

## Supporting information

### Synthesis, DFT Studies on a Series of Tunable Quinolines Derivatives

Nagesh Dhanaji Chavan,<sup>†</sup> Vijayaparthasarathi Vijayakumar<sup>\*†</sup>.

<sup>†</sup>Department of Chemistry, School of Advance Sciences, Vellore Institute of Technology, Vellore- 632014, India

#### Table of Contents

1. General Methods.....	1
2. Synthesis of Functionalized Quinoline.....	2
3. Acid Amine Cross-Coupling Reaction and compound identification data.....	4
4. DFT (FMO, MEP, TD-DFT) Calculations and Diagrams.....	34
5. Absorption and Fluorescent Spectra.....	88
6. IR, <sup>1</sup> H, <sup>13</sup> C, DEPT-135 and 2D NMR and HRMS Spectra.....	102

#### 1. General methods

The reactions were conducted in round bottom flasks, and all solvents and chemical materials were obtained from commercial sources. The preparation of 1-(6-amino-2-methyl-4-phenylquinolin-3-yl)-ethan-1-one followed reported protocols. The <sup>1</sup>H and <sup>13</sup>C NMR spectra were obtained using a Bruker Avance 400 spectrometer and referenced to the residual solvent signal CDCl<sub>3</sub>: (7.26) for <sup>1</sup>H and (77.16) for <sup>13</sup>C NMR; dimethyl sulfoxide-*d*<sub>6</sub> (2.50) for <sup>1</sup>H and (39.50) for <sup>13</sup>C. Chemical shifts (δ) are given in ppm, and coupling constants (*J*) were measured in Hz. The following abbreviations were used: s-singlet, d-doublet, dd-doublet of the doublet, t-triplet, m (multiple), and br-broad. HR ESI-MS values were obtained using Xeo G2-XS QToF (Waters) and given in m/z. Absorption was recorded using a JASCO V-670 spectrometer. Steady-state fluorescence spectra were recorded on

the Hitachi F-7000 FL spectrofluorometer by excitation at the respective absorption maxima. Column chromatography was performed using silica gel (100-200 mesh) packed in glass columns. Analytical TLC was conducted on Macherey-Nagel 60 F245 aluminium-backed silica gel plates.

## 2. Synthesis of Functionalized Quinoline and Nitro to Amine reduction:

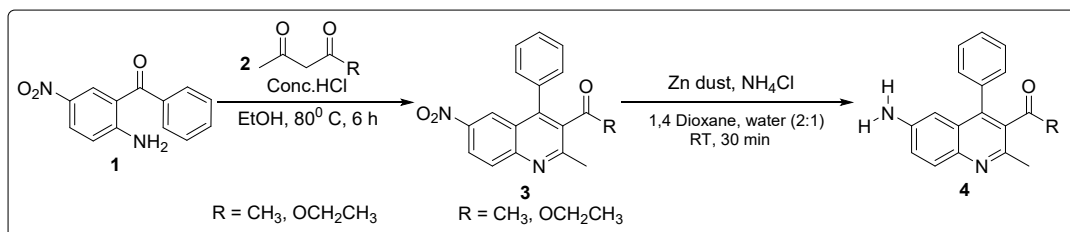
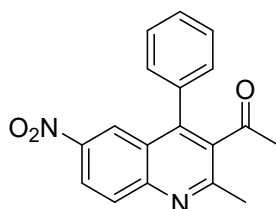


Figure-S1

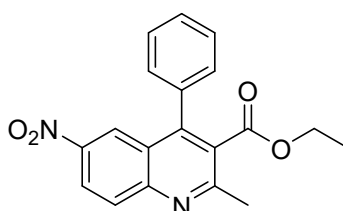
### 2.1; The Preparation of 1-(2-Methyl-6-nitro-4-phenylquinolin-3-yl)ethan-1-one.



(2-Amino-5-nitrophenyl) (phenyl)methanone ( $2 \times 7.5$  g, 0.0309 moles), pentane-2,4-dione (17.41mL, 0.1549 moles), Conc.HCl (1.6 mL) in 200 mL of AR grade EtOH 500 mL round bottom flask was stirred at  $80^{\circ}$  C temperature under the nitrogen gas for 6 hours. Reaction monitored by TLC. After completion of the reaction, the reaction mixture was added to the cold water and formed a precipitate. Precipitate filtered and washed with n-pentane. The crude compound was purified by column chromatography using silica gel (100-200 mesh and Eluent: 25 EtOH in Hexane) a to obtain the Title Product. The product was confirmed by  $^1\text{H}$  NMR, Yield (76.47%).

$^1\text{H}$  NMR:(400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 8.59 (d,  $J = 2.40$  Hz, 1H), 8.51 (dd,  $J = 2.40, 9.20$  Hz, 1H), 8.56 (m, 1H), 7.62-7.61 (m, 3H), 7.40-7.39 (m, 2H), 2.78 (s, 3H), 2.04 (s, 3H).

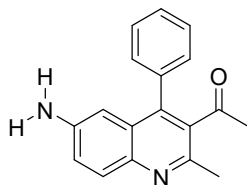
### 2.2; The Preparation of Ethyl 2-methyl-6-nitro-4-phenylquinoline-3-carboxylate.



(2-Amino-5-nitrophenyl) (phenyl)methanone ( $2 \times 10$  g, 0.0413 moles), ethyl 3-oxobutanoate (53.7 mL, 0.04132 moles), Conc.HCl 2.2 mL) in 150 of AR grade EtOH 10 mL round bottom flask was stirred at room temperature under the nitrogen gas for 6 hours. Reaction monitored by TLC. After completion of the reaction, the reaction mixture was added to the cold water and formed a precipitate. Precipitate filtered and washed with n-pentane. The crude compound was purified by column chromatography using silica gel (100-200 mesh and Eluent: 20 EtOH in Hexane) to obtain the Title Product. The product was confirmed by  $^1\text{H NMR}$ , Yield (24.12 g, 86.88 %).

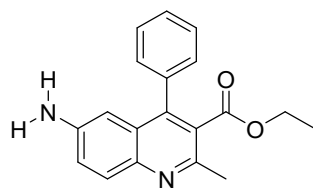
**$^1\text{H NMR}$ :** (400 MHz, DMSO- $d_6$ );  $\delta$  ppm 8.46 (d,  $J = 2.40$  Hz, 1H), 8.40 (dd,  $J = 2.40, 9.20$  Hz, 1H), 8.12 (d,  $J = 9.20$  Hz, 1H), 7.48-7.48 (m, 3H), 7.31-7.30 (m, 2H), 4.02 (q,  $J = 6.80$  Hz, 2H), 2.76 (s, 3H), 0.90 (t,  $J = 6.80$  Hz, 3H).

### 2.3; The Preparation 1-(6-Amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one.



1-(2-Methyl-6-nitro-4-phenylquinolin-3-yl)ethan-1-one (14 g, 0.0457 moles), Zinc dust (17.29 g, 0.2742 moles), Ammonium chloride (14.53 g, 0.2742 moles) in 75 mL dioxane and 75 mL of water in round bottom flask was stirred at room temperature under the nitrogen gas for 30 min. Reaction monitored by TLC, After completion of the reaction, the reaction mixture was added to the water (100mL) and extracted with ethyl acetate ( $2 \times 100$  mL). The organic layer was washed with brine water (100 mL) and distilled under high vacuum to obtain the Title Product. The product was confirmed by  $^1\text{H NMR}$ .  **$^1\text{H NMR}$ :** (400 MHz, DMSO- $d_6$ ),  $\delta$  ppm 7.70 (d,  $J = 8.80$  Hz, 1H), 7.57-7.57 (m, 3H), 7.31-7.31 (m, 2H), 7.16 (dd,  $J = 2.40, 8.80$  Hz, 1H), 6.44 (d,  $J = 2.00$  Hz, 1H), 5.60 (s, 2H), 2.47 (s, 3H), 1.98 (s, 3H).

### 2.4; The Preparation Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate



Ethyl 2-methyl-6-nitro-4-phenylquinoline-3-carboxylate (20 g, 0.0595 moles), Zinc dust (22.5 g, 0.3571 moles), Ammonium chloride (18.92 g, 0.3571 mole in 100 mL dioxane AR grade and 100 mL of water in round bottom flask was stirred at room temperature under the nitrogen gas for 30 min. Reaction monitored by TLC, After completion of the reaction, the reaction mixture was added to the water (100mL) and extracted with ethyl acetate (2 × 100 mL). The organic layer was washed with brine water (100 mL) and distilled under high vacuum to obtain the Title Product. The product was confirmed by <sup>1</sup>H and <sup>13</sup>C NMR,

<sup>1</sup>H NMR: (400 MHz, DMSO-d<sub>6</sub>); δ 7.71 (d, J = 8.80 Hz, 1H), 7.54-7.53 (m, 3H), 7.30-7.30 (m, 2H), 7.18 (dd, J = 2.40, 8.80 Hz, 1H), 6.43 (d, J = 2.40 Hz, 1H), 5.60 (s, 2H), 3.98 (q, J = 6.80 Hz, 2H), 2.54 (s, 3H), 0.86 (t, J = 7.20 Hz, 3H).

### 3: Acid Amine Cross-Coupling Reaction

#### Scheme-1

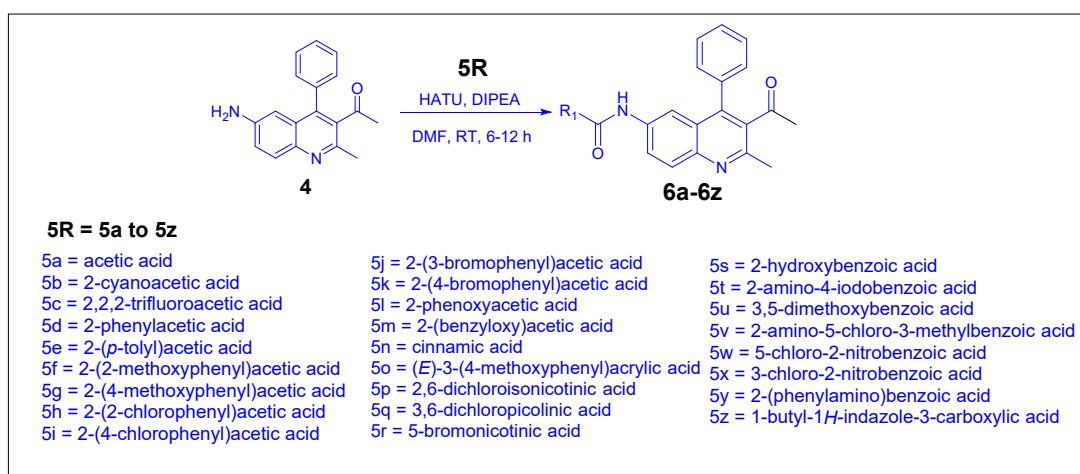


Figure-S2

#### Synthesized Derivatives (6a-6z):

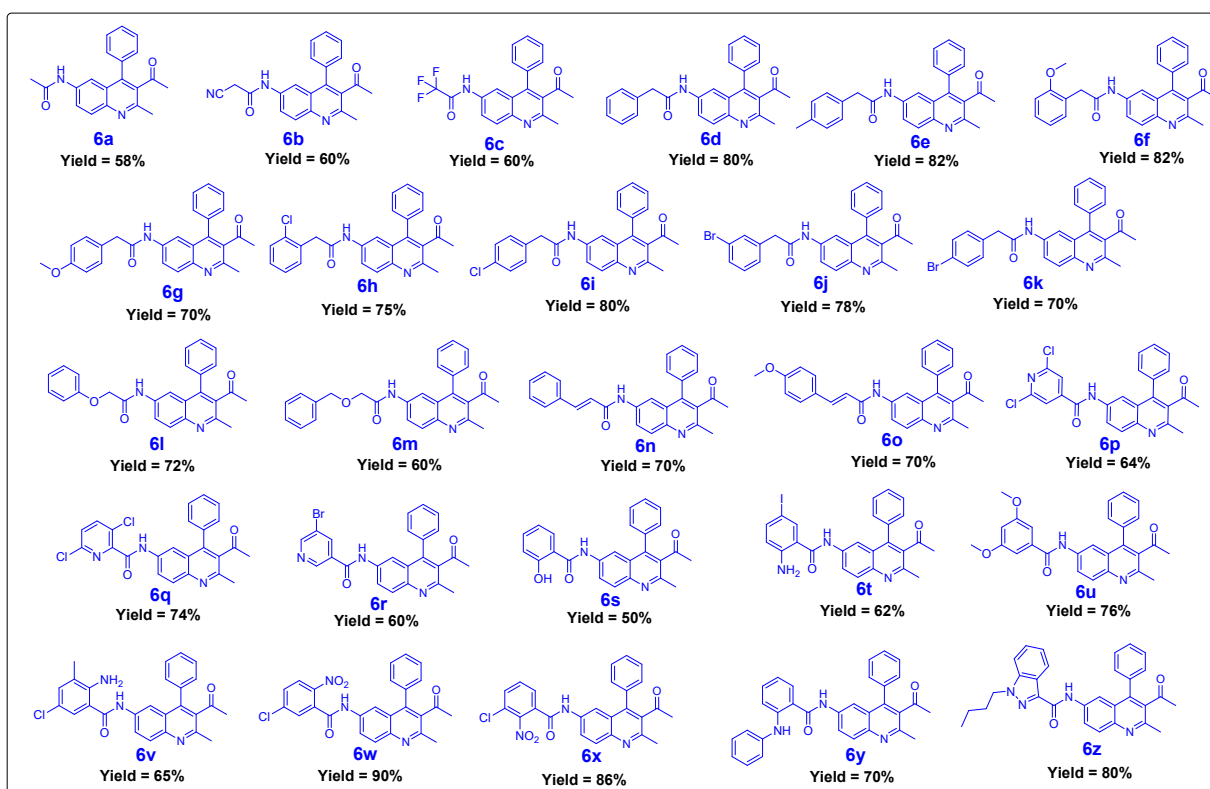


Figure-S3

Scheme-2

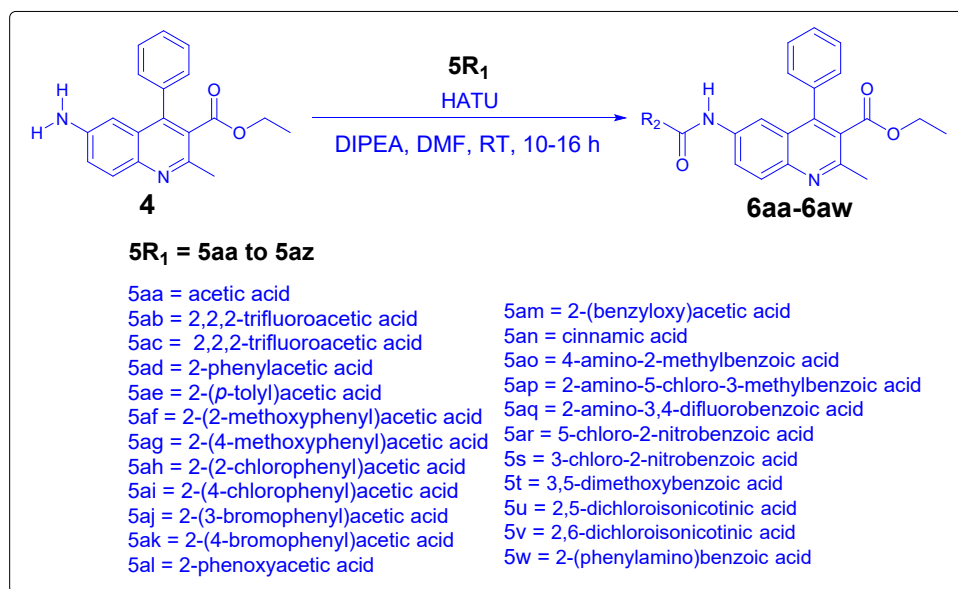
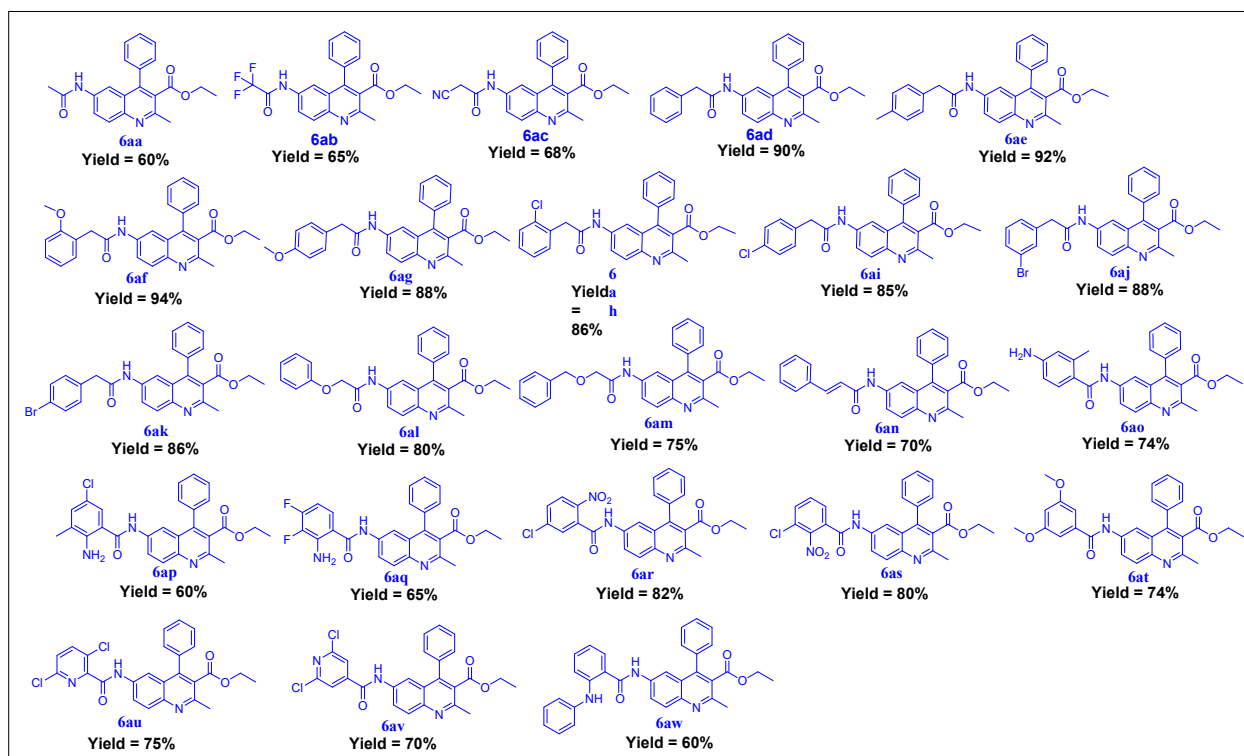


Figure-S4

Synthesized Derivatives (6aa-6aw):z

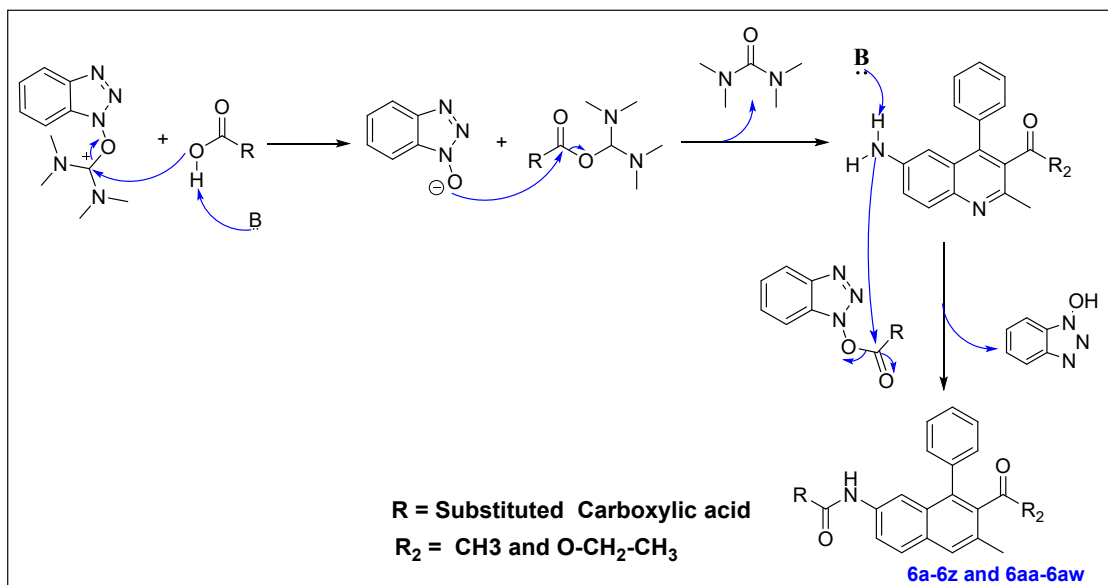


**Figure-S5**

### 3.1 Experimental procedure:

**General procedure for the synthesis of 6a-6z:** 1-(6-amino-2-methyl-4-phenylquinolin-3-yl) ethan-1-one (300-500 mgs), substituted carboxylic acids (1.5 to 5.0 equiv), HATU (2.0 to 2.5 equivalents) and DIPEA (2.5 equivalents) in 10 mL of AR grade DMF 50 mL round bottom flask was stirred at room temperature under the nitrogen gas for 6-12 hours. After completion of the reaction, the reaction mixture was added to the cold water and extracted with ethyl acetate (2 × 25 mL). The organic layer was washed with brine water (25mL). The Organic layer concentrates under a high vacuum to get crude compound. The crude compound was purified by using column chromatography to obtain pure products **6a-6z** and **6aa-6aw**.

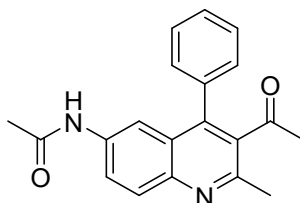
### 3.2 Plausible Mechanism:



**Figure.S6**

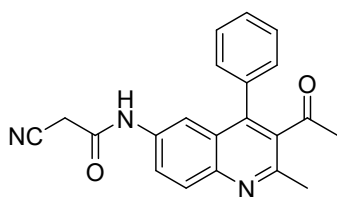
### 3.3 Procedure and Identification Analytical data of the compounds

#### **N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).**



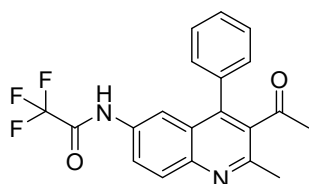
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (300 mg, 1.0869 mmole), acetic acid (130 mg, 2.1739mmole), HATU (1.02 g, 2.7173), DIPEA (304 mg, 4.0869 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 80% ethyl acetate in Hexane). TLC:  $R_f = 0.8$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Brown solid, yield 58%, m.p. 190–192<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz, DMSO- $d_6$ ):  $\delta$  10.21 (s, 1H), 8.01 (dd,  $J = 2.00, 8.80$  Hz, 1H), 7.95 (d,  $J = 9.20$  Hz, 1H), 7.85 (d,  $J = 1.60$  Hz, 1H), 7.58-7.57 (m, 3H), 7.34-7.33 (m, 2H), 2.555 (s, 3H), 2.010 (s, 3H), 2.004 (s, 3H); **<sup>13</sup>C NMR** (100 MHz DMSO- $d_6$ ):  $\delta$  ppm 205.77, 169.10, 151.68, 144.14, 143.01, 138.12, 135.37, 135.33, 130.15, 129.18, 125.43, 124.17, 113.32, 32.24, 24.38, 23.63; **IR Stretching:** N-H (3585  $\text{cm}^{-1}$ ), C=O (1702  $\text{cm}^{-1}$ ). **HRMS (ESI) m/z:** [M + H]<sup>+</sup> Calcd for  $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_2$  319.1446; Found 319.1473.

#### **N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2-cyanoacetic acid (246 mg, 2.8985 mmole), HATU (1.3 g, 3.6231 mmole), DIPEA (467 mg, 3.6231 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.6$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain] Pale yellow solid, yield 60%, m.p. 160–162<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.56 (s, 1H), 8.00 (d,  $J = 9.20$  Hz, 1H), 7.96 (dd,  $J = 2.00, 9.00$  Hz, 1H), 7.82 (d,  $J = 2.00$  Hz, 1H), 7.59-7.58 (m, 3H), 7.35-7.34 (m, 2H), 3.89 (s, 3H), 2.57 (s, 3H), 2.02 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.67, 162.79, 161.82, 152.27, 144.40, 143.11, 137.17, 135.44, 135.21, 130.14, 129.23, 125.38, 123.92, 116.20, 113.94, 32.24, 27.25, 23.66; **IR Stretching**; N-H (3299  $\text{cm}^{-1}$ ), C=O (1686  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{21}\text{H}_{17}\text{N}_3\text{O}_2$  344.1390; Found 344.1410.

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (6c).**



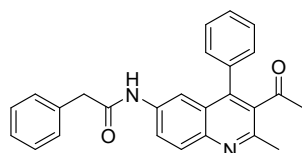
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2,2,2-trifluoroacetic acid (330 mg, 2.8985 mmole), HATU (1.3 g, 3.6231 mmole), DIPEA (467 mg, 3.6231 mmole) in DMF (10 mL) at RT 8 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain] Pale yellow solid Pale yellow solid, yield 60%, m.p. 134–136<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 11.51 (s, 1H), 8.13 (dd,  $J = 2.00, 9.00$  Hz, 1H), 8.06 (d,  $J = 9.20$  Hz, 1H), 7.98 (d,  $J = 2.40$  Hz, 1H), 7.60-7.60 (m, 3H), 7.37-7.37 (m, 2H), 2.60 (s, 3H), 2.03 (s, 3H);



$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.51, 158.79, 157.82, 153.28, 145.04, 143.48, 135.60, 135.26, 134.98, 130.21, 129.25, 124.69, 123.92, 116.20, 113.94, 55.35, 32.21, 23.80;

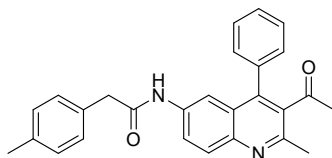
**IR Stretching;** N-H ( $3299\text{ cm}^{-1}$ ), C=O ( $1686\text{ cm}^{-1}$ ); **HRMS (ESI) m/z:** [M + H]<sup>+</sup> Calcd for  $\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}_2$  373.1163; Found 373.1190

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (500 mg, 1.8115 mmole), 2-phenylacetic acid (369 mg, 2.7173 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (584 mg, 4.5289 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid; **yield** 80%, **m.p.** 140–142 $^{\circ}$  C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.45 (s, 1H), 8.02 (d,  $J = 8.80\text{ Hz}$ , 1H), 7.97 (d,  $J = 9.20\text{ Hz}$ , 1H), 7.93 (s, 1H), 7.57–7.55 (m, 3H), 7.34–7.33 (m, 7H), 3.63 (s, 2H), 2.56 (s, 3H), 2.00 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.66, 169.89, 151.79, 144.06, 143.16, 138.10, 136.16, 135.33, 130.14, 129.65, 129.21, 128.75, 127.02, 125.47, 124.20, 113.41, 43.70, 32.23, 23.59; **IR Stretching;** N-H ( $3582\text{ cm}^{-1}$ ), C=O ( $1698\text{ cm}^{-1}$ , C=C ( $1559\text{ cm}^{-1}$ )); **HRMS (ESI) m/z:** [M + H]<sup>+</sup> Calcd for  $\text{C}_{22}\text{H}_{15}\text{N}_2\text{O}$  395.1759; Found 395.1798.

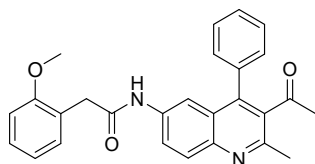
**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl)acetamide (6e).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (200 mg, 0.7246 mmole), 2-(p-tolyl)acetic acid (217 mg, 1.4492 mmole), HATU (550 g, 1.4492 mmole), DIPEA (233 mg, 1.8115 mmole) in DMF (12 mL) at RT 12 h. The title compound was isolated (Eluent 50%

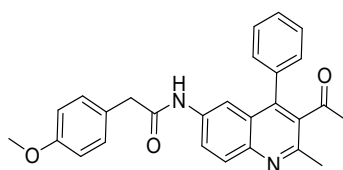
ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 82%, m.p: 112-114<sup>0</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>):  $\delta$  ppm 10.43 (s, 1H), 8.03 (dd,  $J = 1.60, 9.20$  Hz, 1H), 7.97 (d,  $J = 8.80$  Hz, 1H), 7.92 (s, 1H), 7.57-7.55 (m, 3H), 7.34-7.33 (m, 2H), 7.18 (d,  $J = 8.00$  Hz, 2H), 7.10 (d,  $J = 7.60$  Hz, 2H), 3.57 (s, 2H), 2.56 (s, 3H), 2.25 (s, 3H), 2.00 (s, 3H), <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>):  $\delta$  ppm 205.69, 170.04, 151.74, 144.23, 143.23, 138.11, 136.04, 135.39, 133.11, 130.15, 129.55, 129.49, 129.34, 129.30, 129.19, 125.44, 124.15, 113.40, 43.33, 32.22, 23.65, 21.08, **IR Stretching**; N-H (3489 cm<sup>-1</sup>), C=O (1705 cm<sup>-1</sup>, C=C (1540 cm<sup>-1</sup>)), **HRMS (ESI) m/z**: [M + H] + Calculated for C<sub>27</sub>H<sub>25</sub>N<sub>2</sub>O<sub>2</sub> 409.1910; Found 409.1909

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl)acetamide (6f).**



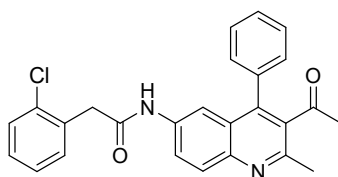
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (200 mg, 0.7246 mmole), 2-(2-methoxyphenyl)acetic acid (180 mg, 1.0869 mmole), HATU (550 g, 1.4492 mmole), DIPEA (233 mg, 1.8115 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 88%, m.p. 158–160<sup>0</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>):  $\delta$  ppm 10.33 (s, 1H), 8.01-7.99 (m, 3H), 7.56-7.54 (m, 3H), 7.33 (d,  $J = 7.20$  Hz, 2H), 7.23 (t,  $J = 8.00$  Hz, 1H), 7.17 (d,  $J = 7.20$  Hz, 1H), 6.95 (d,  $J = 8.00$  Hz, 1H), 6.88 (t,  $J = 7.60$  Hz, 1H), 3.73 (s, 3H), 3.62 (s, 2H), 2.56 (s, 3H), 2.01 (s, 3H); <sup>13</sup>C NMR (100 MHz DMSO-d<sub>6</sub>):  $\delta$  ppm 205.76, 169.88, 157.68, 151.64, 144.16, 143.00, 138.22, 135.41, 135.36, 131.46, 130.15, 129.54, 132.34, 129.18, 128.54, 125.47, 124.36, 124.16, 120.59, 113.21, 111.12, 55.84, 38.11, 32.26, 23.67; **IR Stretching**; N-H (3344 cm<sup>-1</sup>), C=O (1691 cm<sup>-1</sup>, C=C (1540 cm<sup>-1</sup>)); **HRMS (ESI) m/z**: [M + H] + Calculated for C<sub>27</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub> 425.1859; Found 425.1859

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-methoxyphenyl)acetamide (6g).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2-(4-methoxyphenyl)acetic acid (366 mg, 2.1739 mmole), HATU (1.1 g, 2.8985 mmole), DIPEA (560 mg, 4.3478 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield : 70%, m.p. 160–162<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.41 (s, 1H), 7.95-7.95 (m, 3H), 7.54-7.53 (m, 3H), 7.28-7.27 (m, 2H), 7.17 (d,  $J = 8.80$  Hz, 2H), 6.83 (d,  $J = 8.80$  Hz, 2H), 3.68 (s, 3H), 3.51 (s, 2H), 2.52 (s, 3H), 1.97 (s, 3H); **<sup>13</sup>C NMR** (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 206.16, 170.53, 158.48, 151.94, 144.00, 143.31, 137.92, 135.40, 130.65, 130.00, 129.46, 129.31, 129.23, 127.92, 125.44, 124.28, 114.19, 113.49, 55.45, 42.73, 32.21, 23.42 ; **IR Stretching**; N-H (349  $\text{cm}^{-1}$ ), C=O (1686  $\text{cm}^{-1}$ , C=C (1535  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> + Calculated for  $\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}_3$  425.1865; Found 425.1885

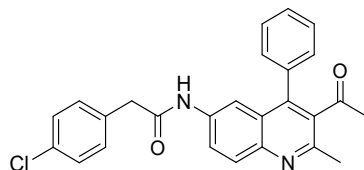
**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl)acetamide (6h).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (200 mg, 0.7246 mmole), 2-(2-chlorophenyl)acetic acid (246 mg, 1.4492 mmole), HATU (550 mg, 1.4492 mmole), DIPEA (233 mg, 1.8115 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield : 75%, m.p. 208–210<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm  $\delta$  10.53 (s, 1H), 8.01 (dd,  $J = 2.00, 9.00$  Hz, 1H), 7.98 (d,  $J = 9.20$  Hz, 1H), 7.94 (s, 1H), 7.56-7.55 (m, 3H), 7.43-7.42 (m,

