**Synthesis of 2,3-dihydroquinazolinones and quinazolin-4(3H)-one catalyzed by Graphene Oxide nanosheets in aqueous medium: “on-water” synthesis accompanied by carbocatalysis and selective C-C bond cleavage**

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Materials and Methods

$^1$H-NMR and $^{13}$C-NMR spectral analysis were carried out on Bruker-Advance Digital 300 MHz and 75 MHz instruments where tetramethylsilane (TMS) was used as internal standard. Infrared spectra were recorded in KBr pallets in reflection mode on a Perkin Elmer RX-1 FTIR spectrophotometer. Suitable single crystal of compound 3h, 5a and 5j was mounted on a Bruker-AXS SMART APEX II diffractometer equipped with a graphite monochromator. All the reactions were monitored by thin layer chromatography carried out on Merck aluminum-blocked silica gel plates coated with silica gel G under UV light and also by exposure to iodine vapor for detection. Melting points were recorded on a Köfler Block apparatus. Synthetic grade chemicals from Sigma-Aldrich, Spectrochem and E-Merck were used for carrying out the organic reactions.
Preparation of GO

Natural graphite powder is used for the synthesis of GO nanosheets. Graphite powder (1000 mg) and NaNO₃ (1000 mg) were added to 35 ml of concentrated H₂SO₄ (98%) under vigorous stirring in a 250 ml conical flask placed in an ice bath. The whole mass was converted to black slurry (it takes 2 min), then KMnO₄ (5000 mg) was added slowly to the slurry maintaining the reaction temperature between 15 °C and 20 °C. After 3 h, the entire system was taken out of the ice bath and diluted with 100 ml water and then further stirred for 3 h at ambient temperature. 200 ml hot water was added to the above reaction mixture followed by 30% H₂O₂ until the excess permanganate and manganese dioxide had been reduced to colourless soluble manganese sulfate. The resultant yellow precipitate was washed with distilled water several times and then was subjected to centrifuge to get the pure graphene oxide powder. After repeated centrifugation, salts and ions results from the oxidation process can be removed from GO suspensions. The GO nanosheets sample was collected and dried at 60 °C for 24 h. The GO nanosheets were characterized using XRD, FTIR, FESEM and TEM images.

General Procedure for the synthesis of 2, 3-dihydroquinazolinones:

Anthranilamide (1 mmol) was added to aldehyde/ketone derivative (1 mmol) in aqueous medium (3 ml water) followed by GO nanosheets (25 mg) at room temperature. The mixture was then stirred for the required period of time (indicated by TLC). After completion of each reaction, product and the catalysts separated from reaction system by simple filtration. The crude product was then dissolved in EtOH (3 ml) and this allows separation of minute quantity of the catalyst through filtration and crystallization of the crude product from EtOH furnished pure compound. All compounds were well characterized by ¹H, ¹³C NMR and FT-IR analysis.
General Procedure for the synthesis of quinazolin-4(3H)-one:

a) Anthanilamide (1 mmol) was added to aldehyde/ketone derivative (1 mmol) in aqueous medium (3 ml water) followed by GO nanosheets (25 mg) and oxone (307 mg) at room temperature. The mixture was then stirred for the required period of time (indicated by TLC). After completion of each reaction, crude product was separated from reaction system by simple filtration. The crude product was then dissolved in EtOH (3 ml) and filtered. Finally crystallization of the crude product from EtOH offered the pure compound. All compounds were well characterized by $^1$H, $^{13}$C NMR and FT-IR analysis.

b) Anthanilamide (1 mmol) was added to 1,3-diketones derivative (1 mmol) in aqueous medium (3 ml water) followed by GO nanosheets (25 mg) at 60 °C. The mixture was then stirred for the required period of time (indicated by TLC). After completion of each reaction, the crude product mixture was extracted with ethyl acetate (2x3ml) and finally purified by column chromatography (eluent- ethyl acetate/petroleum ether: 1:4). All compounds were well characterized by $^1$H, $^{13}$C NMR and FT-IR analysis.
2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3a)

Yield: 94%, (0.211 g); M.p. 224-226 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 5.79 (s, 1H), 5.87 (s, 1H), 6.6 (d, 1H, $J$=7.8 Hz), 6.88 (t, 1H, $J$= 7.5 Hz), 7.23-7.34 (m, 1H), 7.42-7.58 (m, 3H), 7.5-7.6 (m, 2H), 7.9 (dd, 1H, $J$= 7.8 Hz, $J$= 1.5 Hz); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 89.0, 124.7, 127.6, 127.7, 128.6, 128.7, 129.1, 131.2, 131.3, 133.4, 133.5, 139.3, 144.5, 160.1; IR (KBr) cm$^{-1}$: 1615, 1659, 2925, 3061, 3186, 3302.

