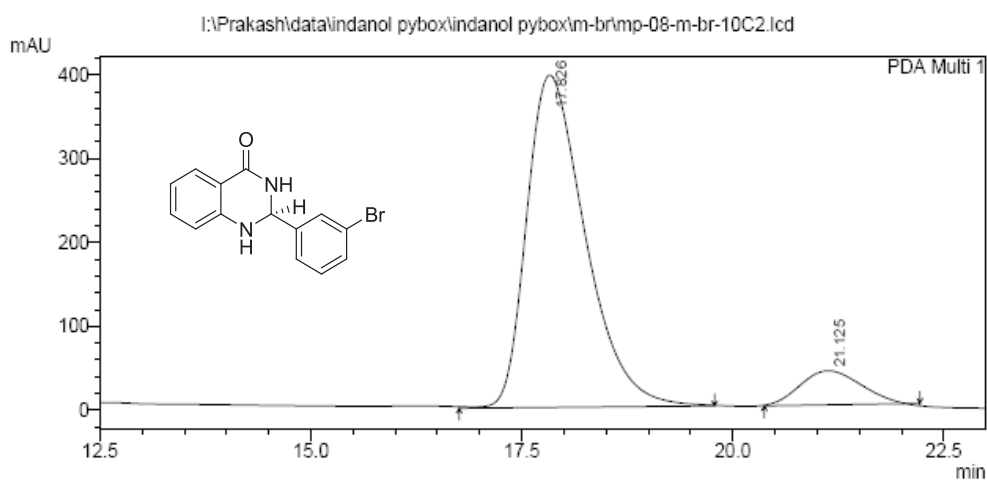
## HPLC Chromatogram of 2-(3-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3d).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.287	866230	17770	50.725	54.943
2	21.392	841455	14572	49.275	45.057
Total		1707684	32342	100.000	100.000

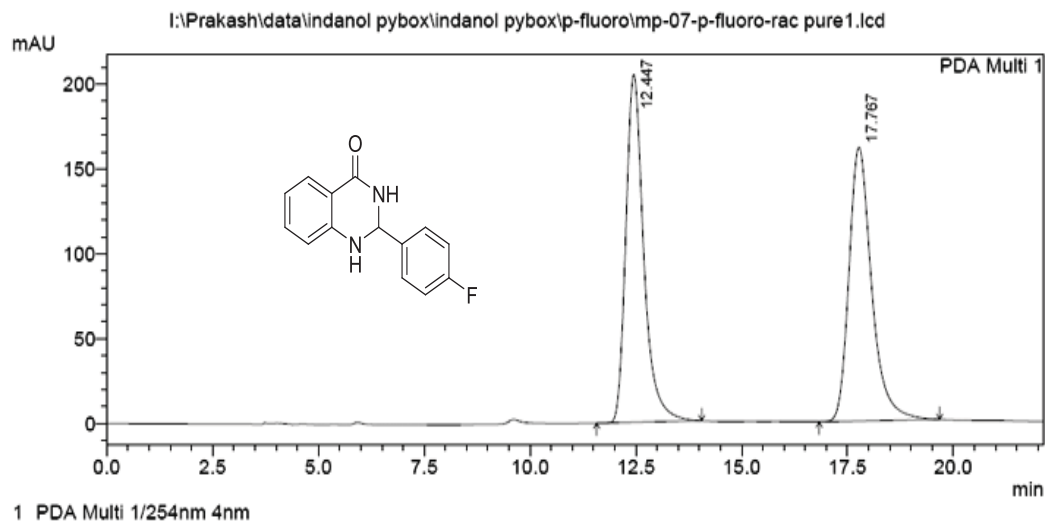


PeakTable

PDA Ch1 254nm 4nm

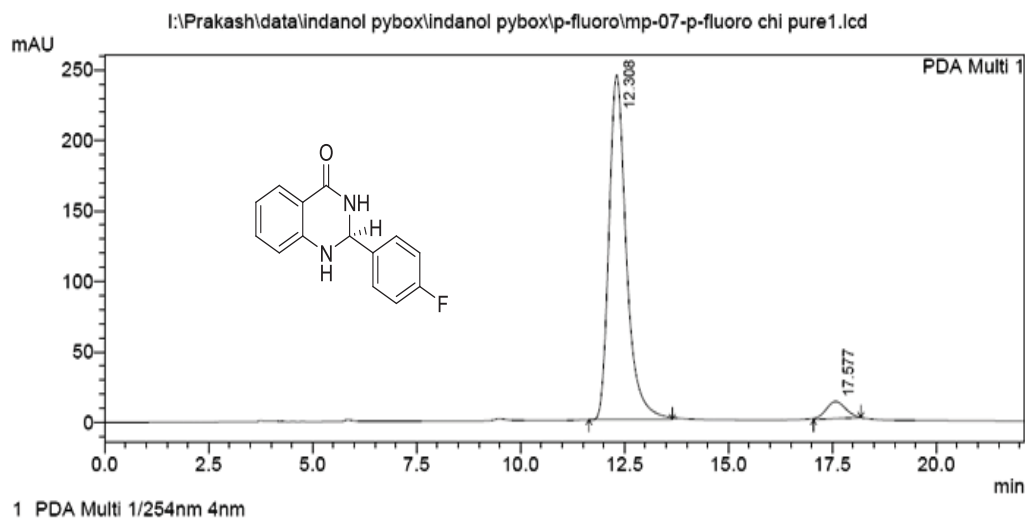
Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.826	19146971	396327	90.440	90.702
2	21.125	2023940	40628	9.560	9.298
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### HPLC Chromatogram of 2-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3e).



PeakTable

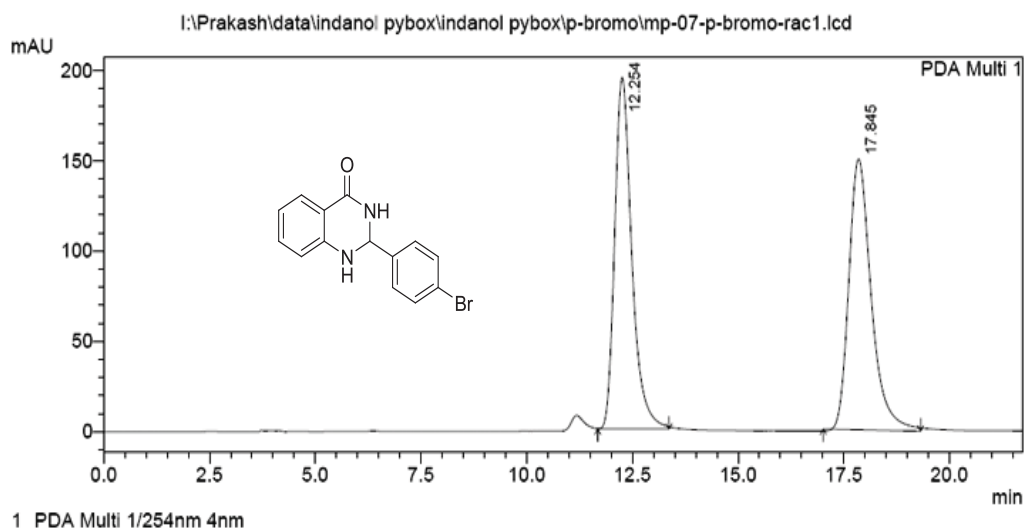
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.447	6023847	204988	49.971	55.937
2	17.767	6030835	161473	50.029	44.063
Total		12054683	366460	100.000	100.000



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.308	7105100	244493	94.728	95.273
2	17.577	395453	12131	5.272	4.727
Total		7500553	256624	100.000	100.000

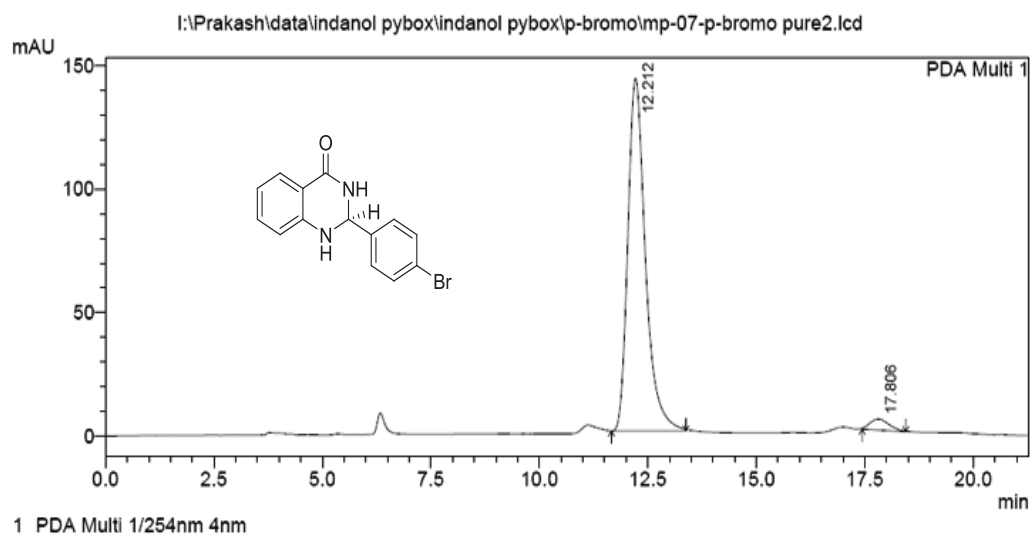
### HPLC Chromatogram of 2-(4-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3f).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.254	5488945	194654	49.867	56.495
2	17.845	5518122	149894	50.133	43.505
Total		11007068	344547	100.000	100.000

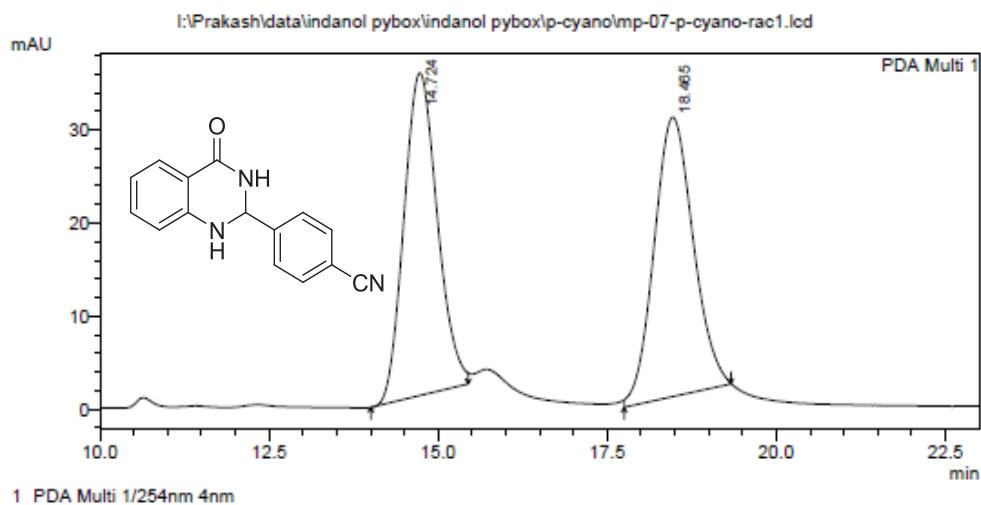


PeakTable

PDA Ch1 254nm 4nm

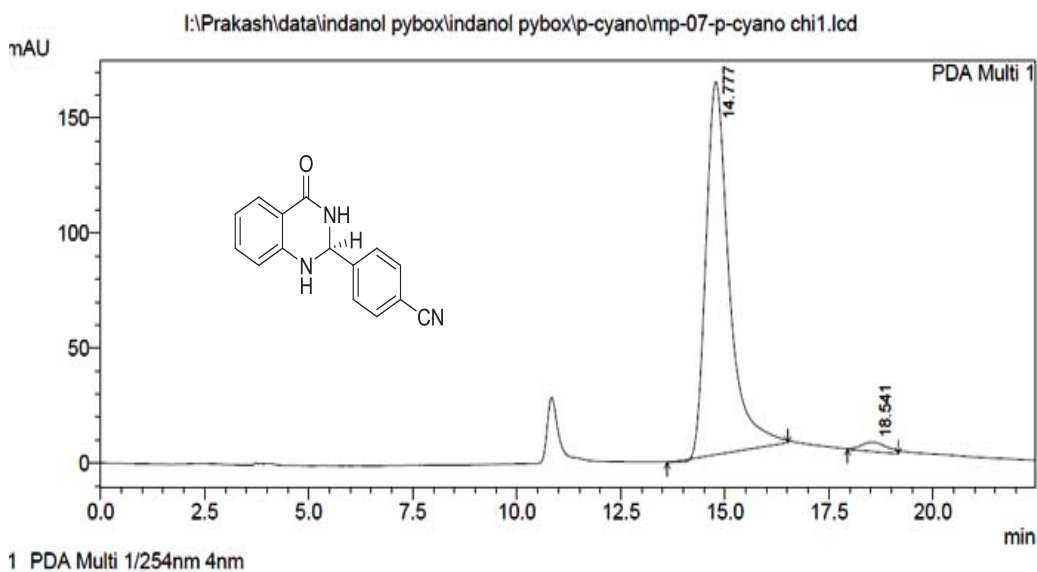
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.212	4020262	142894	96.683	96.976
2	17.806	137929	4456	3.317	3.024
Total		4158191	147350	100.000	100.000