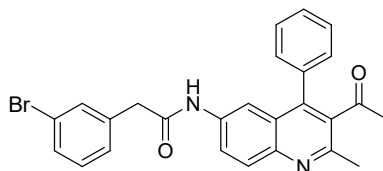
2H), 7.34-7.34 (m, 4H), 3.84 (s, 2H), 2.57 (s, 3H), 2.01 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 206.1, 168.68, 151.76, 144.24, 143.04, 138.04, 135.42, 135.39, 134.17, 134.13, 132.75, 130.14, 129.61, 129.44, 129.36, 129.19, 129.08, 127.51, 125.48, 124.11, 113.34, 41.19, 32.24, 23.66; **IR Stretching**; N-H (3275  $\text{cm}^{-1}$ ), C=O (1704  $\text{cm}^{-1}$ , C=C (1537  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] + Calculated for  $\text{C}_{26}\text{H}_{22}\text{ClN}_2\text{O}_2$  429.1364; Found 429.1362

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-chlorophenyl)acetamide (6i).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (200 mg, 0.7246 mmole), 2-(4-chlorophenyl)acetic acid (246 mg, 1.4492 mmole), HATU (550 mg, 1.4492 mmole), DIPEA (233 mg, 1.8115 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f$  = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield : 80%, m.p. 92–94 $^\circ$  C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.46 (s, 1H), 8.02 (d, J = 9.20 Hz, 1H), 7.97 (d, J = 8.80 Hz, 1H), 7.91 (s, 1H), 7.57-7.55 (m, 3H), 7.37-7.35 (m, 6H), 3.64 (s, 2H), 2.56 (s, 3H), 2.00 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.72, 169.50, 151.82, 144.24, 143.02, 137.97, 135.40, 135.35, 135.14, 131.60, 130.15, 129.21, 128.67, 125.43, 124.09, 113.42, 42.80, 32.24, 23.67; **IR Stretching**; N-H (3579  $\text{cm}^{-1}$ ), C=O (1706  $\text{cm}^{-1}$ , C=C (1494  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] + Calculated for  $\text{C}_{26}\text{H}_{22}\text{ClN}_2\text{O}_2$  429.1364; Found 429.1363

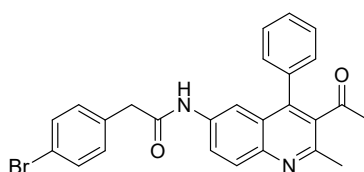
**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl)acetamide (6j).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (200 mg, 0.7246 mmole), 2-(3-bromophenyl)acetic acid (334 mg, 1.4492 mmole), HATU (550 mg, 1.4492 mmole), DIPEA (233 mg, 1.8115 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f$  = 0.5 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White

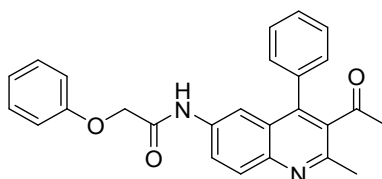
solid, yield : 78%, m.p. 142–144° C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.45 (s, 1H), 8.02 (d, J = 8.40 Hz, 1H), 7.97 (d, J = 9.20 Hz, 1H), 7.90 (s, 1H), 7.56-7.51 (m, 4H), 7.45-7.43 (m, 1H), 7.33 (d, J = 6.80 Hz, 2H), 7.28 (d, J = 8.00 Hz, 2H), 3.66 (s, 2H), 2.56 (s, 3H), 2.00 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 205.71, 169.31, 151.86, 144.26, 143.04, 138.82, 137.92, 135.41, 135.34, 132.48, 130.88, 130.15, 129.93, 129.63, 129.39, 129.22, 128.89, 125.43, 124.10, 121.91, 113.46, 42.98, 32.24, 23.68; **IR Stretching**; N-H (3332 cm<sup>-1</sup>), C=O (1695 cm<sup>-1</sup>), C=C (1534 cm<sup>-1</sup>); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for C<sub>26</sub>H<sub>22</sub>BrN<sub>2</sub>O<sub>2</sub> 473.0859; Found 473.0858

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-bromophenyl)acetamide(6k).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (200 mg, 0.7246 mmole), 2-(4-bromophenyl)acetic acid (334 mg, 1.4492 mmole), HATU (550 mg, 1.4492 mmole), DIPEA (233 mg, 1.8115 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.5 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. White solid, yield : 70%, m.p.: 108–110° C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.50 (s, 1H), 8.02 (dd, J = 1.60, 9.00 Hz, 1H), 7.97 (d, J = 8.80 Hz, 1H), 7.92 (s, 1H), 7.57-7.55 (m, 3H), 7.50-7.48 (m, 2H), 7.33 (d, J = 2.00 Hz, 2H), 7.25 (d, J = 8.00 Hz, 2H), 3.63 (s, 2H), 2.56 (s, 3H), 2.00 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 205.72, 169.44, 151.82, 144.24, 143.03, 137.98, 135.57, 135.39, 135.35, 132.0, 131.59, 130.14, 129.60, 129.37, 129.21, 125.43, 124.10, 120.26, 113.42, 42.86, 32.24, 23.67; **IR Stretching**; N-H (3396 cm<sup>-1</sup>), C=O (1691 cm<sup>-1</sup>), C=C (1485 cm<sup>-1</sup>); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for C<sub>26</sub>H<sub>22</sub>BrN<sub>2</sub>O<sub>2</sub> 473.0859; Found 473.0856

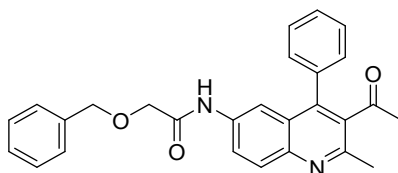
**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (6l).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2-phenoxyacetic

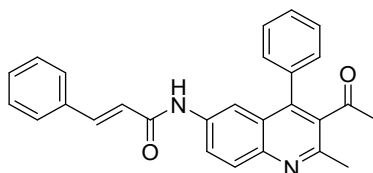
acid (286 mg, 1.8840 mmole), HATU (1.3 g, 3.6231 mmole), DIPEA (476 mg, 3.6231 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane). TLC:  $R_f = 0.6$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid, yield 72%, m.p.: 196–198<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.41 (s, 1H), 8.06 (dd,  $J = 2.00, 9.00$  Hz, 1H), 8.00 (d,  $J = 4.80$  Hz, 1H), 7.95 (d,  $J = 2.00$  Hz, 1H), 7.58-7.57 (m, 3H), 7.36-7.35 (m, 4H), 6.97-6.96 (m, 3H), 4.68 (s, 2H), 2.57 (s, 3H), 2.01 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 210.48, 172.11, 162.99, 156.83, 149.15, 147.88, 142.03, 140.16, 140.04, 134.93, 134.74, 133.97, 130.13, 129.28, 126.38, 119.79, 72.17, 37.00, 28.45; **IR Stretching**; N-H (3394  $\text{cm}^{-1}$ ), C=O (1690  $\text{cm}^{-1}$ ), C=C (1526  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for  $\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}_3$  411.1708; Found 411.1719

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).**



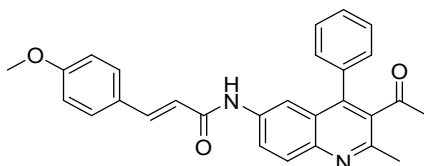
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2-(benzyloxy)acetic acid (360 mg, 2.1739 mmole), HATU (1.1 g, 2.8985 mmole), DIPEA (560 mg, 4.3478 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane). TLC:  $R_f = 0.6$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 62%, m.p. 138–140<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.12 (s, 1H), 8.07 (dd,  $J = 2.40, 9.00$  Hz, 1H), 7.98 (d,  $J = 8.80$  Hz, 1H), 7.96 (d,  $J = 2.00$  Hz, 1H), 7.59-7.57 (m, 3H), 7.37-7.37 (m, 7H), 4.59 (s, 2H), 4.07 (s, 2H), 2.57 (s, 3H), 2.01 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 210.49, 173.54, 156.72, 149.12, 147.87, 142.89, 142.09, 140.13, 140.09, 134.95, 134.12, 133.95, 133.50, 133.01, 132.88, 130.09, 129.45, 119.02, 77.61, 74.57, 37.00, 28.45; **IR Stretching**; N-H (3275  $\text{cm}^{-1}$ ), C=O (1704  $\text{cm}^{-1}$ ) C=C (1537  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for  $\text{C}_{27}\text{H}_{24}\text{N}_2\text{O}_3$  425.1865; Found 425.1888

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)cinnamamide (6n).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (500 mg, 1.8115 mmole), cinnamic acid (536 mg, 3.6231 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (701 mg, 5.4347 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f$  = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid, yield 70%, **m.p.** 188–190° C;  **$^1\text{H NMR}$**  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.49 (s, 1H), 8.10 (dd,  $J$  = 2.40, 7.80 Hz, 1H), 8.06 (d,  $J$  = 1.60 Hz, 1H), 8.01 (d,  $J$  = 8.80 Hz, 1H), 7.61-7.60 (m, 6H), 7.44-7.42 (m, 1H), 6.80 (d,  $J$  = 15.60 Hz, 1H), 2.58 (s, 3H), 2.02 (s, 3H);  **$^{13}\text{C NMR}$**  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.71, 172.45, 164.23, 151.86, 144.32, 143.09, 141.12, 138.11, 135.41, 135.11, 130.20, 129.48, 129.22, 128.21, 125.54, 124.20, 122.31, 121.18, 113.71, 32.27, 23.69; **IR Stretching**; N-H (3317  $\text{cm}^{-1}$ ), C=O (1688  $\text{cm}^{-1}$ ), C=C (1551  $\text{cm}^{-1}$ ); **HRMS (ESI)  $m/z$** : [M + H]<sup>+</sup> + Calculated for  $\text{C}_{27}\text{H}_{22}\text{N}_2\text{O}_2$  407.1759; Found 407.1785

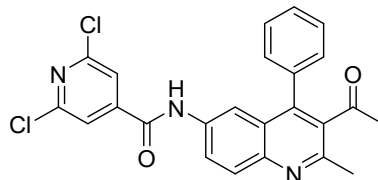
**(E)-N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-methoxyphenyl)acrylamide(6o).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (450 mg, 1.6304 mmole), (E)-3-(4-methoxyphenyl)acrylic acid (435 mg, 3.6231 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (701 mg, 5.4347 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f$  = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid, yield 64%, **m.p.** 228–230° C;  **$^1\text{H NMR}$**  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.39 (s, 1H), 8.10 (dd,  $J$  = 2.40, 9.00 Hz, 1H), 8.04 (d,  $J$  = 2.00 Hz, 1H), 7.97 (d,  $J$  = 11.60 Hz, 1H), 7.60-7.30 (m, 3H), 7.56-7.55 (m, 3H), 7.38-7.37 (m, 2H), 7.00 (d,  $J$  = 8.80 Hz, 2H), 6.65 (d,  $J$  = 15.60 Hz, 1H), 3.80 (s, 3H), 2.57 (s, 3H), 2.02 (s, 3H);  **$^{13}\text{C NMR}$**  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.74, 164.56, 161.14, 151.75, 144.25, 143.04, 140.89, 138.26, 135.43, 135.38, 130.20, 129.87, 129.21, 127.67, 125.54, 124.19,

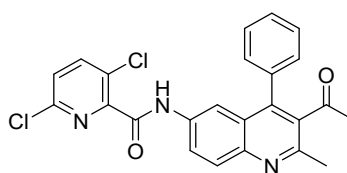
119.68, 114.94, 113.53, 55.37, 32.27, 23.69; **IR Stretching**; N-H (3369 cm<sup>-1</sup>), C=O (1678 cm<sup>-1</sup>), C=C (1493 cm<sup>-1</sup>); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for C<sub>28</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub> 437.1865; Found 437.1895

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2,6-dichloroisonicotinic acid (333 mg, 1.7309 mmole), HATU (1.3 g, 3.6231 mmole), DIPEA (476 mg, 3.6231 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.5 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Brown solid, yield 70%, **m.p.** 179–181<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.85 (bs, 1H), 8.17 (dd, J = 2.40, 8.80 Hz, 1H), 8.05 (d, J = 9.20 Hz, 2H), 7.98 (s, 2H), 7.60-7.59 (m, 3H), 7.38-7.37 (m, 2H), 2.59 (s, 3H), 2.03 (s, 3H); **<sup>13</sup>C NMR** (100 MHz DMSO-, d<sub>6</sub>): δ ppm 205.66, 172.49, 161.99, 152.62, 150.22, 148.46, 144.73, 143.33, 173.06, 135.52, 135.20, 130.19, 129.26, 125.29, 124.89, 122.40, 115.45, 32.24, 23.75; **IR Stretching**; N-H (3337 cm<sup>-1</sup>), C=O (1690 cm<sup>-1</sup>), C=C (1535 cm<sup>-1</sup>); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for C<sub>24</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub> 450.0776 Found 450.0777

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-3,6-dichloropicolinamide (6q).**

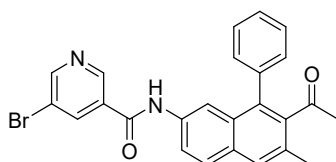


1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (500 mg, 1.8115 mmole), 3,6-dichloropicolinic acid (519 mg, 2.7173 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (584 mg, 4.5289 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.5 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Pale Yellow solid, yield 74%, **m.p.** 248–250<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.02 (bs, 1H), 8.16 (dd, J = 8.80, 12.80 Hz, 2H), 8.06 (d, J = 9.20 Hz, 1H), 7.99 (d, J = 2.00 Hz, 1H), 7.75 (d, J = 8.40 Hz, 1H), 7.59-7.58 (m, 3H), 7.39-7.39 (m, 2H), 2.60 (s, 3H), 2.03 (s, 3H); **<sup>13</sup>C NMR** (100 MHz,



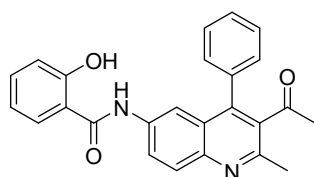
DMSO-d<sub>6</sub>):  $\delta$  ppm 205.66, 162.50, 151.80, 148.20, 144.63, 143.26, 142.33, 137.11, 135.52, 135.21, 130.21, 129.24, 127.93, 127.53, 125.42, 124.23, 114.67, 32.26, 23.76; **IR Stretching**; N-H (3217 cm<sup>-1</sup>), C=O (1680 cm<sup>-1</sup>), C=C (1503 cm<sup>-1</sup>); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> + Calculated for C<sub>24</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub> 450.0776; Found 450.077

**N-(7-Acetyl-6-methyl-8-phenylquinolin-2-yl)-5-bromonicotinamide (6r).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 5-bromonicotinic acid (434 mg, 2.1739 mmole), HATU (1.3 g, 3.6231 mmole), DIPEA (467 mg, 3.6231 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 70% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.3 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Yellow solid, yield 60%, m.p.: 152–154<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  ppm 10.74 (s, 1H), 9.03 (s, 1H), 8.87 (s, 1H), 8.50 (s, 1H), 8.18 (d, J = 5.20 Hz, 1H), 8.07-8.04 (m, 2H), 7.58 (s, 3H), 7.38 (s, 2H), 2.58 (s, 3H), 2.02 (s, 3H); **<sup>13</sup>C NMR** (100 MHz, DMSO-d<sub>6</sub>):  $\delta$  ppm 205.69, 163.27, 162.78, 153.23, 152.34, 147.88, 144.62, 143.24, 138.23, 137.50, 135.46, 135.29, 132.36, 130.21, 129.53, 129.43, 129.23, 125.30, 124.96, 120.38, 115.11, 32.22, 23.73; **IR Stretching**; N-H (3436 cm<sup>-1</sup>), C=O (1686 cm<sup>-1</sup>); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> + Calculated for C<sub>24</sub>H<sub>19</sub>BrN<sub>3</sub>O<sub>2</sub> 460.0660 ; Found 460.0657

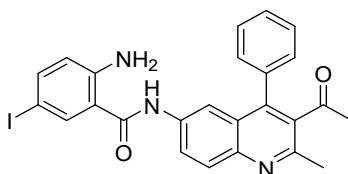
**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2-hydroxybenzoic acid (300 mg, 2.1739 mmole), HATU (1.1 g, 2.8985 mmole), DIPEA (373 mg, 2.8985 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.5 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Yellow solid, yield 50%, m.p.: 168–170<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  ppm 11.563 (bs, 400 MHz, CDCl<sub>3</sub>:  $\delta$  11.563 (bs, 1H),

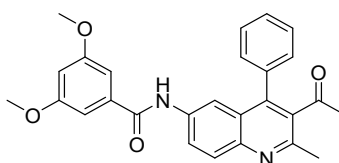
10.605 (bs, 1H), 8.11 (dd, J = 2.40, 9.00 Hz, 1H), 8.04-8.02 (m, 2H), 7.87 (dd, J = 1.20, 8.00 Hz, 1H), 7.60-7.60 (m, 3H), 7.44-7.44 (m, 3H), 6.98-6.96 (m, 2H), 2.592 (s, 3H), 2.026 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.68, 172.44, 167.20, 158.62, 152.29, 144.62, 143.25, 137.15, 135.45, 135.30, 134.09, 130.25, 129.22, 125.59, 125.35, 119.49, 117.59, 115.49, 32.24, 23.73; **IR Stretching**; N-H (3331  $\text{cm}^{-1}$ ), C=O (1694  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for  $\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_3$  397.1552; Found 397.1584

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-iodobenzamide (6t).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (450 mg, 1.6304 mmole), 2-amino-4-iodobenzoic acid (514 mg, 1.9565 mmole), HATU (1.5 g, 4.0760 mmole), DIPEA (525 mg, 4.0760 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane). TLC:  $R_f$  = 0.6 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Yellow solid, yield 62%, m.p.: 108–110 $^\circ$  C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ppm  $\delta$  10.36 (s, 1H), 8.15 (dd, J = 2.40, 9.20 Hz, 1H), 8.00 (d, J = 9.20 Hz, 1H), 7.92 (d, J = 2.40 Hz, 1H), 7.84 (d, J = 2.00 Hz, 1H), 7.60-7.58 (m, 3H), 7.52 (dd, J = 2.00, 51.60 Hz, 1H), 7.38-7.38 (m, 2H), 6.60 (d, J = 8.40 Hz, 1H), 6.42 (s, 2H), 2.70 (s, 3H), 2.01 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.77, 167.10, 151.99, 149.76, 144.46, 143.11, 140.65, 137.97, 136.90, 135.37, 130.28, 129.23, 125.67, 125.25, 119.34, 117.69, 115.17, 32.25, 23.73; **IR Stretching**; N-H (3471  $\text{cm}^{-1}$ ), C=O (1696  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> Calculated for  $\text{C}_{25}\text{H}_{20}\text{IN}_3\text{O}_2$  522.0878; Found 522.0685

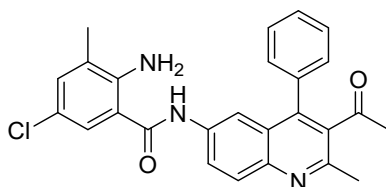
**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (500 mg, 1.8115 mmole), 3,5-dimethoxybenzoic acid (494 mg, 2.7173 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (584 mg,

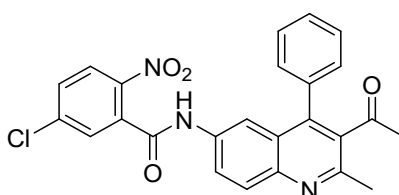
4.5289 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Yellow solid, yield 76%, m.p.: 179–181 $^\circ$  C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ) ppm  $\delta$  10.45 (s, 1H), 8.18-8.17 (m, 2H), 8.02 (d,  $J = 9.20$  Hz, 1H), 7.06 (d,  $J = 2.00$  Hz, 1H), 6.70 (s, 1H), 3.81 (s, 6H), 2.58 (s, 3H), 2.02 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.76, 172.47, 165.84, 160.81, 152.08, 144.49, 143.23, 137.91, 137.16, 135.41, 135.38, 130.23, 129.41, 129.33, 129.22, 125.38, 125.32, 115.01, 160.14, 103.95, 55.97, 32.25, 23.71; **IR Stretching**; N-H (3369  $\text{cm}^{-1}$ ), C=O (1678  $\text{cm}^{-1}$ ) C=C (1493  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] Calculated for  $\text{C}_{28}\text{H}_{25}\text{NO}_2$  441.1814; Found 441.1838

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).**



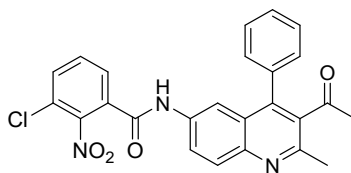
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (500 mg, 1.8115 mmole), 2-amino-5-chloro-3-methylbenzoic acid (435 mg, 2.3550 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (584 mg, 4.5289 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane). TLC:  $R_f = 0.6$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Yellow solid, yield 65%, m.p.: 130–132 $^\circ$  C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.32 (s, 1H), 8.10 (dd,  $J = 2.00, 9.00$  Hz, 1H), 7.93 (d,  $J = 8.80$  Hz, 1H), 7.87 (d,  $J = 2.40$  Hz, 1H), 7.53-7.51 (m, 4H), 7.30 (dd,  $J = 2.00, 7.40$  Hz, 2H), 7.12 (d,  $J = 2.00$  Hz, 1H), 5.69 (s, 2H), 2.51 (s, 3H), 2.04 (s, 3H), 1.94 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.76, 172.46, 167.73, 152.03, 147.12, 144.47, 143.14, 137.94, 135.35, 132.82, 130.27, 129.39, 129.21, 126.18, 126.06, 125.64, 125.25, 118.18, 116.07, 115.26, 55.37, 32.25, 23.73, 21.51; **IR Stretching**; N-H (3355  $\text{cm}^{-1}$ ), C=O (1692  $\text{cm}^{-1}$ ) C=C (1539  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] Calculated for  $\text{C}_{26}\text{H}_{23}\text{ClN}_3\text{O}_2$  444.1473; Found 444.1473

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-5-chloro-2-nitrobenzamide (6w).**



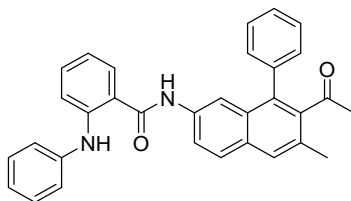
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (500 mg, 1.8115 mmole), 5-chloro-2-nitrobenzoic acid (543 mg, 2.3550 mmole), HATU (1.7 g, 4.5289 mmole), DIPEA (584 mg, 4.5289 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Brown solid, yield 50%, m.p.: 118–120° C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  ppm 10.98 (s, 1H), 8.18 (d,  $J = 8.80$  Hz, 1H), 8.13 (dd,  $J = 2.00, 9.00$  Hz, 1H), 8.05 (d,  $J = 9.20$  Hz, 1H), 7.97 (d,  $J = 2.40$  Hz, 1H), 7.91 (d,  $J = 2.00$  Hz, 1H), 7.84 (dd,  $J = 2.40, 8.80$  Hz, 1H), 7.59-7.57 (m, 3H), 7.38-7.38 (m, 2H), 2.60 (s, 3H), 2.04 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.67, 172.47, 163.23, 152.36, 145.29, 144.56, 143.21, 139.31, 137.51, 135.50, 135.23, 134.44, 131.33, 130.18, 129.82, 129.74, 129.42, 129.23, 126.80, 125.41, 124.22, 114.42, 32.27, 23.75; **IR Stretching**; N-H ( $3266\text{ cm}^{-1}$ ), C=O ( $1688\text{ cm}^{-1}$ ), C=C ( $1519\text{ cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] Calculated for  $\text{C}_{26}\text{H}_{22}\text{ClN}_3\text{O}_2$  460.1064; Found 460.1076

**N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)-3-chloro-2-nitrobenzamide (6x).**



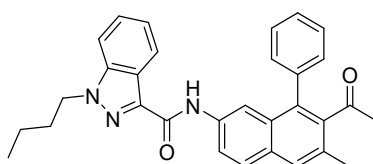
1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (450 mg, 1.6304 mmole), 3-chloro-2-nitrobenzoic acid (456 mg, 2.2826 mmole), HATU (1.5 g, 4.0760 mmole), DIPEA (525 mg, 4.0760 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale Yellow solid, yield 86 %, m.p.: 124–126° C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  ppm 11.15 (s, 1H), 8.21 (d,  $J = 8.40$  Hz, 1H), 8.09 (d,  $J = 9.20$  Hz, 1H), 7.95-7.93 (m, 4H), 7.59 (s, 3H), 7.29 (s, 2H), 2.63 (s, 3H), 2.03 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.03, 162.76, 162.64, 152.60, 147.40, 144.68, 143.12, 137.63, 135.61, 134.86, 133.67, 132.78, 131.38, 130.15, 129.71, 129.32, 128.80, 128.53, 125.58, 125.24, 125.18, 115.15, 31.22, 23.13; **IR Stretching**; N-H ( $3393\text{ cm}^{-1}$ ), C=O ( $1688\text{ cm}^{-1}$ ), C=C ( $1534\text{ cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] Calculated for  $\text{C}_{28}\text{H}_{25}\text{NO}_2$  460.1064; Found 460.1064

**N-(7-Acetyl-6-methyl-8-phenyl-naphthalen-2-yl)-2-(phenylamino)benzamide(6y).**



1-(6-amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 2-(phenylamino)benzoic acid (401 mg, 1.8840 mmole), HATU (1.1 g, 3.6231 mmole), DIPEA (476 mg, 3.6231 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 80%, m.p.: 208–208<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  ppm 10.61 (s, 1H), 8.949 (s, 1H), 8.20 (dd,  $J = 1.60, 9.00$  Hz, 1H), 8.01 (d,  $J = 9.20$  Hz, 1H), 7.94 (d,  $J = 1.60$  Hz, 1H), 7.72 (d,  $J = 7.20$  Hz, 1H), 7.59-7.57 (m, 3H), 7.37-7.36 (m, 3H), 7.30-7.28 (m, 3H), 7.13 (d,  $J = 7.60$  Hz, 2H), 6.97-6.95 (m, 2H), 2.59 (s, 3H), 2.01 (s, 3H); **<sup>13</sup>C NMR** (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 205.76, 168.25, 152.11, 144.53, 144.38, 143.15, 142.12, 137.84, 135.37, 135.33, 132.68, 130.27, 129.80, 129.21, 125.56, 125.26, 122.22, 120.93, 119.85, 119.04, 116.27, 115.34, 32.23, 23.73; **IR Stretching**; N-H (3328  $\text{cm}^{-1}$ ), C=O (1710  $\text{cm}^{-1}$ ), C=C (1591  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] Calculated for  $\text{C}_{31}\text{H}_{25}\text{N}_3\text{O}_2$  472.2025; Found 472.2027

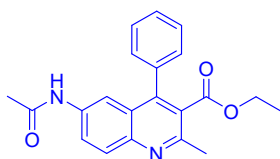
**N-(7-Acetyl-6-methyl-8-phenylnaphthalen-2-yl)-1-butyl-1H-indazole-3-carboxamide (6z).**



1-(6-Amino-2-methyl-4-phenylquinolin-3-yl)ethan-1-one (400 mg, 1.4492 mmole), 1-butyl-1H-indazole-3-carboxylic acid (379 mg, 1.7391 mmole), HATU (1.1 g, 2.8985 mmole), DIPEA (560 mg, 4.3478 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 90%, m.p.: 180–182<sup>o</sup> C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  ppm 10.60 (s, 1H), 8.33 (dd,  $J = 2.00, 9.00$  Hz, 1H), 8.23 (d,  $J = 2.00$  Hz, 1H), 8.17 (d,  $J = 8.40$  Hz, 1H), 8.02 (d,  $J = 9.20$  Hz, 1H), 7.81 (d,  $J = 8.40$  Hz, 1H), 7.62-7.60 (m, 3H), 7.48 (t,  $J = 7.20$  Hz, 1H), 7.37 (dd,  $J = 2.00, 27.40$  Hz,

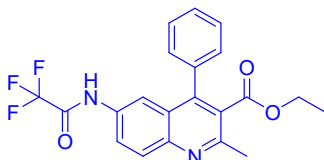
2H), 7.30 (t,  $J = 7.60$  Hz, 1H), 4.53 (t,  $J = 7.20$  Hz, 2H), 2.59 (s, 3H), 2.02 (s, 3H), 1.880 (qt, 3H), 1.2765 (sext, 2H), 0.89 (t,  $J = -7.20$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 205.80, 161.28, 151.91, 144.45, 143.19, 141.12, 137.71, 137.26, 135.46, 135.39, 130.30, 129.38, 129.25, 127.19, 125.47, 125.34, 123.11, 122.88, 122.19, 115.01, 110.97, 49.09, 32.22, 31.97, 23.71, 19.90, 13.98; **IR Stretching**; N-H (3335  $\text{cm}^{-1}$ ), C=O (1698  $\text{cm}^{-1}$ ), C=C (1543  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H] Calculated for  $\text{C}_{31}\text{H}_{29}\text{N}_3\text{O}_2$  477.2290; Found 477.2280

### Ethyl 6-Acetamido-2-methyl-4-phenylquinoline-3-carboxylate (6aa).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (500 mg, 1.6339 mmole), acetic acid (980 mg, 16.3398 mmole), HATU (1.2 g, 3.2679 mmole), DIPEA (526 mg, 4.0849 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 80% ethyl acetate in Hexane). TLC:  $R_f = 0.3$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Brown solid, yield 60%, m.p.: 158–160 $^\circ$  C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ): ppm  $\delta$  10.20 (s, 1H), 8.04 (dd,  $J = 2.00, 9.00$  Hz, 1H), 7.97 (d,  $J = 9.20$  Hz, 1H), 7.84 (d,  $J = 2.00$  Hz, 1H), 7.55-7.55 (m, 3H), 7.34-7.33 (m, 2H), 4.01 (q,  $J = 7.20$  Hz, 2H), 2.63 (s, 3H), 2.01 (s, 3H), 0.87 (t,  $J = 7.20$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO-,  $d_6$ ):  $\delta$  ppm 169.07, 168.16, 152.41, 145.20, 144.42, 138.20, 135.70, 129.55, 129.01, 128.84, 127.70, 125.32, 124.48, 113.48, 61.45, 24.41, 23.52, 12.88. **HRMS (ESI) m/z**: [M + H] + Calcd for  $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}_3$  349.1547; Found 349.1543.

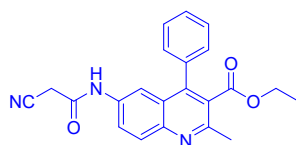
### Ethyl 2-Methyl-4-phenyl-6-(2,2,2-trifluoroacetamido)quinoline-3-carboxylate (6ab).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (500 mg, 1.6339 mmole), trifluoroacetic acid (745 mg, 6.5359 mmole), HATU (993 mg, 2.6143 mmole), DIPEA (421 mg, 3.2679 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 80% ethyl acetate in Hexane).

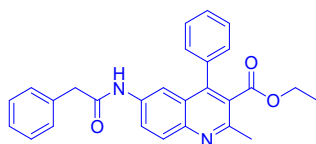
TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Brown solid, yield 65%, m.p.: 138–140 $^\circ$  C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 11.52 (s, 1H), 8.15 (dd,  $J = 2.00, 9.20$  Hz, 1H), 8.08 (d,  $J = 9.20$  Hz, 1H), 7.98 (d,  $J = 2.00$  Hz, 1H), 7.58–7.57 (m, 3H), 7.37–7.36 (m, 2H), 4.03 (q,  $J = 6.80$  Hz, 2H), 2.67 (s, 3H), 0.88 (t,  $J = 7.20$  Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 167.94, 153.99, 145.73, 145.30, 135.37, 135.28, 130.0, 129.58, 129.22, 128.93, 128.02, 125.05, 116.75, 61.59, 3.66, 13.87; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{21}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_3$  403.1264; Found 403.1257

### Ethyl 6-(2-Cyanoacetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ac).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (500 mg, 1.6339 mmole), 2-cyanoacetic acid (416 mg, 4.9019 mmole), HATU (1.2 gm, 2.6143 mmole), DIPEA (526 mg, 4.0849 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Brown solid, yield 68%, m.p.: 198–200 $^\circ$  C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.60 (s, 1H), 8.01 (dd,  $J = 9.20, 11.00$  Hz, 1H), 7.97 (d,  $J = 1.60$  Hz, 1H), 7.82 (d,  $J = 8.00$  Hz, 1H), 7.57–7.55 (m, 3H), 7.35–7.34 (m, 2H), 4.02 (q,  $J = 6.80$  Hz, 2H), 3.89 (s, 2H), 2.64 (s, 3H), 0.88 (t,  $J = 7.20$  Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 168.05, 161.88, 152.99, 145.35, 144.69, 137.25, 135.52, 129.90, 129.54, 129.12, 128.90, 127.84, 125.28, 124.29, 116.19, 114.16, 61.51, 27.25, 23.58, 13.88; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{22}\text{H}_{20}\text{N}_3\text{O}_3$  374.1499; Found 374.1495

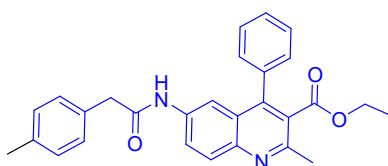
### Ethyl 2-Methyl-4-phenyl-6-(2-Phenylacetamido)quinoline-3-carboxylate (6ad).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (650 mg, 2.1241 mmole), 2-phenylacetic acid (577 mg, 4.2483 mmole), HATU (1.6 gm, 4.2483 mmole), DIPEA (685 mg, 5.3104 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane).

TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid, yield 90%, m.p.: 150–152 $^\circ$  C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.37 (s, 1H), 7.97 (dd,  $J = 1.60, 9.20$  Hz, 1H), 7.91 (d,  $J = 9.20$  Hz, 1H), 7.84 (s, 1H), 7.47-7.46 (m, 3H), 7.26-7.25 (m, 6H), 3.93 (q,  $J = 7.20$  Hz, 2H), 3.55 (s, 2H), 2.56 (s, 3H), 0.80 (t,  $J = 6.80$  Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 169.89, 168.13, 152.51, 145.24, 144.50, 138.12, 136.16, 135.67, 129.66, 129.54, 129.04, 128.87, 128.76, 127.02, 125.33, 124.44, 113.57, 61.46, 55.38, 43.70, 23.53, 13.88; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  + Calcd for  $\text{C}_{27}\text{H}_{25}\text{N}_2\text{O}_3$  425.1859; Found 425.1854

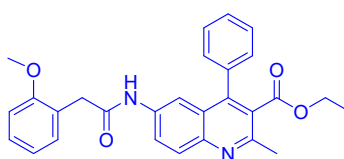
**Ethyl 2-Methyl-4-phenyl-6-(2-(p-tolyl)acetamido)quinoline-3-carboxylate (6ae).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (700 mg, 2.2875 mmole), 2-(p-tolyl)acetic acid (514 mg, 4.2483 mmole), HATU (1.7 gm, 4.5751 mmole), DIPEA (737 mg, 5.7189 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 92%, m.p.: 162–1164 $^\circ$  C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.41 (s, 1H), 8.04 (d,  $J = 9.20$  Hz, 1H), 7.98 (d,  $J = 9.20$  Hz, 1H), 7.91 (s, 1H), 7.53-0.00 (m, 3H), 7.32 (d,  $J = 5.60$  Hz, 2H), 7.17 (d,  $J = 7.60$  Hz, 2H), 7.10 (d,  $J = 7.60$  Hz, 2H), 4.01 (q,  $J = 5.60$  Hz, 2H), 3.57 (s, 2H), 2.63 (s, 3H), 2.26 (s, 3H), 0.87 (t,  $J = 7.20$  Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 170.06, 168.14, 152.48, 145.23, 144.47, 138.15, 136.05, 135.67, 133.08, 129.53, 129.50, 129.31, 128.87, 127.77, 125.32, 124.44, 113.54, 61.46, 43.32, 23.53, 21.10, 13.88; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  + Calculated for  $\text{C}_{28}\text{H}_{27}\text{N}_2\text{O}_3$  439.2016; Found 439.2009

**Ethyl-6-(2-(2-Methoxyphenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate**

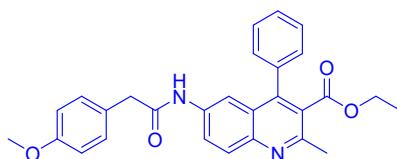
**(6af)**





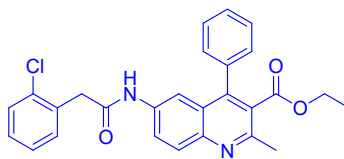
Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (600 mg, 1.9607 mmole), 2-(2-methoxyphenyl)acetic acid (488 mg, 2.9411 mmole), HATU (1.4 gm, 3.9215 mmole), DIPEA (632 mg, 4.9019 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield 94%, m.p.: 164–166<sup>o</sup> C;  $^1\text{H NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.37 (s, 1H), 8.02 (dd,  $J = 2.00, 9.20$  Hz, 1H), 7.99 (d,  $J = 9.20$  Hz, 1H), 7.96 (d,  $J = 1.60$  Hz, 1H), 7.54-7.52 (m, 3H), 7.33-7.33 (m, 2H), 7.25-7.25 (m, 2H), 6.95 (d,  $J = 8.00$  Hz, 1H), 6.88 (t,  $J = 7.60$  Hz, 1H), 4.01 (q,  $J = 6.80$  Hz, 2H), 3.73 (s, 3H), 3.62 (s, 2H), 3.62 (s, 3H), 2.64 (s, 3H), 0.87 (t,  $J = 7.20$  Hz, 3H),  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 169.92, 168.17, 157.67, 152.37, 145.22, 144.44, 138.28, 135.72, 131.46, 129.63, 129.53, 129.02, 128.84, 128.54, 127.74, 125.37, 124.49, 124.34, 120.58, 113.41, 111.09, 61.45, 55.83, 38.12, 23.53, 13.88; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calculated for  $\text{C}_{28}\text{H}_{27}\text{N}_2\text{O}_4$  455.1965; Found 455.1962

**Ethyl 6-(2-(4-Methoxyphenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ag)**



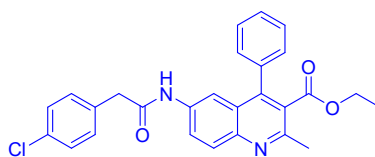
Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (700 mg, 2.2875 mmole), 2-(4-methoxyphenyl)acetic acid (569 mg, 3.4315 mmole), HATU (1.7 gm, 4.5751 mmole), DIPEA (737 mg, 5.7189 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f = 0.5$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. White solid, yield : 92 %, m.p.: 138–140<sup>o</sup> C;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.29 (s, 1H), 8.05 (dd,  $J = 2.00, 9.00$  Hz, 1H), 7.98 (d,  $J = 9.20$  Hz, 1H), 7.91 (s, 1H), 7.55-7.53 (m, 3H), 7.33-7.33 (m, 2H), 7.21 (d,  $J = 8.40$  Hz, 2H), 6.86 (d,  $J = 8.40$  Hz, 2H), 4.01 (q,  $J = 6.80$  Hz, 2H), 3.71 (s, 3H), 3.55 (s, 2H), 2.63 (s, 3H), 0.87 (t,  $J = 7.20$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 170.24, 168.14, 158.53, 145.22, 144.49, 138.18, 135.70, 130.62, 129.63, 129.54, 129.02, 128.85, 128.06, 127.78, 125.34, 124.46, 114.20, 61.44, 55.48, 42.83, 23.51, 13.87; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calculated for  $\text{C}_{28}\text{H}_{27}\text{N}_2\text{O}_4$  455.1965; Found 455.1960

**Ethyl 6-(2-(2-Chlorophenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ah).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (700 mg, 2.2875 mmole), 2-(2-chlorophenyl)acetic acid (583 mg, 3.4313 mmole), HATU (1.7 gm, 4.5751 mmole), DIPEA (737 mg, 5.7189 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC:  $R_f$ =0.5 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid, yield : 86%, m.p.: 152–154<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.56-0.00 (m, 1H), 8.07 (dd,  $J$  = 2.00, 8.80 Hz, 1H), 8.04 (d,  $J$  = 8.80 Hz, 1H), 7.98 (d,  $J$  = 1.60 Hz, 1H), 7.58-7.56 (m, 3H), 7.48-7.47 (m, 2H), 7.36-7.36 (m, 4H), 4.05 (q,  $J$  = 7.20 Hz, 2H), 3.88 (s, 2H), 2.68 (s, 3H), 0.91 (t,  $J$  = 7.20 Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 168.72, 168.14, 152.50, 145.25, 144.48, 138.09, 135.67, 134.14, 134.12, 132.80, 129.72, 129.52, 129.44, 129.11, 129.05, 128.87, 127.79, 127.52, 125.36, 124.40, 113.47, 61.47, 41.20, 23.54, 13.88; **IR Stretching**; N-H (3354  $\text{cm}^{-1}$ ), C=O (1701  $\text{cm}^{-1}$ , C=C (1539  $\text{cm}^{-1}$ ); **HRMS (ESI) m/z**: [M + H]<sup>+</sup> + Calculated for  $\text{C}_{27}\text{H}_{24}\text{ClN}_2\text{O}_3$  459.1470; Found 459.1465

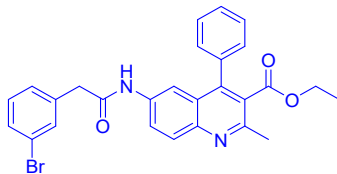
**Ethyl 6-(2-(4-Chlorophenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ai).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (650 mg, 2.1241 mmole), 2-(4-chlorophenyl)acetic acid (541 mg, 3.1862 mmole), HATU (1.6 gm, 4.2483 mmole), DIPEA (685 mg, 5.3104 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f$ =0.4 (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. pale yellow solid, yield : 85%, m.p ; 158–160<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  ppm 10.46 (s, 1H), 8.03 (dd,  $J$  = 2.00, 9.20 Hz, 1H), 7.99 (d,  $J$  = 9.20 Hz, 1H), 7.90 (d,  $J$  = 1.60 Hz, 1H), 7.55-7.53 (m, 3H), 7.36 (d,  $J$  = 8.40 Hz, 2H), 7.33-7.32 (m, 4H), 4.01 (q,  $J$  = 6.80 Hz, 2H), 3.64 (s, 2H), 2.63 (s, 3H), 0.87 (t,  $J$  = 7.20 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 169.53, 168.13, 152.56, 145.25,

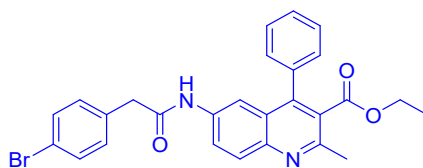
144.50, 138.03, 135.65, 135.12, 131.61, 129.53, 128.87, 128.68, 125.32, 124.42, 113.61, 61.47, 42.79, 23.54, 13.88; **HRMS (ESI) m/z:** [M + H]<sup>+</sup> Calculated for C<sub>27</sub>H<sub>24</sub>ClN<sub>2</sub>O<sub>3</sub> 459.1470; Found 459.1465

**Ethyl 6-(2-(3-Bromophenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aj).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (700 mg, 2.2875 mmole), 2-(3-bromophenyl)acetic acid (730 mg, 3.4313 mmole), HATU (1.7 gm, 4.5751 mmole), DIPEA (737 mg, 5.7189 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. White solid, yield: 88%, m.p. 144–146<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.46 (s, 1H), 8.04 (d, J = 8.80 Hz, 1H), 7.99 (d, J = 9.20 Hz, 1H), 7.90 (s, 1H), 7.55-7.53 (m, 4H), 7.44 (d, J = 6.80 Hz, 1H), 7.33-7.31 (m, 4H), 4.01 (q, J = 7.20 Hz, 2H), 3.66 (s, 1H), 2.63 (s, 3H), 0.87 (t, J = 7.20 Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 169.33, 168.12, 152.58, 145.25, 144.53, 138.81, 137.98, 135.66, 132.49, 130.87, 129.71, 129.53, 129.06, 128.88, 127.79, 125.32, 124.44, 121.91, 113.66, 61.46, 55.38, 42.98, 23.54, 13.88; **HRMS (ESI) m/z:** [M + H]<sup>+</sup> Calculated for C<sub>27</sub>H<sub>24</sub>BrN<sub>2</sub>O<sub>3</sub> 503.0964; Found 503.0959

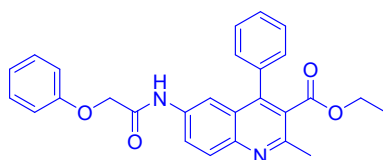
**Ethyl 6-(2-(4-Bromophenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ak).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (650 mg, 2.1241 mmole), 2-(4-bromophenyl)acetic acid (678 mg, 3.1862 mmole), HATU (1.6 gm, 4.2483 mmole), DIPEA (685 mg, 5.3104 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Pale yellow solid, yield : 86%, m.p. 160–162<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.45 (s, 1H), 8.04 (dd, J = 1.60, 9.20 Hz, 1H), 7.98 (d, J = 9.20 Hz, 1H), 7.90 (s, 1H), 7.54-7.53 (m, 3H), 7.49 (d, J = 8.40

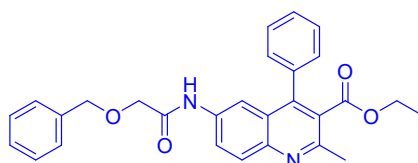
Hz, 2H), 7.32 (d, J = 7.60 Hz, 2H), 7.25 (d, J = 8.40 Hz, 2H), 4.01 (q, J = 6.80 Hz, 2H), 3.62 (s, 2H), 2.63 (s, 3H), 0.87 (t, J = 7.20 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 169.44, 168.13, 152.56, 145.24, 144.52, 138.02, 135.66, 135.54, 131.99, 131.60, 129.53, 129.05, 128.87, 127.78, 125.32, 124.42, 120.27, 113.62, 61.46, 42.87, 23.54, 13.88;

**Ethyl 2-methyl-6-(2-Phenoxyacetamido)-4-phenylquinoline-3-carboxylate (6al).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (500 mg, 1.6339 mmole), 2-phenoxyacetic acid (496 mg, 3.2679 mmole), HATU (1.2 g, 4.2483 mmole), DIPEA (526 mg, 4.0849 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.6 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. White solid, yield 80%, m.p.: 196–198<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.41 (s, 1H), 8.08 (dd, J = 1.60, 9.00 Hz, 1H), 8.01 (d, J = 9.20 Hz, 1H), 7.94 (d, J = 1.60 Hz, 1H), 7.55-7.54 (m, 3H), 7.34-7.34 (m, 4H), 6.97-6.96 (m, 3H), 4.67 (s, 2H), 4.01 (q, J = 6.80 Hz, 2H), 2.64 (s, 3H), 0.88 (t, J = 7.20 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 168.11, 167.38, 158.25, 152.80, 145.35, 144.68, 137.35, 135.60, 129.98, 129.68, 129.56, 129.08, 128.88, 127.81, 125.27, 124.87, 121.63, 115.04, 114.44, 67.42, 61.49, 23.57, 13.89; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calculated for C<sub>27</sub>H<sub>25</sub>N<sub>2</sub>O<sub>4</sub> 441.1808; Found 414.1804

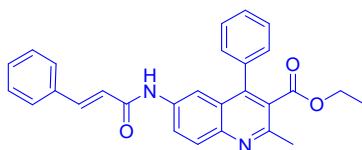
**Ethyl 6-(2-(Benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (500 mg, 1.6339 mmole), 2-(benzyloxy)acetic acid (542 mg, 3.2679 mmole), HATU (1.2 g, 3.2679 mmole), DIPEA (526 mg, 4.0849 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 70% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.3 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. White solid, yield 75%, m.p.: 118–120<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.14 (s, 1H), 8.09 (dd, J

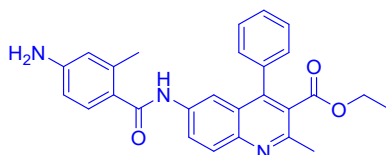
= 2.40, 9.20 Hz, 1H), 7.99 (d, J = 9.20 Hz, 1H), 7.96 (d, J = 2.40 Hz, 1H), 7.56-7.55 (m, 3H), 7.37-7.37 (m, 7H), 4.58 (s, 2H), 4.08 (s, 2H), 4.02 (q, J = 7.20 Hz, 2H), 2.64 (s, 3H), 0.88 (t, J = 7.20 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 168.82, 168.14, 152.69, 145.32, 144.64, 138.15, 137.42, 135.65, 129.57, 129.54, 129.05, 128.86, 128.75, 128.26, 128.12, 127.77, 125.24, 125.04, 114.46, 72.85, 69.81, 61.47, 23.56, 13.89; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calculated for C<sub>28</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub> 455.1965; Found 4505.1961

### Ethyl 6-Cinnamamido-2-methyl-4-phenylquinoline-3-carboxylate (6an).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (400 mg, 1.3071 mmole), cinnamic acid (383 mg, 2.6143 mmole), HATU (993 mg, 2.6143 mmole), DIPEA (412 mg, 3.2679 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Brown solid, yield 70%, **m.p.**: 194–196° C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.50 (s, 1H), 8.12 (dd, J = 2.00, 9.20 Hz, 1H), 8.05 (d, J = 1.60 Hz, 1H), 8.02 (d, J = 9.20 Hz, 1H), 7.61-7.60 (m, 6H), 7.44-7.42 (m, 3H), 7.38-7.37 (m, 2H), 6.80 (d, J = 15.60 Hz, 1H), 4.02 (q, J = 7.20 Hz, 2H), 2.59 (s, 3H), 0.89 (t, J = 7.20 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 168.16, 164.25, 152.60, 145.30, 144.59, 141.16, 138.17, 135.09, 130.34, 129.72, 129.59, 129.48, 129.05, 128.88, 128.22, 127.77, 125.42, 124.53, 122.26, 113.91, 61.47, 23.56, 13.89; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calculated for C<sub>28</sub>H<sub>26</sub>N<sub>2</sub>O<sub>3</sub> 437.1859; Found 437.1853

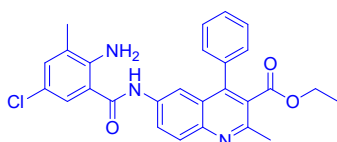
### Ethyl 6-(4-Amino-2-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ao).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (360 mg, 1.1764 mmole), 4-amino-2-methylbenzoic acid (355 mg, 2.3529 mmole), HATU (894 mg, 2.33529 mmole), DIPEA (379 mg, 3.2679 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 70% ethyl

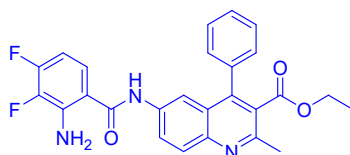
acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale yellow solid, yield 74%, **m.p.** 104–106<sup>0</sup> C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm  $\delta$  8.83-8.82 (m, 1H), 8.74-8.73 (m, 1H), 8.12 (d,  $J = 8.80$  Hz, 1H), 7.72 (d,  $J = 8.80$  Hz, 1H), 7.54-7.53 (m, 3H), 7.29 (d,  $J = 7.60$  Hz, 2H), 7.19 (d,  $J = 8.80$  Hz, 1H), 6.58 (s, 2H), 6.44 (s, 1H), 3.98 (q,  $J = 7.20$  Hz, 2H), 2.54 (s, 2H), 2.43 (s, 3H), 0.86 (t,  $J = 7.20$  Hz, 3H). **<sup>13</sup>C NMR** (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 168.60, 161.95, 155.92, 152.79, 151.34, 148.00, 147.85, 145.86, 142.80, 141.77, 140.90, 136.51, 134.97, 134.42, 130.12, 129.78, 129.54, 129.20, 128.75, 128.60, 127.29, 126.71, 122.81, 121.94, 121.05, 116.47, 111.65, 107.00, 103.60, 61.16, 23.12, 22.53, 13.89; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calculated for  $\text{C}_{27}\text{H}_{26}\text{N}_3\text{O}_3$  440.1969; Found 440.1960

**Ethyl-6-(2-Amino-5-chloro-3-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ap).**



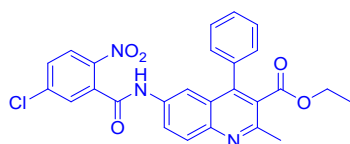
Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (360 mg, 1.1764 mmole), 2-amino-5-chloro-3-methylbenzoic acid (435 mg, 2.3529 mmole), HATU (849 mg, 2.3529 mmole), DIPEA (379 mg, 2.3529 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 70% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Brown solid, yield 60%, **m.p.:** 178–180<sup>0</sup> C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 10.38 (s, 1H), 8.76 (s, 1H), 8.53 (d,  $J = 7.20$  Hz, 1H), 8.20 (d,  $J = 8.40$  Hz, 1H), 8.03-8.01 (m, 2H), 7.55-7.38 (m, 7H), 6.20 (s, 2H), 4.03 (d,  $J = 5.20$  Hz, 2H), 2.66 (s, 3H), 2.12 (s, 6H), 0.90 (s, 3H); **<sup>13</sup>C NMR** (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  ppm 169.44, 168.17, 167.75, 152.76, 151.52, 149.14, 147.11, 145.34, 144.75, 140.10, 138.02, 135.69, 135.10, 134.19, 132.82, 129.64, 125.98, 125.16, 121.15, 117.84, 116.07, 115.48, 115.48, 61.47, 23.58, 17.86, 13.89; **HRMS (ESI) m/z**:  $[\text{M} + \text{H}]^+$  Calculated for  $\text{C}_{27}\text{H}_{25}\text{ClN}_3\text{O}_3$  474.1579; Found 474.1573

**Ethyl 6-(2-Amino-3,4-difluorobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aq).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (400 mg, 1.3071 mmole), 2-amino-3,4-difluorobenzoic acid (452 mg, 2.6143 mmole), HATU (993 mg, 2.6143 mmole), DIPEA (421 mg, 3.2679 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 70% ethyl acetate in Hexane). TLC:  $R_f = 0.3$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Pale Yellow solid, yield 70%, m.p. : 188–190<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ );  $\delta$  ppm 10.20 (s, 1H), 8.10 (dd,  $J = 1.60, 9.20$  Hz, 1H), 7.95 (d,  $J = 9.20$  Hz, 1H), 7.84 (d,  $J = 1.60$  Hz, 1H), 7.69-7.67 (m, 1H), 7.50-7.48 (m, 3H), 7.30-7.30 (m, 2H), 6.66-6.64 (m, 1H), 6.42 (s, 2H), 3.95 (q,  $J = 6.80$  Hz, 2H), 2.58 (s, 3H), 0.82 (t,  $J = 7.20$  Hz, 3H); <sup>13</sup>C NMR (100 MHz DMSO-,  $d_6$ ):  $\delta$  ppm 168.16, 166.75, 152.77, 145.32, 144.72, 137.93, 135.65, 129.76, 129.62, 129.53, 129.31, 129.09, 128.89, 128.76, 128.62, 122.82, 115.35, 61.49, 23.56, 13.89; HRMS (ESI) m/z: [M + H] + Calculated for  $\text{C}_{26}\text{H}_{22}\text{F}_2\text{N}_3\text{O}_3$  462.1623; Found 462.1617

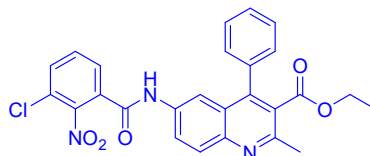
**Ethyl 6-(5-Chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ar).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (300 mg, 1.3071 mmole), 5-chloro-2-nitrobenzoic acid (294 mg, 1.4705 mmole), HATU (745 mg, 1.9607 mmole), DIPEA (316 mg, 2.4509 mmole) in DMF (8 mL) at RT 10 h. The title compound was isolated (Eluent 70% ethyl acetate in Hexane). TLC:  $R_f = 0.3$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Yellow solid, yield 82%, m.p.: 210–212<sup>o</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ )  $\delta$  ppm 10.99 (s, 1H), 8.19-8.16 (m, 2H), 8.06 (d,  $J = 9.20$  Hz, 1H), 7.96 (d,  $J = 2.00$  Hz, 1H), 7.91 (s, 1H), 7.56-7.54 (m, 3H), 7.37-7.35 (m, 2H), 4.03 (q,  $J = 7.20$  Hz, 2H), 2.66 (s, 3H), 0.89 (t,  $J = 7.20$  Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 168.06, 163.24, 153.08, 145.44, 145.29, 144.84, 139.31, 137.57, 135.54, 134.43, 131.34, 129.91, 129.75, 129.56, 129.10, 128.89, 128.75, 127.91, 126.79, 125.30,

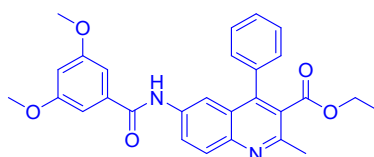
124.57, 114.64, 61.52, 23.60, 13.89; **HRMS (ESI) m/z:** [M + H]<sup>+</sup> + Calculated for C<sub>26</sub>H<sub>21</sub>ClN<sub>3</sub>O<sub>5</sub> 490.1165; Found 490.1159

**Ethyl 6-(3-Chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6as).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (400 mg, 1.3071 mmole), 3-chloro-2-nitrobenzoic acid (394 mg, 1.9607 mmole), HATU (993 mg, 2.6143 mmole), DIPEA (421 mg, 3.2679 mmole) in DMF (10 mL) at RT 10 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Yellow solid, yield 80%, m.p. : 124–126° C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ ppm 8.14 (dd, J = 1.60, 9.20 Hz, 1H), 8.03 (d, J = 9.20 Hz, 1H), 7.93 (d, J = 8.00 Hz, 2H), 7.86 (s, 1H), 7.75 (t, J = 8.00 Hz, 1H), 7.56-7.54 (m, 3H), 7.36-7.36 (m, 2H), 4.02 (q, J = 7.20 Hz, 2H), 2.66 (s, 3H), 0.88 (t, J = 7.20 Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 168.10, 162.63, 152.95, 147.47, 145.37, 144.85, 138.37, 135.58, 133.30, 132.60, 132.02, 129.67, 129.58, 129.09, 128.88, 127.84, 125.42, 125.24, 125.01, 115.37, 61.50, 23.59, 13.89; **HRMS (ESI) m/z:** [M + H]<sup>+</sup> + Calculated for C<sub>26</sub>H<sub>21</sub>ClN<sub>3</sub>O<sub>5</sub> 490.1164; Found 490.1155

**Ethyl 6-(3,5-Dimethoxybenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6at).**

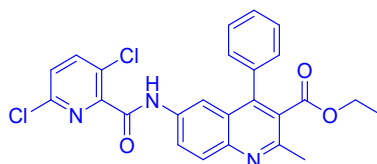


Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (500 mg, 1.3071 mmole), 3,5-dimethoxybenzoic acid (446 mg, 2.4509 mmole), HATU (1.2 mg, 3.2679 mmole), DIPEA (526 mg, 4.0849 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 50% ethyl acetate in Hexane). TLC: R<sub>f</sub> = 0.4 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. Yellow solid, yield 74%, m.p.: 170–172° C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ ppm 10.46 (s, 1H), 8.19 (dd, J = 2.00, 9.20 Hz, 1H), 8.14 (d, J = 2.00 Hz, 1H), 8.03 (d, J = 9.20 Hz, 1H), 7.57-7.56 (m, 3H), 7.38-



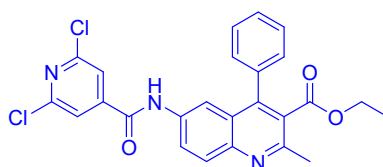
7.37 (m, 2H), 7.07 (d,  $J = 2.00$  Hz, 2H), 6.71 (s, 1H), 4.04 (q,  $J = 3.60$  Hz, 2H), 3.81 (s, 6H), 2.66 (s, 3H), 0.89 (t,  $J = 7.20$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 168.17, 165.87, 160.80, 152.79, 145.42, 144.78, 137.98, 137.14, 135.70, 129.61, 129.42, 129.07, 128.88, 127.81, 125.70, 125.22, 115.19, 106.14, 103.95, 61.48, 55.96, 23.57, 13.89; **HRMS (ESI) m/z:**  $[\text{M} + \text{H}]^+$  Calculated for  $\text{C}_{28}\text{H}_{27}\text{N}_2\text{O}_5$  471.1914; Found 471.1912

**Ethyl 6-(3,6-Dichloropicolinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6au).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (300 mg, 0.9803 mmole), 3,6-dichloropicolinic acid (279 mg, 1.4705 mmole), HATU (745 mg, 1.9607 mmole), DIPEA (316 mg, 2.4509 mmole) in DMF (8 mL) at RT 12 h. The title compound was isolated (Eluent 40% ethyl acetate in Hexane). TLC:  $R_f = 0.6$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Yellow solid, yield 76%, m.p.: 174–176 $^\circ$  C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  ppm 11.06 (s, 1H), 8.18-8.16 (m, 2H), 8.07 (d,  $J = 9.20$  Hz, 1H), 7.99 (s, 1H), 7.74 (d,  $J = 8.80$  Hz, 1H), 7.57-7.55 (m, 3H), 7.38-7.36 (m, 2H), 4.03 (q,  $J = 6.80$  Hz, 2H), 2.66 (s, 3H), 0.88 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  ppm 168.07, 162.56, 153.18, 151.84, 148.19, 145.48, 144.89, 142.31, 137.28, 135.52, 129.95, 129.59, 129.11, 128.90, 127.91, 127.50, 125.30, 124.64, 114.91, 61.53, 23.62, 13.89; **HRMS (ESI) m/z:**  $[\text{M} + \text{H}]$  Calculated for  $\text{C}_{25}\text{H}_{20}\text{Cl}_2\text{N}_3\text{O}_3$  480.0871; Found 480.0872

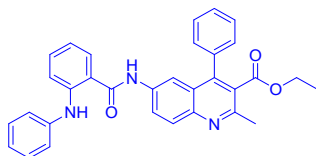
**Ethyl 6-(2,6-Dichloroisonicotinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6av).**



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (400 mg, 1.3071 mmole), 2,6-dichloroisonicotinic acid (372 mg, 1.9607 mmole), HATU (993 mg, 2.6143 mmole), DIPEA (421 mg, 3.2679 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 60% ethyl acetate in Hexane). TLC:  $R_f = 0.4$  (EtOAc/Hexane 5:5) [silica gel, UV and  $\text{KMnO}_4$  stain]. Yellow

solid, yield 70%, m.p. : 238–240<sup>0</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm 10.87 (s, 1H), 8.18 (dd, J = 1.20, 9.00 Hz, 1H), 8.07 (d, J = 2.40 Hz, 2H), 7.98-0.00 (m, 2H), 7.56-0.00 (m, 2H), 7.37-7.36 (m, 2H), 4.03 (q, J = 6.80 Hz, 2H), 2.66 (s, 3H), 0.88 (t, J = 6.80 Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 168.04, 162.03, 153.33, 150.22, 145.55, 145.01, 137.15, 135.51, 129.75, 129.57, 129.16, 128.93, 128.76, 127.93, 125.24, 122.42, 115.65, 61.54, 23.62, 13.89;

#### Ethyl 2-methyl-4-phenyl-6-(2-(Phenylamino)benzamido)quinoline-3-carboxylate (**6aw**).



Ethyl 6-amino-2-methyl-4-phenylquinoline-3-carboxylate (400 mg, 1.3071 mmole), 2-(phenylamino)benzoic acid (427 mg, 1.9607 mmole), HATU (993 mg, 2.6143 mmole), DIPEA (421 mg, 3.2679 mmole) in DMF (10 mL) at RT 12 h. The title compound was isolated (Eluent 70% ethyl acetate in Hexane). TLC: R<sub>f</sub>=0.2 (EtOAc/Hexane 5:5) [silica gel, UV and KMnO<sub>4</sub> stain]. White yield 60%, m.p.: 78–80<sup>0</sup> C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ ppm 10.54 (s, 1H), 8.84 (s, 1H), 8.13 (dd, J = 2.00, 9.20 Hz, 1H), 7.95 (d, J = 9.20 Hz, 1H), 7.86 (d, J = 2.00 Hz, 1H), 7.65-7.65 (m, 1H), 7.50-7.48 (m, 3H), 7.30-7.30 (m, 3H), 7.23-7.21 (m, 2H), 7.07-7.05 (m, 2H), 6.90-6.88 (m, 2H), 3.95 (q, J = 7.20 Hz, 2H), 2.58 (s, 3H), 0.82 (t, J = 7.20 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ ppm 168.25, 168.16, 152.83, 145.35, 144.79, 144.31, 142.13, 137.91, 135.62, 132.68, 130.09, 129.80, 129.63, 129.36, 129.08, 128.88, 127.77, 125.90, 125.15, 122.20, 121.01, 119.83, 119.06, 116.28, 115.51, 61.50, 23.59, 13.90; MS (ESI) m/z: [M + H] Calculated for C<sub>32</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub> 502.2; Found 502.2

#### 4. DFT Calculations for all Quinoline Derivatives (**6a-6az**) and (**6aa-6aw**)

DFT calculations were conducted at B3LYP/6-31+ G'(d,p) level using the Gaussian 09 program package. The results were related to compounds **6a** (also depicted in the main text), **6b-6w**, **6aa-6aw**, and related compounds. Figure 7(1)–V(49) illustrates the HOMO and LUMO molecular orbitals of the molecules **6a-6z** and **6a-6aw**. While all LUMOs are essentially identical and delocalize primarily on the quinoline ring and carboxylic amide groups regardless of the substitution, the geometries of the HOMOs show clearly how the substituent at C4 has an impact. The table made it abundantly evident

that the substituent at quinoline's C6 position has a significant impact on the HOMO levels of each derivative. In compound **6a-6m**, the transition from the quinoline ring to the carboxylic amide group is prominently visible. Compound **6n**'s entire quinoline moiety contribution towards the amide group, while compound (**6q,6p**)'s pyridine ring's **6q** LUMO (-2.41 eV) contribution only the coupling substituent of the quinoline moiety's HOMO (-5.79 eV) and  $\Delta E$  is 3.37 eV. The HOMO and LUMO orbitals are frontier orbitals that govern reactivity. EHOMO and ELUMO are important parameters that determine electron donation ease and electron acceptance, respectively. Apart from these, there are several other reactivity parameters that play a crucial role in understanding the electron behavior of a molecule. Some of these parameters are global hardness (h), softness (S), electronegativity (c), chemical potential (m), electrophilicity index (w), electron-donating power (w-), and electron-accepting power (w+). The global reactivity descriptors of a molecule, including the HOMO and LUMO values, are listed in Table VIII. In a specific analysis, it was found that compound - **6c** has the highest HOMO energy (-6.31 eV), indicating strong electron-donating ability, while molecule **6w** has the lowest LUMO energy (-3.90 eV), indicating superior electron-accepting properties. By studying these descriptors, we can gain insights into the molecular behavior, facilitating our understanding of chemical reactivity. reactivity parameters include global calculated formulae:  $\Delta E = \text{LUMO-HOMO}$  (eV),  $I = -\text{EHOMO}$  (eV),  $A = -\text{ELUMO}$  (eV),  $\chi = (I + A)/2$  (eV),  $\mu = -\chi$  (eV),  $\eta = (I - A)/2$  (eV),  $S = 1/\eta$  (eV),  $\omega = \mu^2/2\eta$  (eV),  $\omega^- = (3I + A)^2/16(I - A)$ ,  $\omega^+ = (I + 3A)^2/16(I - A)$ .