2-(m-tolyl)-2,3-dihydroquinazolin-4(1H)-one (3b)

Yield: 92%, (0.219 g); M.p. 185-187 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, DMSO-d$_6$): $\delta$ 2.32 (s, 3H), 5.72 (s, 1H), 6.65-6.76 (m, 2H), 7.08 (s, 1H), 7.18-7.32 (m, 5H), 7.6 (d, 1H, $J$= 6.9 Hz), 8.26 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-d$_6$): $\delta$ 21.5, 67.00, 114.8, 117.5, 124.4, 127.7, 127.9, 128.6, 129.5, 133.7, 137.8, 141.9, 148.3, 164.0; IR (KBr) cm$^{-1}$: 1610, 1655, 2920, 3063, 3185, 3305.
2-(3-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (3c)

Yield: 96%, (0.258 g); M.p. 192-194 °C; Characteristics: Yellow crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): δ 5.39 (s, 1H), 5.82 (s, 1H), 6.65 (t, 2H, $J$=8.1 Hz), 7.13-7.18 (m, 1H), 7.34-7.44 (m, 1H), 7.62-7.69 (m, 2H), 8.1 (d, 2H, $J$=6.9 Hz); $^{13}$C NMR (75 MHz, DMSO-D$_6$): δ 82.6, 114.9, 117.9, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.0, 147.8, 163.9; HRMS (ESI-TOF) m/z Calculated for $[C_{14}H_{11}N_3O_3+Na]^+$: 292.0693, found: 292.0695; IR (KBr) cm$^{-1}$: 1345, 1461, 1520, 1608, 1647, 2855, 2922, 3032, 3174, 3278.

2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3d)

Yield: 95%, (0.236 g); M.p. 200-202 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): δ 6.13 (s, 1H), 6.36 (s, 1H), 6.67 (d, 1H, $J$= 8.1 Hz), 6.89 (t, 1H, $J$= 7.5Hz), 7.31-7.44 (m, 4H), 7.73-7.77 (m, 1H), 7.93 (d, 1H, $J$= 7.5 Hz); $^{13}$C NMR (75 MHz, CDCl$_3$): δ 66.2, 114.9, 115.4, 117.7, 127.8, 128.8, 129.2, 133.4, 133.9, 141.1, 148.1, 163.9; IR (KBr) cm$^{-1}$: 1618, 1650, 2922, 3051, 3176, 3307.
2-(4-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3e)

Yield: 95%, (0.287 g); M.p. 203-205 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 5.74 (s, 1H), 6.02 (s, 1H), 6.55-6.71 (m, 2H), 7.17-7.44 (m, 6H), 7.74 (s, 1H) ; $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 66.3, 114.9, 115.5, 117.8, 127.8, 128.8, 129.2, 133.4, 133.9, 141.2, 148.1, 163.9; IR (KBr) cm$^{-1}$: 16012, 1662, 2932, 3062, 3180, 3310.

2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3f)

Yield: 95%, (0.245 g); M.p. 197-198 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 5.82 (s, 1H), 5.90(s, 1H), 6.69 (d, 1H, $J$= 8.1 Hz), 6.92 (t, 1H, $J$= 7.7 Hz) 7.33-7.44(m, 2H), 7.43 (d, 2H, $J$= 8.4 Hz), 7.55 (d, 2H, $J$= 8.4 Hz), 7.93-7.96 (m, 1H); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 66.2, 114.9, 115.4, 117.7, 127.8, 128.8, 129.2, 133.4, 133.9, 141.1, 148.1, 163.9 ; IR (KBr) cm$^{-1}$: 1607, 1658, 2927, 3060, 3188, 3306.
2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (3g)

Yield: 92%, (0.219 g); M.p. 232-233 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 2.39 (s, 3H), 5.78 (s, 1H), 5.87 (s, 1H), 6.67 (d, 1H, $J$ = 8.1 Hz), 6.90 (t, 1H, $J$ = 7.5Hz), 7.26-7.42 (m, 5H), 7.95 (d, 1H, $J$ = 7.8Hz) ; $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 21.4, 67.10, 114.8, 117.5, 124.4, 127.7, 127.9, 128.6, 129.5, 133.7, 137.8, 141.9, 148.3, 154.1, 164.1; IR (KBr) cm$^{-1}$: 1512, 1607, 1908, 2855, 2924, 3060, 3189, 3312.

2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (3h)

Yield: 97%, (0.261 g); M.p. 200-202 °C; Characteristics: Yellow crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 6.05 (s, 1H), 6.09 (s, 1H) 6.71 (d, 1H, $J$= 7.8 Hz), 6.94 (t, 1H, $J$= 7.5Hz), 7.37 (t, 1H, $J$= 7.8Hz), 7.79 (d, 2H, $J$= 8.1 Hz), 7.94 (d, 1H, $J$= 7.8 Hz), 8.30 (d, 2H, $J$= 7.8 Hz) ; $^{13}$C NMR (75 MHz, DMSO-D$_6$): $\delta$ 79.9, 114.9, 117.9, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.0, 147.7, 163.9; IR (KBr) cm$^{-1}$: 1525, 1615, 1643, 2856, 2923, 3030, 3179, 3288.
2-(4-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3i)

Yield: 88%, (0.211 g); M.p. 210-212 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 4.43 (s, 1H), 5.78 (s, 1H), 5.86 (s, 1H), 6.67 (d, 1H, $J$=8.1 Hz), 6.90 (t, 1H, $J$=7.5 Hz), 7.26-7.42 (m, 5H), 7.95 (d, 1H, $J$=7.8 Hz), 8.33 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-d$_6$): $\delta$ 66.8, 114.0, 114.8, 115.5, 117.5, 127.7, 128.6, 133.7, 133.9, 148.4 159.8, 164.1; IR (KBr) cm$^{-1}$: 1622, 1655, 2930, 3062, 3179, 3302, 3342.