# HPLC Chromatogram of 4-(4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzonitrile (3g).



PeakTable

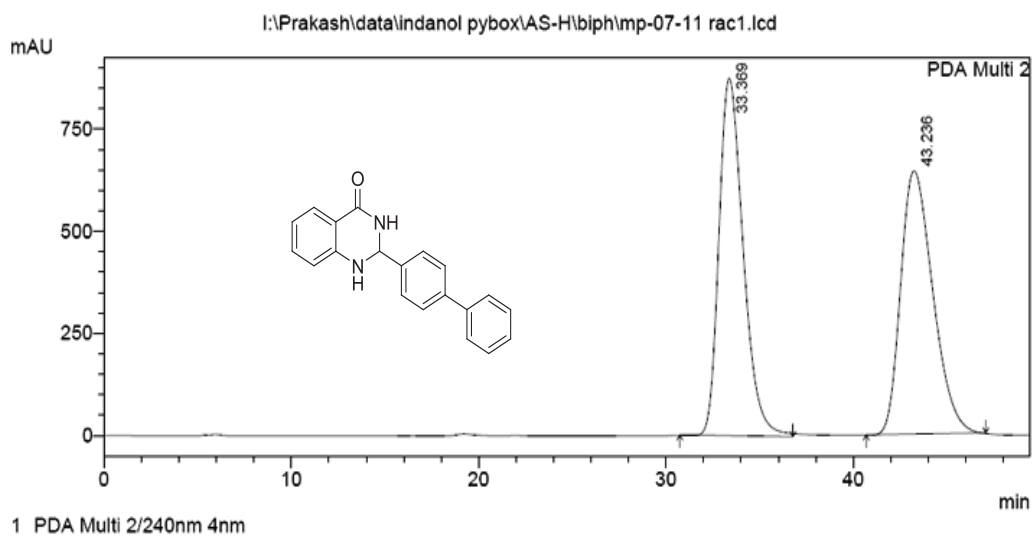
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.724	1189996	34693	49.625	53.581
2	18.465	1207976	30056	50.375	46.419
Total		2397972	64748	100.000	100.000



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.777	6315885	162164	97.217	97.539
2	18.541	180835	4092	2.783	2.461
Total		6496720	166256	100.000	100.000

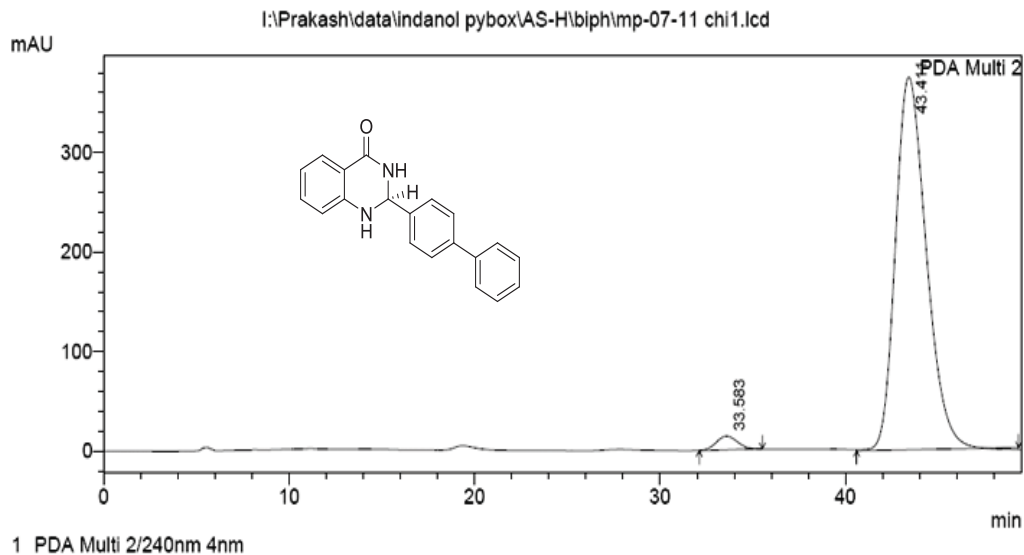
## HPLC Chromatogram of 2-(Biphenyl-4-yl)-2,3-dihydroquinazolin-4(1H)-one (3h).



PeakTable

PDA Ch2 240nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	33.369	78642633	874572	50.599	57.587
2	43.236	76781637	644129	49.401	42.413
Total		155424271	1518700	100.000	100.000

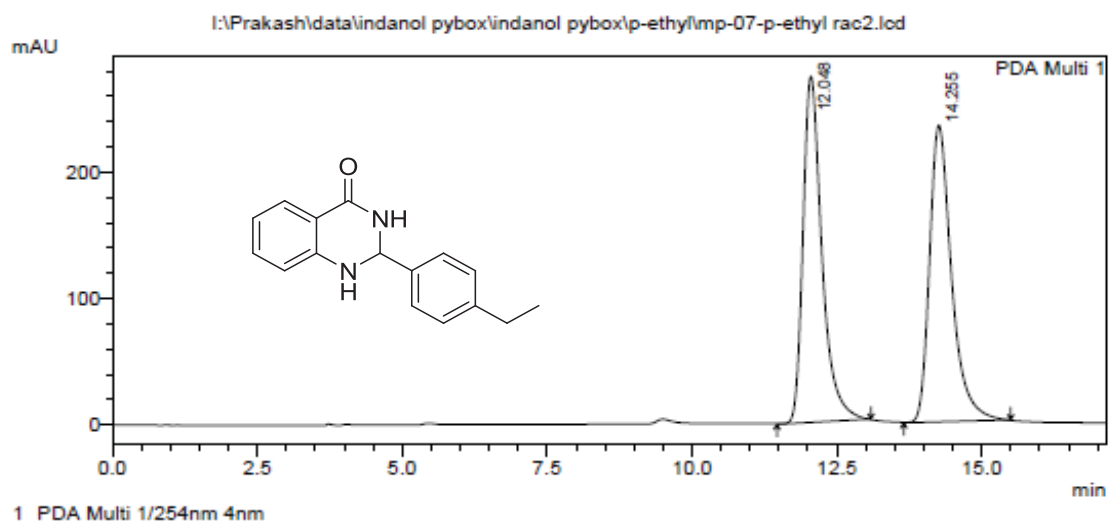


PeakTable

PDA Ch2 240nm 4nm

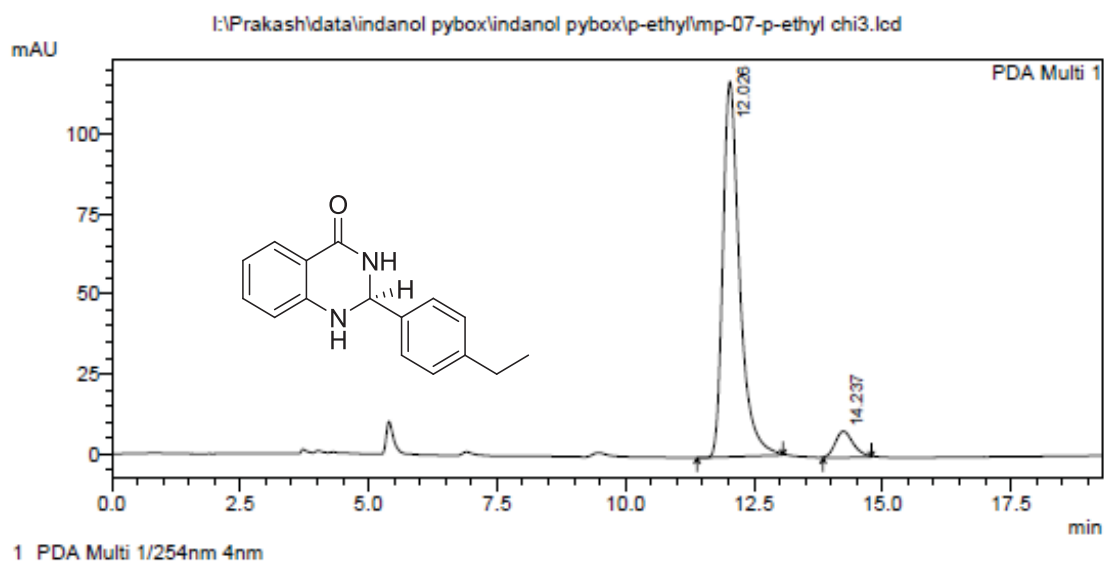
Peak#	Ret. Time	Area	Height	Area %	Height %
1	33.583	1100695	13834	2.491	3.564
2	43.411	43085907	374283	97.509	96.436
Total		44186602	388118	100.000	100.000

### HPLC Chromatogram of 2-(4-ethylphenyl)-2,3-dihydroquinazolin-4(1H)-one (3i)



PeakTable

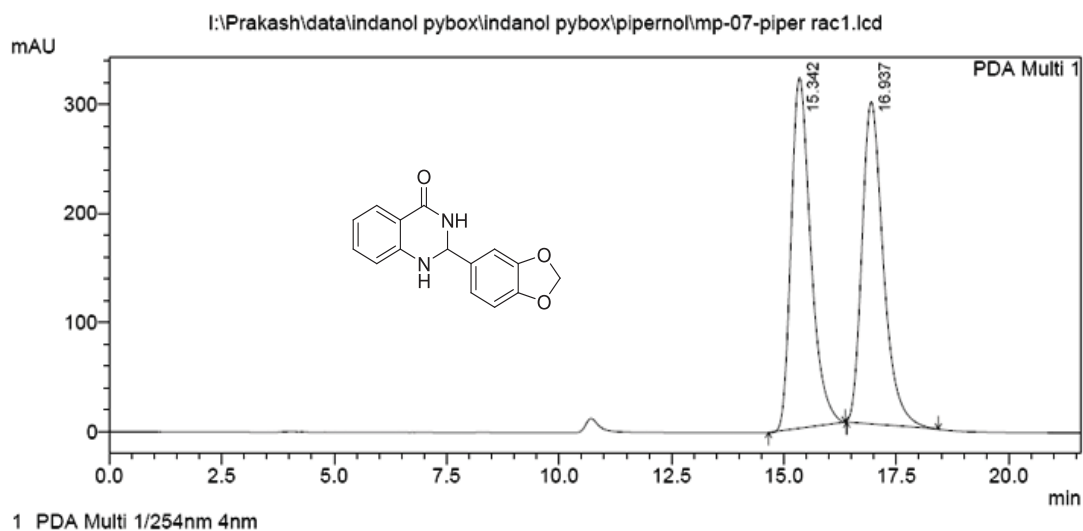
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.048	6220345	274011	50.065	53.855
2	14.255	6204146	234784	49.935	46.145
Total		12424491	508796	100.000	100.000



PeakTable

PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.026	2661665	117493	92.874	93.447
2	14.237	204220	8239	7.126	6.553
Total		2865886	125733	100.000	100.000

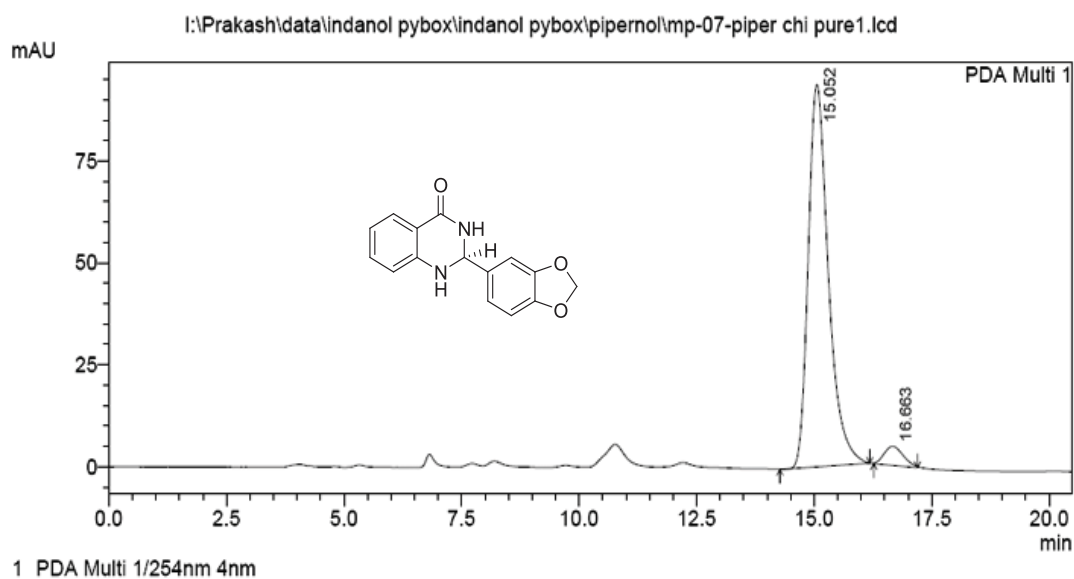
## HPLC Chromatogram of 2-(Benzo[d][1,3]dioxol-5-yl)-2,3-dihydroquinazolin-4(1H)-one (3j)



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.342	9748483	321566	49.976	52.133
2	16.937	9757747	295251	50.024	47.867
Total		19506230	616818	100.000	100.000