The electronic chemical potentials of acid amine cross-coupling reactions with some reagents used have tabulated in Table VIII. Compound **6w**, for example, has an electronic chemical potential of 4.87 eV and acts as a strong electron-donating molecule. However, as the substituent present becomes more electron-withdrawing, the electronic chemical potential of the corresponding quinoline derivative decreases, as seen in the order  $6w < 6x < 6ar < 6as$ . This causes an increase in the polar character of the reactions towards compounds **6t**, **6v**, **6ap**, **6aq** and **6a**

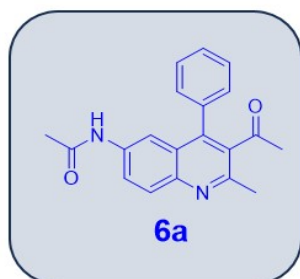
**Table S1: FMO parameters and Global reactivity Description of the compounds.**

S No.	Code	HOMO	LUMO	$\Delta E$	I	A	$\chi$	$\mu$	$\eta$	S	$\omega$	$\omega^-$	$\omega^+$
1	6a	-5.954	-2.234	3.720	5.954	2.234	4.094	-4.094	1.86	0.538	4.506	6.785	2.691
2	6b	-6.173	-2.341	3.832	6.173	2.341	4.257	-4.257	1.916	0.522	4.729	7.097	2.84
3	6c	-6.317	-2.377	3.940	6.317	2.377	4.347	-4.347	1.97	0.508	4.796	7.215	2.868
4	6d	-5.837	-2.084	3.753	5.837	2.084	3.9605	-3.961	1.877	0.533	4.179	6.394	2.433
5	6e	-5.818	-2.071	3.747	5.818	2.071	3.9445	-3.945	1.874	0.534	4.152	6.358	2.414
6	6f	-5.755	-2.059	3.696	5.755	2.059	3.907	-3.907	1.848	0.541	4.13	6.314	2.407
7	6g	-5.893	-2.159	3.734	5.893	2.159	4.026	-4.026	1.867	0.536	4.341	6.587	2.561
8	6h	-5.893	-2.063	3.830	5.893	2.063	3.978	-3.978	1.915	0.522	4.132	6.36	2.382
9	6i	-5.91	-2.114	3.796	5.91	2.114	4.012	-4.012	1.898	0.527	4.24	6.483	2.471
10	6j	-5.901	-2.106	3.795	5.901	2.106	4.0035	-4.004	1.898	0.527	4.223	6.462	2.458
11	6k	-5.903	-2.108	3.795	5.903	2.108	4.0055	-4.006	1.898	0.527	4.228	6.467	2.462
12	6l	-5.964	-2.191	3.773	5.964	2.191	4.0775	-4.078	1.887	0.53	4.407	6.681	2.603
13	6m	-5.912	-2.156	3.756	5.912	2.156	4.034	-4.034	1.878	0.532	4.333	6.584	2.55
14	6n	-5.756	-2.159	3.597	5.756	2.159	3.9575	-3.958	1.799	0.556	4.354	6.557	2.6
15	6o	-5.702	-2.122	3.580	5.702	2.122	3.912	-3.912	1.79	0.559	4.275	6.454	2.542
16	6p	-6.211	-2.603	3.608	6.211	2.603	4.407	-4.407	1.804	0.554	5.383	7.811	3.404
17	6q	-5.794	-2.417	3.377	5.794	2.417	4.1055	-4.106	1.689	0.592	4.991	7.254	3.149
18	6r	-6.065	-2.315	3.750	6.065	2.315	4.19	-4.19	1.875	0.533	4.682	7.011	2.821
19	6s	-6.001	-2.192	3.809	6.001	2.192	4.0965	-4.097	1.905	0.525	4.406	6.692	2.595
20	6t	-5.772	-2.132	3.640	5.772	2.132	3.952	-3.952	1.82	0.549	4.291	6.494	2.542
21	6u	-5.851	-2.177	3.674	5.851	2.177	4.014	-4.014	1.837	0.544	4.385	6.622	2.608
22	6v	-5.67	-2.268	3.402	5.67	2.268	3.969	-3.969	1.701	0.588	4.631	6.827	2.858
23	6w	-5.844	-3.908	1.936	5.844	3.908	4.876	-4.876	0.968	1.033	12.28	14.84	9.963
24	6x	-5.779	-3.851	1.928	5.779	3.851	4.815	-4.815	0.964	1.037	12.03	14.55	9.738
25	6y	-5.415	-2.069	3.346	5.415	2.069	3.742	-3.742	1.673	0.598	4.185	6.264	2.522
26	6z	-5.597	-1.939	3.658	5.597	1.939	3.768	-3.768	1.829	0.547	3.881	5.993	2.225

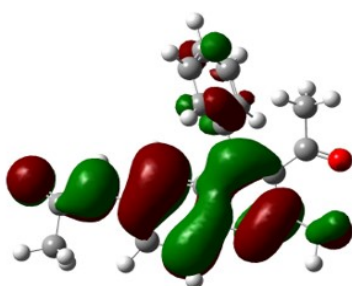
27	6aa	-5.856	-2.114	3.742	5.856	2.114	3.985	-3.985	1.871	0.534	4.244	6.47	2.485
28	6ab	-6.198	-2.259	3.939	6.198	2.259	4.2285	-4.229	1.97	0.508	4.539	6.899	2.671
29	6ac	-6.067	-2.225	3.842	6.067	2.225	4.146	-4.146	1.921	0.521	4.474	6.787	2.641
30	6ad	-5.747	-1.961	3.786	5.747	1.961	3.854	-3.854	1.893	0.528	3.923	6.086	2.232
31	6ae	-5.736	-1.968	3.768	5.736	1.968	3.852	-3.852	1.884	0.531	3.938	6.099	2.247
32	6af	-5.682	-1.977	3.705	5.682	1.977	3.8295	-3.83	1.853	0.54	3.958	6.104	2.274
33	6ag	-5.629	-1.823	3.806	5.629	1.823	3.726	-3.726	1.903	0.525	3.648	5.748	2.022
34	6ah	-5.639	-1.801	3.838	5.639	1.801	3.72	-3.720	1.919	0.521	3.606	5.705	1.985
35	6ai	-5.806	-1.991	3.815	5.806	1.991	3.898	-3.898	1.908	0.524	3.983	6.171	2.273
36	6aj	-5.782	-1.967	3.815	5.782	1.967	3.8745	-3.875	1.908	0.524	3.935	6.11	2.236
37	6ak	-5.798	-1.985	3.813	5.798	1.985	3.8915	-3.892	1.907	0.525	3.972	6.155	2.264
38	6al	-5.866	-2.072	3.794	5.866	2.072	3.969	-3.969	1.897	0.527	4.152	6.373	2.404
39	6am	-5.817	-2.039	3.778	5.817	2.039	3.928	-3.928	1.889	0.529	4.084	6.284	2.356
40	6an	-5.669	-2.071	3.598	5.669	2.071	3.87	-3.87	1.799	0.556	4.163	6.322	2.452
41	6ao	-5.494	-1.884	3.610	5.494	1.884	3.689	-3.689	1.805	0.554	3.77	5.839	2.15
42	6ap	-5.623	-2.149	3.474	5.623	2.149	3.886	-3.886	1.737	0.576	4.347	6.506	2.62
43	6aq	-5.925	-2.164	3.761	5.925	2.164	4.0445	-4.045	1.881	0.532	4.349	6.606	2.562
44	6ar	-5.701	-3.822	1.879	5.701	3.822	4.7615	-4.762	0.94	1.064	12.07	14.56	9.802
45	6as	-5.563	-3.721	1.842	5.563	3.721	4.642	-4.642	0.921	1.086	11.7	14.13	9.492
46	6at	-5.761	-2.056	3.705	5.761	2.056	3.9085	-3.909	1.853	0.54	4.123	6.308	2.4
47	6au	-5.81	-2.415	3.395	5.81	2.415	4.1125	-4.113	1.698	0.589	4.982	7.25	3.137
48	6av	-6.107	-2.551	3.556	6.107	2.551	4.329	-4.329	1.778	0.562	5.27	7.656	3.327
49	6aw	-5.341	-1.946	3.395	5.341	1.946	3.6435	-3.644	1.698	0.589	3.91	5.944	2.3

**FMO Diagrams (Figure S7):**

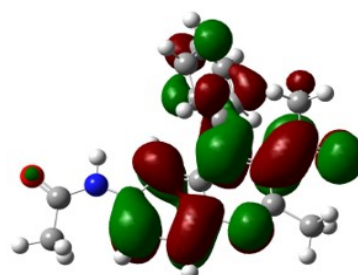
**Figure S7.1:**



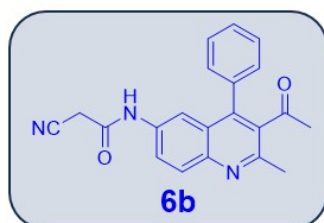
**HOMO (6a)**



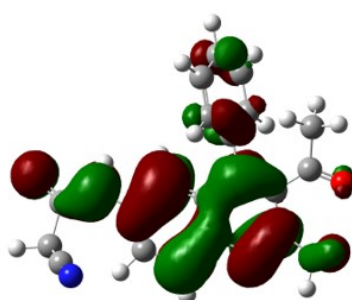
**LUMO (6a)**



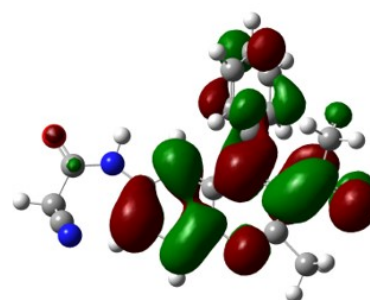
**Figure S7.2:**



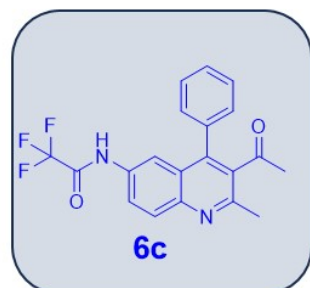
**HOMO (6b)**



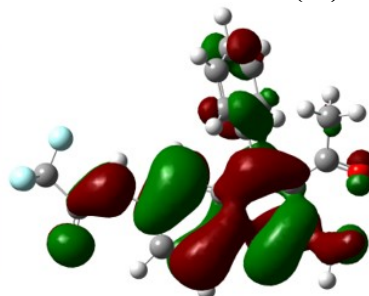
**LUMO (6b)**



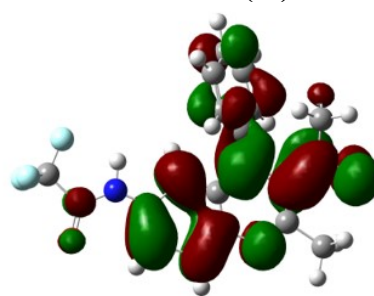
**Figure S7.3:**



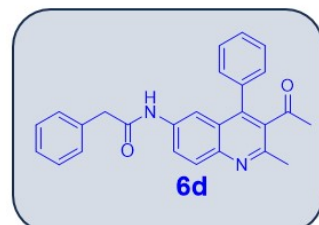
**HOMO (6c)**



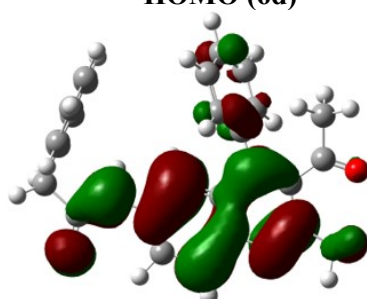
**LUMO (6c)**



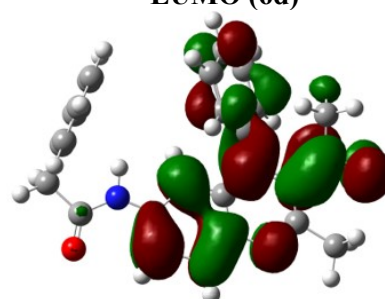
**Figure S7.4:**



**HOMO (6d)**



**LUMO (6d)**



**Figure S7.5:**

**HOMO (6e)**

**LUMO (6e)**

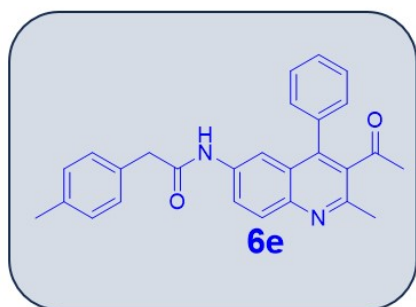
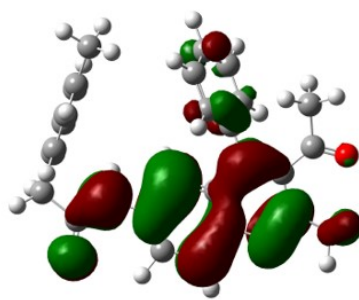
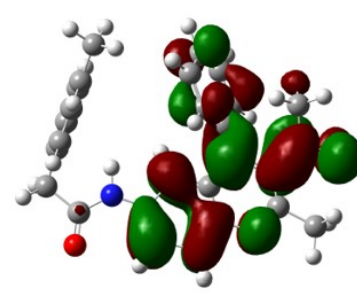


Figure S7.6:



HOMO (6e)



LUMO (6e)

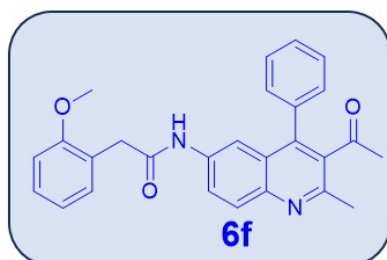
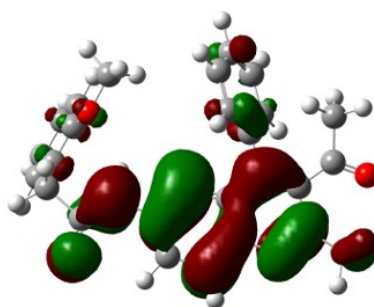
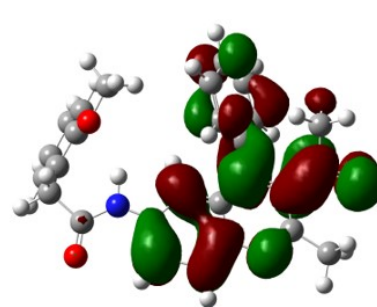


Figure S7.7:



HOMO (6f)



LUMO (6f)

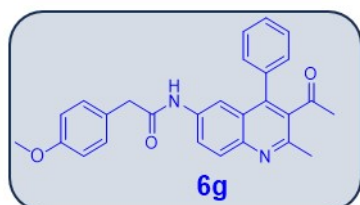
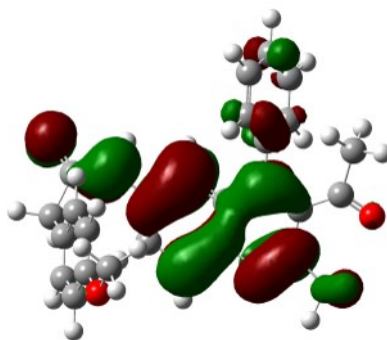
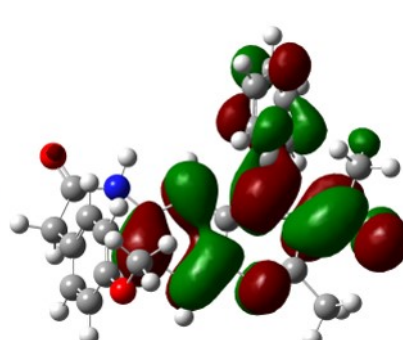


Figure S7.8:



HOMO (6g)



LUMO (6g)

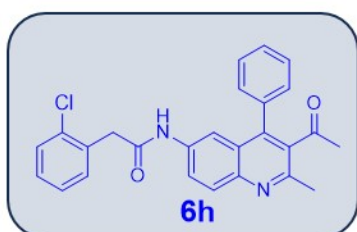
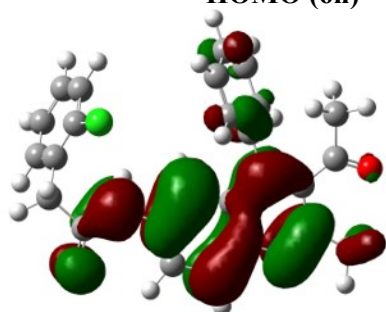
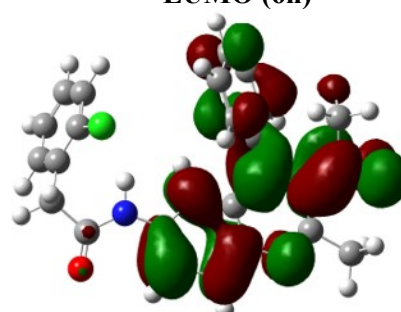


Figure S7.9:



HOMO (6h)



LUMO (6h)

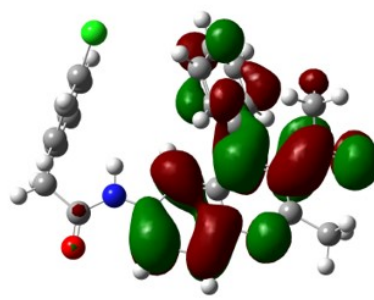
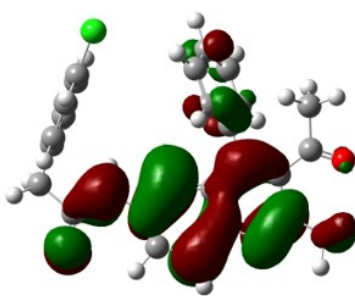
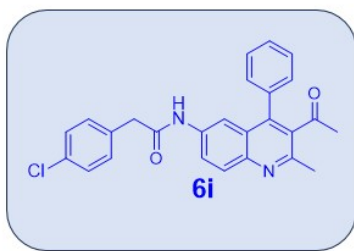


Figure S7.10:

HOMO (6j)

LUMO (6j)

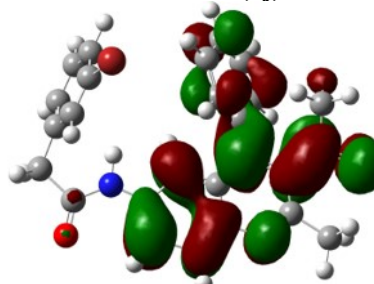
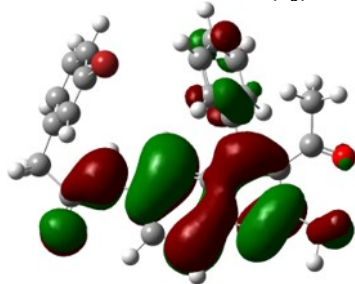
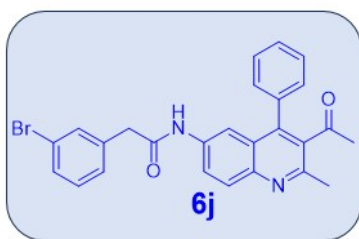


Figure S7.11:

HOMO (6k)

LUMO (6k)

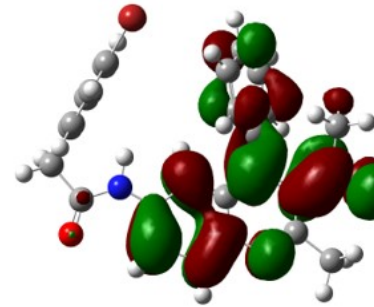
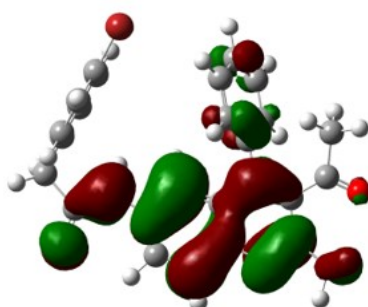
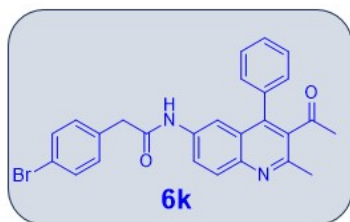


Figure S7.12:

HOMO (6l)

LUMO (6l)

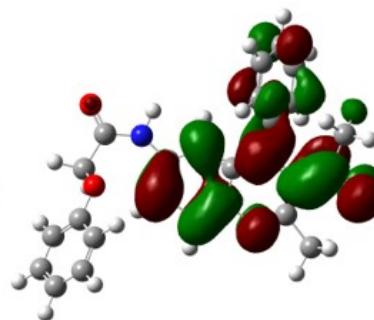
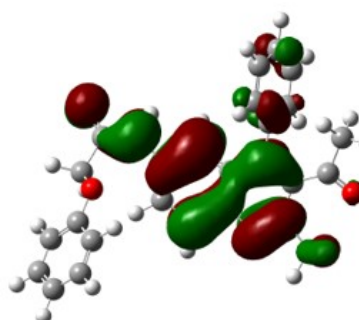
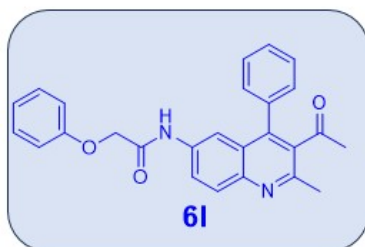


Figure S7.13:

HOMO (6m)

LUMO (6m)



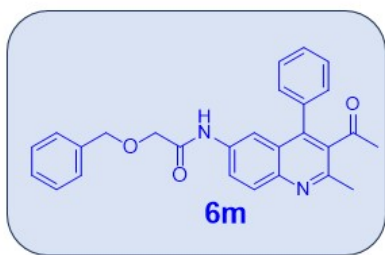
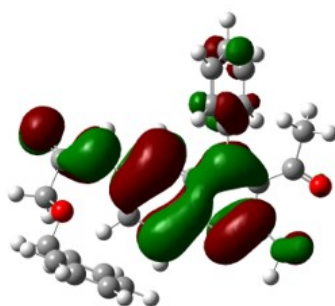
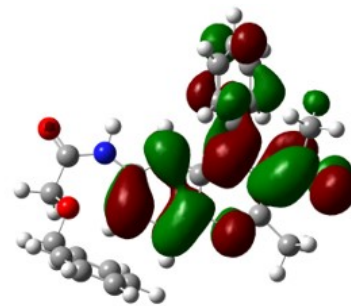


Figure S7.14:



HOMO (6m)



LUMO (6m)

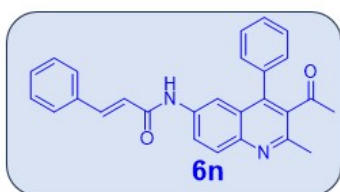
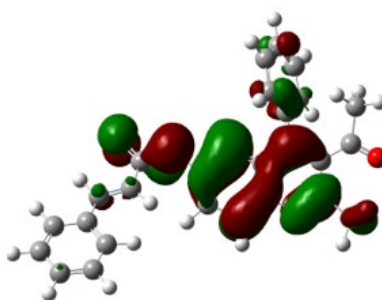
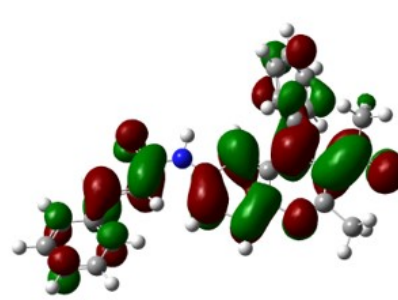


Figure S7.15:



HOMO (6n)



LUMO (6n)

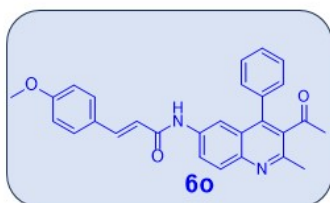
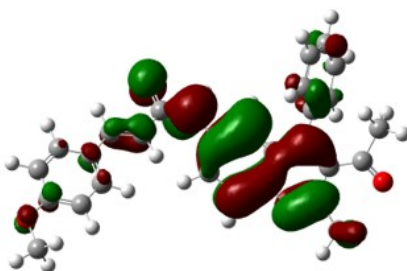
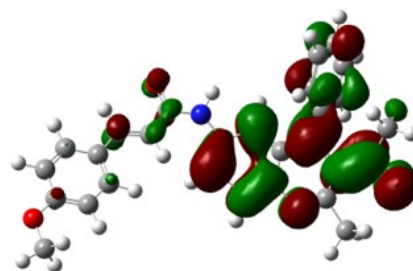


Figure S7.16:



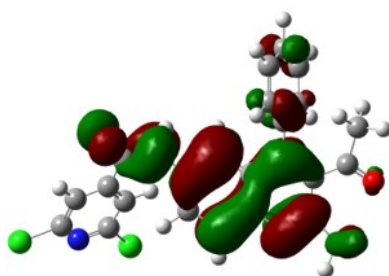
HOMO (6o)



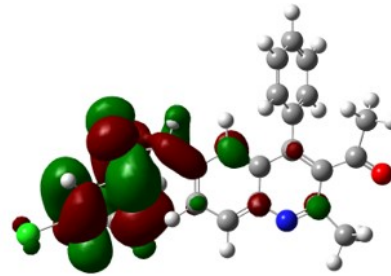
LUMO (6o)



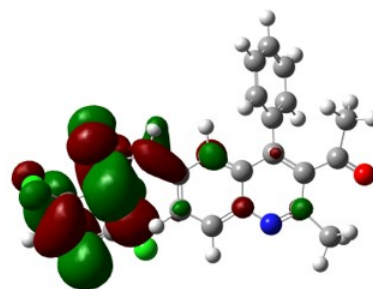
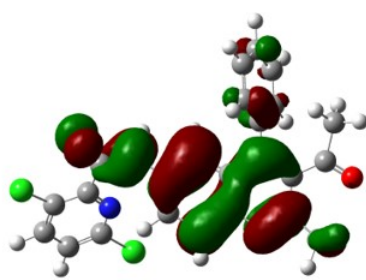
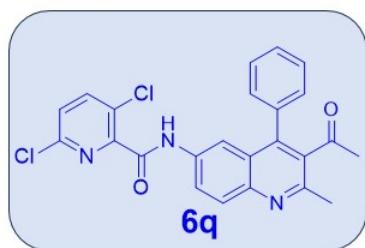
Figure S7.17:



HOMO (6p)



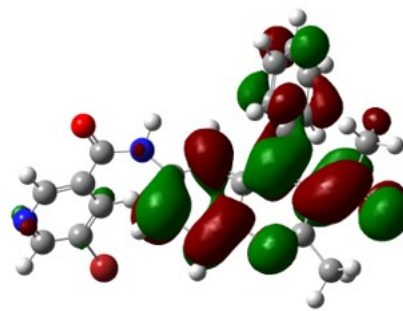
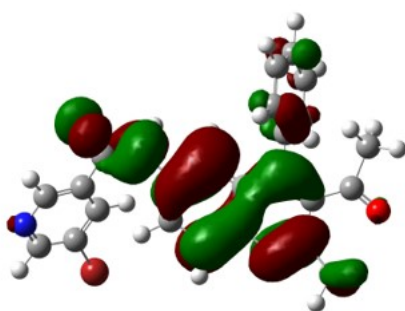
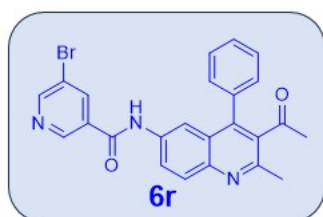
LUMO (6p)



**Figure S7.18:**

**HOMO (6r)**

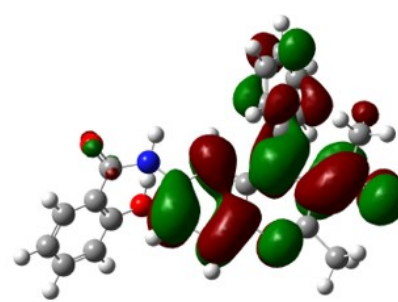
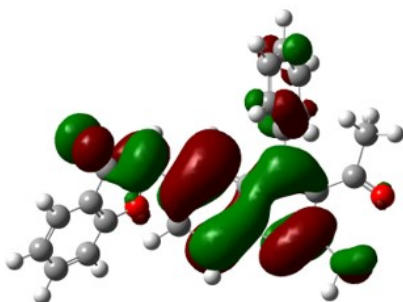
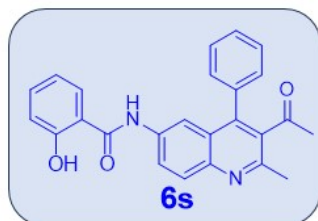
**LUMO (6r)**



**Figure S7.19:**

**HOMO (6s)**

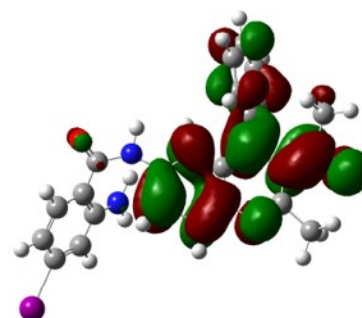
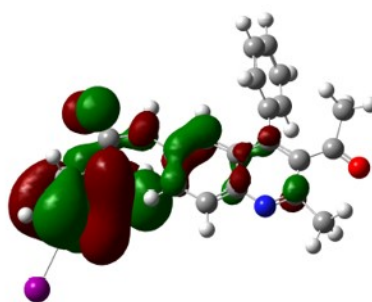
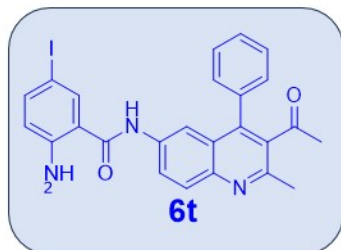
**LUMO (6s)**



**Figure S7.20:**

**HOMO (6t)**

**LUMO (6t)**



**Figure S7.21:**

**HOMO (6u)**

**LUMO (6u)**

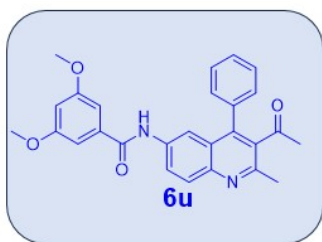
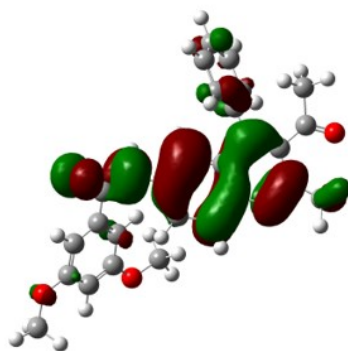
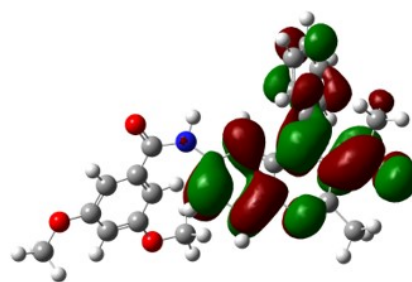


Figure S7.22:



HOMO (6v)



LUMO (6v)

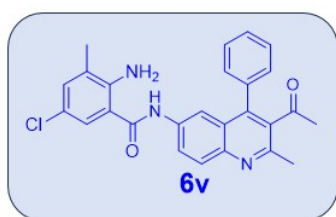
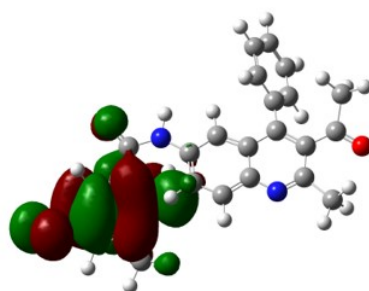
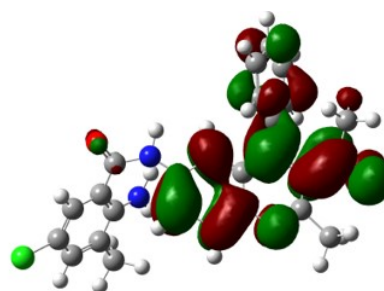


Figure S7.23:



HOMO (6w)



LUMO (6w)

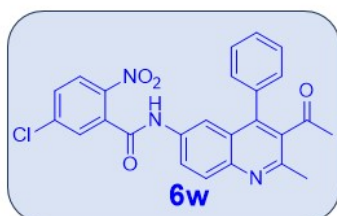
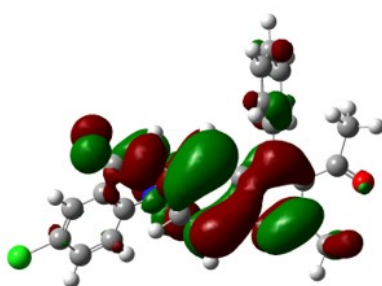
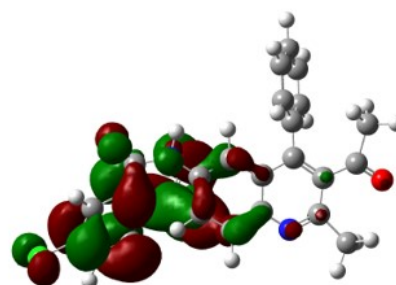