2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3j)

Yield: 89%, (0.226 g); M.p. 177-178 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, DMSO-D$_6$): $\delta$ 3.77 (s, 3H), 5.72 (s, 1H), 6.65-6.76 (m, 2H), 7.17-7.32 (m, 6H), 7.61 (d, 1H, $J$=6.9 Hz) 8.26 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-D$_6$): $\delta$ 55.6, 66.7, 114.0, 114.8, 115.4, 117.5, 127.7, 128.6, 133.6, 133.9, 148.4 159.8, 164.1; IR (KBr) cm$^{-1}$: 1473, 1599, 1676, 2923, 3183, 3315, 3448.
2-(2-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3k)

Yield: 89%, (0.214 g); M.p. 220-221 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 4.61 (s, 1H), 5.92 (s, 1H), 5.98 (s, 1H), 6.54-6.72 (m, 4H), 6.77 (d, 1H, $J$=7.8 Hz), 7.02 (d, 1H, $J$=7.5 Hz), 7.11-7.33 (m, 2H), 8.91 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-D$_6$): $\delta$ 69.9, 128.4, 128.5, 128.6, 129.0, 132.1, 132.7, 133.9, 135.8, 140.5, 156.7, 166.6; IR (KBr) cm$^{-1}$: 1618, 1663, 2932, 3056, 3176, 3306, 3340.

2-(thiophen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (3l)

Yield: 90%, (0.207 g); M.p. 191-193 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 5.95 (s, 1H), 6.21 (s, 1H), 6.71 (d, 1H, $J$=7.5 Hz), 6.93 (t, 1H, $J$=8.1 Hz), 7.02-7.05 (m, 1H), 7.23-7.42 (m, 3H), 7.95 (d, 1H, $J$=5.7); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 62.1, 112.9, 113.9, 121.0, 126.5, 126.7, 127.6, 134.9, 143.4, 145.4, 146.2, 160.0; IR (KBr) cm$^{-1}$: 1376, 1457, 1651, 1763, 2853, 2923, 3448.
2-isopropyl-2,3-dihydroquinazolin-4(1H)-one (3m)

Yield: 88%, (0.167 g); M.p. 180-182 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 0.93 (d, 6H, \(J=6.9\) Hz), 1.89 (m, 1H), 4.59 (d, 1H, \(J=6.9\) Hz), 6.59-6.69 (m, 4H), 7.18 (s, 1H), 7.74 (s, 1H); \(^{13}\)C NMR (75 MHz, DMSO-D\(_6\)): \(\delta\) 16.9, 17.3, 33.2, 69.6, 114.5, 115.1, 116.9, 127.6, 133.4, 148.9, 164.3; IR (KBr) cm\(^{-1}\): 1372, 1457, 1656, 1763, 2853, 2923, 3206, 3448.

2-(2-hydroxy-4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3n)

Yield: 87%, (0.235 g); M.p. 227-228 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, DMSO-D\(_6\)): \(\delta\) 3.72 (s, 3H), 4.92 (s, 1H), 5.42 (s, 1H), 5.94 (s, 1H), 6.58-6.70 (m, 3H), 7.03-7.16 (m, 2H), 7.19 (t, 1H, \(J=7.2\) Hz), 7.53 (d, 1H, \(J=7.5\) Hz); \(^{13}\)C NMR (75 MHz, DMSO-D\(_6\)): \(\delta\) 55.7, 66.8, 114.0, 114.8, 115.4, 117.5, 127.7, 128.6, 133.6, 133.9, 148.4 159.8, 164.2; IR (KBr) cm\(^{-1}\): 1473, 1592, 1676, 2937, 3182, 3312, 3320, 3445.

4-(4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzonitrile (3o)
Yield: 92%, (0.229 g); M.p. 178-180 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): 5.78 (s, 1H), 5.86 (s, 1H), 6.67 (d, 1H, \(J=8.1\) Hz), 6.90 (t, 1H, \(J=7.5\) Hz), 7.26-7.42 (m, 6H), 8.49 (s, 1H); \(^13\)C NMR (75 MHz, DMSO-d\(_6\)): \(\delta\) 76.9, 114.9, 118.1, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.1, 147.7, 1653.0; IR (KBr) cm\(^{-1}\): 1475, 1595, 1676, 2208, 2923, 3180, 3316, 3445.

2-(furan-2-yl)-2,3-dihydroquinazolin-4(1H)-one (3p)

Yield: 90%, (0.193 g); M.p. 166-167 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 5.76 (s, 1H), 6.72 (s, 1H), 7.25-7.49 (m, 3H), 7.61 (s, 1H), 7.73 (d, 2H, \(J=6.9\) Hz), 8.24 (d, 2H, \(J=6.9\) Hz); \(^13\)C NMR (75 MHz, CDCl\(_3\)): \(\delta\) 60.0, 112.9, 113.9, 121.0, 126.5, 126.7, 127.6, 134.9, 143.4, 145.4, 146.2, 149.2; IR (KBr) cm\(^{-1}\): 1673, 2928, 3174, 3309, 3446.