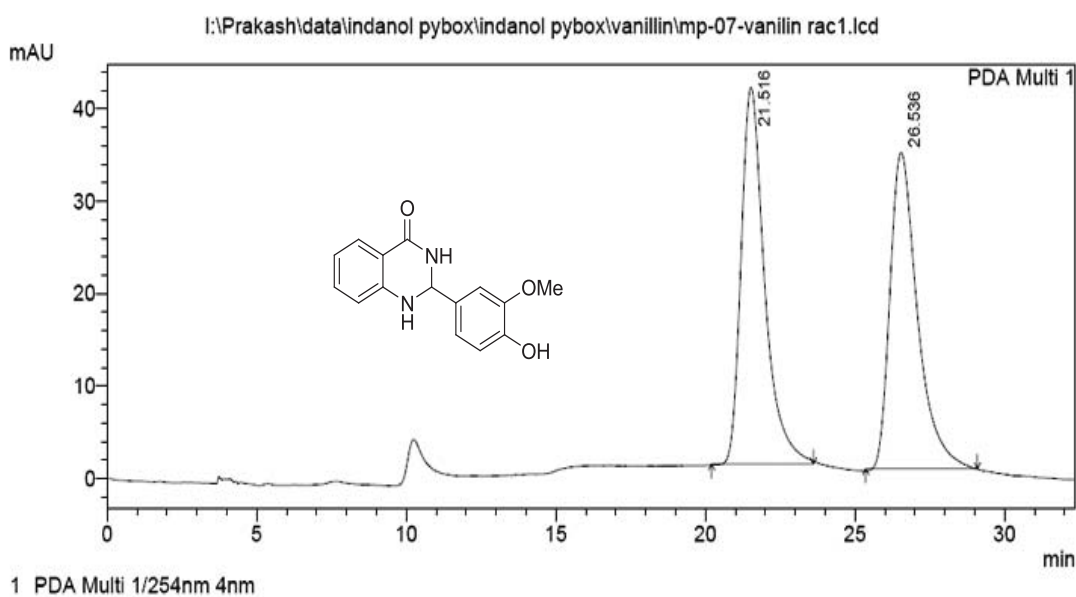
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.052	2794749	93817	95.460	95.229
2	16.663	132910	4700	4.540	4.771
Total		2927659	98517	100.000	100.000



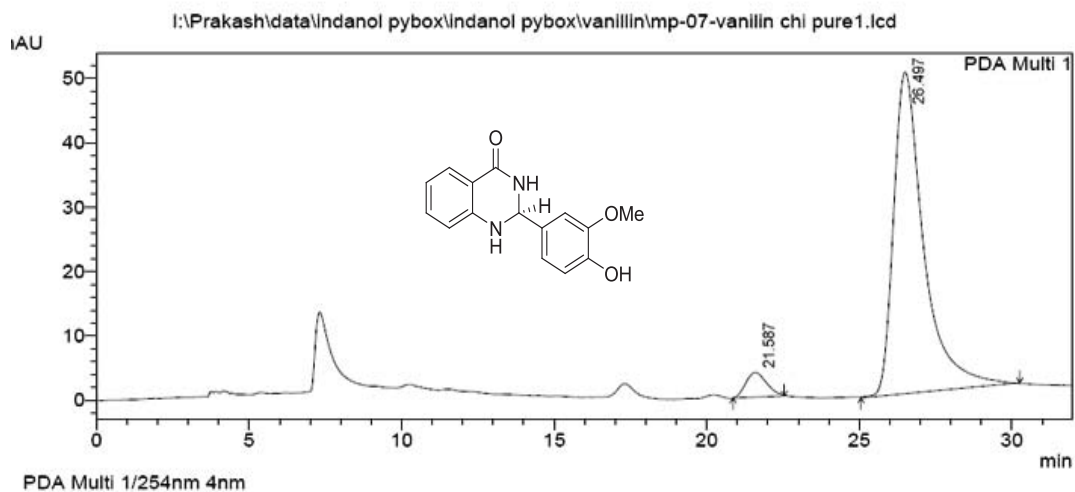
# HPLC Chromatogram of 2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3k).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.516	2230650	40760	50.528	54.366
2	26.536	2184007	34213	49.472	45.634
Total		4414657	74972	100.000	100.000

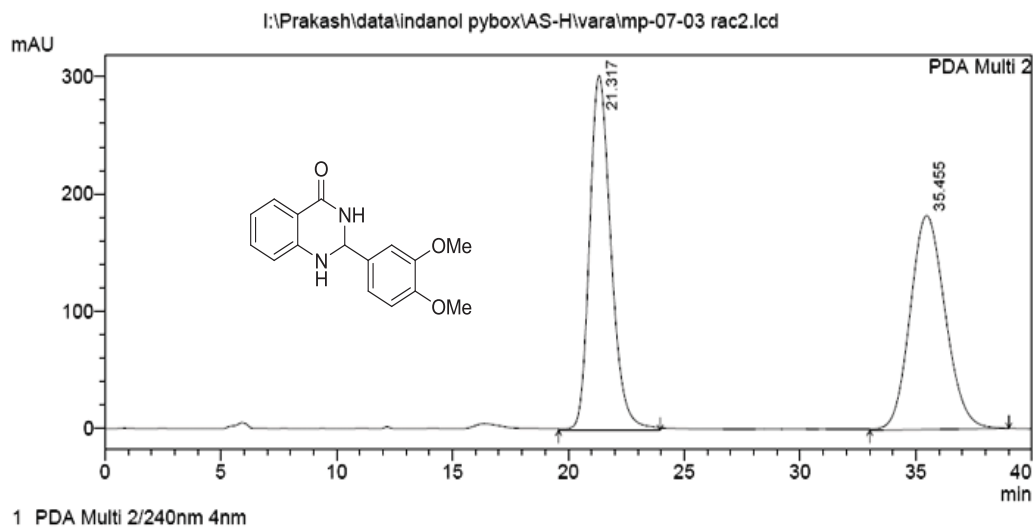


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.587	182105	3819	5.029	7.103
2	26.497	3439039	49947	94.971	92.897
Total		3621144	53766	100.000	100.000

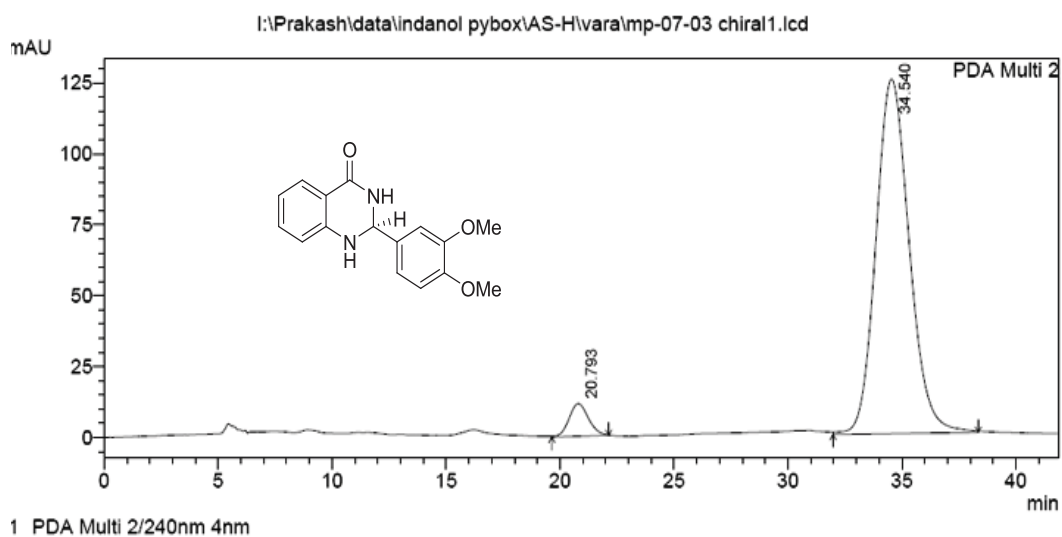
# HPLC Chromatogram of 2-(3,4-Dimethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (31).



PeakTable

PDA Ch2 240nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.317	19528012	302607	50.388	62.399
2	35.455	19226888	182346	49.612	37.601
Total		38754899	484953	100.000	100.000

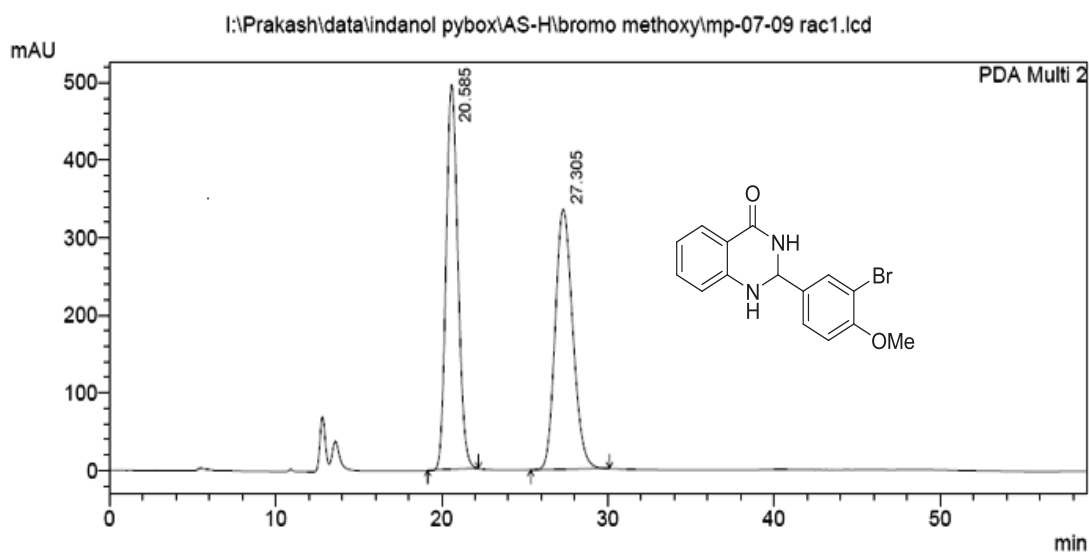


PeakTable

PDA Ch2 240nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.793	684513	11507	5.094	8.425
2	34.540	12754271	125072	94.906	91.575
Total		13438784	136578	100.000	100.000

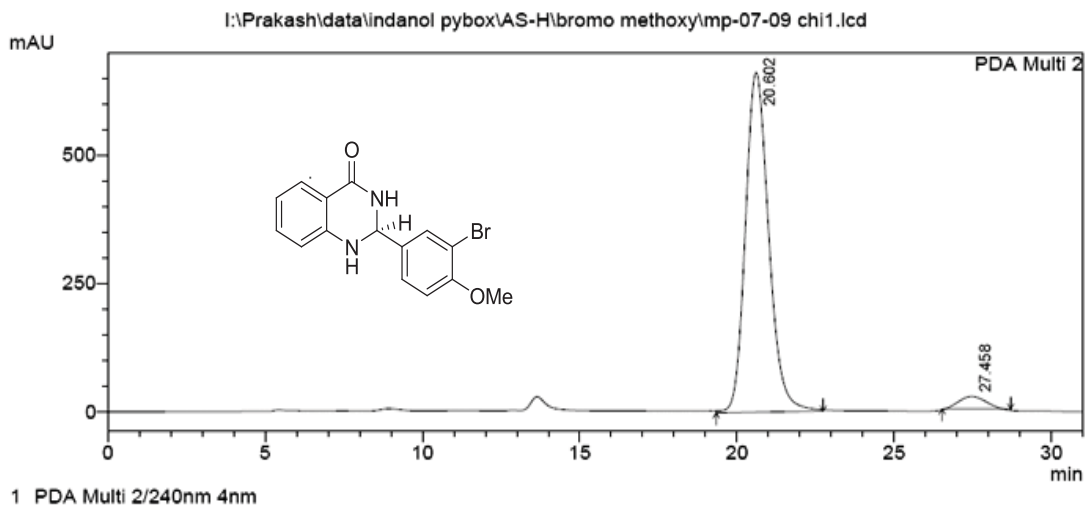
# HPLC Chromatogram of 2-(3-Bromo-4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3m).