Figure S7.24:



HOMO (6x)



LUMO (6x)

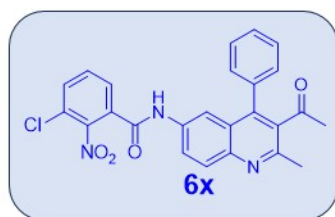
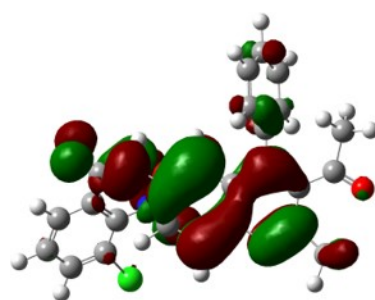
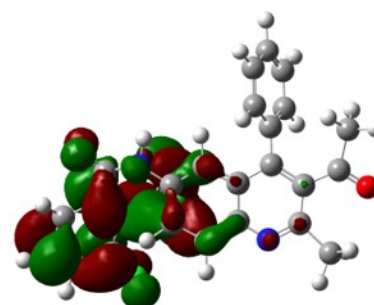


Figure S7.25:



HOMO (6y)



LUMO (6y)

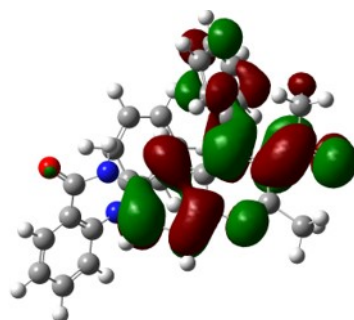
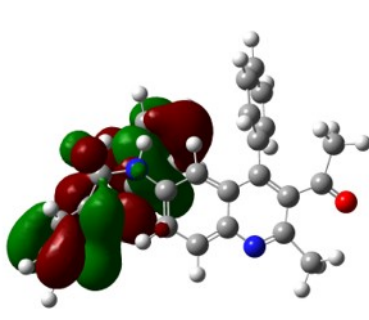
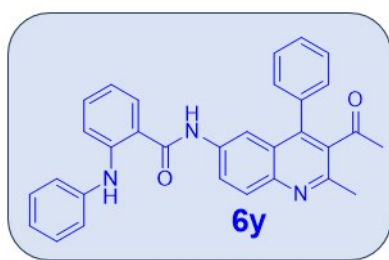


Figure S7.26:

HOMO (6z)

LUMO (6z)

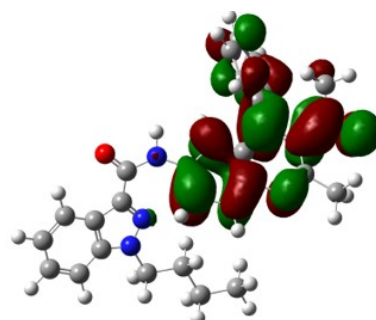
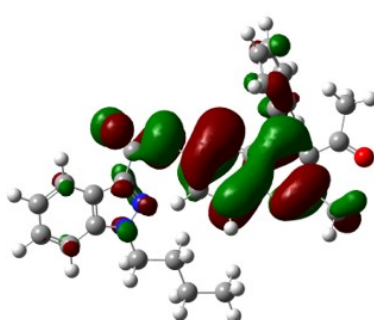
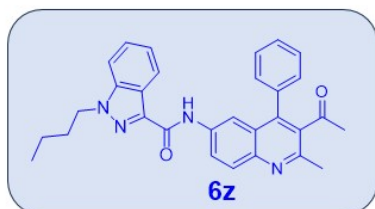


Figure S7.27:

HOMO (6aa)

LUMO (6aa)

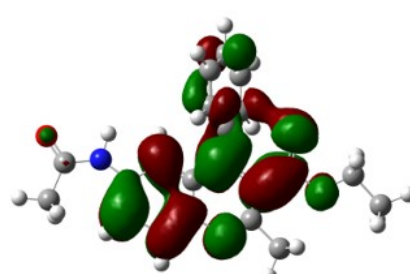
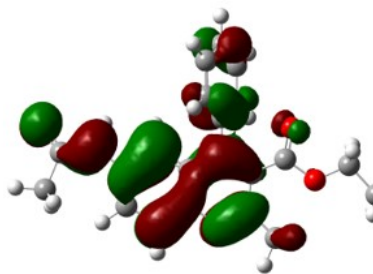
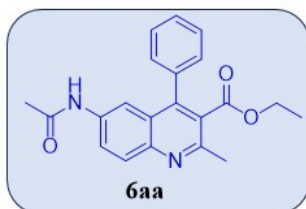


Figure S7.28:

HOMO (6ab)

LUMO (6ab)

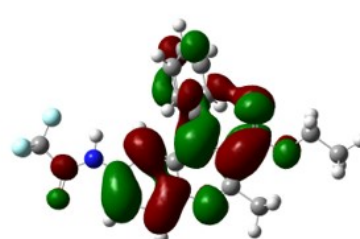
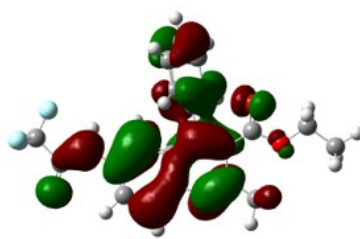
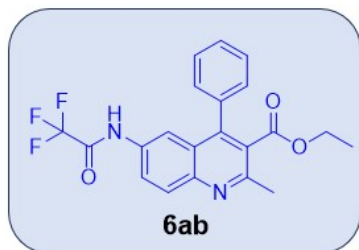


Figure S7.29:

HOMO (6ac)

LUMO (6ac)

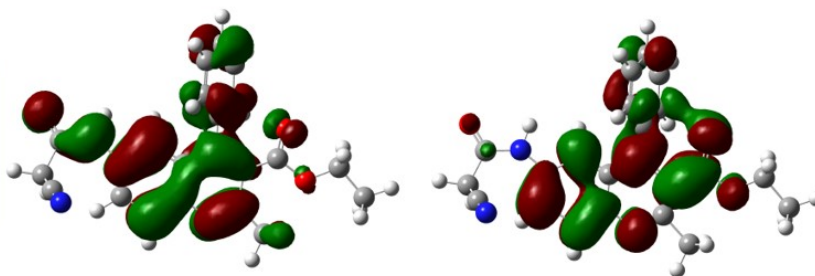
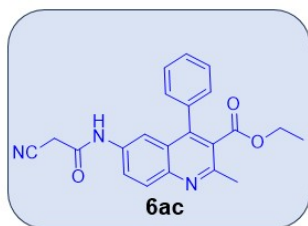


Figure S7.30:

HOMO (6ad)

LUMO (6ad)

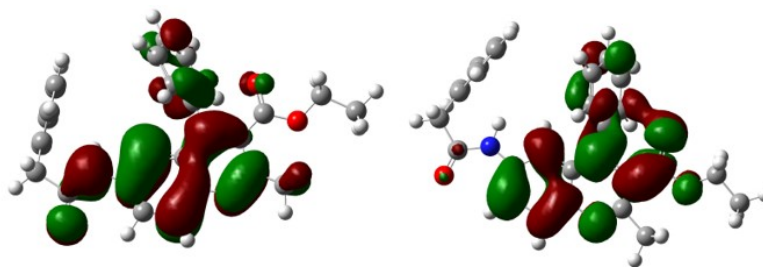
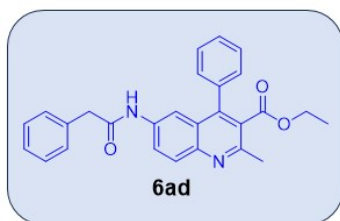


Figure S7.31:

HOMO (6ae)

LUMO (6ae)

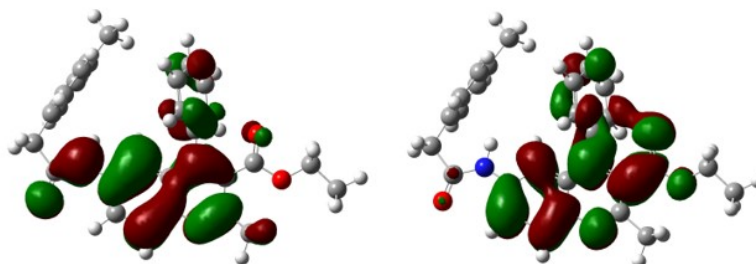
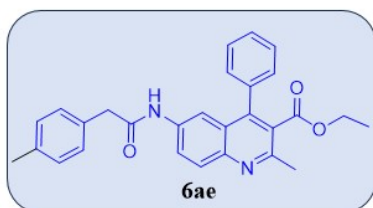


Figure S7.32:

HOMO (6af)

LUMO (6af)

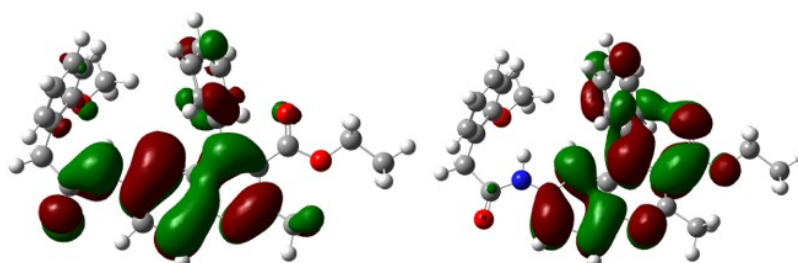
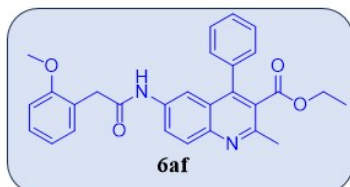


Figure S7.33:

HOMO (6ag)

LUMO (6ag)

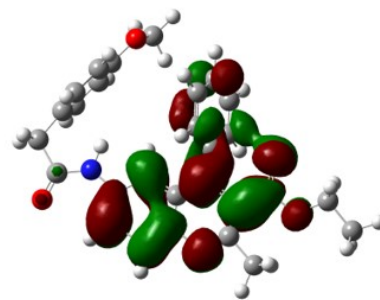
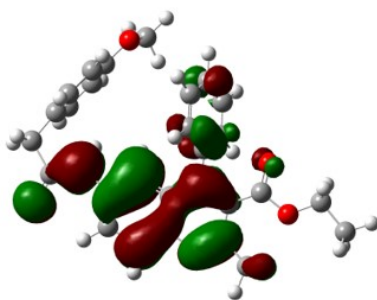
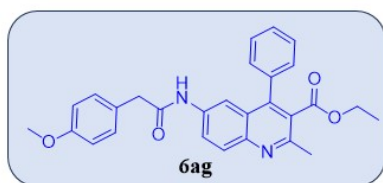


Figure S7.34:

HOMO (6ah)

LUMO (6ah)

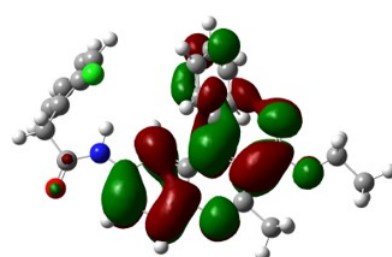
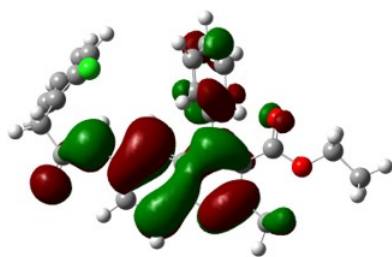
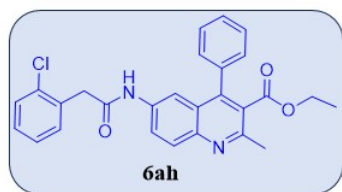


Figure S7.35:

HOMO (6ai)

LUMO (6ai)

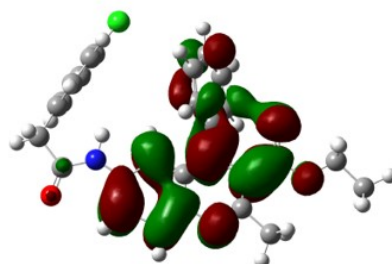
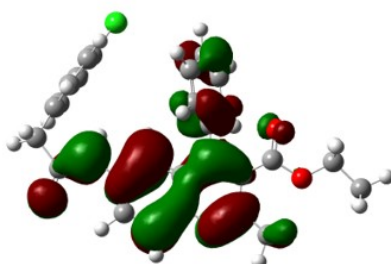
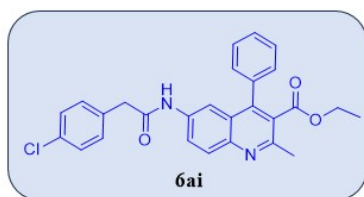


Figure S7.36:

HOMO (6aj)

LUMO (6aj)

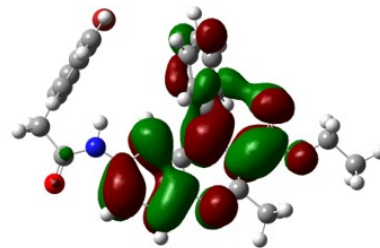
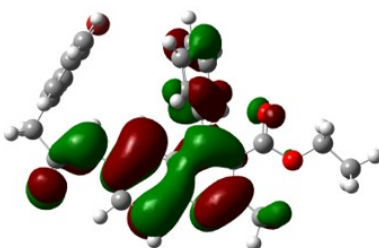
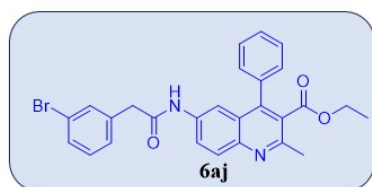


Figure S7.37:

HOMO (6ak)

LUMO (6ak)

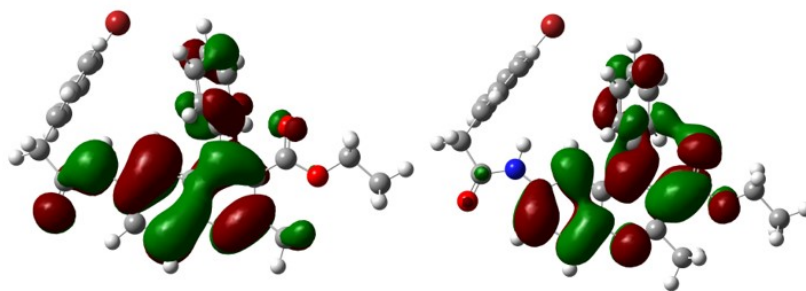
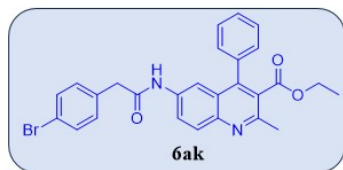


Figure S7.38:

HOMO (6al)

LUMO (6al)

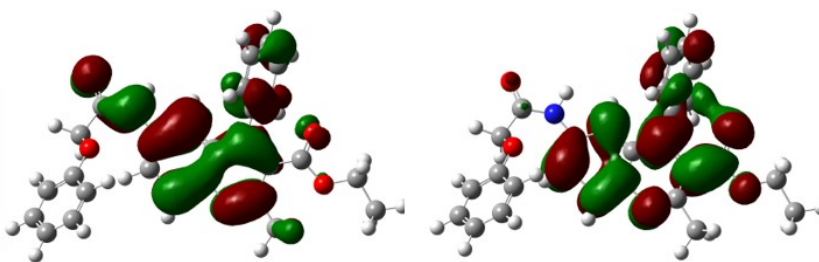
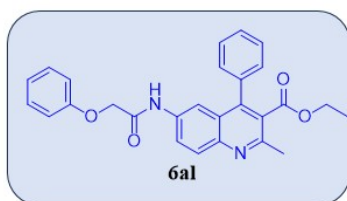


Figure S7.39:

HOMO (6am)

LUMO (6am)

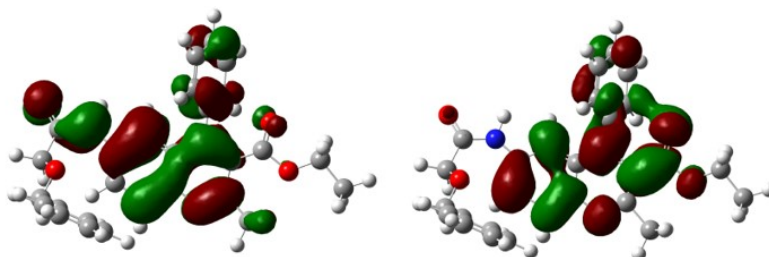
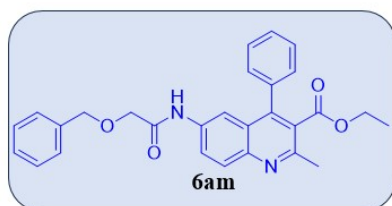


Figure S7.40:

HOMO (6an)

LUMO (6an)

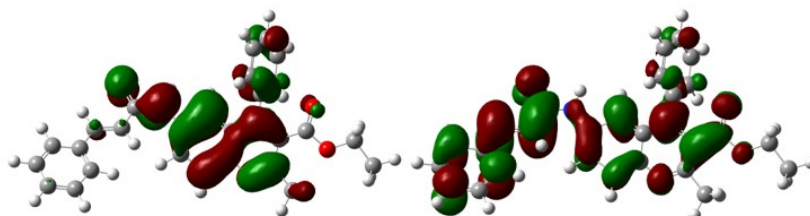
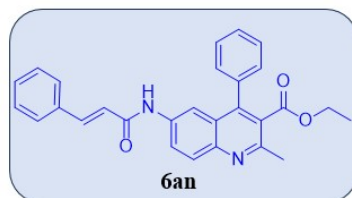


Figure S7.41:

HOMO (6ao)

LUMO (6ao)

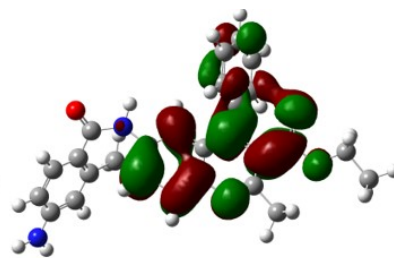
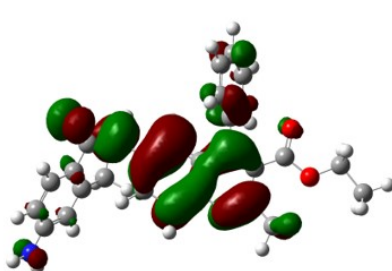
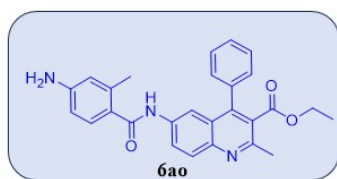


Figure S7.42:

HOMO (6ap)

LUMO (6ap)

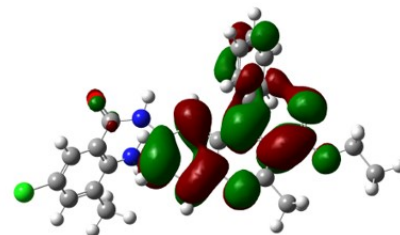
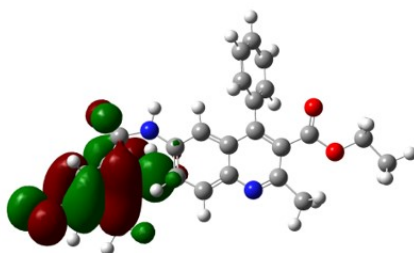
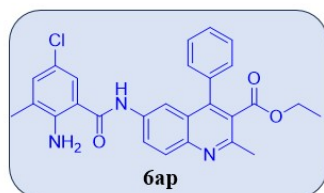


Figure S7.43:

HOMO (6aq)

LUMO (6aq)

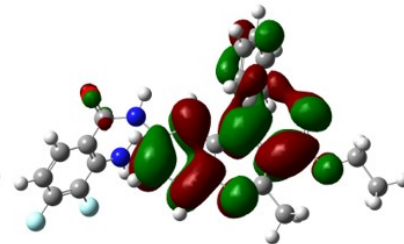
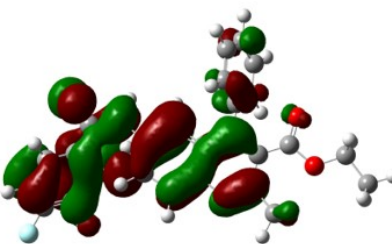
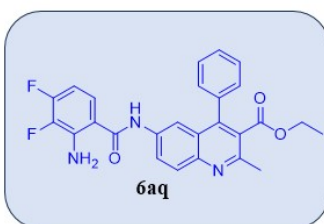


Figure S7.44:

HOMO (6ar)

LUMO (6ar)

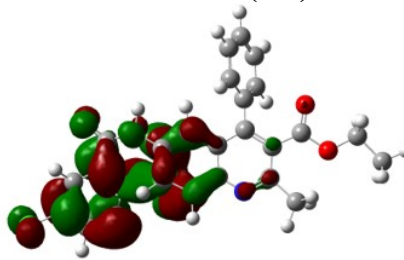
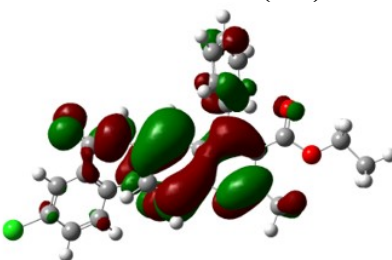
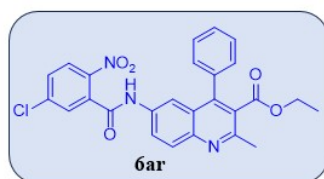


Figure S7.45:

HOMO (6as)

LUMO (6as)

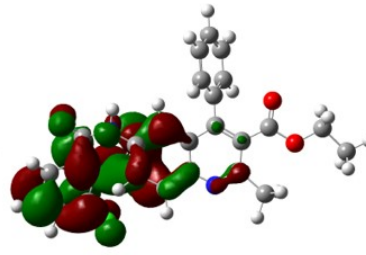
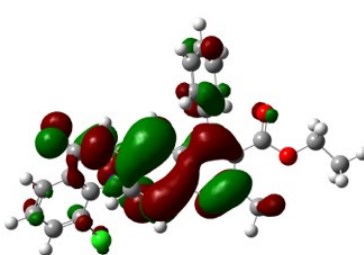
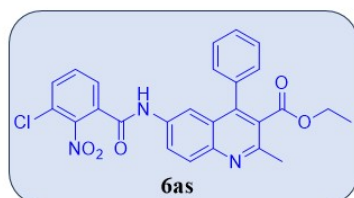


Figure S7.46:

HOMO (6at)

LUMO (6at)



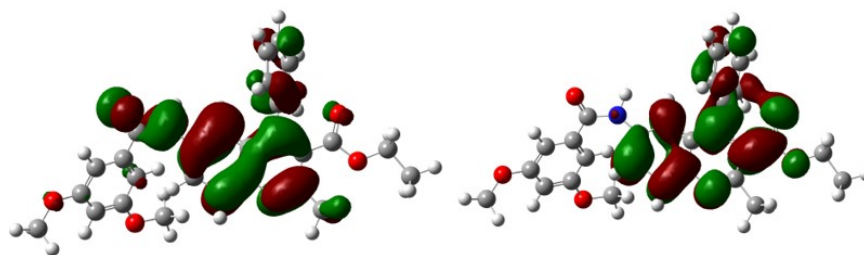
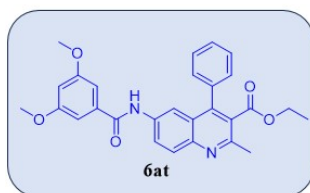


Figure S7.47:

HOMO (6au)

LUMO (6au)

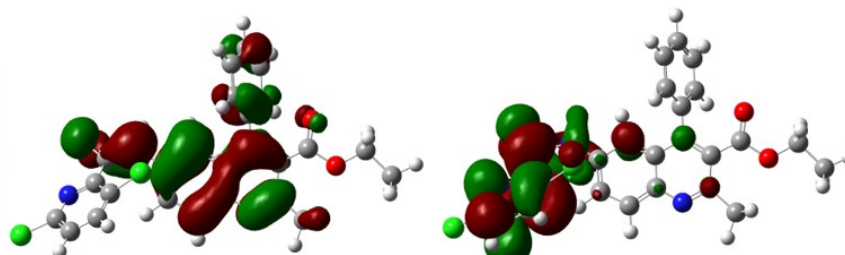
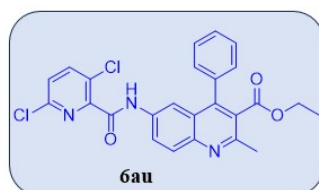


Figure S7.48:

HOMO (6av)

LUMO (6av)

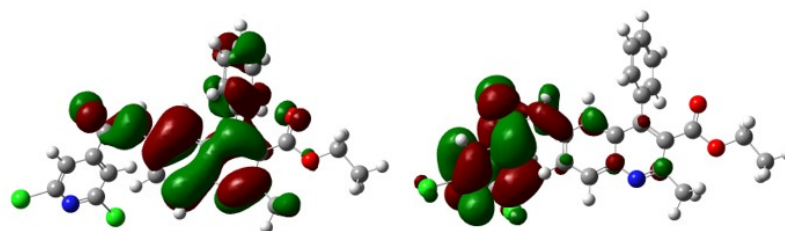
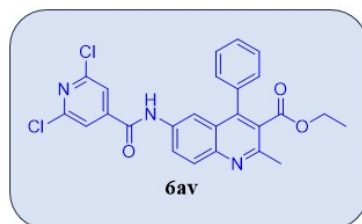
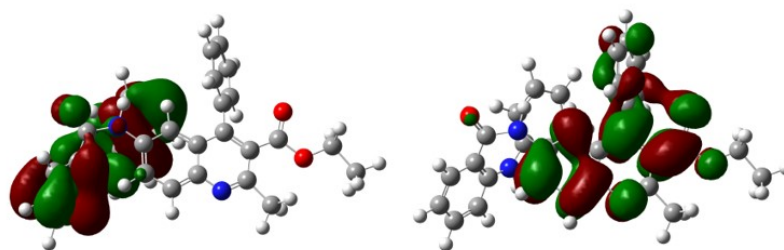
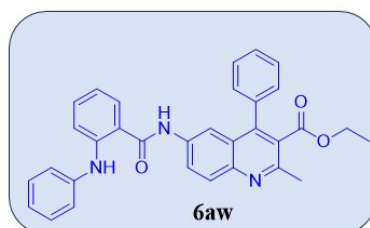


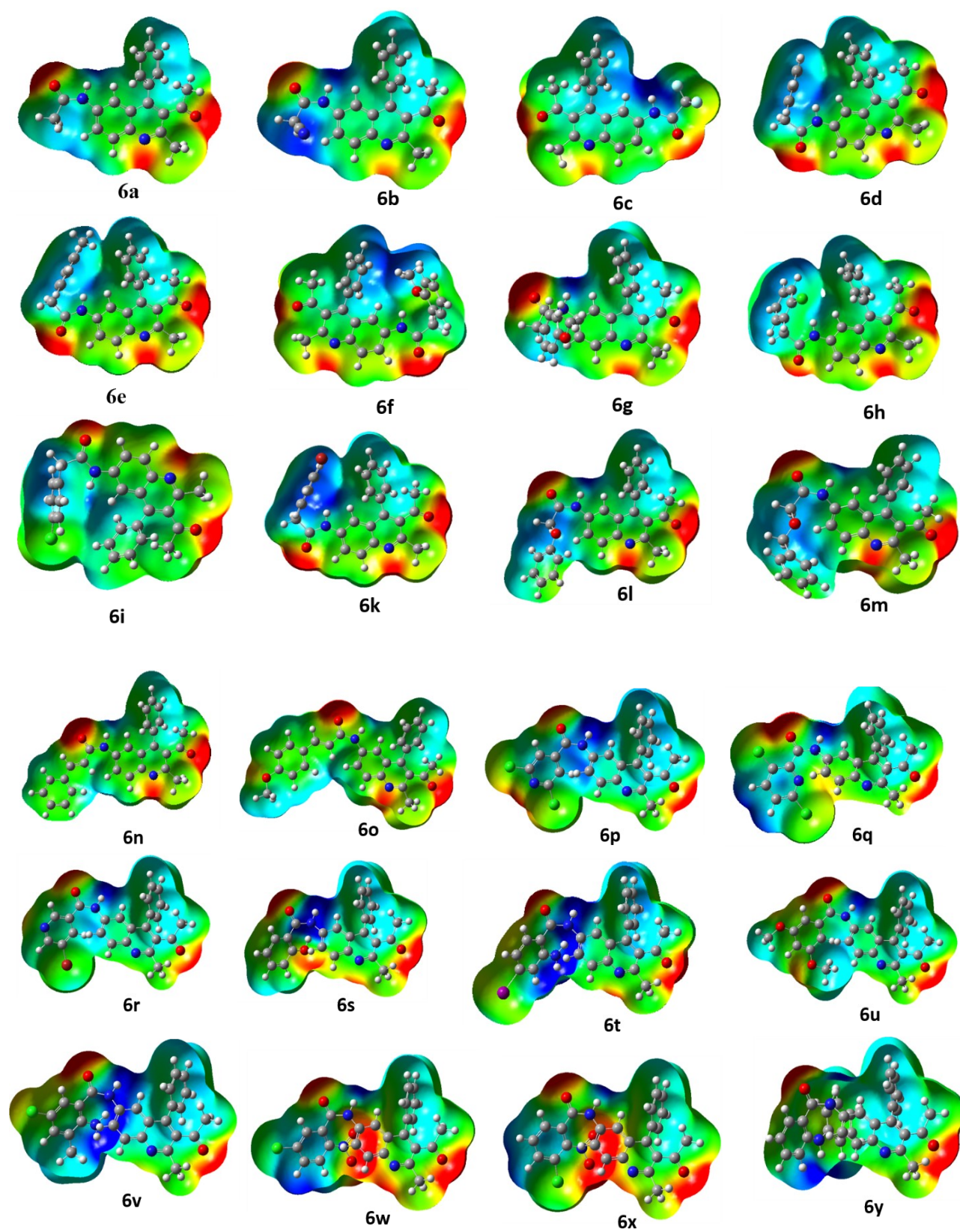
Figure S7.49:

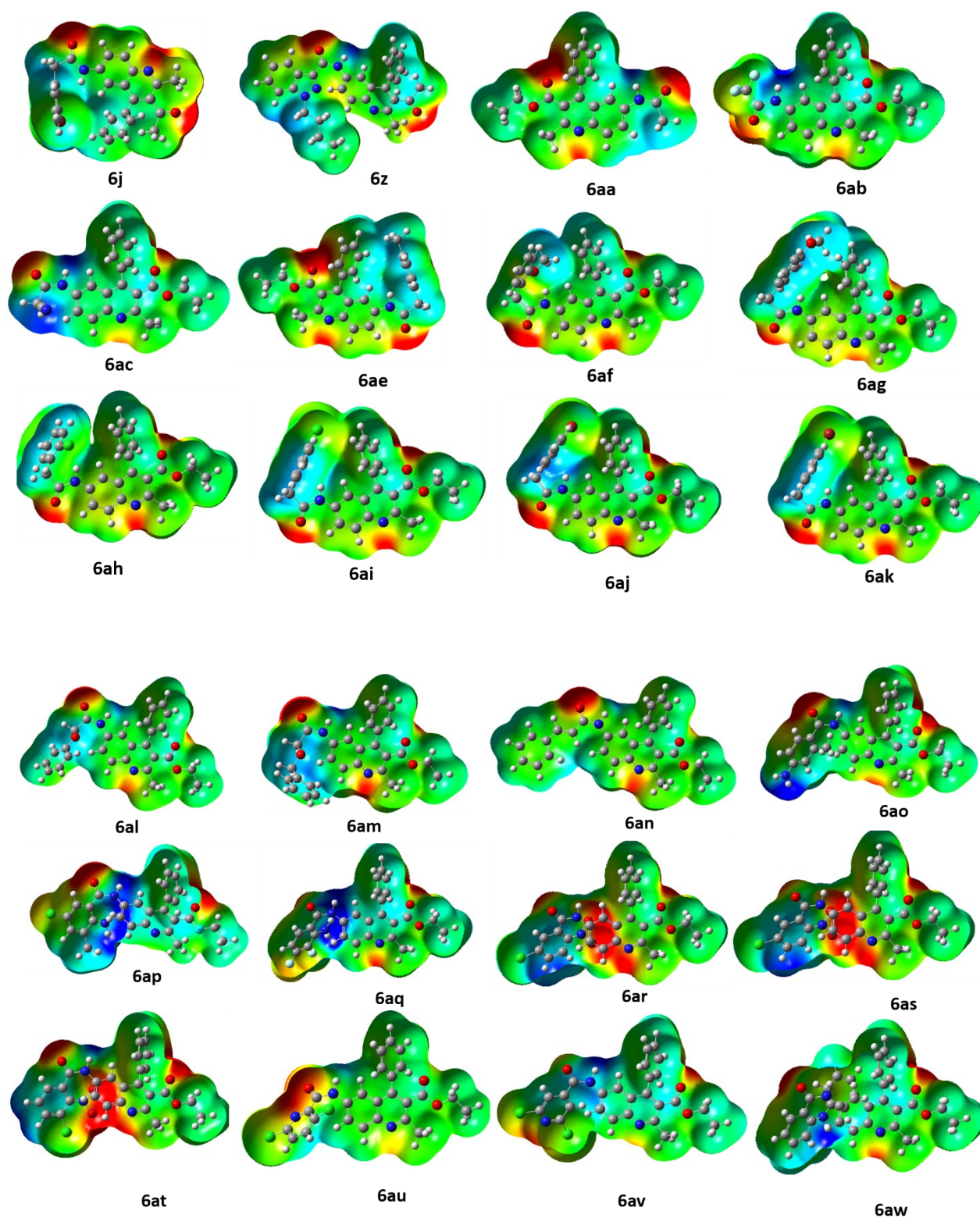
HOMO (6aw)

LUMO (6aw)



**Figure S8:** MEP Diagrams of compounds 6a-6z and 6aa-6aw.





## TD-DFT

TD-DFT empowers investigations into various processes involving excited states, offering insights into phenomena such as molecular transitions and optical properties. This methodological synergy between DFT and TD-DFT furnishes a robust toolkit for comprehensively analyzing molecular

behavior, thereby advancing our understanding of chemical reactivity, spectroscopy, and materials science applications. Time-Dependent Density Functional Theory (TD-DFT) serves as a prevalent computational method for predicting absorption spectra in molecules. Subsequently, UV-vis spectra were calculated using the TD-DFT approach employing the B3LYP functional and 6-31G' (d,p) basis sets. These findings underscore the importance of meticulous analysis to reconcile theoretical predictions with experimental observations in spectral studies. All 31 compounds theoretical and experimental UV-vis spectra and  $\lambda_{\text{max}}$ , Oscillation strength f, Energy.