2-(2,3-dichlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3q)
Yield: 94%, (0.274 g); M.p. 182-184 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 6.16 (s, 1H), 6.62-6.66 (m, 2H), 7.11-7.17 (m, 2H), 7.35 (dd, 1H, \(J=8.1\) Hz, \(J=1.5\) Hz), 7.44 (s, 1H), 7.49-7.53 (m, 2H), 7.68 (dd, 1H, \(J=7.9\) Hz, \(J=1.5\) Hz); \(^13\)C NMR (75 MHz, DMSO-D\(_6\)): \(\delta\) 64.7, 114.9, 117.9, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.1, 147.7, 163.8; IR (KBr) cm\(^{-1}\): 1618, 1656, 2922, 3178, 3311, 3439.

**2-octyl-2,3-dihydroquinazolin-4(1H)-one (3r)**

![Diagram of 2-octyl-2,3-dihydroquinazolin-4(1H)-one (3r)](image)

Yield: 85%, (0.221 g); M.p. 238-240 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 0.92 (t, 3H, \(J=6.9\) Hz), 1.10-1.38 (m, 14H), 6.00 (s, 1H), 6.73 (t, 1H, \(J=7.5\) Hz), 7.19-7.24 (m, 3H), 8.49 (s, 1H); \(^13\)C NMR (75 MHz, CDCl\(_3\)): \(\delta\) 16.9, 17.3, 23.9, 26.2, 29.6, 33.2, 69.9, 114.5, 115.1, 116.9, 127.6, 133.4, 148.9, 164.3; IR (KBr) cm\(^{-1}\): 1617, 2928, 3174, 3309, 3443.

**2-(2,3-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3s)**

![Diagram of 2-(2,3-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3s)](image)

Yield: 89%, (0.253 g); M.p. 211-213 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, DMSO-D\(_6\)): \(\delta\) 3.75 (s, 6H), 5.94 (s, 1H), 6.58-6-70 (m, 3H), 6.98 (s, 1H), 7.16 (t, 2H, \(J=7.5\) Hz), 7.53 (d, 2H, \(J=7.5\) Hz), 7.9 (s, 1H); \(^13\)C NMR (75 MHz, DMSO-D\(_6\)): \(\delta\) 56.2, 61.1, 61.6,
113.4, 114.8, 115.1, 119.5, 124.3, 127.7, 133.6, 134.9, 146.5, 148.4, 152.7, 164.1; IR (KBr) cm⁻¹: 1622, 2924, 3170, 3319, 3438.

2-methyl-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (5a)

Yield: 86%, (0.205 g); M.p. 227-228 °C; Characteristics: White crystalline solid;

¹H NMR (300 MHz, DMSO-D₆): δ 1.63 (s, 3H), 6.55 (t, 1H, J=7.5 Hz ), 6.76 (d, 1H, J=8.1 Hz), 7.19 (d, 1H, J=7.2 Hz), 7.28 (t, 2H, J=7.2 Hz), 7.46-7.50 (m, 3H), 7.66 (s, 1H), 8.79 (s, 1H); ¹³C NMR (75 MHz, DMSO-D₆): δ 31.1, 70.5, 114.7, 115.4, 117.2, 125.6, 127.4, 127.6, 128.3, 133.7, 147.6, 148.1, 164.2; IR (KBr) cm⁻¹: 1622, 1477, 1658, 2933, 3060, 3181, 3310.

2-ethyl-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5b)

Yield: 85%, (0.162 g); M.p. 180-182 °C; Characteristics: White crystalline solid;

¹H NMR (300 MHz, CDCl₃): δ 0.97 (t, 3H, J=6.5 Hz ), 1.42 (s, 3H), 1.73 (q, 2H, J=7.5 Hz ), 6.37 (s, 1H), 6.54 (d, 1H, J=8.1 Hz ), 6.73 (t, 1H, J=7.5 Hz ), 7.19-7.24 (m, 2H), 7.79 (d, 1H, J=6.6 Hz); ¹³C NMR (75 MHz, CDCl₃): δ 8.1, 27.5, 34.8, 70.1, 114.4, 118.5, 128.3, 133.9, 160.6; IR (KBr) cm⁻¹: 1612, 1489, 1653, 2925, 3186, 3300.

2-isopropyl-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5c)
Yield: 89%, (0.182 g); M.p. 189-190 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 0.81 (d, 6H, \(J=6.6\) Hz), 1.29 (s, 3H), 1.74-1.78 (m, 1H), 6.47-6.55 (m, 2H), 7.08-7.16 (m, 1H), 7.47 (t, 1H, \(J=6.8\) Hz), 7.78 (s, 1H), 7.83 (s, 1H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): \(\delta\) 18.9, 27.5, 34.8, 70.1, 114.5, 118.5, 128.3, 133.9, 143.8, 160.6; IR (KBr) cm\(^{-1}\): 1610, 1485, 1513, 1658, 2931, 3186, 3301.

2-(2-hydroxyphenyl)-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5d)

Yield: 84%, (0.213 g); M.p. 255-257 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 1.35 (s, 3H), 6.42-6.66 (m, 4H), 7.09 (t, 1H, \(J=7.7\) Hz), 7.20 (t, 1H, \(J=7.5\) Hz), 7.49-7.57 (m, 2H), 7.68 (s, 1H), 7.90 (s, 1H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): \(\delta\) 24.1, 70.5, 114.7, 115.4, 117.2, 125.6, 127.4, 127.6, 128.3, 133.7, 147.6, 148.1, 164.3; IR (KBr) cm\(^{-1}\): 1616, 1482, 1518, 1656, 2929, 3060, 3187, 3310, 3361.