PeakTable

PDA Ch2 240nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.585	24488968	496173	49.862	59.682
2	27.305	24624561	335195	50.138	40.318
Total		49113529	831368	100.000	100.000

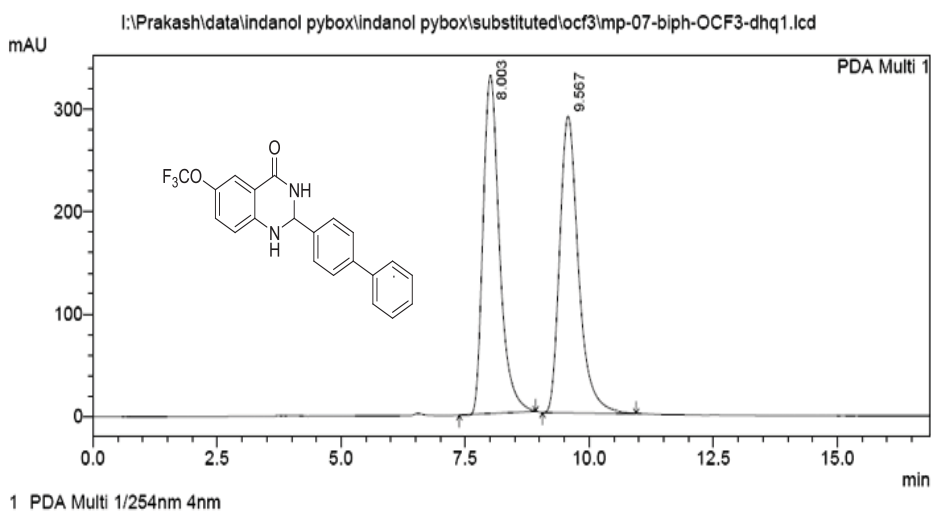


PeakTable

PDA Ch2 240nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.602	34178963	661843	95.999	96.431
2	27.458	1424327	24498	4.001	3.569
Total		35603289	686341	100.000	100.000

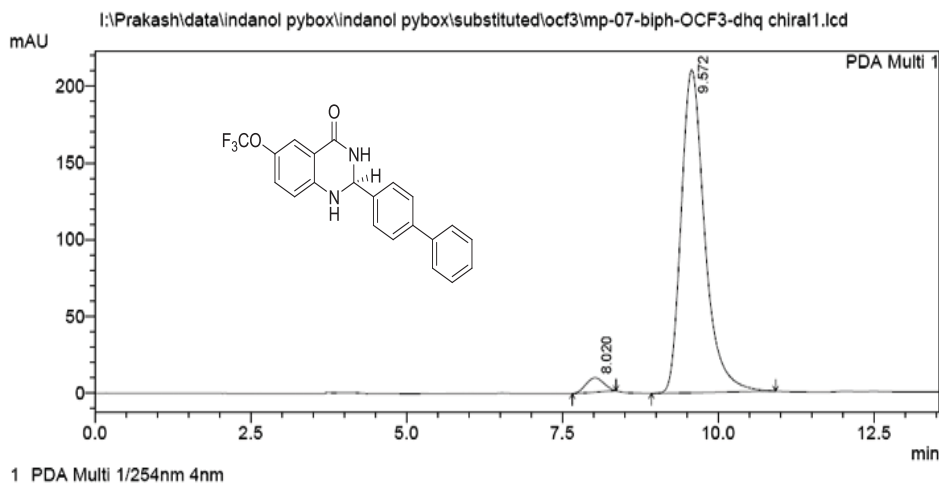
## HPLC Chromatogram of 2-(biphenyl-4-yl)-6-(trifluoromethoxy)-2,3-dihydroquinazolin-4(1H)-one (3n).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.003	7570252	330386	49.786	53.279
2	9.567	7635313	289719	50.214	46.721
Total		15205565	620105	100.000	100.000

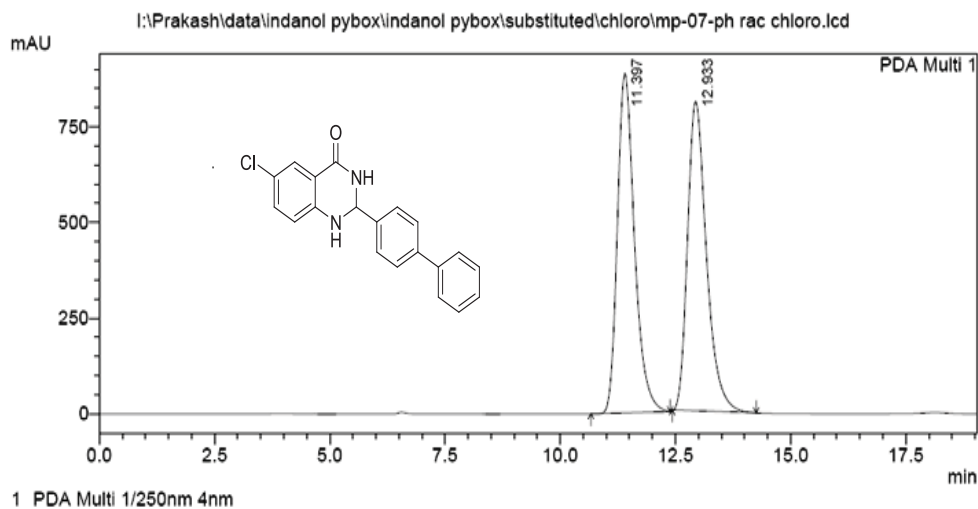


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.020	186784	9311	3.260	4.240
2	9.572	5542939	210263	96.740	95.760
Total		5729723	219574	100.000	100.000

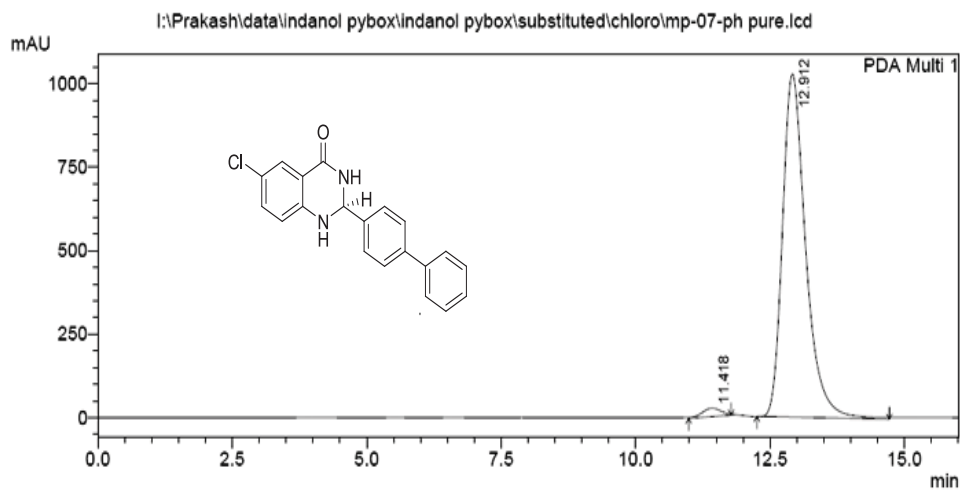
## HPLC Chromatogram of 2-(biphenyl-4-yl)-6-chloro-2,3-dihydroquinazolin-4(1H)-one (3o).



PeakTable

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.397	22896731	887075	49.873	52.341
2	12.933	23013333	807734	50.127	47.659
Total		45910064	1694809	100.000	100.000



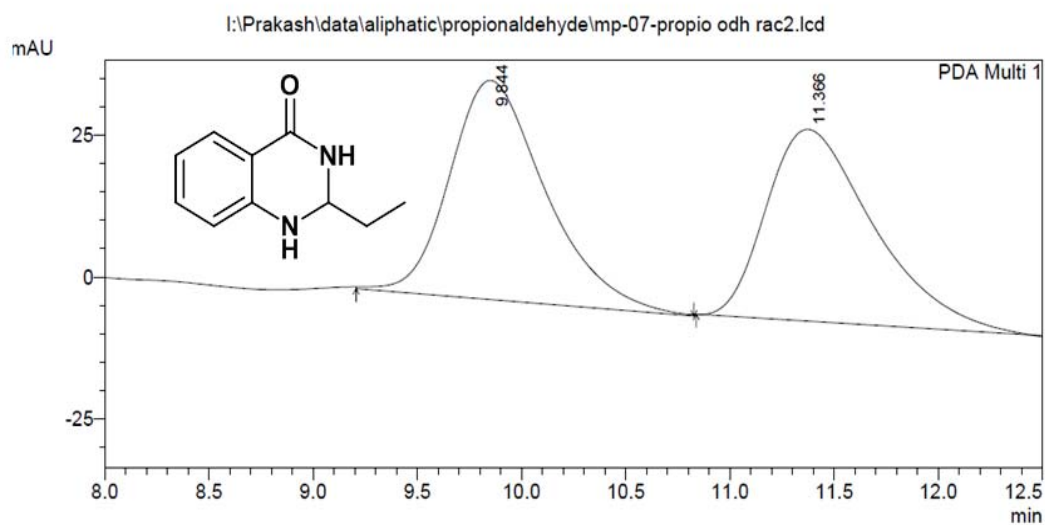
PeakTable

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.418	627000	25390	1.996	2.412
2	12.912	30786789	1027438	98.004	97.588
Total		31413789	1052829	100.000	100.000

**Table 7**

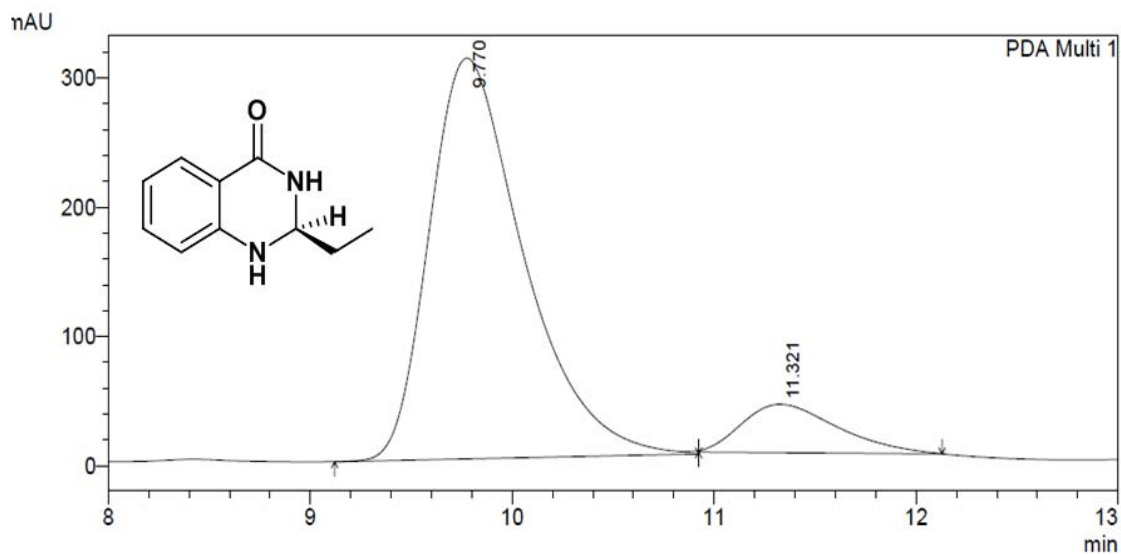
**HPLC Chromatogram of 2-ethyl-2,3-dihydroquinazolin-4(1H)-one (13a)**



**Peak Table**

PDA Ch1 250nm 4nm

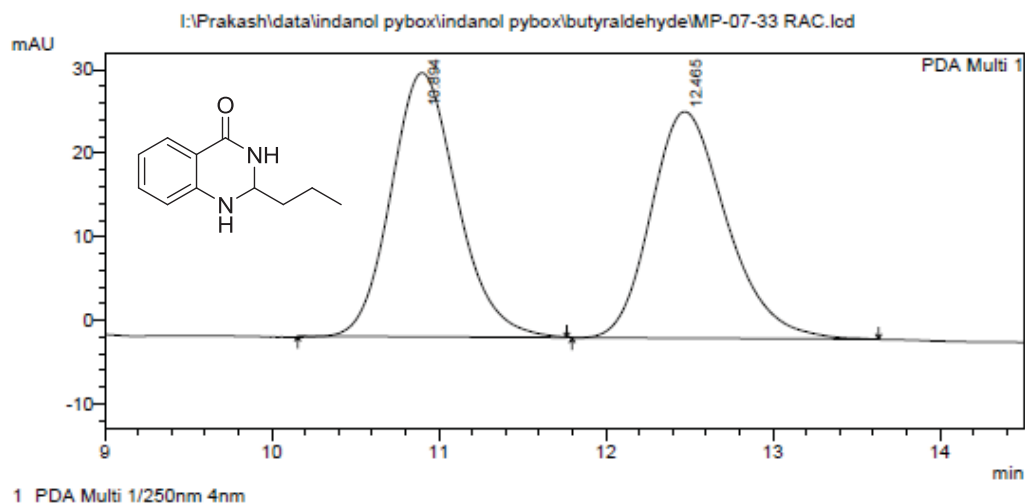
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.844	1235909	38608	50.626	53.329
2	11.366	1205349	33788	49.374	46.671
Total		2441257	72396	100.000	100.000