**Table S2:** Theoretical  $\lambda_{\text{max}}$ , experimental  $\lambda_{\text{max}}$ , Oscillation strength,  $\Delta E$  of compounds.

Sr. No.	Compound code	Experimental $\lambda_{\text{max}}$ nm	Theoretical $\lambda_{\text{max}}$ nm	Oscillation strength, f	Energy eV
1	6a	341.12	374.55	0.0328	3.3102
2	6b	338.22	364.20	0.0657	3.403
3	6d	340.38	373.20	0.0356	3.3222
4	6e	342.76	373.72	0.0323	3.3176
5	6f	341.45	376.92	0.0139	3.2894
6	6g	343.51	373.09	0.0324	3.3232
7	6h	340.28	372.44	0.0373	3.329
8	6i	344.68	369.36	0.0458	3.3568
9	6j	341.09	369.49	0.0452	3.3555
10	6k	340.29	369.37	0.0453	3.3566
11	6l	338.87	370.21	0.0481	3.349
12	6m	337.12	368.49	0.042	3.3647
13	6s	352.83	368.85	0.0632	3.3614
14	6u	352.63	375.31	0.0045	3.3035
15	6v	347.33	380.24	0.0416	3.2607
16	6z	309.18	371.00	0.0013	3.3419
17	6aa	338.87	341.23	0.0030	3.6335
18	6ab	372.65	359.51	0.0775	3.1749
19	6ac	339.11	339.97	0.0020	3.6469
20	6ad	342.78	335.07	0.0037	3.3143
21	6ae	341.95	334.9	0.0004	3.7021
22	6af	340.42	332.86	0.0077	3.7249
23	6ag	342.67	335.54	0.0042	3.6951
24	6ah	340.22	335.19	0.0032	3.6989
25	6ai	340.43	335.73	0.0014	3.693
26	6aj	339.17	336.72	0.0018	3.6821
27	6ak	340.54	336.32	0.0021	3.6865
28	6al	337.72	338.72	0.0018	3.6604
29	6am	338.16	338.24	0.0023	3.6656
30	6ao	370.32	374.17	0.0023	3.3135
31	6ap	350.27	373.76	0.0728	3.3172

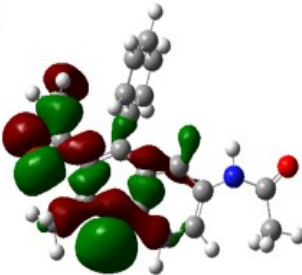
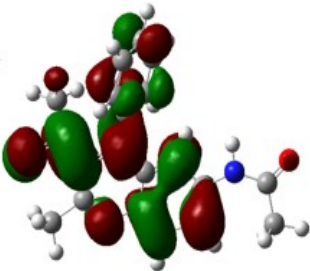
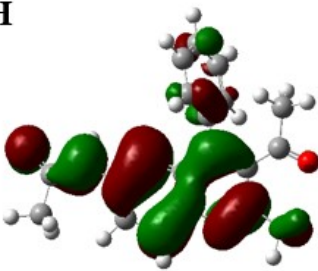
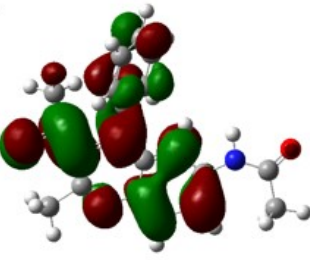
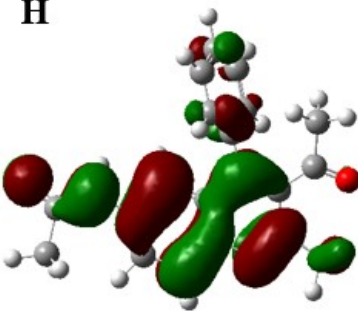
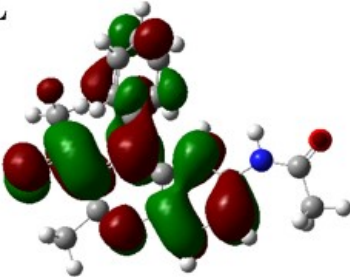
**Table S3.** Selected electronic transitions contribution obtained from TD-DFT calculation with B3LYP/6-31 G' (d, p) basic level of Compounds.

Sr. No.	Compound code	$\lambda_{\text{max}}$ (nm)	Oscillation strength, f	Energy (eV)	Selected Major Contribution
<b>1</b>	<b>6a</b>	414.28 nm	0.0004	2.9927 eV	H-1 -> L (66 %)
		383.65 nm	0.0343	3.2317 eV	H -> L (53 %)
		374.55 nm	0.0328	3.3102 eV	H -> L (42 %)
<b>2</b>	<b>6b</b>	417.23 nm	0.0002	2.9716 eV	H-1 -> L (70 %)
		382.29 nm	0.0076	3.2432 eV	H-2 -> L (65 %)
		364.20 nm	0.0657	3.4043 eV	H -> L (79 %)
<b>3</b>	<b>6d</b>	409.82 nm	0.0005	3.0253 eV	H-1 ->L (54 %)
		383.11 nm	0.0211	3.2362 eV	H ->L (40 %)
		373.20 nm	0.0356	3.3222 eV	H ->L (54 %)
<b>4</b>	<b>6e</b>	409.43 nm	0.0005	3.0282 eV	H-1 ->L (53 %)
		383.27 nm	0.0231	3.2349 eV	H ->L (44 %)
		373.72 nm	0.0323	3.3176 eV	H ->L (50 %)
<b>5</b>	<b>6f</b>	408.64 nm	0.0009	3.0340 eV	H-1 ->L+1 (52 %)
		386.27 nm	0.0393	3.2098 eV	H ->L (73 %)
		376.92 nm	0.0139	3.2894 eV	H-1 ->L (42 %)
<b>6</b>	<b>6g</b>	411.70 nm	0.0004	3.0115 eV	H-1 ->L (61 %)
		383.10 nm	0.0318	3.2363 eV	H->L (53 %)
		373.09 nm	0.0324	3.3232 eV	H ->L (42 %)
<b>7</b>	<b>6h</b>	409.61 nm	0.0005	3.0269 eV	H-1 ->L+1 (54 %)
		382.31 nm	0.0194	3.2431 eV	H-2 ->L (41 %)
		372.44 nm	0.0373	3.3290 eV	H ->L (57 %)
<b>8</b>	<b>6i</b>	410.87 nm	0.0003	3.0176 eV	H-1 ->L (56 %)
		381.52 nm	0.0122	3.2497 eV	H-2 ->L (48 %)
		369.36 nm	0.0458	3.3568 eV	H ->L (69 %)
<b>9</b>	<b>6j</b>	410.58 nm	0.0004	3.0197 eV	H-1 ->L (56 %)
		381.66 nm	0.0123	3.2485 eV	H-2 ->L (48 %)
		369.49 nm	0.0452	3.3555 eV	H ->L (69 %)

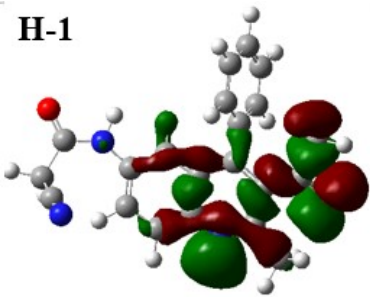
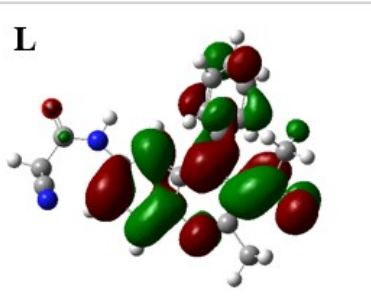
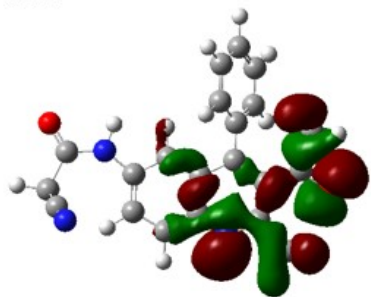
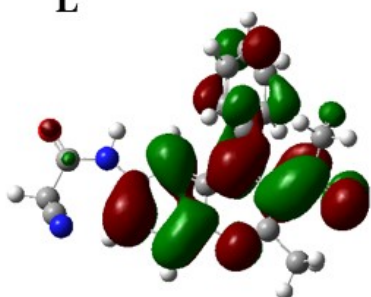
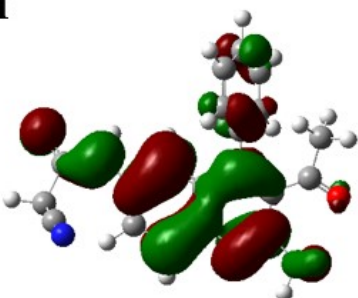
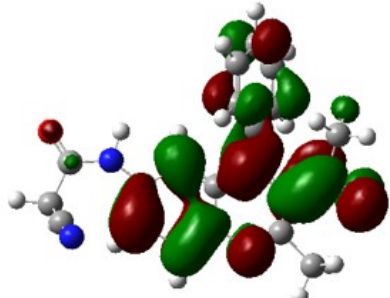
<b>10</b>	<b>6k</b>	410.76 nm	0.0003	3.0184 eV	H-1 ->L (56 %)
		381.39 nm	0.0124	3.2509 eV	H-2 ->L (48 %)
		369.37 nm	0.0453	3.3566 eV	H ->L (69 %)
<b>11</b>	<b>6l</b>	412.60 nm	0.0003	3.0049 eV	H-1 ->L (64 %)
		380.95 nm	0.0225	3.2546 eV	H-2 ->L (47 %)
		370.21 nm	0.0481	3.3490 eV	H ->L (59 %)
<b>12</b>	<b>6m</b>	418.60 nm	0.0003	2.9619 eV	H-1 ->L (82 %)
		378.81 nm	0.0263	3.2730 eV	H-2 ->L (53 %)
		368.49 nm	0.0452	3.3647 eV	H ->L (55 %)
<b>13</b>	<b>6s</b>	412.70 nm	0.0004	3.0042 eV	H-1 ->L (61 %)
		379.63 nm	0.0110	3.2659 eV	H-2 ->L (57 %)
		368.85 nm	0.0632	3.3614 eV	H ->L (78 %)
<b>14</b>	<b>6u</b>	411.77 nm	0.0009	3.0110 eV	H-2 ->L (62 %)
		387.23 nm	0.0644	3.2018 eV	H ->L (89 %)
		375.31 nm	0.0045	3.3035 eV	H-3 ->L (59 %)
<b>15</b>	<b>6v</b>	416.32 nm	0.0133	2.9781 eV	H ->L (94 %)
		412.71 nm	0.0021	3.0041 eV	H-2 ->L (62 %)
		380.24 nm	0.0416	3.2607 eV	H-1 ->L (54 %)
<b>16</b>	<b>6z</b>	405.20 nm	0.0021	3.0599 eV	H-1 ->L (56 %)
		389.29 nm	0.0626	3.1849 eV	H ->L (91 %)
		371.00 nm	0.0013	3.3419 eV	H-2 ->L (55 %)
<b>17</b>	<b>6aa</b>	389.26 nm	0.0138	3.1851 eV	H-1 -> L (86 %)
		377.12 nm	0.0669	3.2877 eV	H -> L (83 %)
		341.23 nm	0.0030	3.6335 eV	H-2 -> L (91 %)
<b>18</b>	<b>6ab</b>	390.51 nm	0.0058	3.1749 eV	H-1 ->L (86 %)
		359.51 nm	0.0775	3.4486 eV	H ->L (68 %)
		334.90 nm	0.0080	3.7021 eV	H-2 ->L (76 %)
<b>19</b>	<b>6ac</b>	391.08 nm	0.0079	3.1703 eV	H-1 -> L (89 %)
		367.69 nm	0.0772	3.3719 eV	H -> L (80 %)
		339.97 nm	0.0020	3.6469 eV	H-2 -> L (85 %)
<b>20</b>	<b>6ad</b>	386.39 nm	0.0046	3.2087 eV	H-1 ->L (95 %)
		374.09 nm	0.0634	3.3143 eV	H ->L (92 %)
		335.07 nm	0.0037	3.7003 eV	H-2 ->L (89 %)
<b>21</b>	<b>6ae</b>	386.77 nm	0.0042	3.2057 eV	H-1 ->L (95 %)
		376.27 nm	0.0617	3.2951 eV	H ->L (93 %)
		334.90 nm	0.0044	3.7021 eV	H-2 ->L (83 %)

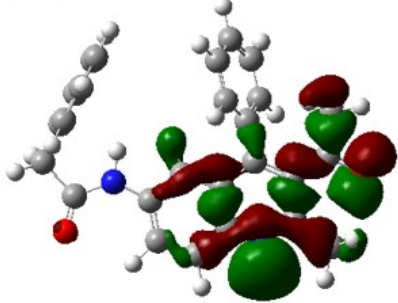
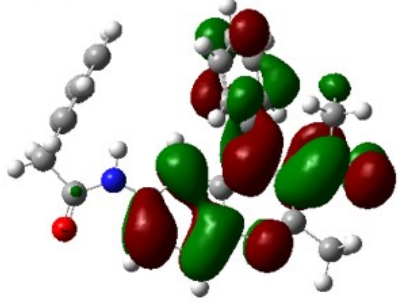
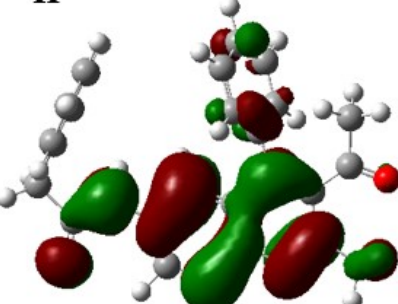
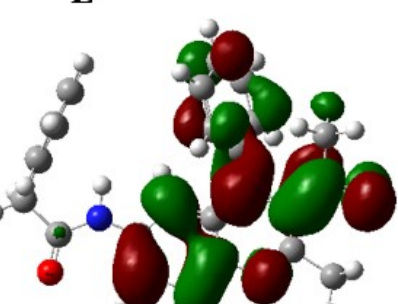
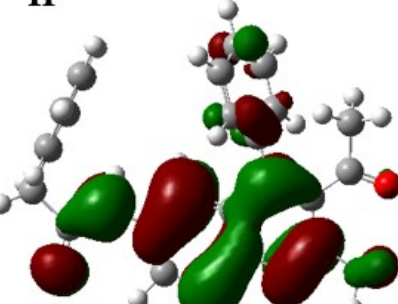
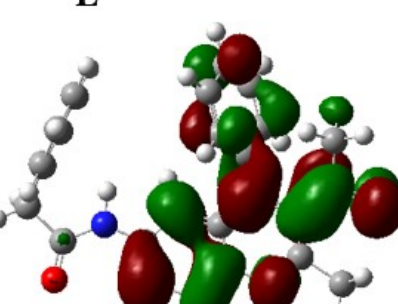
<b>22</b>	<b>6af</b>	386.60 nm	0.0043	3.2071 eV	H-1 ->L (96 %)
		383.60 nm	0.0566	3.2321 eV	H-3 ->L (94 %)
		332.86 nm	0.0077	3.7249 eV	H-2 ->L (72 %)
<b>23</b>	<b>6ag</b>	386.59 nm	0.0047	3.2072 eV	H-1 ->L (95 %)
		376.06 nm	0.0612	3.2969 eV	H ->L (93 %)
		335.54 nm	0.0042	3.6951 eV	H-3 ->L (88 %)
<b>24</b>	<b>6ah</b>	386.06 nm	0.0050	3.2115 eV	H-1 ->L (94 %)
		373.50 nm	0.0640	3.3195 eV	H ->L (92 %)
		335.19 nm	0.0032	3.6989 eV	H-2 ->L (90 %)
<b>25</b>	<b>6ai</b>	390.42 nm	0.0038	3.1757 eV	H-1 ->L (94 %)
		365.56 nm	0.0652	3.3916 eV	H ->L (90 %)
		335.73 nm	0.0014	3.6930 eV	H-2 ->L (80 %)
<b>26</b>	<b>6aj</b>	386.71 nm	0.0063	3.2061 eV	H-1 ->L (92 %)
		371.15 nm	0.0634	3.3405 eV	H ->L (88 %)
		336.72 nm	0.0018	3.6821 eV	H-2 ->L (89 %)
<b>27</b>	<b>6ak</b>	386.78 nm	0.0053	3.2055 eV	H ->L (93 %)
		371.41 nm	0.0631	3.3382 eV	H ->L (90 %)
		336.32 nm	0.0021	3.6865 eV	H-2 ->L (90 %)
<b>28</b>	<b>6al</b>	387.18 nm	0.0104	3.2022 eV	H-1 ->L (89 %)
		372.38 nm	0.0742	3.3295 eV	H ->L (85 %)
		338.72 nm	0.0018	3.6604 eV	H-3 ->L (90 %)
<b>29</b>	<b>6am</b>	385.51 nm	0.0145	3.2161 eV	H-1 ->L (86 %)
		373.92 nm	0.0680	3.3158 eV	H ->L (82 %)
		338.24 nm	0.0023	3.6656 eV	H-2 ->L (90 %)
<b>30</b>	<b>6ao</b>	394.79 nm	0.0756	3.1405 eV	H ->L (93 %)
		383.47 nm	0.0015	3.2333 eV	H-2 ->L (91 %)
		374.17 nm	0.0023	3.3135 eV	H-1 ->L (96 %)
<b>31</b>	<b>6ap</b>	408.41 nm	0.0154	3.0358 eV	H ->L (98 %)
		386.31 nm	0.0151	3.2094 eV	H-2 ->L (83 %)
		373.76 nm	0.0728	3.3172 eV	H-1 ->L (81 %)

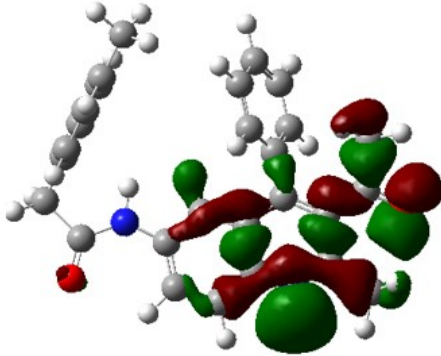
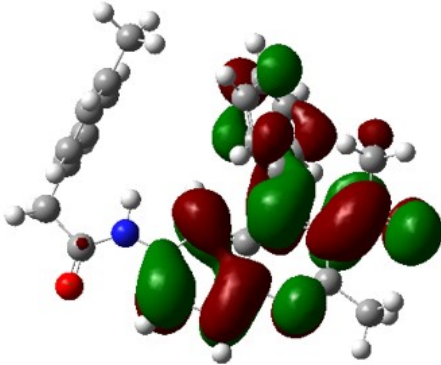
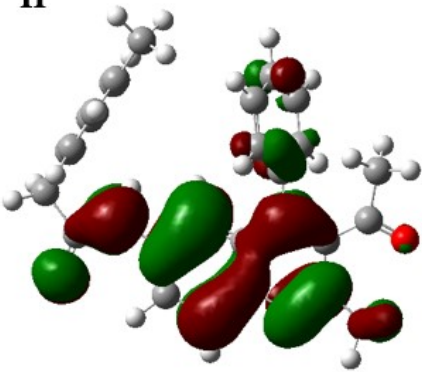
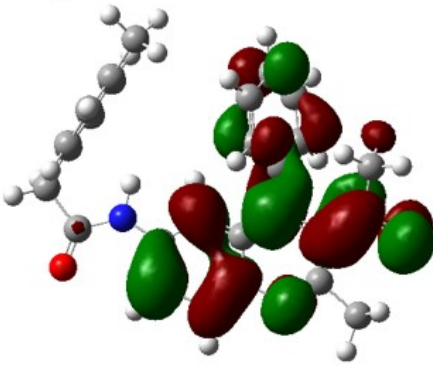
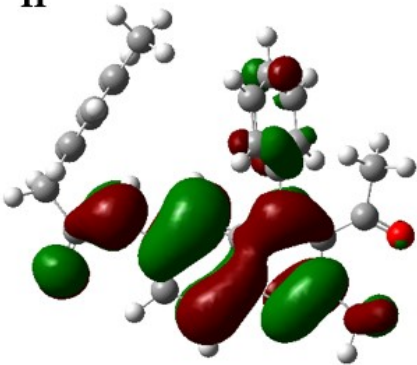
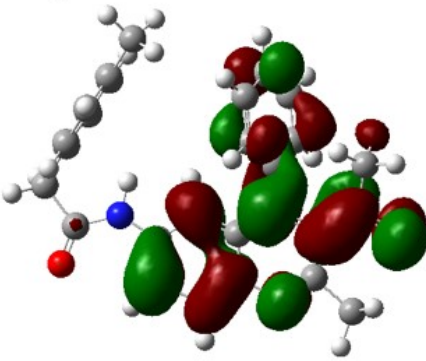
**Table S4.** Density surface of the selected major contributions of compounds frontier molecular orbitals involved in electronic transitions of at Basic set level of B3LYP/6-31+ G'(d,p) using iso-surface value of 0.02 au.

Sr. No.	Comp. Code	HOMO	LUMO
1	6a	<p data-bbox="387 434 579 465">Excited state-1</p> <p data-bbox="453 499 512 530"><b>H-1</b></p> 	<p data-bbox="1015 521 1042 553"><b>L</b></p> 
		<p data-bbox="387 916 579 947">Excited state-2</p> <p data-bbox="424 1066 451 1097"><b>H</b></p> 	<p data-bbox="1015 1066 1042 1097"><b>L</b></p> 
		<p data-bbox="387 1449 579 1480">Excited state-3</p> <p data-bbox="435 1612 462 1644"><b>H</b></p> 	<p data-bbox="986 1612 1013 1644"><b>L</b></p> 



2	6b	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L-1</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

3	6d	<p>Excited state-1</p> <p><b>H-1</b></p> 	<p><b>L</b></p> 
		<p>Excited state-2</p> <p><b>H</b></p> 	<p><b>L</b></p> 
		<p>Excited state-3</p> <p><b>H</b></p> 	<p><b>L</b></p> 

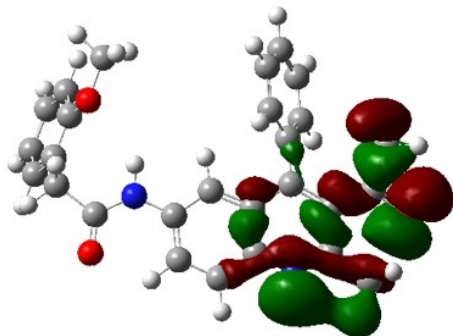
		<p>Excited state-1</p> <p><b>H-1</b> </p> <p><b>L</b> </p> <p>Excited state-2</p> <p><b>H</b> </p> <p><b>L</b> </p> <p>Excited state-3</p> <p><b>H</b> </p> <p><b>L</b> </p>
4	6e	

5

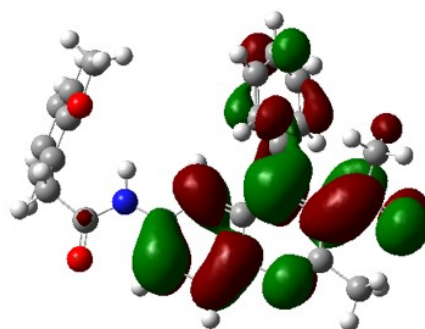
6f

Excited state-1

H-1

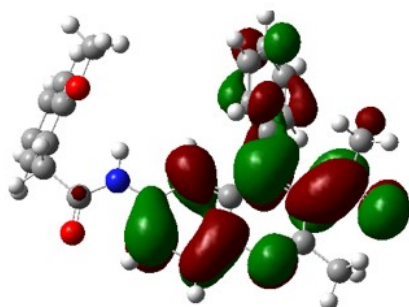


L

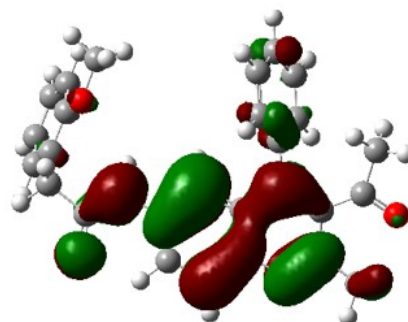


Excited state-2

H

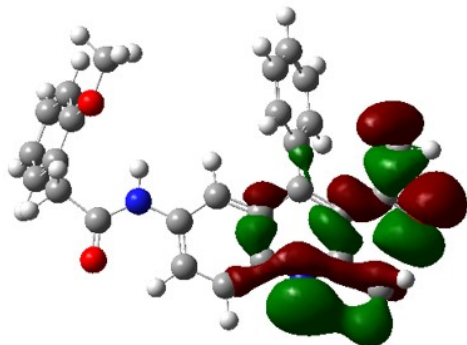


L

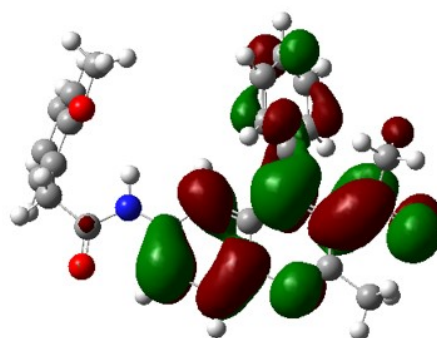


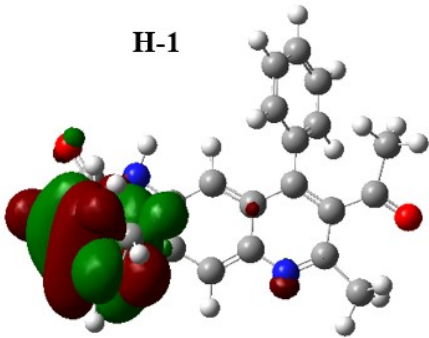
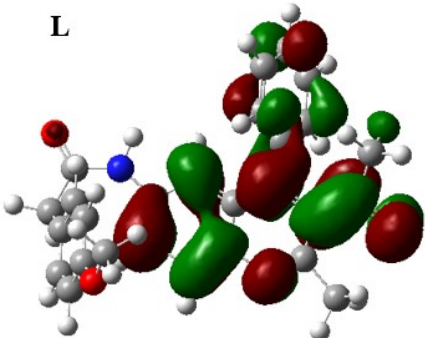
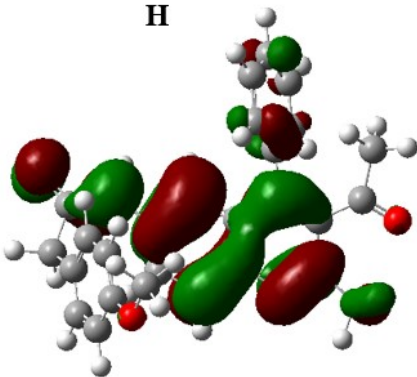
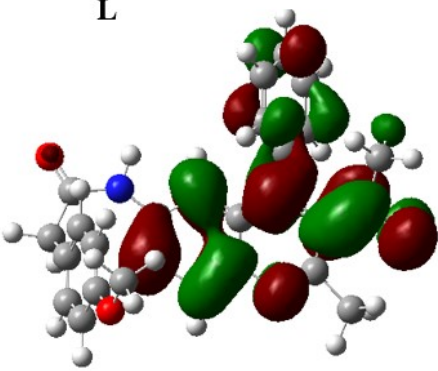
Excited state-3

H-1



L

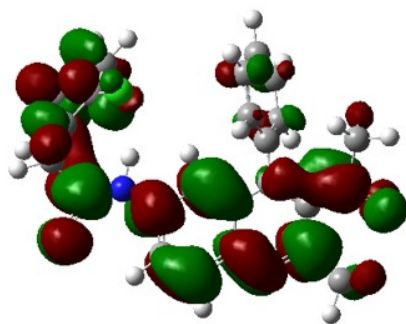


6	6g	<p>Excited state-1</p> <p><b>H-1</b></p>  <p><b>L</b></p>  <p>Excited state-2</p> <p><b>H</b></p>  <p><b>L</b></p>  <p>Excited state-3</p>

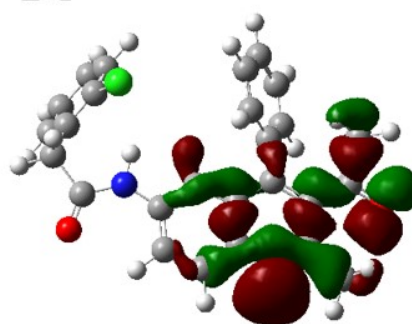


Excited state-1

**H-1**

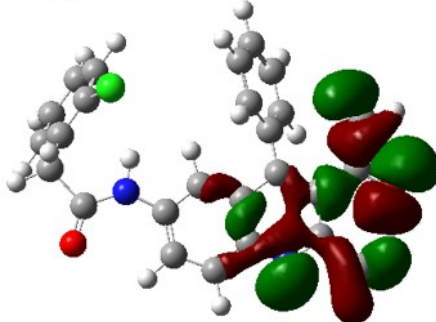


**L+1**

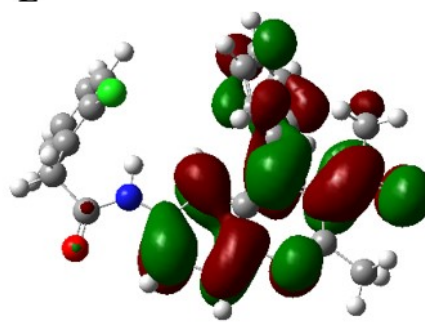


Excited state-2

**H-2**



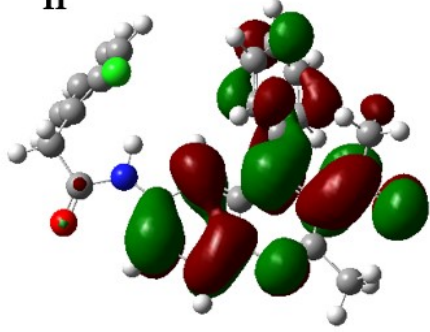
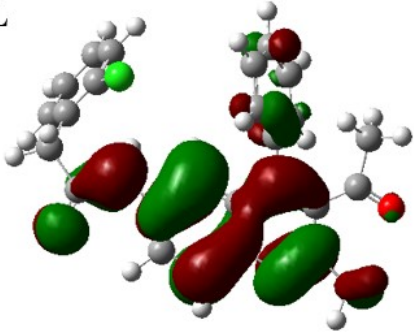
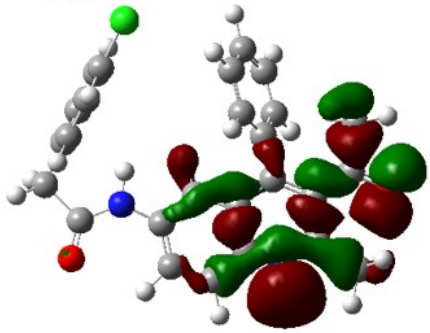
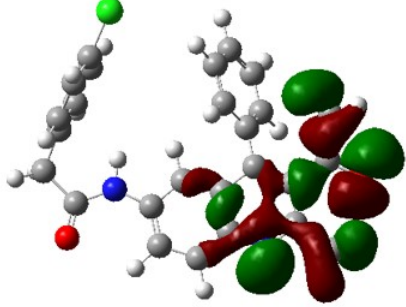
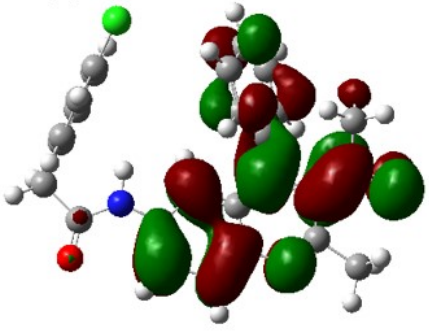
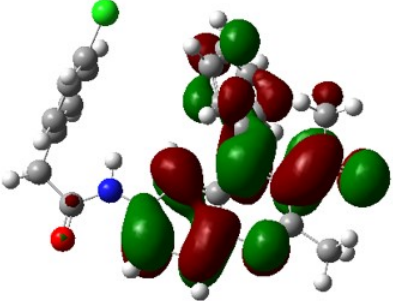
**L**