2-methyl-2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (5e)
Yield: 83%, (0.209 g); M.p. 228-230; Characteristics: White crystalline solid;

\[ ^1H \text{ NMR (300 MHz, CDCl}_3\text{)}: \delta 1.78 (s, 3H), 2.38 (s, 3H), 6.53-6.73 (m, 2H), 6.89 (s, 1H), 7.03 (d, 1H, \text{ J}=7.5 \text{ Hz}), 7.16-7.24 (m, 2H), 7.34 (d, 2H, \text{ J}=8.4 \text{ Hz}), 7.75-7.82 (m, 1H); \]
\[ ^{13}C \text{ NMR (75 MHz, CDCl}_3\text{)}: \delta 21.4, 29.5, 70.6, 114.5, 114.6, 115.2, 118.5, 118.8, 125.0, 128.2, 129.0, 133.8, 137.7, 141.9, 145.6, 164.5; \]
\[ \text{IR (KBr) cm}^{-1}: 1612, 1482, 1508, 1658, 2929, 3062, 3178, 3303. \]

2-(4-bromophenyl)-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5f)

Yield: 85%, (0.269 g); M.p. 238-240 °C; Characteristics: White crystalline solid;

\[ ^1H \text{ NMR (300 MHz, CDCl}_3\text{)}: \delta 1.69 (s, 3H), 5.82 (s, 1H), 6.68 (d, 1H, \text{ J}=8.1 \text{ Hz }), 6.92 (t, 1H, \text{ J}=7.7 \text{ Hz}), 7.33-7.44 (m, 1H), 7.43 (d, 2H, \text{ J}=8.4 \text{ Hz}), 7.55 (d, 2H, \text{ J}=8.4 \text{ Hz}), 7.94 (d, 1H, \text{ J}=7.8 \text{ Hz}); \]
\[ ^{13}C \text{ NMR (75 MHz, CDCl}_3\text{)}: \delta 27.9, 84.8, 114.9, 117.9, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.1, 147.7, 163.9; \text{IR (KBr) cm}^{-1}: 1614, 1488, 1510, 1655, 2931, 3066, 3180, 3302. \]

2-methyl-2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (5g)
Yield: 89%, (0.252 g); M.p. 239-241 °C; Characteristics: Yellow crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 1.72 (s, 3H), 5.88 (s, 1H), 6.67 (d, 1H, \(J=8.1\) Hz), 6.90 (t, 1H, \(J=7.5\) Hz), 7.33-7.42 (m, 5H), 7.95 (d, 1H, \(J=7.8\) Hz); \(^{13}\)C NMR (75 MHz, DMSO-d\(_6\)): \(\delta\) 25.7, 82.7, 114.9, 117.9, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.1, 147.7, 163.8; IR (KBr) cm\(^{-1}\): 1615, 1479, 1508, 1658, 2926, 3066, 3182, 3306.

2-(4-fluorophenyl)-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5h)

Yield: 87%, (0.223 g); M.p. 233-236 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 1.72 (s, 3H), 6.39 (s, 1H), 6.60 (d, 1H, \(J=7.8\) Hz), 6.76 (t, 1H, \(J=7.5\) Hz), 6.94 (t, 2H, \(J=8.6\) Hz), 7.07 (s, 1H), 7.23 (t, 2H, \(J=8.1\) Hz), 7.44-7.48 (m, 2H), 7.93; \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): \(\delta\) 28.8, 70.6, 114.9, 117.9, 127.6, 127.8, 128.8, 130.3, 130.9, 132.4, 133.9, 141.1, 147.7, 163.8; IR (KBr) cm\(^{-1}\): 1610, 1482, 1508, 1658, 2929, 3066, 3183, 3300.

1'H-spiro[cyclohexane-1,2'-quinazolin]-4'(3'H)-one (5i)
Yield: 95%, (0.205 g); M.p. 224-226 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, DMSO-\(D_6\)): \(\delta\) 1.26-1.74 (m, 10H), 6.64 (s, 1H), 6.82 (d, 1H, \(J=8.1\) Hz), 7.23 (m, 2H), 7.57 (d, 1H, \(J=7.5\) Hz), 7.94 (s, 1H); \(^{13}\)C NMR (75 MHz, DMSO-\(D_6\)): \(\delta\) 21.3, 25.1, 68.2, 114.9, 116.9, 127.5, 133.5, 147.2, 163.6; IR (KBr) cm\(^{-1}\): 1618, 1658, 2927, 3183, 3311.

\textit{1'H-spiro[cyclopentane-1,2'-quinazolin]-4'(3'H)-one (5j)}

Yield: 95%, (0.192 g); M.p. 210-212 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, DMSO-\(D_6\)): 1.67-1.79 (m, 8H), 6.61-6.74 (m, 2H), 7.19-7.25 (m, 1H), 7.75 (d, 1H, \(J=7.8\) Hz), 7.94 (s, 1H), 8.09 (s, 1H); \(^{13}\)C NMR (75 MHz, DMSO-\(D_6\)): \(\delta\) 22.4, 29.4, 67.2, 77.5, 115.0, 116.8, 127.6, 133.4, 147.9, 163.8; IR (KBr) cm\(^{-1}\): 1616, 1655, 2933, 3178, 3310.