PDA Ch1 250nm 4nm

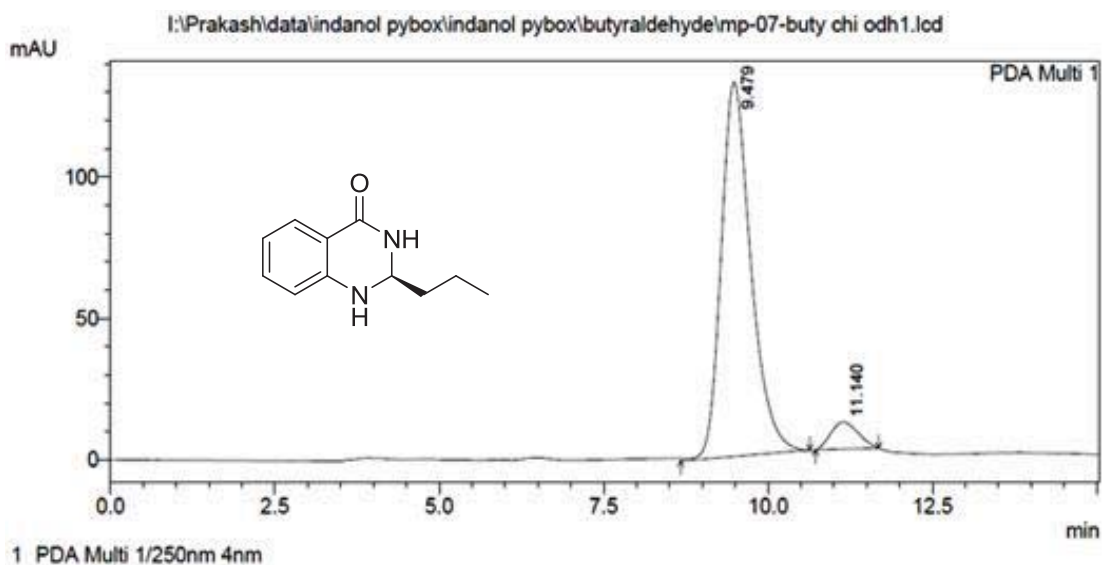
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.770	10066333	309950	89.053	89.237
2	11.321	1237408	37383	10.947	10.763
Total		11303740	347333	100.000	100.000

## HPLC Chromatogram of 2-propyl-2,3-dihydroquinazolin-4(1H)-one (13b)



PeakTable

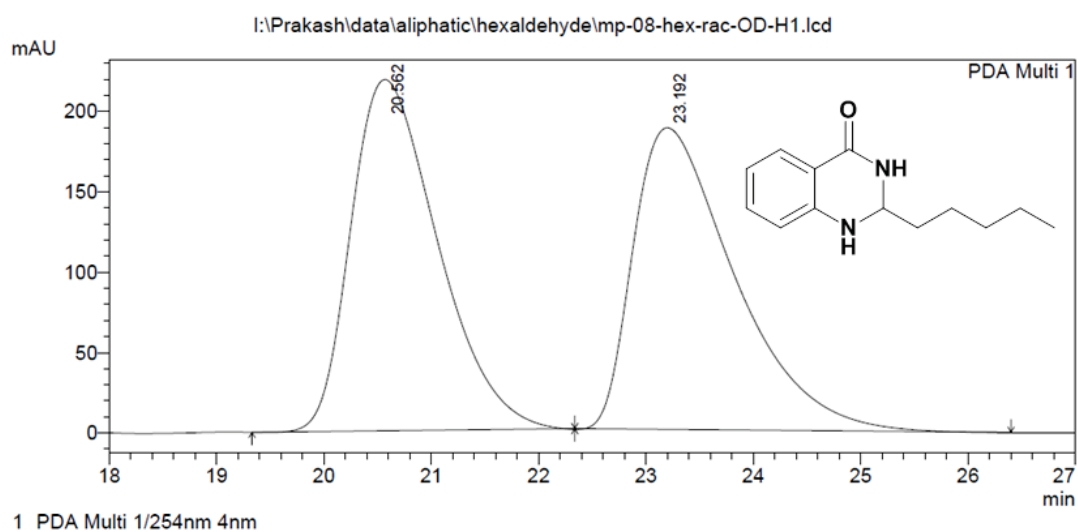
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.894	871161	31582	50.472	53.819
2	12.465	854878	27099	49.528	46.181
Total		1726040	58682	100.000	100.000



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.479	4177310	132485	93.790	93.297
2	11.140	276576	9519	6.210	6.703
Total		4453886	142004	100.000	100.000

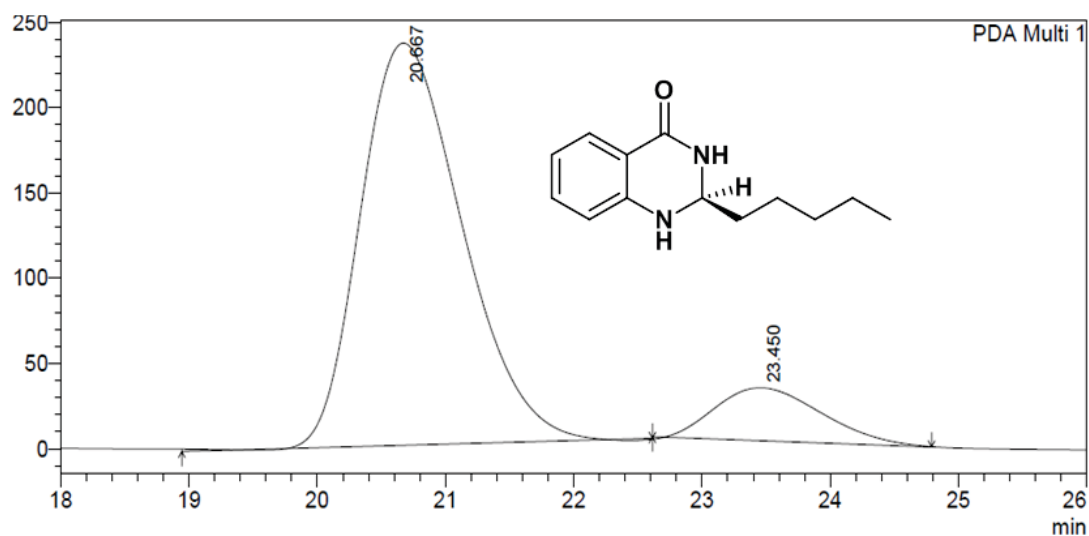
# HPLC Chromatogram of 2-pentyl-2,3-dihydroquinazolin-4(1H)-one (13c)



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.562	12273994	218544	49.977	53.804
2	23.192	12285213	187644	50.023	46.196
Total		24559208	406188	100.000	100.000



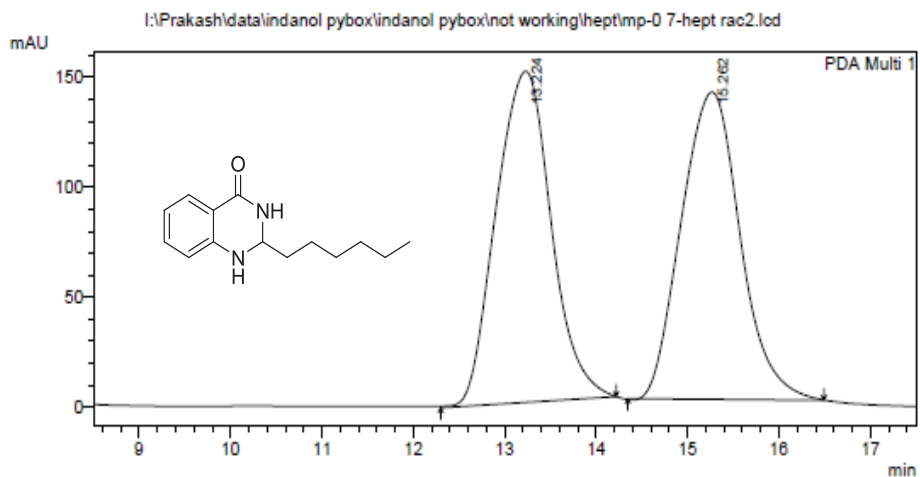
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.667	12967244	235805	87.881	88.363
2	23.450	1788272	31055	12.119	11.637
Total		14755516	266860	100.000	100.000



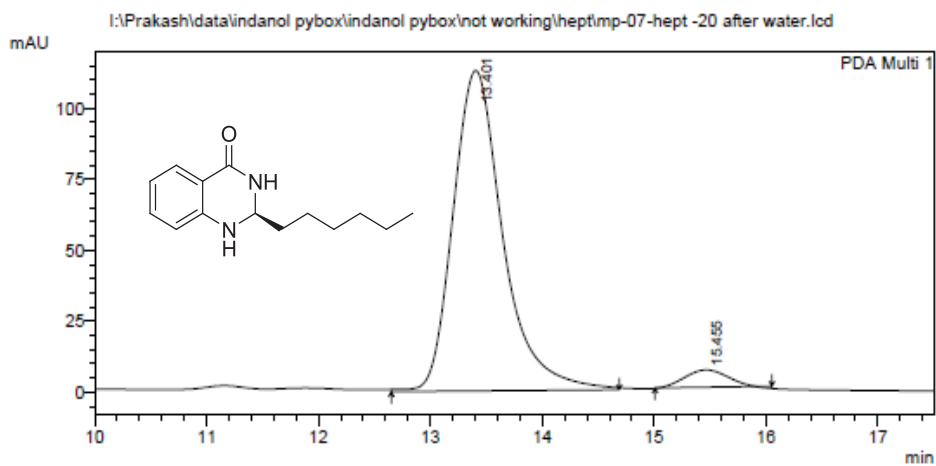
## HPLC Chromatogram of 2-hexyl-2,3-dihydroquinazolin-4(1H)-one (13d)



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.224	6329226	150741	50.265	51.882
2	15.262	6262376	139806	49.735	48.118
Total		12591602	290547	100.000	100.000

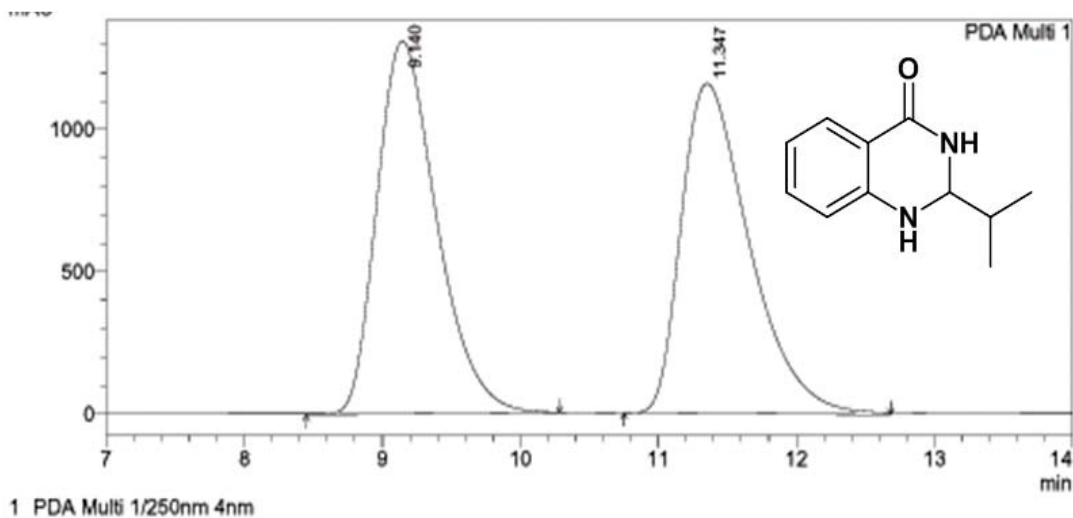


PeakTable

PDA Ch1 254nm 4nm

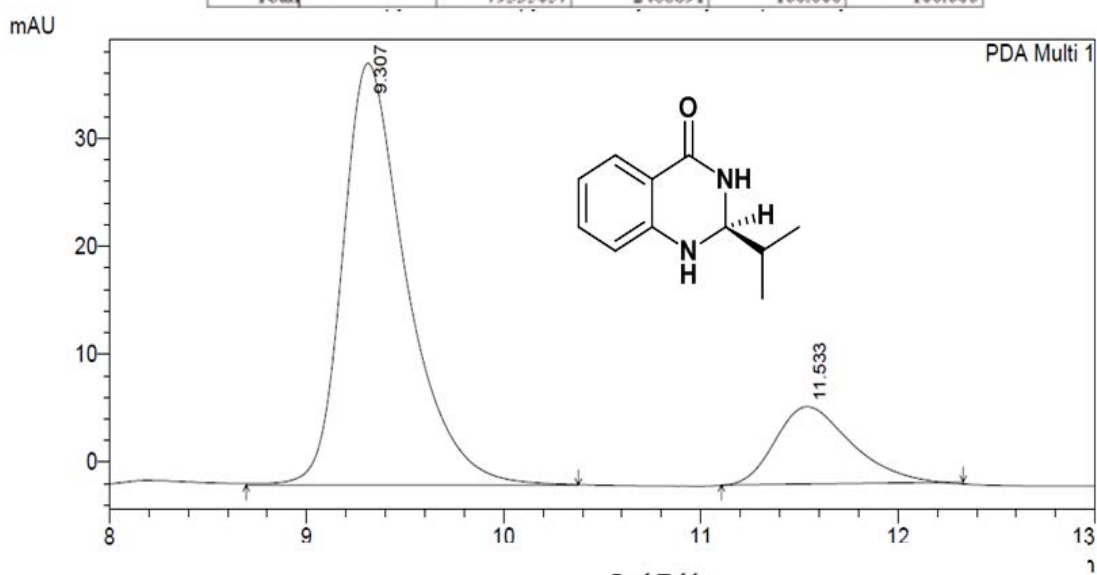
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.401	3500185	112909	95.710	94.874
2	15.455	156881	6101	4.290	5.126
Total		3657066	119010	100.000	100.000