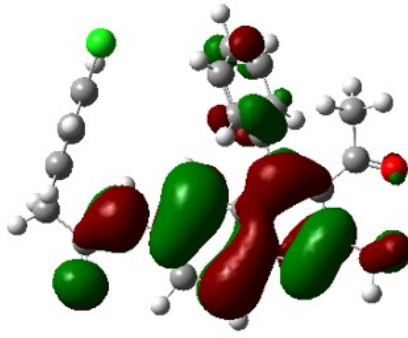
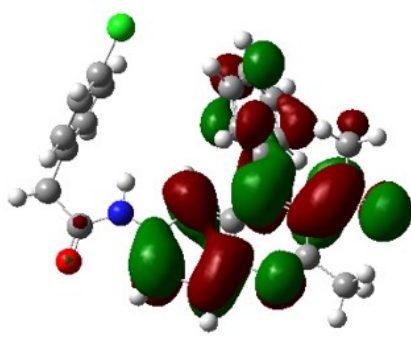
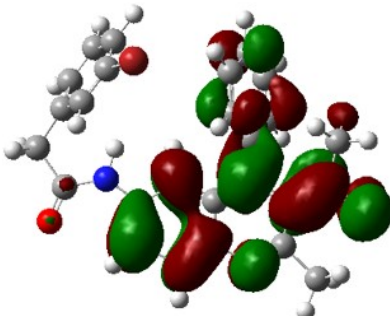
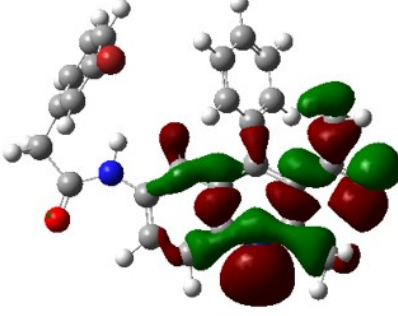
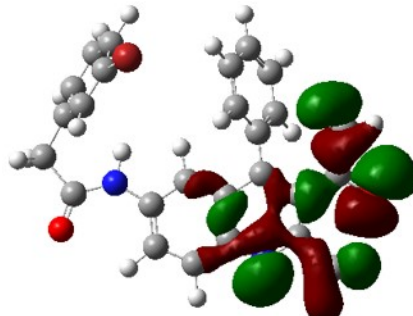
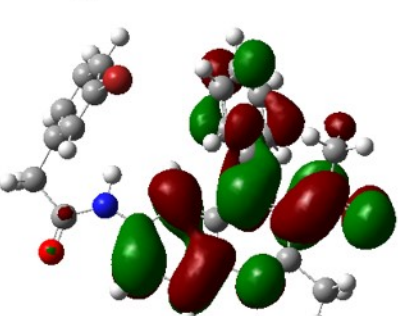


7

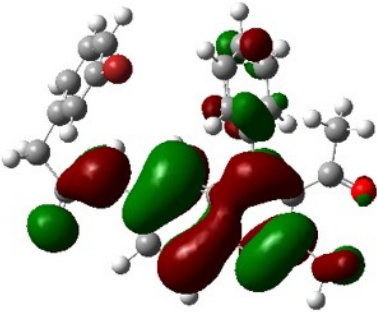
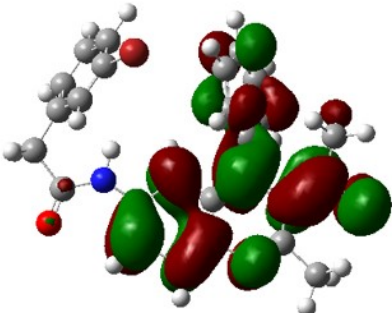
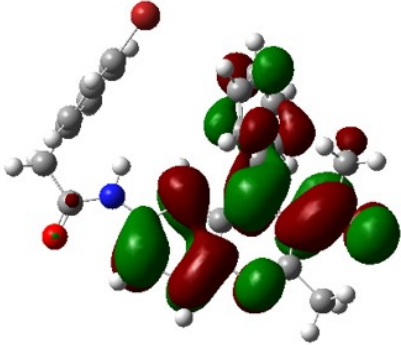
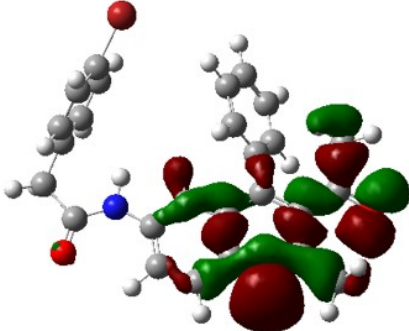
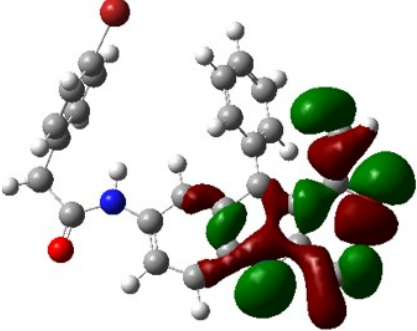
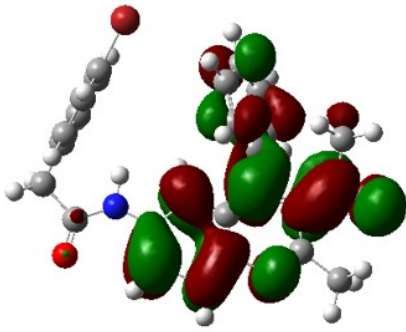
6h

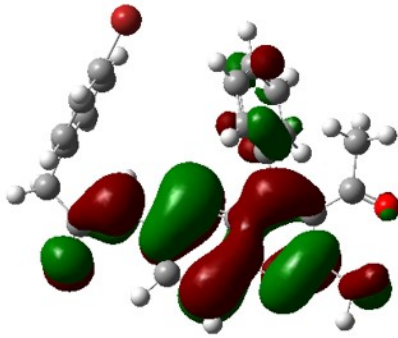
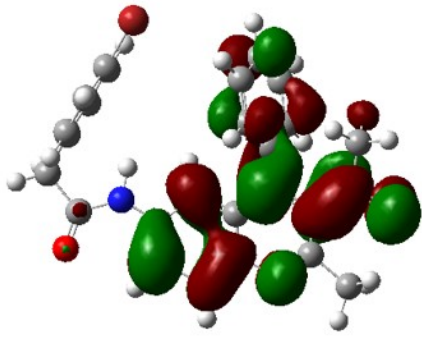
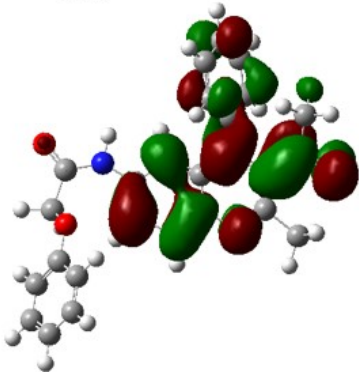
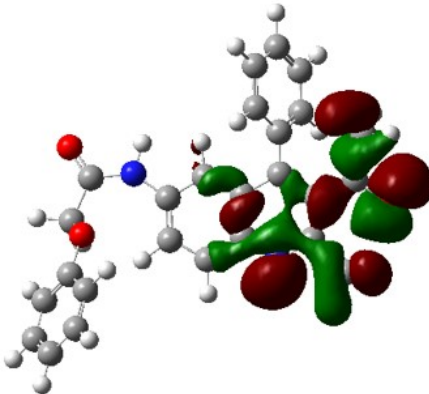
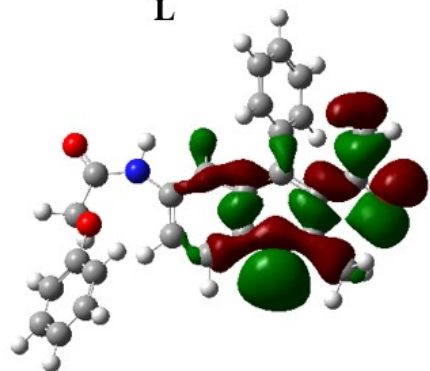
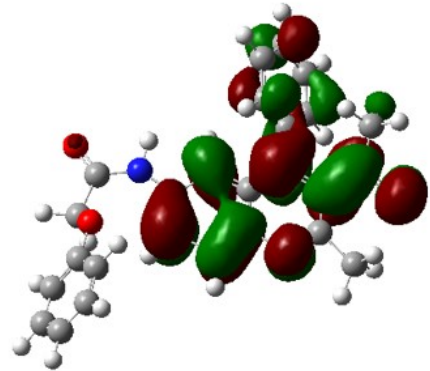
Excited state-3

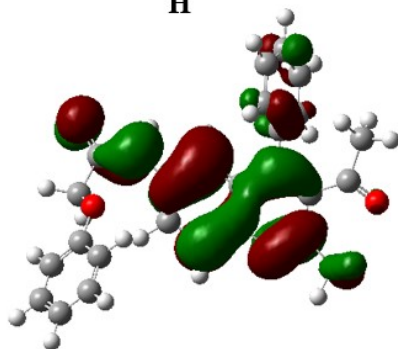
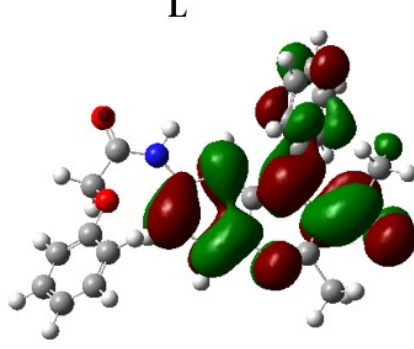
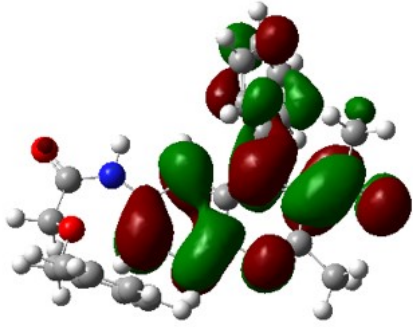
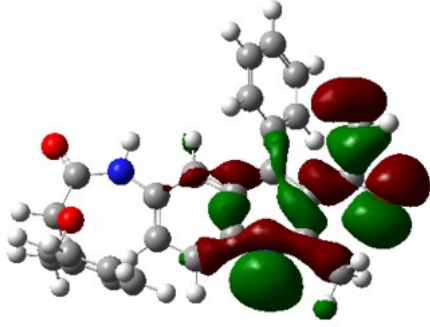
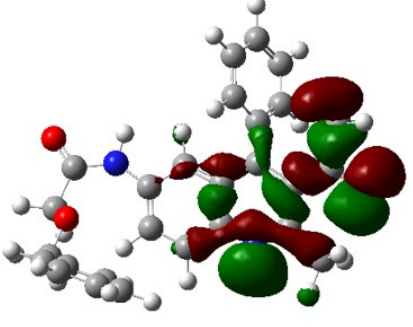
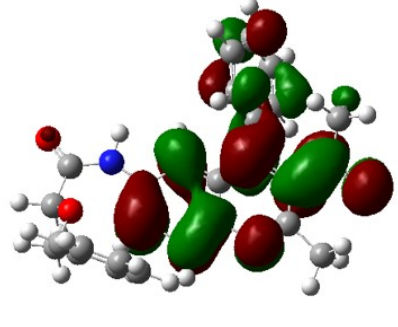
		<p><b>H</b></p> 	<p><b>L</b></p> 
<p>8</p>	<p>6i</p>	<p>Excited state-1</p> <p><b>H-1</b></p>  <p>Excited state-2</p> <p><b>H-2</b></p>  <p>Excited state-3</p>	<p><b>L</b></p>  <p><b>L</b></p> 

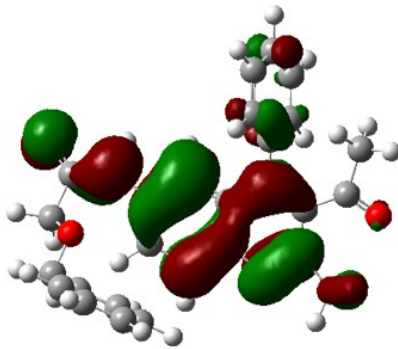
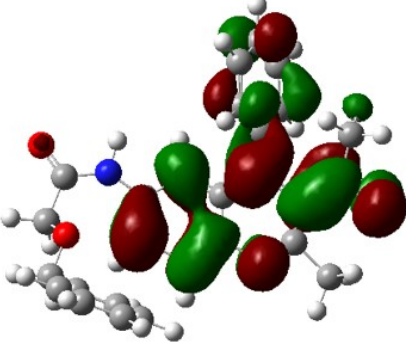
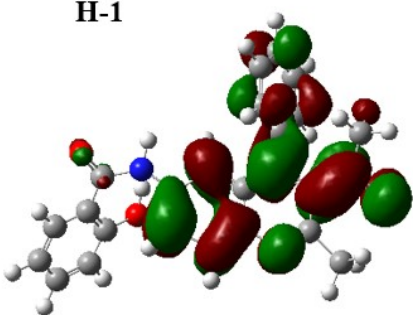
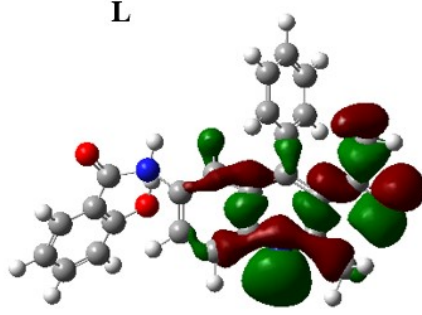
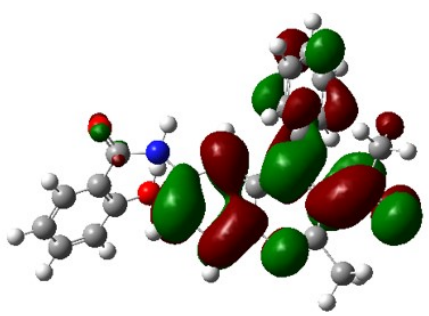
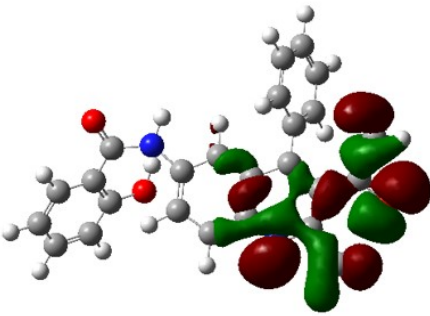
		<p><b>H</b></p> 	<p><b>L</b></p> 
<p>9</p>	<p>6j</p>	<p>Excited state-1</p> <p><b>H-1</b></p>  <p><b>L</b></p>  <p>Excited state-2</p> <p><b>H-2</b></p>  <p><b>L</b></p>  <p>Excited state-3</p>	

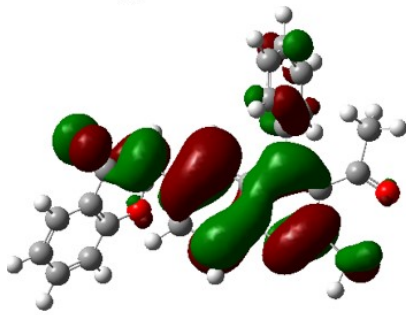
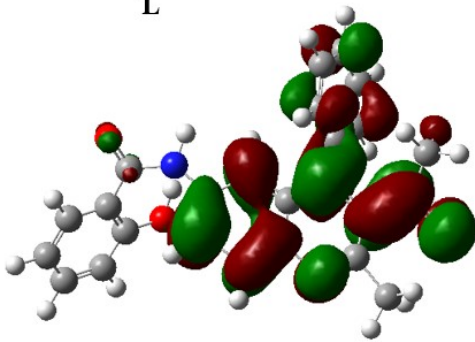
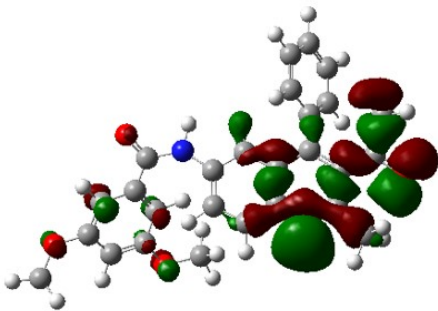
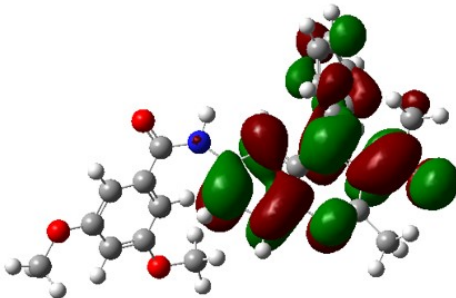
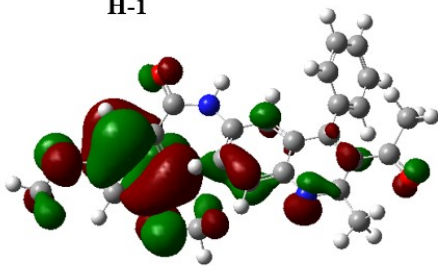
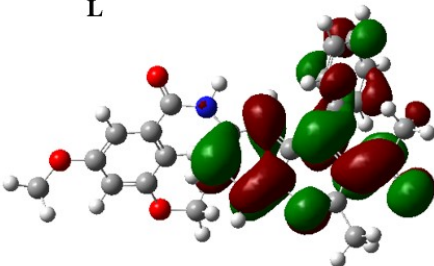


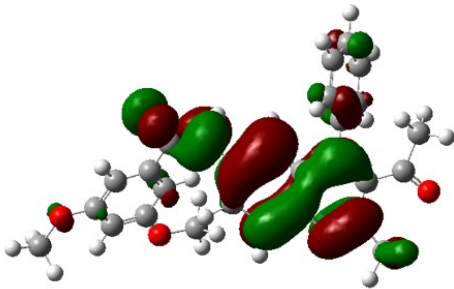
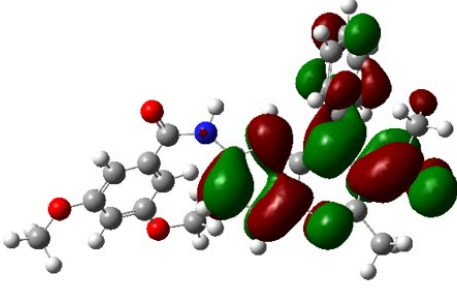
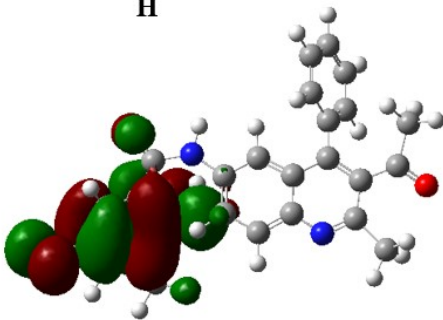
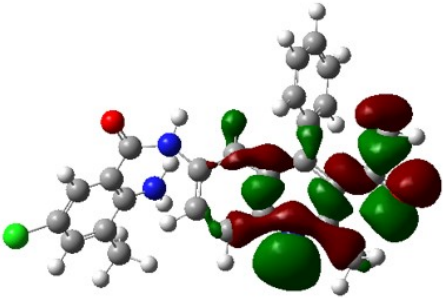
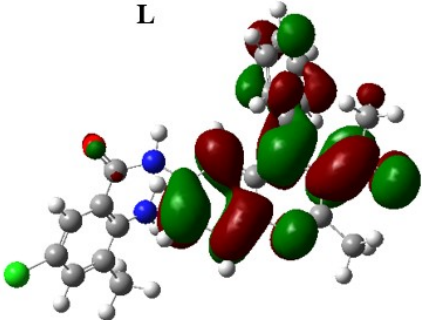
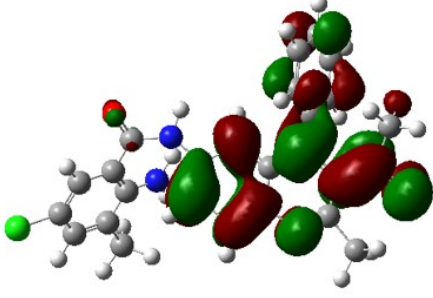
		<p><b>H</b></p>  <p><b>L</b></p> 
<p>10</p>	<p>6k</p>	<p>Excited state-1</p> <p><b>H-1</b></p>  <p><b>L</b></p>  <p>Excited state-2</p> <p><b>H-2</b></p>  <p><b>L</b></p>  <p>Excited state-3</p>

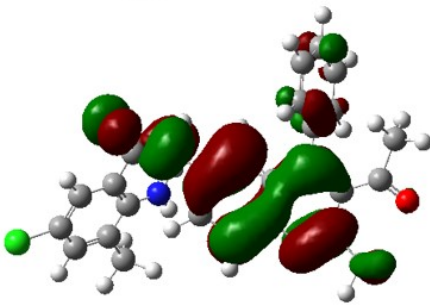
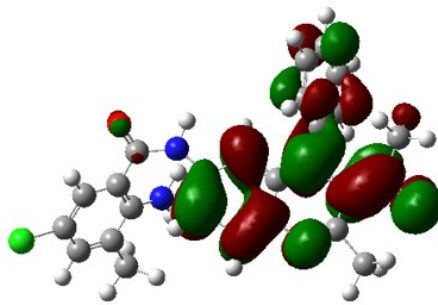
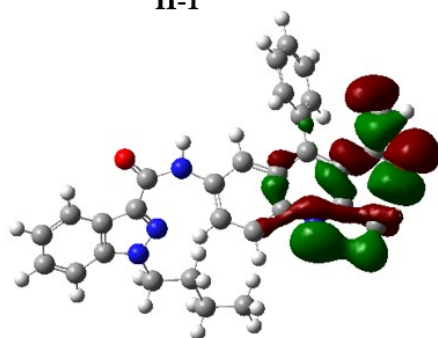
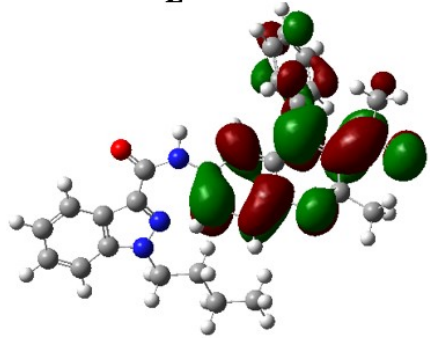
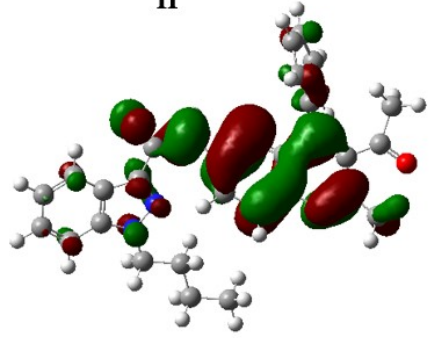
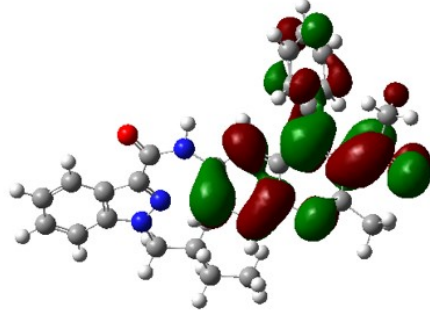
		<p><b>H</b></p> 	<p><b>L</b></p> 
11	6l	<p>Excited state-1</p> <p><b>H-1</b></p>  <p>Excited state-2</p> <p><b>H-2</b></p>  <p>Excited state-3</p>	<p><b>L</b></p>  <p><b>L</b></p> 

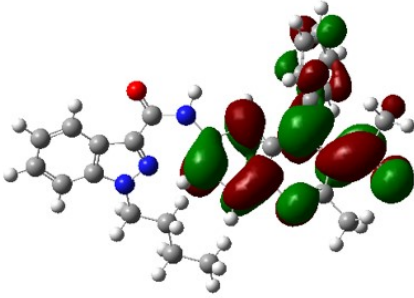
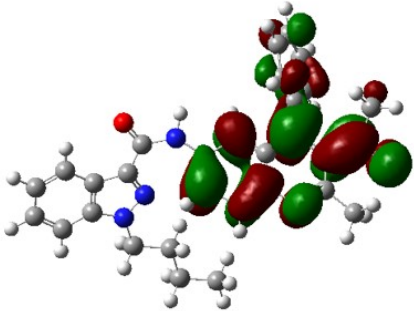
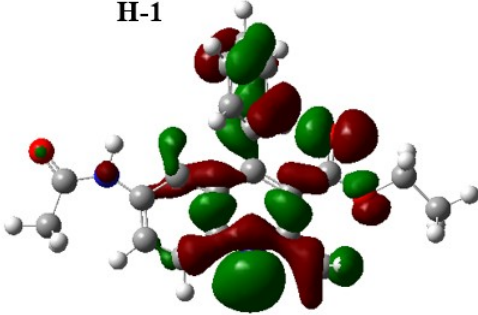
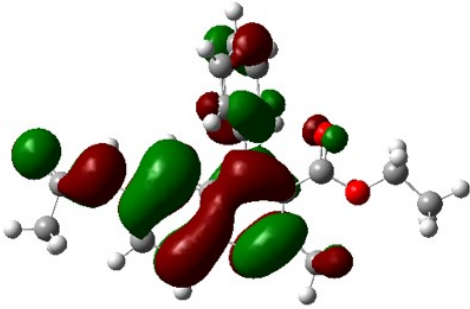
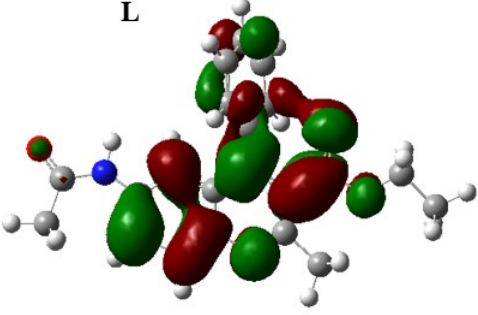
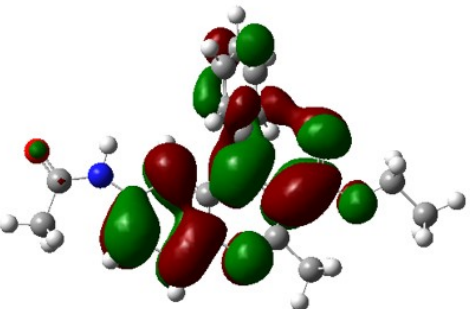
		<p style="text-align: center;"><b>H</b></p>  <p style="text-align: center;"><b>L</b></p> 
12	6m	<p>Excited state-1</p> <p style="text-align: center;"><b>H-1</b></p>  <p style="text-align: center;"><b>L</b></p>  <p>Excited state-2</p> <p style="text-align: center;"><b>H-2</b></p>  <p style="text-align: center;"><b>L</b></p>  <p>Excited state-3</p>

		<p style="text-align: center;"><b>H</b></p>  <p style="text-align: center;"><b>L</b></p> 
<p style="text-align: center;"><b>13</b></p>	<p style="text-align: center;"><b>6s</b></p>	<p style="text-align: center;">Excited state-1</p> <p style="text-align: center;"><b>H-1</b></p>  <p style="text-align: center;"><b>L</b></p>  <p style="text-align: center;">Excited state-2</p> <p style="text-align: center;"><b>H-2</b></p>  <p style="text-align: center;"><b>L</b></p>  <p style="text-align: center;">Excited state-3</p>

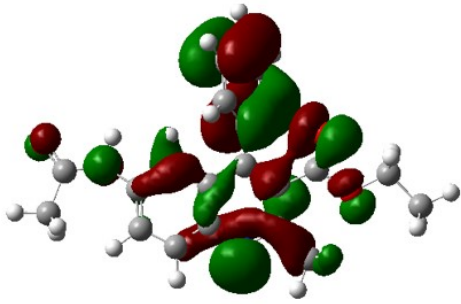
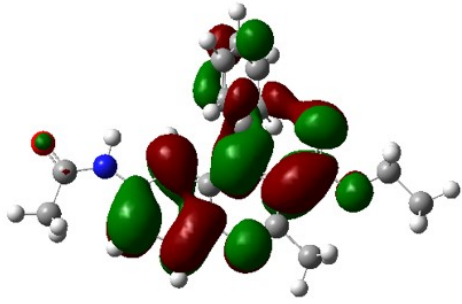
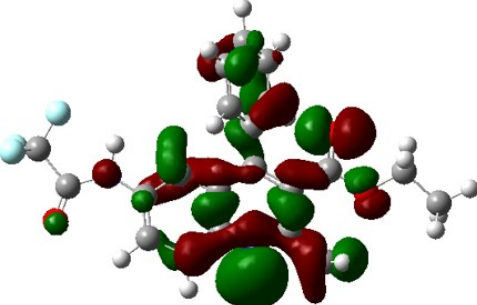
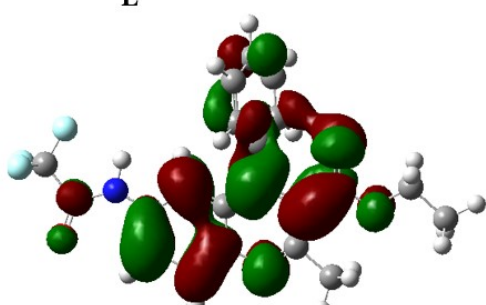
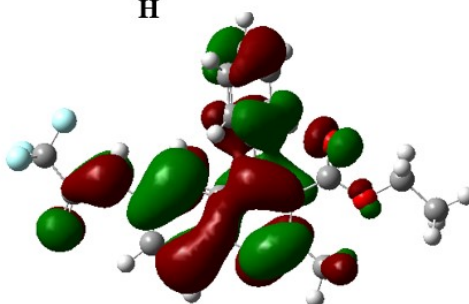
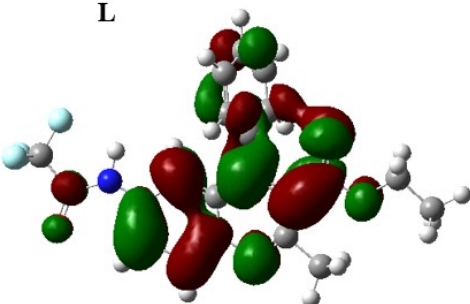
		<p><b>H</b></p> 	<p><b>L</b></p> 
14	6u	<p>Excited state-1</p> <p><b>H-2</b></p> 	<p><b>L</b></p> 
		<p>Excited state-2</p> <p><b>H-1</b></p> 	<p><b>L</b></p> 
		<p>Excited state-3</p>	

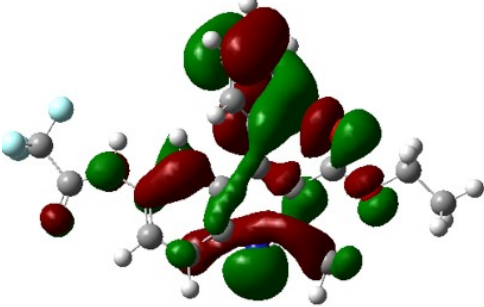
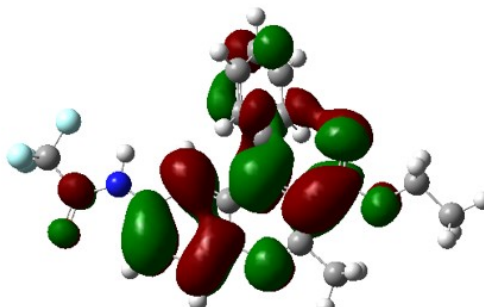
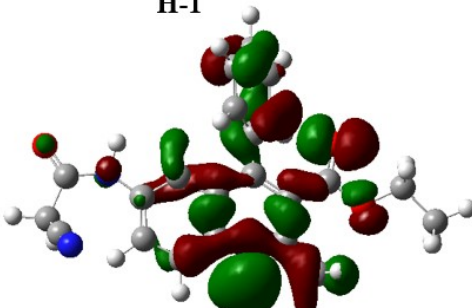
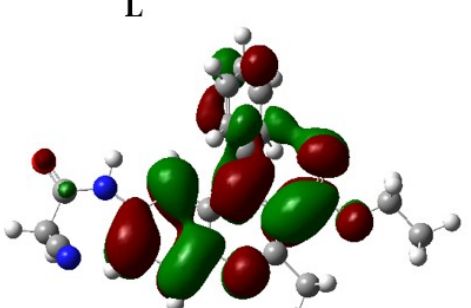
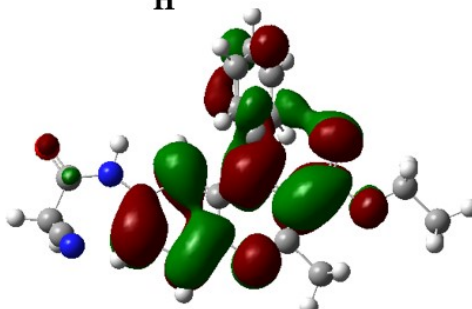
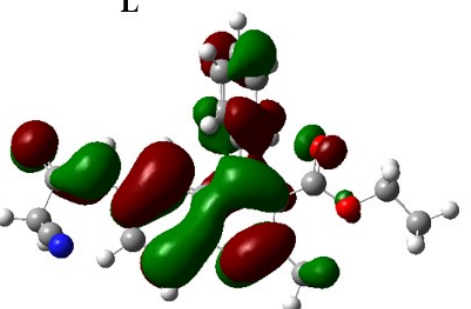
		<p style="text-align: center;"><b>H</b></p> 	<p style="text-align: center;"><b>L</b></p> 
15	6v	<p>Excited state-1</p> <p style="text-align: center;"><b>H</b></p>  <p>Excited state-2</p> <p style="text-align: center;"><b>H-2</b></p>  <p>Excited state-3</p>	<p style="text-align: center;"><b>L</b></p>  <p style="text-align: center;"><b>L</b></p> 