\textit{2-(2-methoxyphenyl)-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5k)}

Yield: 87%, (0.192233 g); M.p. 220-2212 °C; Characteristics: White crystalline solid;

\(^1\)H NMR (300 MHz, DMSO-\(D_6\)): 1.69 (s, 3H), 3.87 (s, 3H), 5.69 (s, 1H), 6.65-6.73 (m, 3H), 7.16-7.24
(m, 2H), 7.35 (d, 2H, J=7.8 Hz), 7.59 (d, 1H, J=7.5 Hz), 8.20 (s, 1H) ; $^1$C NMR (75 MHz, DMSO-D$_6$): δ 28.9, 56.9, 73.1, 114.9, 116.5, 121.6, 123.5, 131.7, 140.4, 147.8, 161.5, 162.9 ; IR (KBr) cm$^{-1}$: 1618, 1657, 2933, 3175, 3312.

2-(2,4-dichlorophenyl)-2-methyl-2,3-dihydroquinazolin-4(1H)-one (5I)

Yield: 89%, (0.269 g); M.p. 215-2172 °C; Characteristics: White crystalline solid;

$^1$H NMR (300 MHz, DMSO-D$_6$): 1.67 (s, 3H), 5.88 (s, 1H), 7.20 (d, 2H, J=7.2 Hz), 7.44 (d, 1H, J=7.5 Hz), 7.57-7.62 (m, 2H), 7.87 (dd, 2H, J=7.9 Hz, J=1.4 Hz), 9.69 (s, 1H) ; $^1$C NMR (75 MHz, DMSO-D$_6$): δ 21.1, 66.8, 114.8, 115.4, 117.5, 127.1, 127.8, 129.2, 133.7, 138.1, 139.1, 148.2, 164.1; IR (KBr) cm$^{-1}$: 1615, 1659, 2930, 31878, 3309.

2-(4-nitrophenyl)quinazolin-4(3H)-one (6a)

Yield: 97%, (0.259 g); M.p. 280-282 °C; Characteristics: White solid;

$^1$H NMR (300 MHz, CDCl$_3$): 7.53 (d, 1H, J=6.6 Hz), 7.73-7.85 (m, 4H), 8.09-8.14 (m, 3H), 12.61 (s, 1H); $^1$C NMR (75 MHz, DMSO-D$_6$): δ 114.8, 114.9, 117.8, 127.7, 127.8, 129.0, 129.9, 130.6, 132.1, 133.7, 138.2, 147.9, 163.9; HRMS (ESI-TOF) m/z Calculated for [C$_{14}$H$_9$N$_3$O$_3$+Na]$^+$: 290.0536, found:
290.0536; IR (KBr) cm\(^{-1}\): 1663, 3178.

2-phenylquinazolin-4(3\(H\))-one (6b)

Yield: 94\%, (0.208 g); M.p. 122-123 \(^{\circ}\)C; Characteristics: White solid;

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta\) 7.52 (t, 2H, \(J=\) 7.1 Hz), 7.71-7.86 (m, 5H), 8.09-8.15 (m, 2H), 12.59 (s, 1H); \(^{13}\)C NMR (75 MHz, DMSO-D\(_6\)): \(\delta\) 117.7, 127.8, 128.8, 129.2, 133.4, 133.9, 141.1, 148.1, 152.0, 158.1, 163.9; IR (KBr) cm\(^{-1}\): 1661, 3175.

2-(3-nitrophenyl)quinazolin-4(3\(H\))-one (6c)

Yield: 96\%, (0.256 g); M.p. 292-294 \(^{\circ}\)C; Characteristics: White solid;

\(^1\)H NMR (300 MHz, DMSO-D\(_6\)): \(\delta\) 6.65-6.73 (m, 2H), 7.22 (t, 1H, \(J=\) 7.7 Hz), 7.34-7.38 (m, 2H), 7.43-7.47 (m, 1H), 7.61 (dd, 2H, \(J=\) 6.0 Hz, \(J=\) 2.7 Hz); \(^{13}\)C NMR (75 MHz, DMSO-D\(_6\)): 114.8, 114.9, 117.8, 127.7, 127.8, 129.1, 129.8, 130.6, 132.1, 133.7, 138.2, 147.9, 163.9; IR (KBr) cm\(^{-1}\): 1659, 3180.
2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (6d)

Yield: 95%, (0.243 g); M.p. 295-296 °C; Characteristics: White solid;

$^1$H NMR (300 MHz, DMSO-D$_6$): 6.13-6.77 (m, 2H), 7.25 (t, 1H, $J$= 7.7 Hz), 7.38-7.41 (m, 2H), 7.48-7.51 (m, 1H), 7.65 (d, 2H, $J$=6.6 Hz) ; $^{13}$C NMR (75 MHz, DMSO-D$_6$): δ 117.9, 127.8, 127.9, 129.2, 130.1, 130.7, 133.9, 148.1, 157.1, 164.1; HRMS (ESI-TOF) m/z Calculated for [C$_{14}$H$_9$ClN$_2$O$^+$K]$^+$: 295.0035, found: 295.0035. IR (KBr) cm$^{-1}$: 1653, 3138.