# HPLC Chromatogram of 2-isopropyl-2,3-dihydroquinazolin-4(1H)-one (13e)



PeakTable

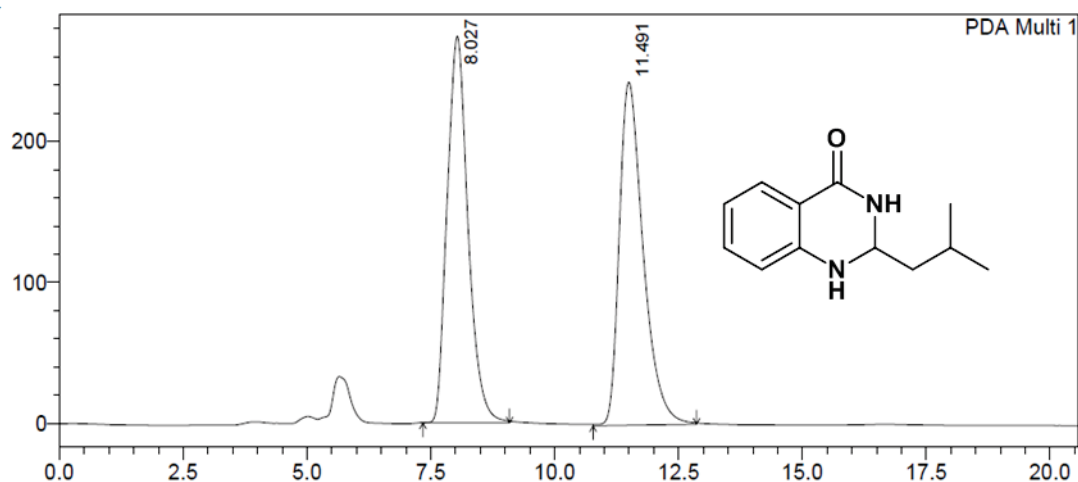
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.140	39548386	1309219	49.850	53.072
2	11.347	39786671	1157672	50.150	46.928
Total		79335057	2466891	100.000	100.000



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.307	880771	39103	82.157	84.503
2	11.533	191285	7171	17.843	15.497
Total		1072056	46275	100.000	100.000

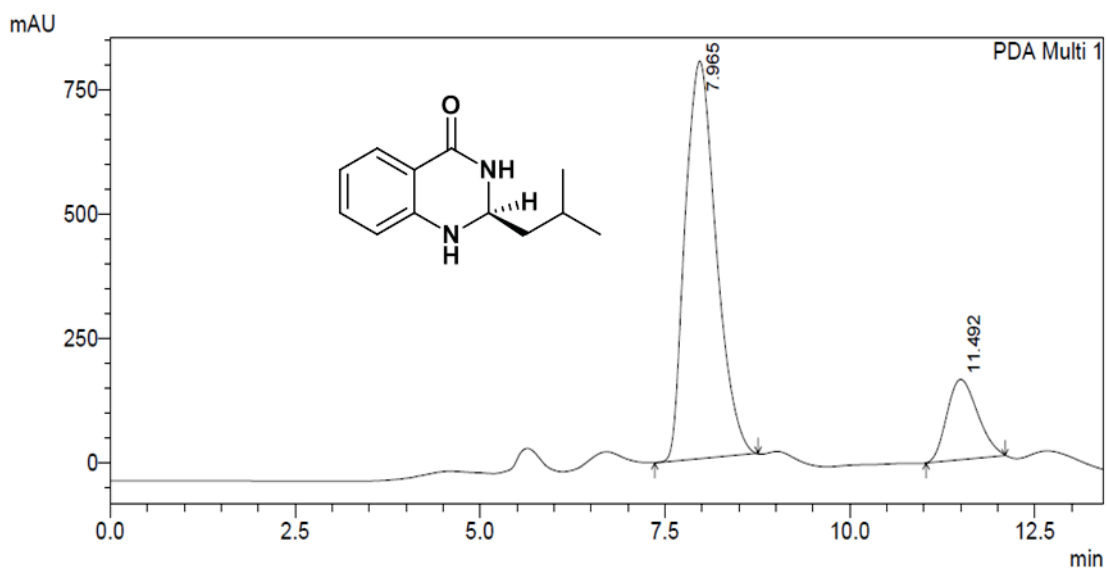
# HPLC Chromatogram of 2-isobutyl-2,3-dihydroquinazolin-4(1H)-one (13f)



PeakTable

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.027	8045027	273955	49.597	52.979
2	11.491	8175745	243142	50.403	47.021
Total		16220772	517097	100.000	100.000



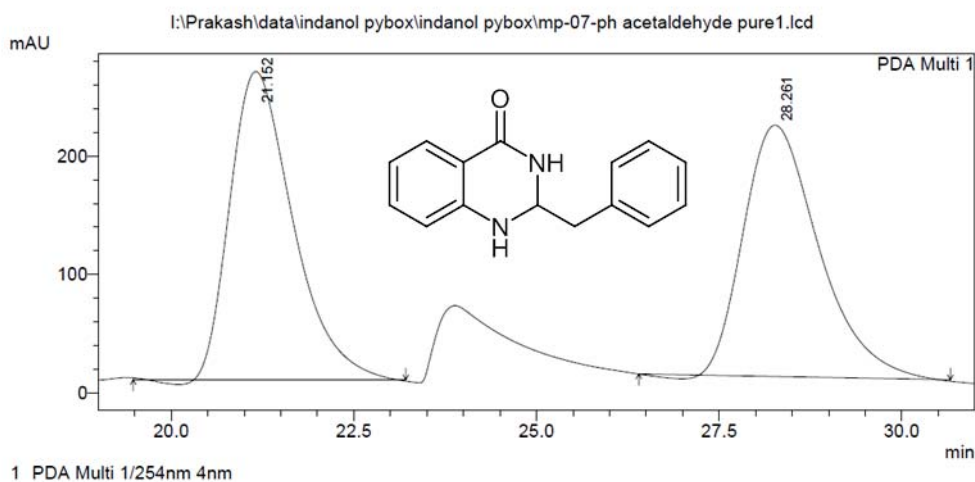
1 PDA Multi 1/250nm 4nm

PeakTable

PDA Ch1 250nm 4nm

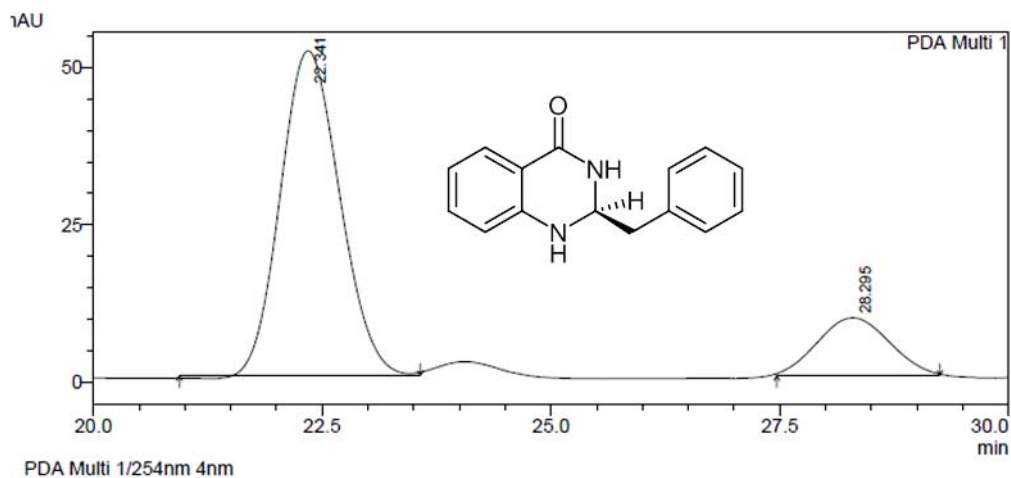
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.965	23396075	800045	83.319	83.190
2	11.492	4684196	161667	16.681	16.810
Total		28080271	961712	100.000	100.000

# HPLC Chromatogram of 2-benzyl-2,3-dihydroquinazolin-4(1H)-one (13g)



PeakTable

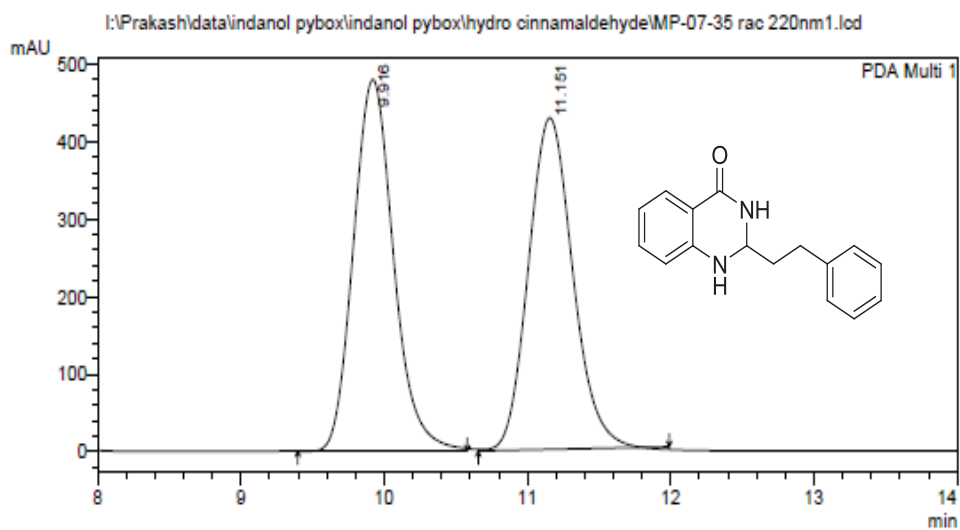
Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.152	15525413	260558	50.645	55.078
2	28.261	15129825	212514	49.355	44.922
Total		30655237	473072	100.000	100.000



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.341	2317537	51652	82.179	84.909
2	28.295	502566	9180	17.821	15.091
Total		2820103	60833	100.000	100.000

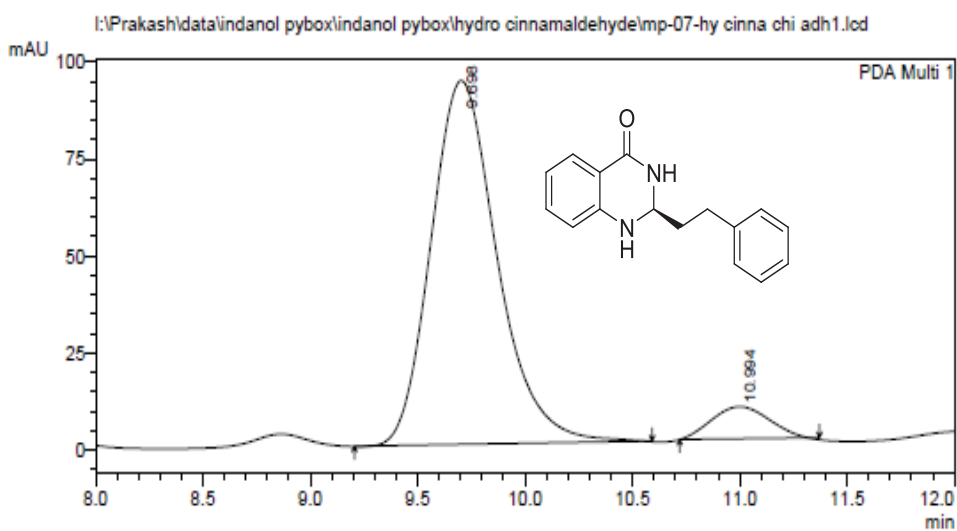
## HPLC Chromatogram of 2-phenethyl-2,3-dihydroquinazolin-4(1H)-one (13h)



Peak Table

PDA Ch1 254nm 4nm

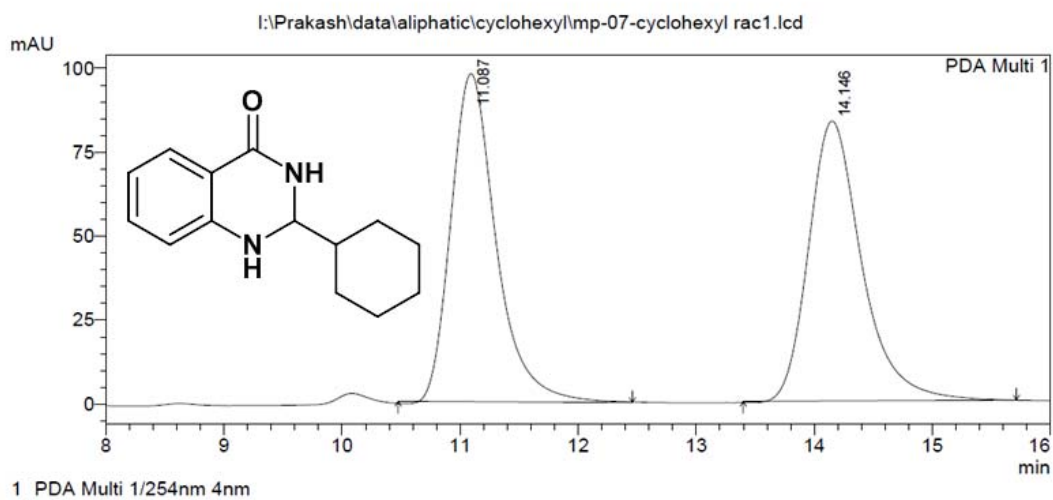
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.916	9328728	478924	50.456	52.844
2	11.151	9160058	427377	49.544	47.156
Total		18488786	906301	100.000	100.000



PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.698	2009802	93732	92.988	91.943
2	10.994	151544	8213	7.012	8.057
Total		2161346	101945	100.000	100.000

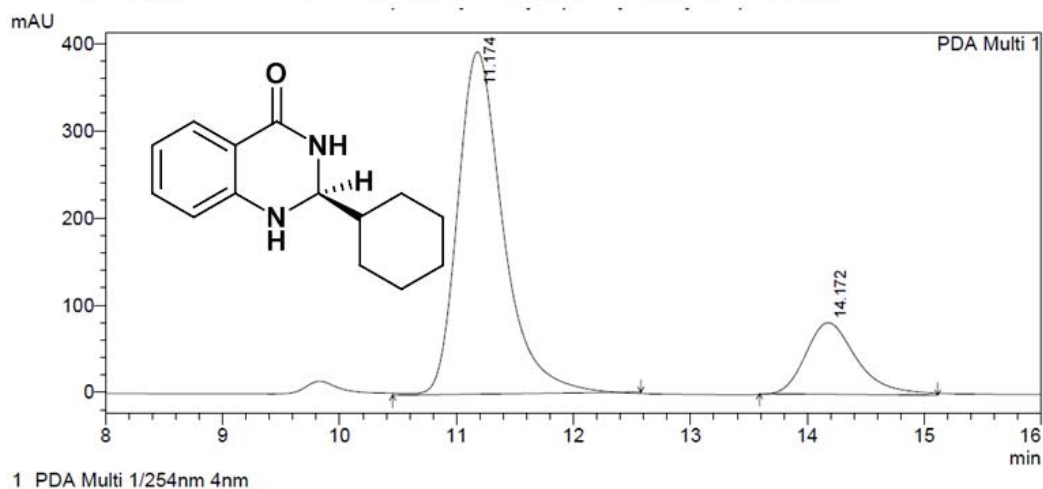
# HPLC Chromatogram of 2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (13i)



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.087	2593183	97749	49.900	53.975
2	14.146	2603564	83352	50.100	46.025
Total		5196747	181101	100.000	100.000

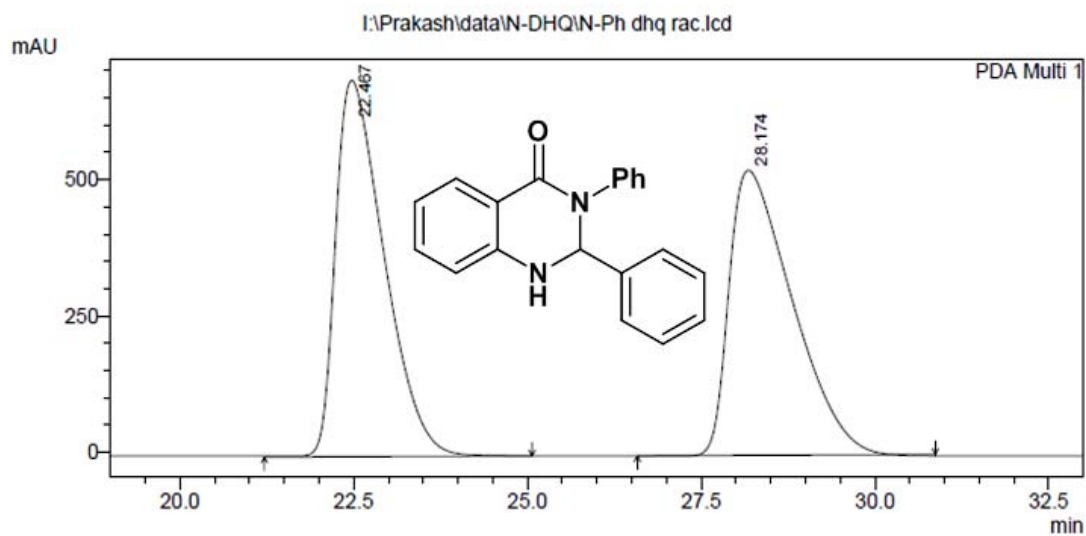


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.174	10572063	392641	80.909	82.712
2	14.172	2494578	82069	19.091	17.288
Total		13066641	474710	100.000	100.000

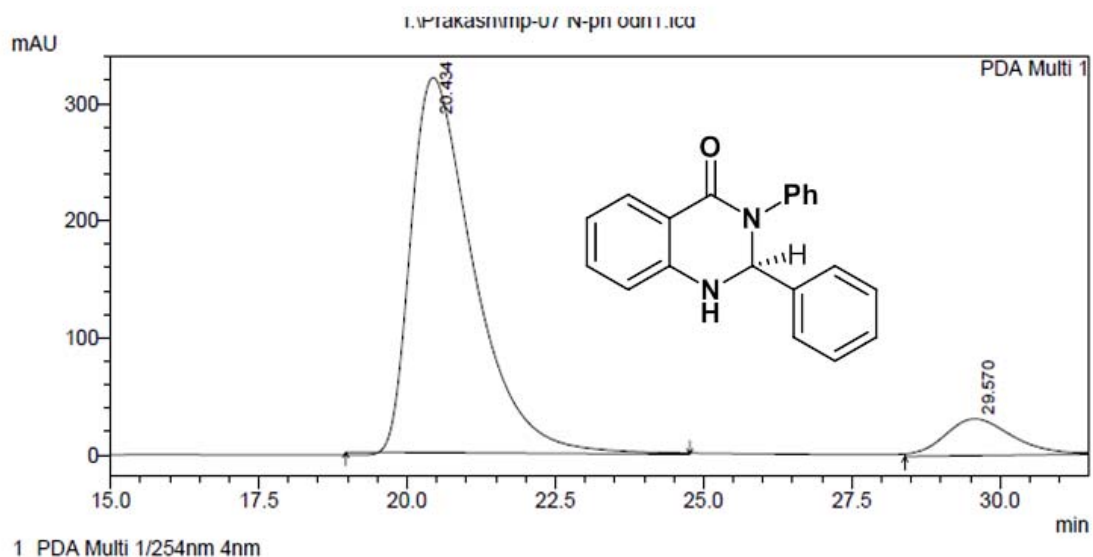
**Table 9**  
**HPLC Chromatogram of 2,3-diphenyl-2,3-dihydroquinazolin-4(1H)-one (15a)**



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.467	33480158	690113	50.471	56.925
2	28.174	32855845	522214	49.529	43.075
Total		66336003	1212327	100.000	100.000

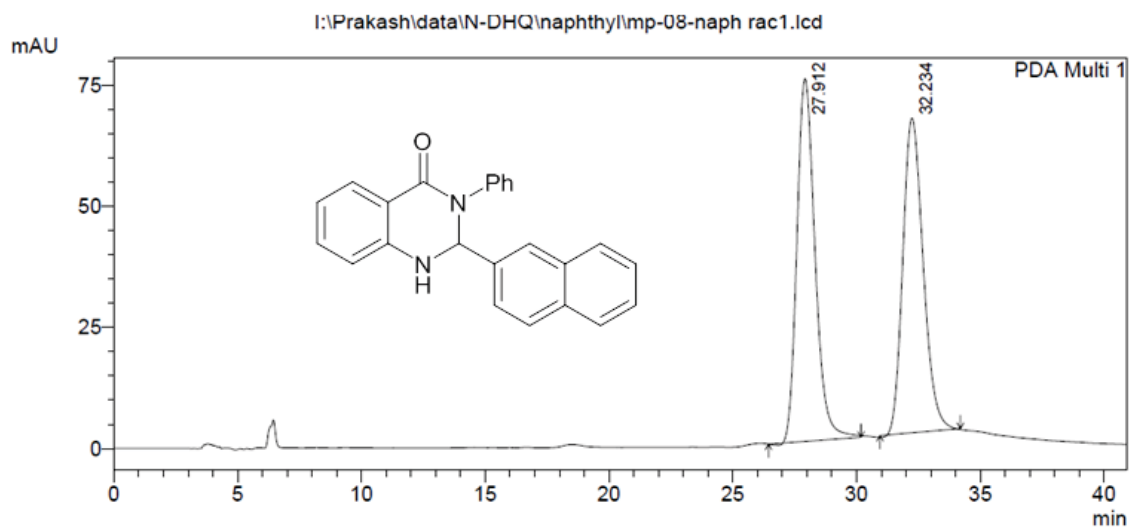


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.434	23499496	320290	90.309	91.064
2	29.570	2521762	31428	9.691	8.936
Total		26021258	351718	100.000	100.000

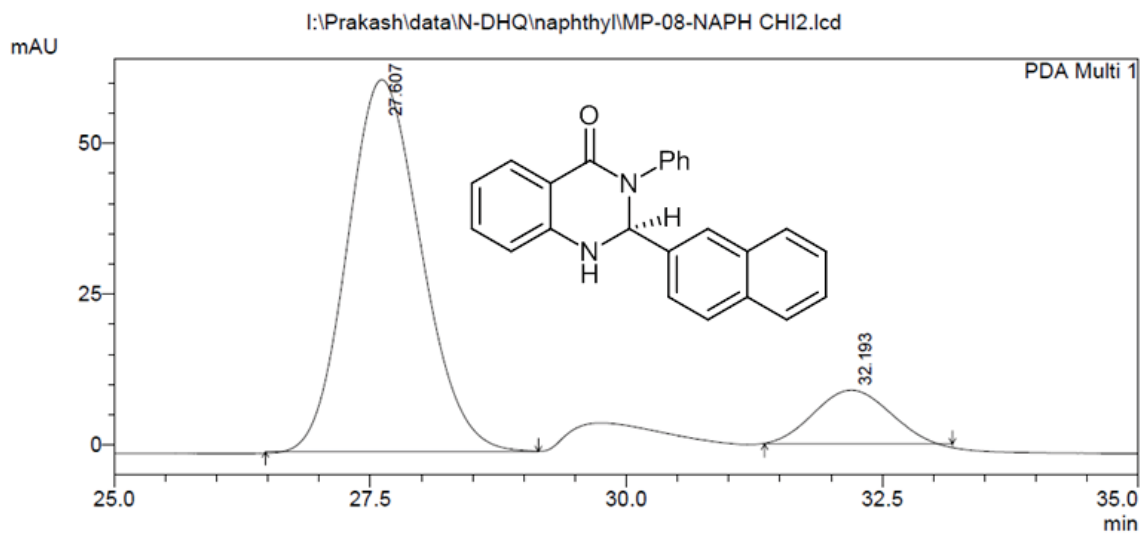
### HPLC Chromatogram of 2-(naphthyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15b).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.912	3816075	74930	50.698	53.551
2	32.234	3711001	64993	49.302	46.449
Total		7527076	139923	100.000	100.000



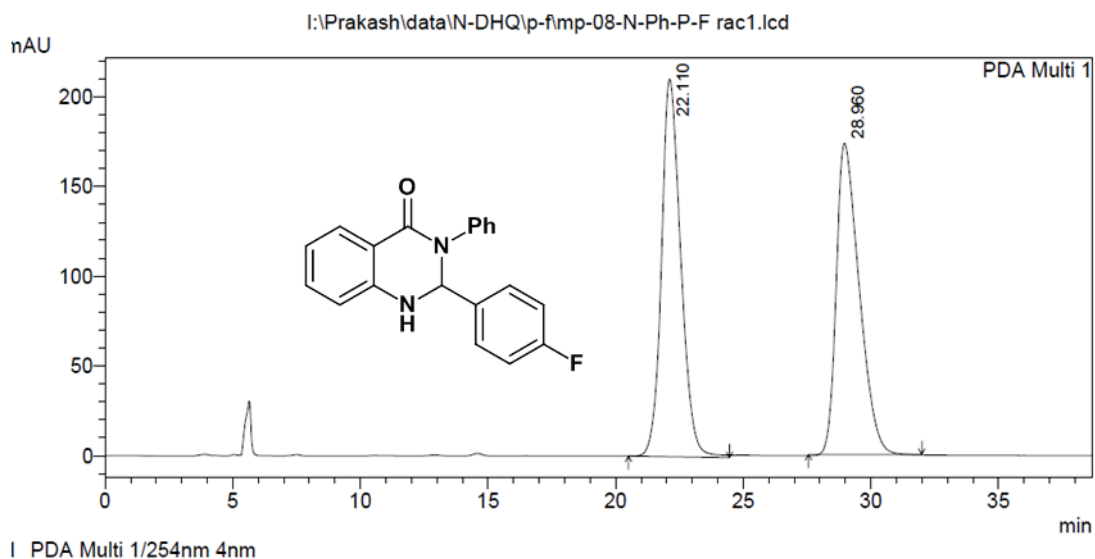
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.607	3092768	61700	87.169	87.347
2	32.193	455239	8938	12.831	12.653
Total		3548007	70638	100.000	100.000