2-(thiophen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (6e)

Yield:90%, (0.205 g); M.p. 244-246 °C; Characteristics: White solid;

$^1$H NMR (300 MHz, DMSO-D$_6$): 6.64-6.73 (m, 2H), 6.92-6.94 (m, 1H), 7.07-7.08 (m, 1H), 7.20-7.24 (m, 1H), 7.40 (d, 1H, $J$=5.1), 7.57 (d, 1H, $J$=7.5); $^{13}$C NMR (75 MHz, DMSO-D$_6$): δ 117.6, 125.7, 125.9, 126.6, 127.4, 133.5, 146.6, 147.2, 163.2; HRMS (ESI-TOF) m/z Calculated for [C$_{12}$H$_9$N$_2$OS$^+$K]$^+$: 266.9989, found: 266.9986; IR (KBr) cm$^{-1}$: 1637, 3166.

2-isopropylquinazolin-4(3H)-one (6f)
Yield: 88%, (0.165 g); M.p. 180-182 °C; Characteristics: White solid;

$^1$H NMR (300 MHz, DMSO-D$_6$): $\delta$ 0.83 (d, 6H, $J=6.6$Hz), 1.77-1.79 (m, 1H), 6.53 (t, 1H, $J=7.4$Hz), 6.67 (d, 1H, $J=8.1$Hz), 7.12 (t, 1H, $J=7.5$Hz), 7.48 (d, 1H, $J=7.5$Hz), 9.07 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-D$_6$): $\delta$ 30.7, 32.8, 114.2, 114.8, 116.6, 127.3, 133.1, 148.6, 163.9. IR (KBr) cm$^{-1}$: 1250, 1369, 1457, 1651, 3160.

2-(furan-2-yl)quinazolin-4(3H)-one (6g)

Yield: 90%, (0.190 g); M.p. 210-212 °C; Characteristics: White solid;

$^1$H NMR (300 MHz, DMSO-D$_6$): $\delta$ 6.64-6.73 (m, 2H), 6.92-6.94 (m, 1H), 7.07-7.08 (m, 1H), 7.20-7.24 (m, 1H), 7.40 (d, 1H, $J=5.1$), 7.57 (d, 1H, $J=7.5$); $^{13}$C NMR (75 MHz, DMSO-D$_6$): $\delta$ 117.6, 125.7, 125.9, 126.6, 127.4, 133.5, 146.6, 147.2, 163.2; IR (KBr) cm$^{-1}$: 1370, 1457, 1652, 3155.

2-(1H-indol-3-yl)quinazolin-4(3H)-one (6h)

Yield: 95%, (0.247 g); M.p. 302-304 °C; Characteristics: Yellow solid;
$^1$H NMR (300 MHz, DMSO-$d_6$): $\delta$ 6.82-7.04 (m, 4H), 7.29-7.41 (m, 5H), 9.75 (s, 1H), 10.69 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-$d_6$): $\delta$ 111.8, 118.3, 118.7, 119.6, 121.0, 123.6, 127.2, 136.9, 149.6, 162.9; IR (KBr) cm$^{-1}$: 1376, 1457, 1651, 3160.

2-(quinolin-2-yl)quinazolin-4(3$H$)-one (6i)

Yield: 95%, (0.259 g); M.p. 188-190 $^\circ$C; Characteristics: White solid;

$^1$H NMR (300 MHz, DMSO-$d_6$): $\delta$ 7.62-7.89 (m, 5H), 8.12 (d, 1H, $J=7.5$), 8.25 (t, 2H, $J=7.6$), 8.54-8.65 (m, 2H), 12.05 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-$d_6$): $\delta$ 115.2, 119.6, 122.5, 122.6, 124.1, 127.5, 130.6, 140.2, 145.2, 152.5, 168.1; IR (KBr) cm$^{-1}$: 1675, 3140.

2-(2,2-dimethyl-4-oxopentyl)quinazolin-4(3$H$)-one (7a)

Yield: 69%, (0.178 g); M.p. 160-162 $^\circ$C; Characteristics: White solid

$^1$H NMR (300 MHz, DMSO-$d_6$): $\delta$ 1.00 (s, 6H), 2.31 (s, 2H), 2.52 (s, 2H), 2.71 (s, 3H), 7.50 (t, 1H, $J=7.1$), 7.58 (d, 1H, $J=7.8$), 7.77 (d, 1H, $J=7.5$), 8.08 (d, 1H, $J=7.8$), 12.22 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-$d_6$): $\delta$ 26.2, 30.1, 33.2, 43.9, 53.6, 121.1, 127.1, 133.5, 142.6, 148.9, 153.9, 164.2; IR (KBr) cm$^{-1}$: 1659, 3150.

2-(4-oxopentyl)quinazolin-4(3$H$)-one (7b)
Yield: 85%, (0.195 g); M.p. 144-145 °C; Characteristics: White solid

$^1$H NMR (300 MHz, DMSO-D$_6$): δ 1.49 (t, 2H, $J$=5.1), 1.65 (m, 2H), 1.98 (s, 3H), 2.63 (t, 2H, $J$=5.1) 7.46-7.54 (m, 1H), 7.69 (d, 1H, $J$=7.8), 7.79 (t, 1H, $J$=7.7), 8.29 (d, 1H, $J$=7.8), 11.74 (s, 1H) ; $^{13}$C NMR (75 MHz, DMSO-D$_6$): δ 22.1, 30.1, 33.2, 43.4, 120.6, 127.1, 133.4, 142.6, 148.9, 153.9, 164.3; IR (KBr) cm$^{-1}$: 1659, 3133.