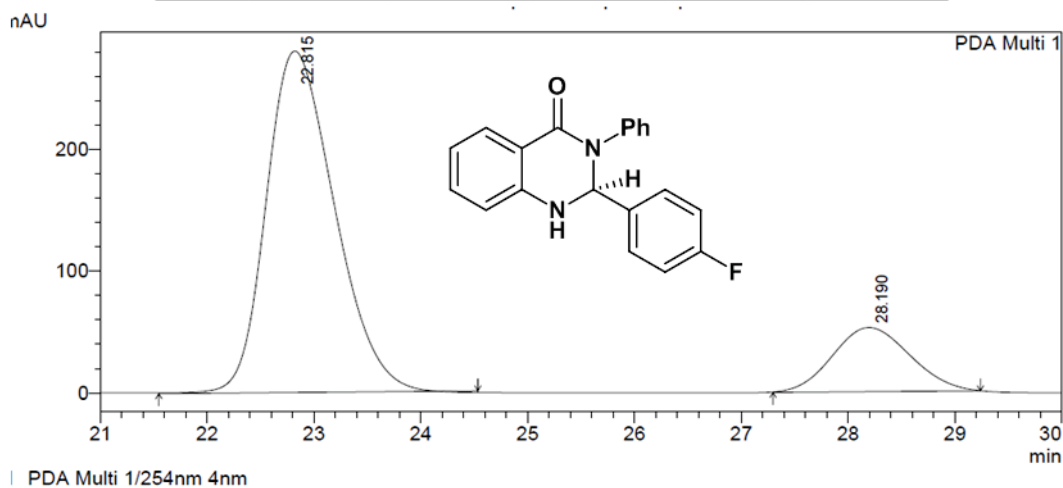
# HPLC Chromatogram of 2-(4-fluorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15c).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.110	11070741	210340	50.620	54.827
2	28.960	10799579	173303	49.380	45.173
Total		21870320	383642	100.000	100.000

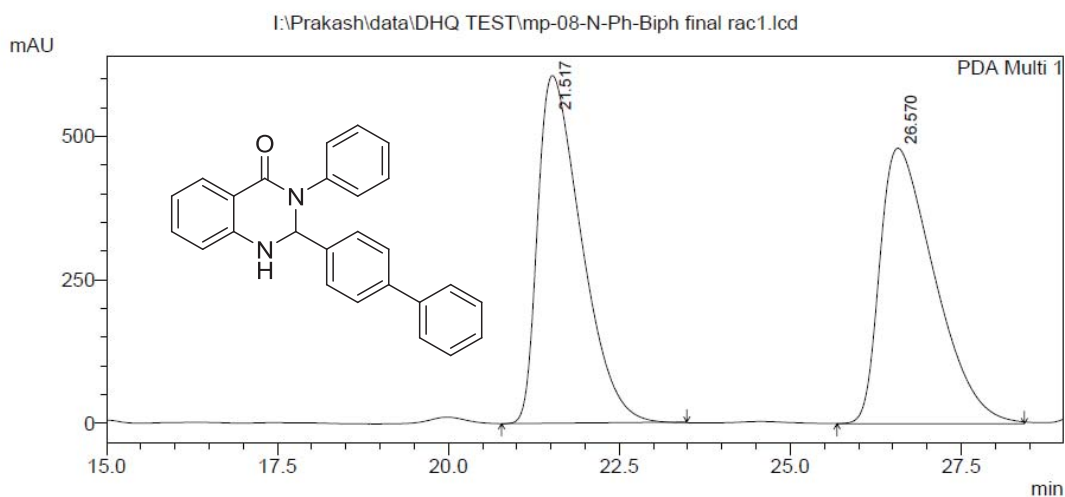


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.815	12479250	280847	82.454	84.196
2	28.190	2655595	52716	17.546	15.804
Total		15134846	333563	100.000	100.000

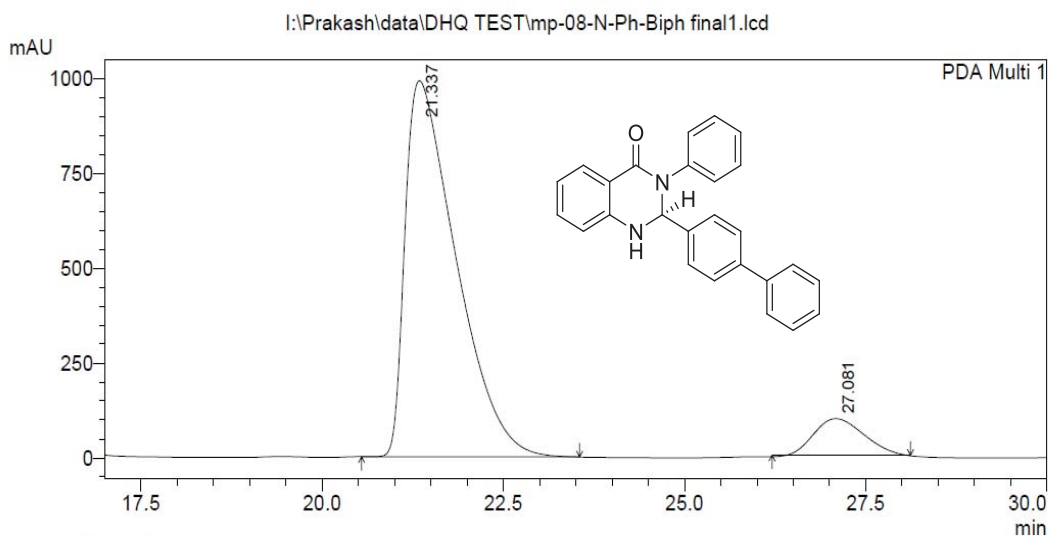
### HPLC Chromatogram of 2-(biphenyl-4-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15d).



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.517	26917561	605778	50.127	55.796
2	26.570	26781701	479923	49.873	44.204
Total		53699262	1085700	100.000	100.000

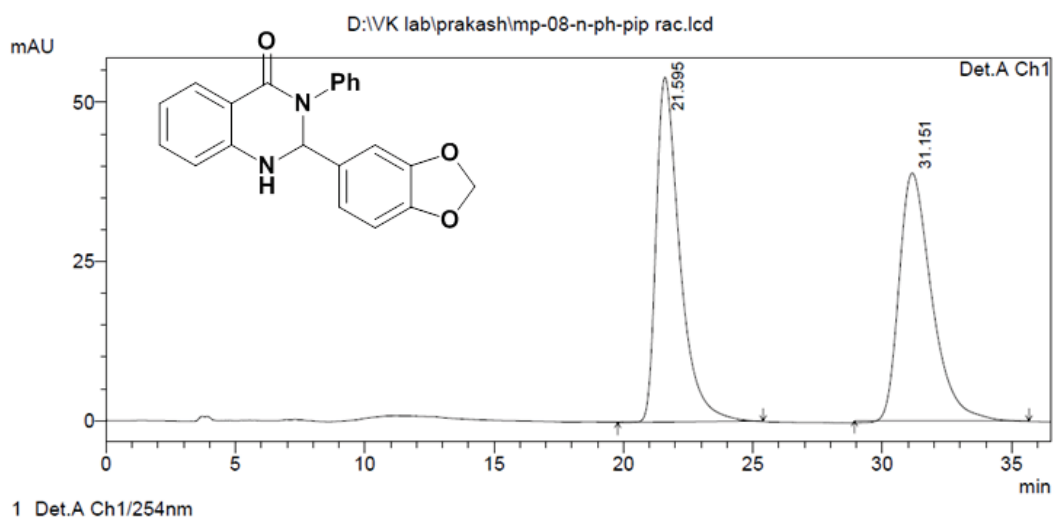


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.337	48453686	990674	91.411	91.135
2	27.081	4552747	96361	8.589	8.865
Total		53006433	1087035	100.000	100.000

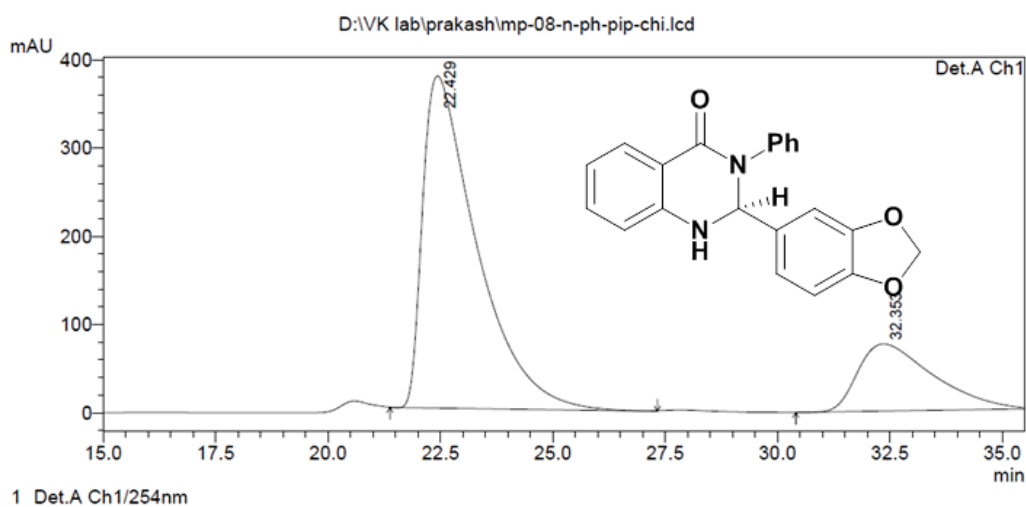
# HPLC Chromatogram of 2-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15e).



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.595	3446001	54148	50.398	58.187
2	31.151	3391586	38911	49.602	41.813
Total		6837587	93059	100.000	100.000

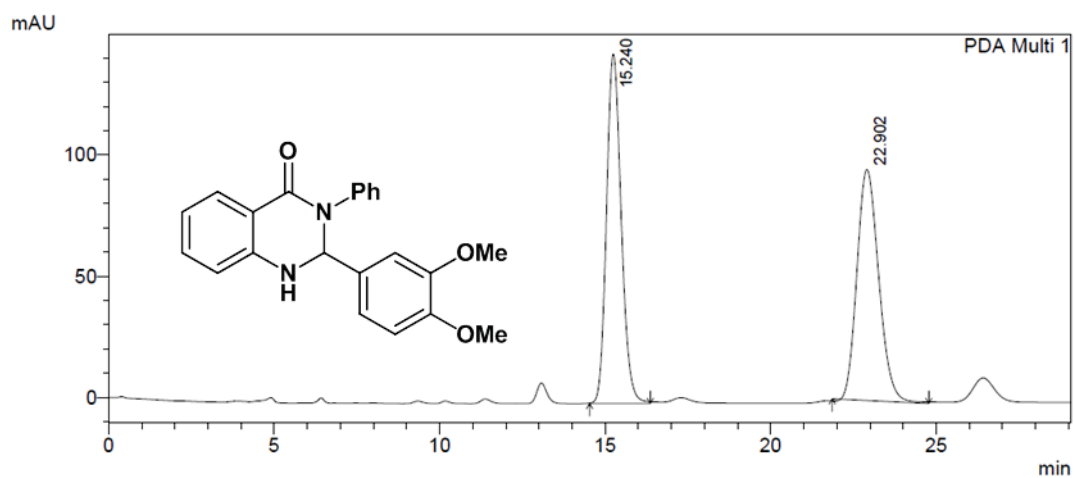


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.429	31519066	376301	78.036	83.191
2	32.353	8871438	76031	21.964	16.809
Total		40390504	452332	100.000	100.000

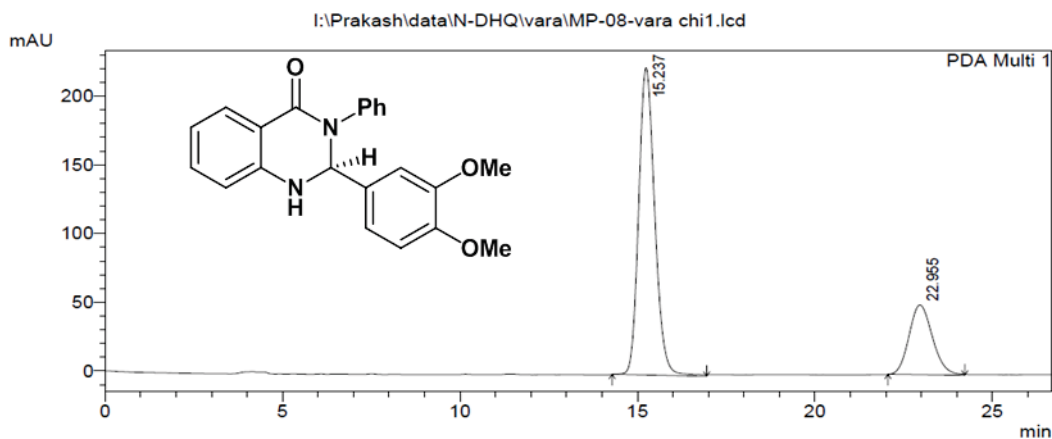
# HPLC Chromatogram of 2-(3,4-dimethoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (15f)



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.240	4454910	144102	50.633	60.218
2	22.902	4343578	95200	49.367	39.782
Total		8798488	239303	100.000	100.000



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.237	7031820	223506	75.174	81.525
2	22.955	2322294	50650	24.826	18.475
Total		9354114	274156	100.000	100.000