2-methylquinazolin-4(3H)-one (8a)/(8b)/(8c)

Yield: 98%, (0.156 g); M.p. 175-176 °C; Characteristics: White solid

$^1$H NMR (300 MHz, CDCl$_3$): δ 2.61 (s, 3H), 7.33-7.54 (m, 1H), 7.69 (d, 1H, $J$=7.8), 7.78 (t, 1H, $J$=7.7), 8.29 (d, 1H, $J$=7.8), 12.03 (s, 1H); $^{13}$C NMR (75 MHz, DMSO-D$_6$): δ 22.4, 120.5, 127.6, 133.4, 138.5, 147.9, 154.9, 163.8; IR (KBr) cm$^{-1}$: 1665, 3137.
$^{1}$HNMR, $^{13}$CNMR Spectra of the Compounds (3a-3i):

$^{1}$H NMR of Compound 3a

$^{13}$C NMR of Compound 3a
$^1$H NMR of Compound 3b

$^{13}$C NMR of Compound 3b
$^1$H NMR of Compound 3c

$^{13}$C NMR of Compound 3c
$^1$H NMR of Compound 3d

$^{13}$C NMR of Compound 3d
\(^1\text{H} \text{NMR of Compound 3e}\)

\(^{13}\text{C} \text{NMR of Compound 3e}\)
$^1$H NMR of Compound 3f

$^{13}$C NMR of Compound 3f
$^{1}H$ NMR of Compound 3g

$^{13}C$ NMR of Compound 3g
$^1$H NMR of Compound 3h

$^{13}$C NMR of Compound 3h
$^1$H NMR of Compound 3i

$^{13}$C NMR of Compound 3i
$^1$H NMR of Compound 3j

$^{13}$C NMR of Compound 3j
$^1$H NMR of Compound 3k

$^{13}$C NMR of Compound 3k
$\text{H NMR of Compound 3l}$

$\text{C NMR of Compound 3l}$
$^1$H NMR of Compound 3m

$^{13}$C NMR of Compound 3m
$^1$H NMR of Compound 3n

$^{13}$C NMR of Compound 3n
$^1$H NMR of Compound 3o

$^{13}$C NMR of Compound 3o
$^1$H NMR of Compound 3p

$^{13}$C NMR of Compound 3p
$^1$H NMR of Compound 3q

$^{13}$C NMR of Compound 3q

41
$^1$H NMR of Compound 3r

$^{13}$C NMR of Compound 3r
$^1$H NMR of Compound 3r

$^{13}$C NMR of Compound 3s
$^1$HNMR, $^{13}$CNMR Spectra of the Compounds (5a-5l):

$^1$H NMR of Compound 5a

$^{13}$C NMR of Compound 5a
$^1$H NMR of Compound 5b

$^{13}$C NMR of Compound 5b
\(^1\)H NMR of Compound 5c

\(^{13}\)C NMR of Compound 5c
$^1$H NMR of Compound 5d

$^{13}$C NMR of Compound 5d
$^1$H NMR of Compound 5e

$^{13}$C NMR of Compound 5e
$^1$H NMR of Compound 5f

$^{13}$C NMR of Compound 5f
$^1$H NMR of Compound 5g

$^{13}$C NMR of Compound 5g

50
$^1$H NMR of Compound 5h

$^{13}$H CMR of Compound 5h
$^1$H NMR of Compound 5i

$^{13}$C NMR of Compound 5i
$^1$H NMR of Compound 5j

$^{13}$C NMR of Compound 5j
$^1$H NMR of Compound 5k

$^{13}$C NMR of Compound 5k
$^1$H NMR of Compound 5l

$^{13}$C NMR of Compound 5l
$^1$HNMR, $^{13}$CNMR Spectra of the Compounds (6a-6i):

$^1$H NMR of Compound 6a

$^{13}$C NMR of Compound 6a
$^1$H NMR of Compound 6b

$^{13}$C NMR of Compound 6b
$^1$H NMR of Compound 6c

$^{13}$C NMR of Compound 6c
$^1$H NMR of Compound 6d

$^{13}$C NMR of Compound 6d
$^1$H NMR of Compound 6e

$^{13}$C NMR of Compound 6e
$^1$H NMR of Compound 6f

$^{13}$C NMR of Compound 6f
$^1$H NMR of Compound 6g

$^{13}$C NMR of Compound 6g
$^1$H NMR of Compound 6h

$^{13}$C NMR of Compound 6h
$^1$H NMR of Compound 6i

$^{13}$C NMR of Compound 6i
$^1$H NMR of Compound 7a

$^{13}$C NMR of Compound 7a
$^1$H NMR of Compound 7b

$^{13}$C NMR of Compound 7b
$^{1}$H NMR of Compound 8a/8b/8c

$^{13}$C NMR of Compound 8a/8b/8c
HRMS of Compound 3c

HRMS of Compound 6a
HRMS of Compound 6d

HRMS of Compound 6e
HRMS of compound 8a