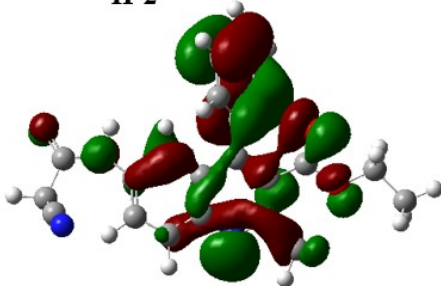
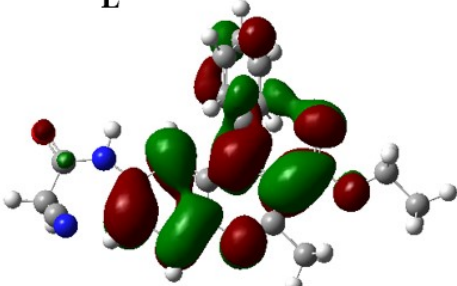
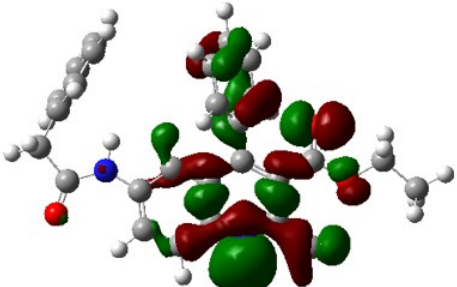
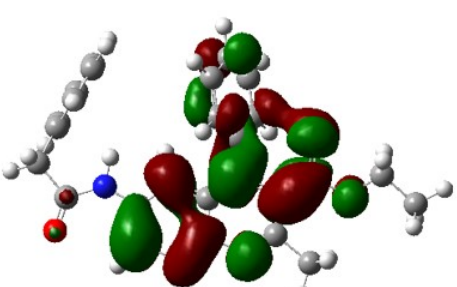
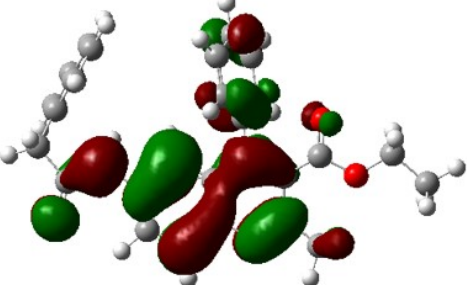
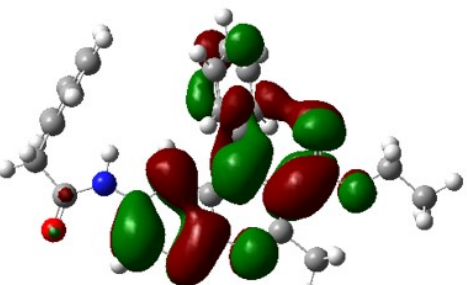
		<p style="text-align: center;"><b>H-1</b></p> 	<p style="text-align: center;"><b>L</b></p> 
<p style="text-align: center;"><b>16</b></p>	<p style="text-align: center;"><b>6z</b></p>	<p style="text-align: center;">Excited state-1</p> <p style="text-align: center;"><b>H-1</b></p> 	<p style="text-align: center;"><b>L</b></p> 
		<p style="text-align: center;">Excited state-2</p> <p style="text-align: center;"><b>H</b></p> 	<p style="text-align: center;"><b>L</b></p> 
		<p style="text-align: center;">Excited state-3</p>	

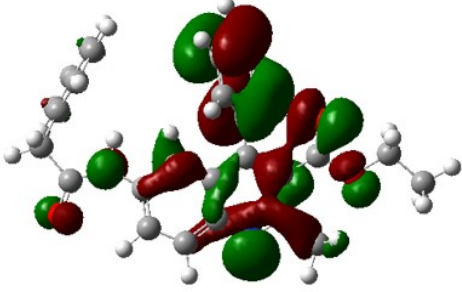
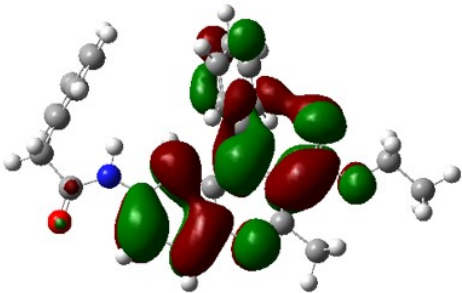
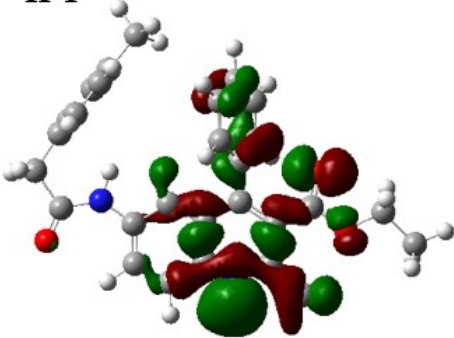
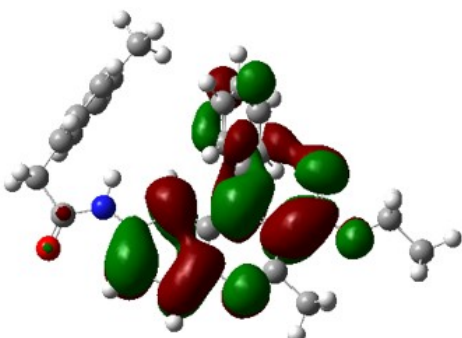
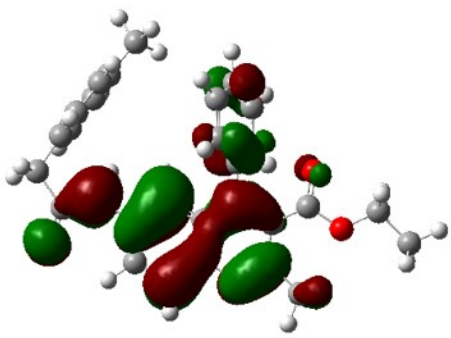
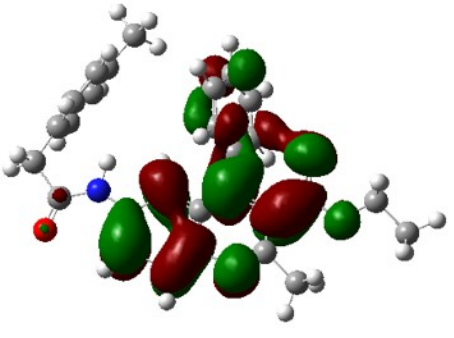
		<p style="text-align: center;"><b>H-2</b></p> 	<p style="text-align: center;"><b>L</b></p> 
17	6aa	<p>Excited state-1</p> <p style="text-align: center;"><b>H-1</b></p>  <p>Excited state-2</p> <p style="text-align: center;"><b>H</b></p> 	<p style="text-align: center;"><b>L</b></p>  <p style="text-align: center;"><b>L</b></p> 

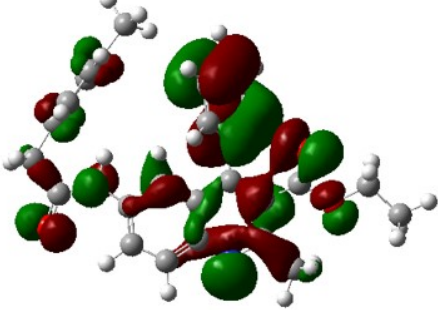
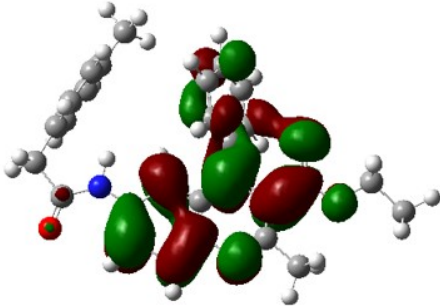
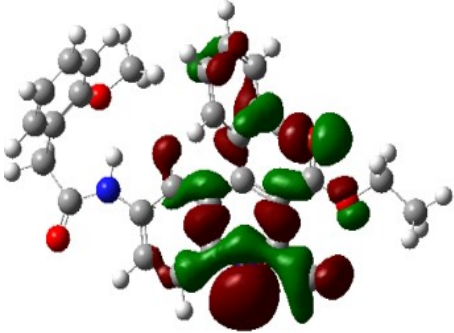
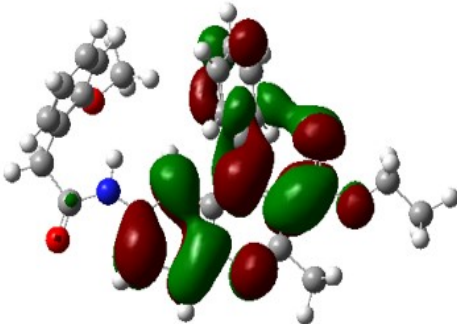
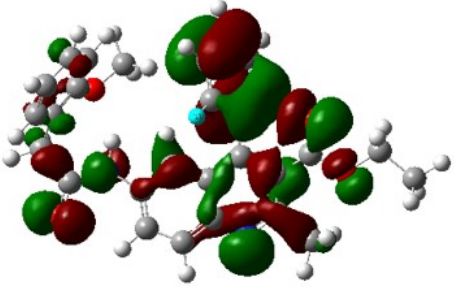
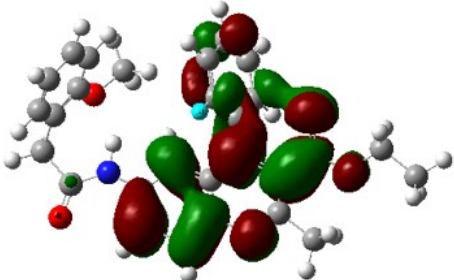


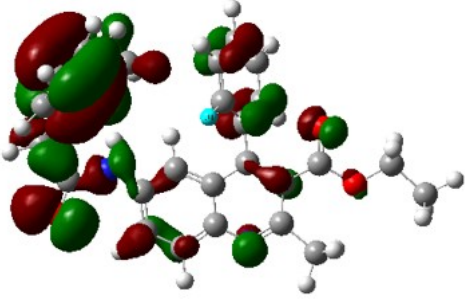
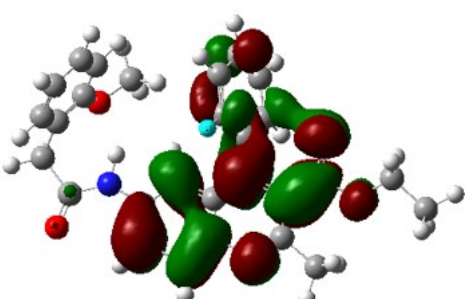
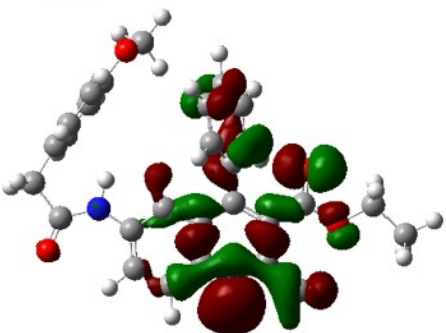
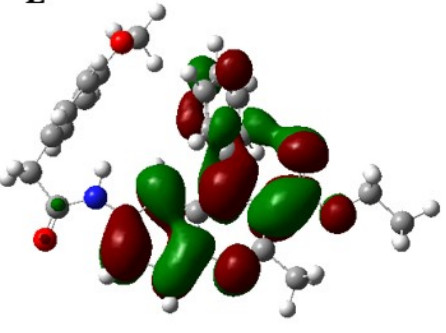
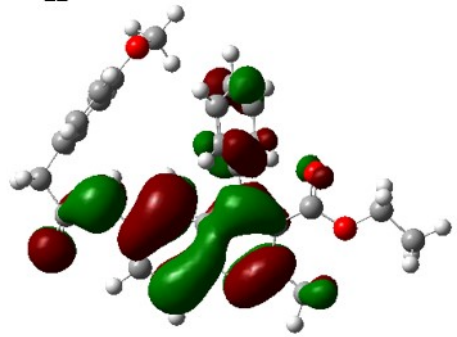
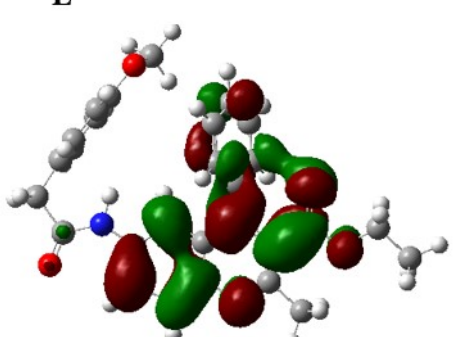
		<p>Excited state-3</p> <p style="text-align: center;"><b>H-2</b></p>  <p style="text-align: center;"><b>L</b></p> 
<p>18</p>	<p>6ab</p>	<p>Excited state-1</p> <p style="text-align: center;"><b>H-1</b></p>  <p style="text-align: center;"><b>L</b></p>  <p>Excited state-2</p> <p style="text-align: center;"><b>H</b></p>  <p style="text-align: center;"><b>L</b></p> 

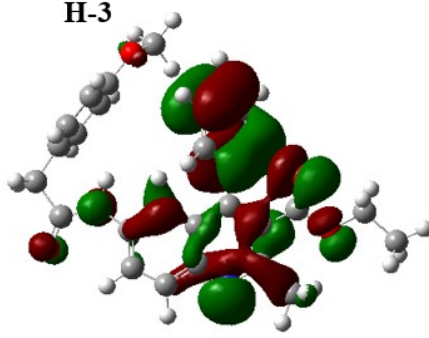
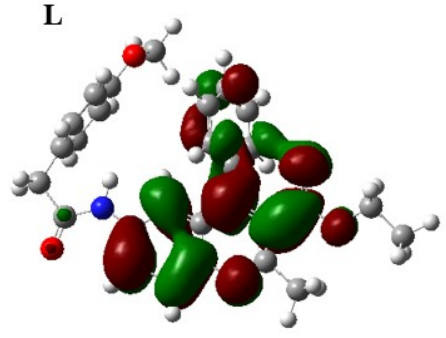
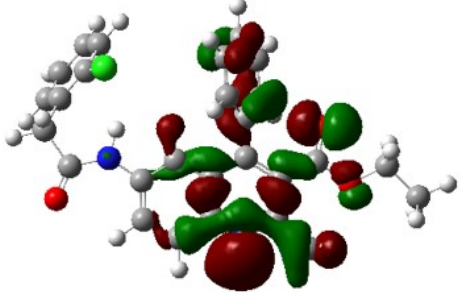
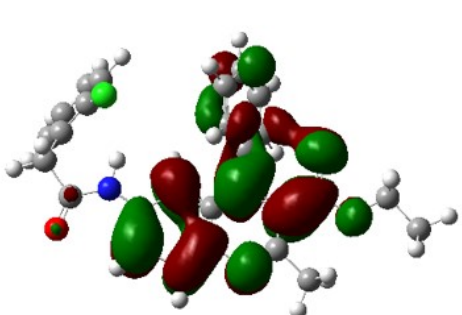
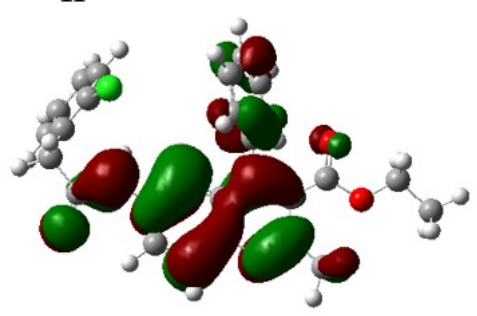
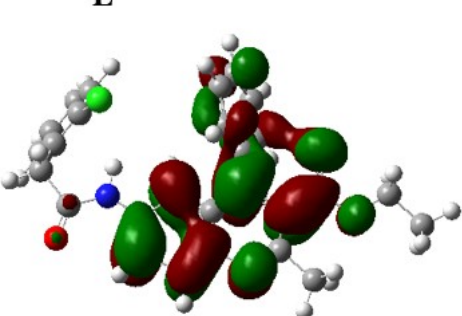
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
19	6ac	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

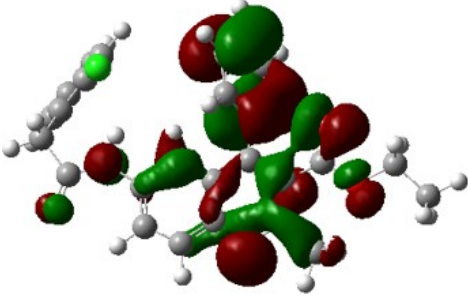
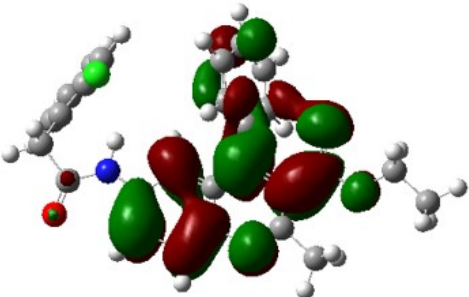
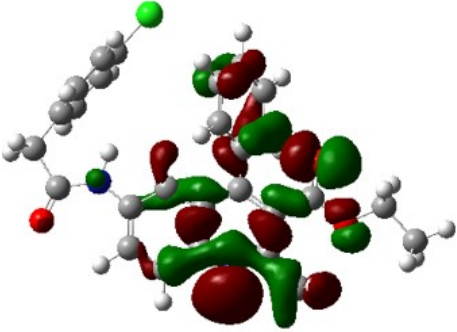
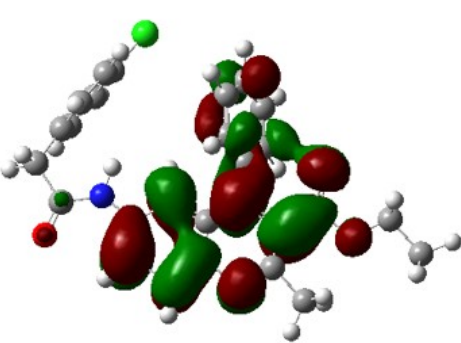
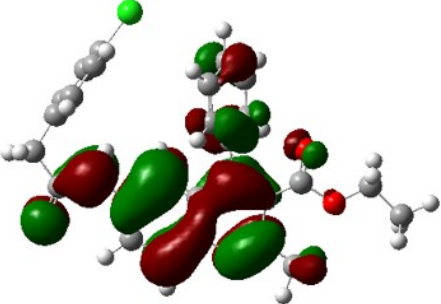
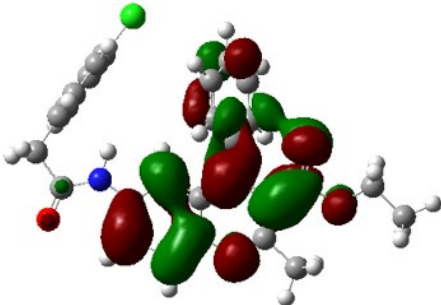
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
20	6ad	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
21	6ae	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

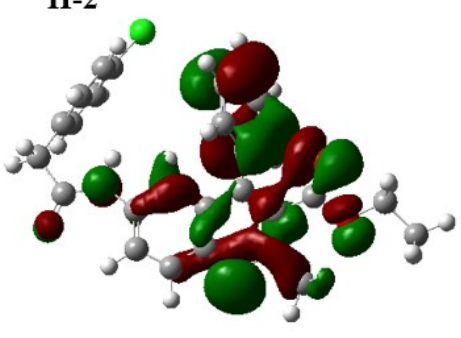
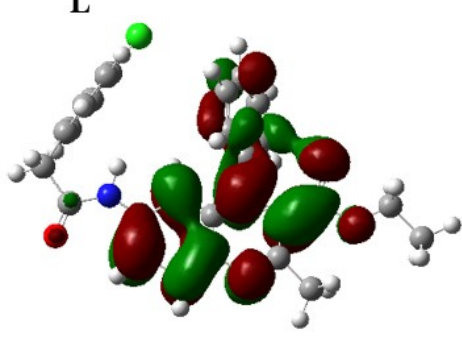
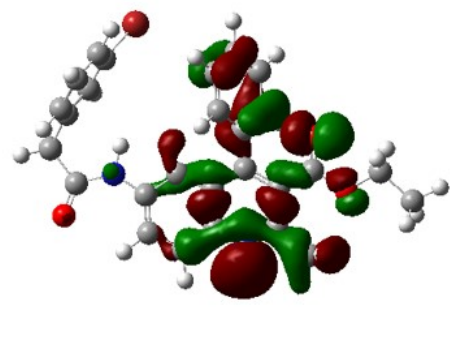
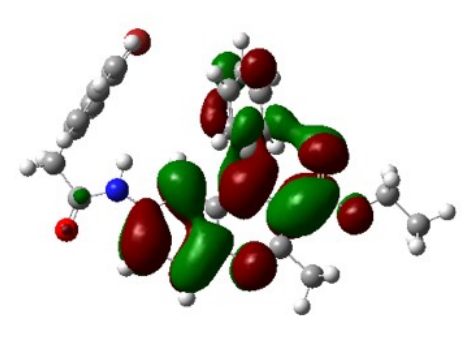
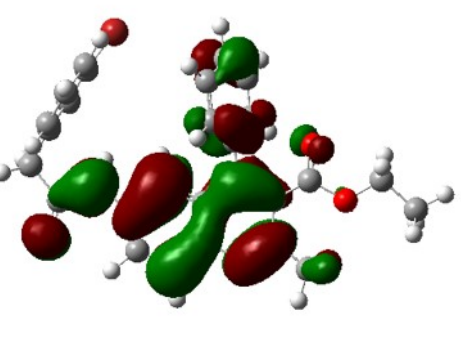
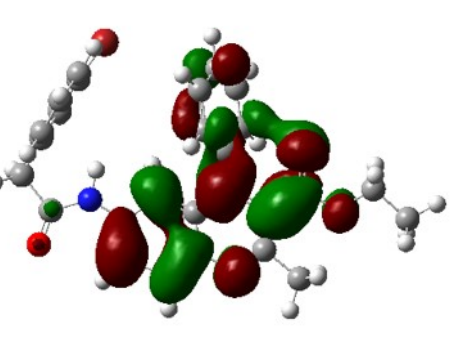
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
22	6af	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-3</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

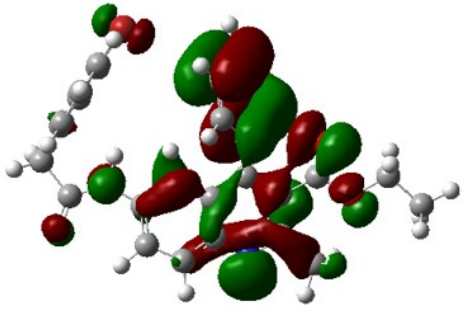
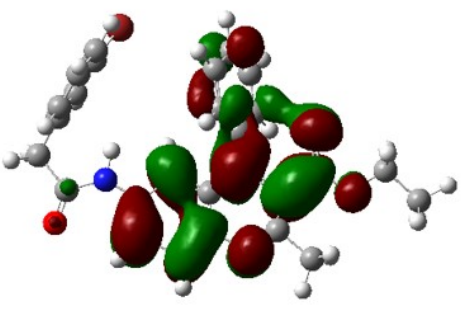
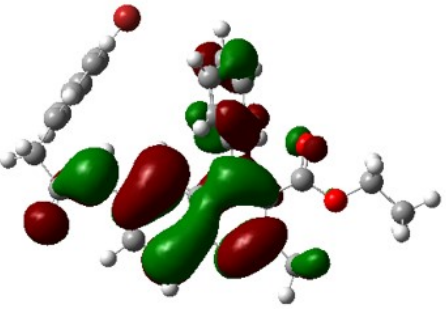
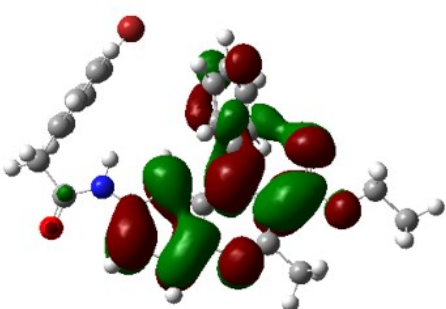
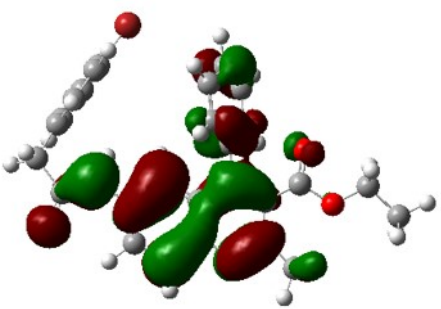
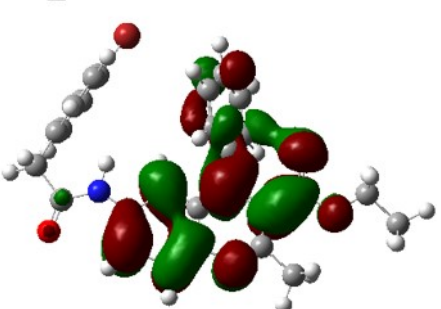
		<p>Excited state-3</p> <p><b>H-2</b></p>  <p><b>L</b></p> 
23	6ag	<p>Excited state-1</p> <p><b>H-1</b></p>  <p><b>L</b></p>  <p>Excited state-2</p> <p><b>H</b></p>  <p><b>L</b></p> 

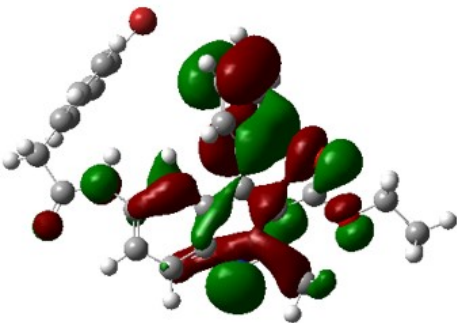
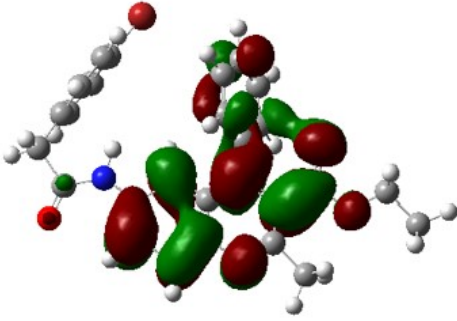
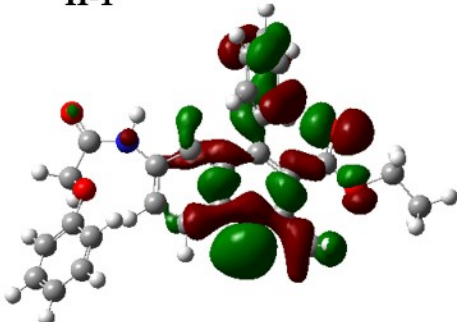
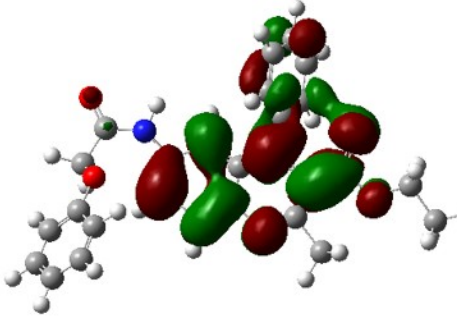
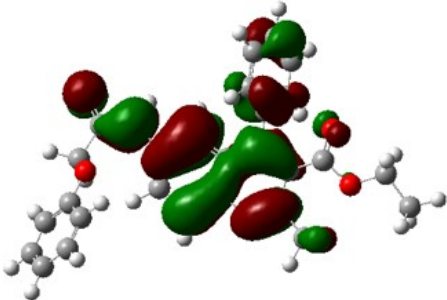
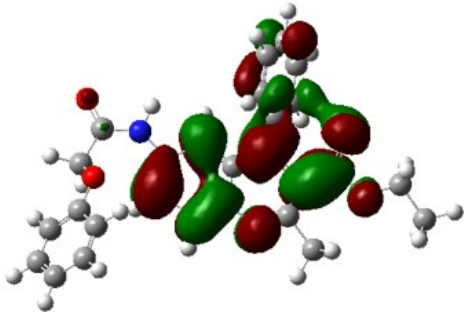
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p><b>H-3</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
24	6ah	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

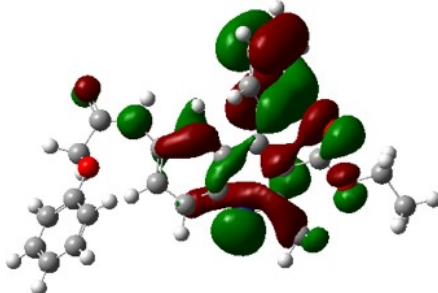
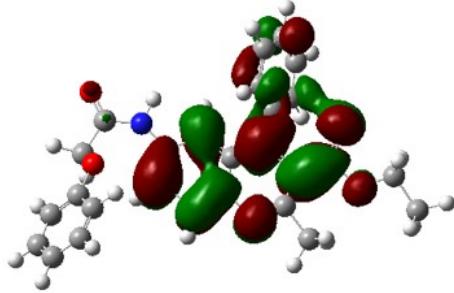
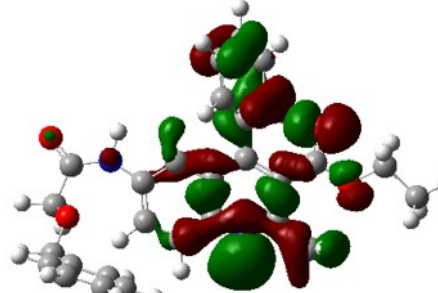
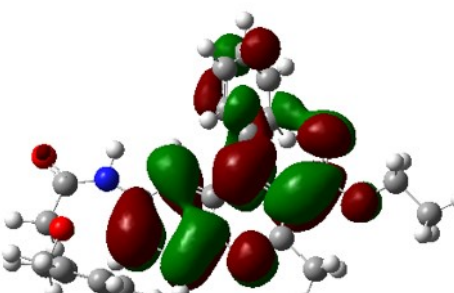
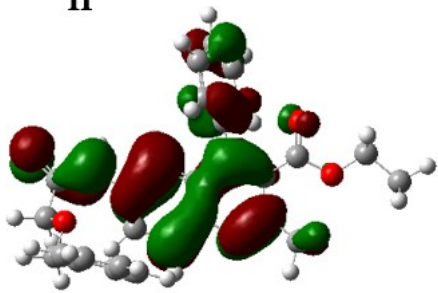
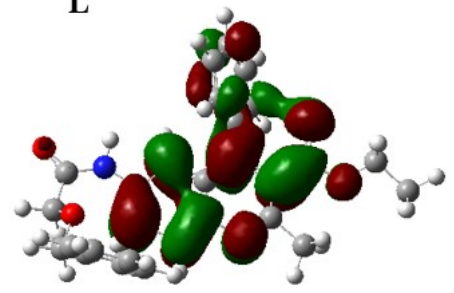
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
25	6ai	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>



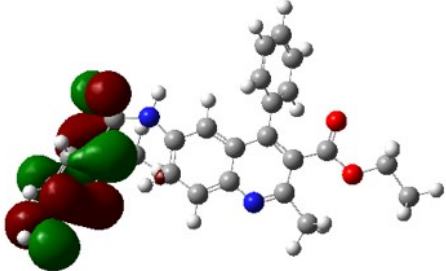
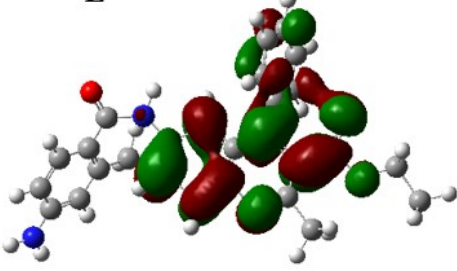
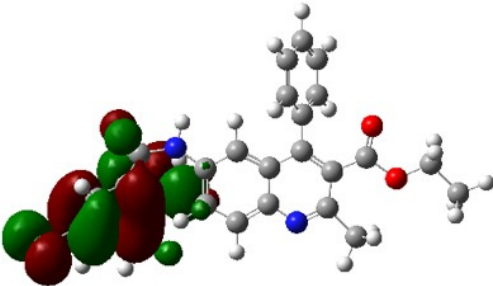
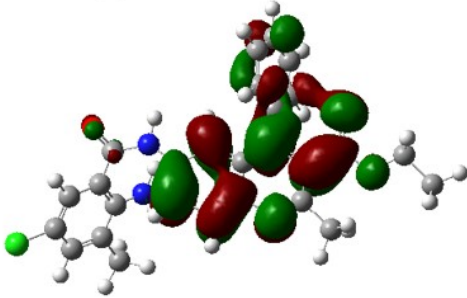
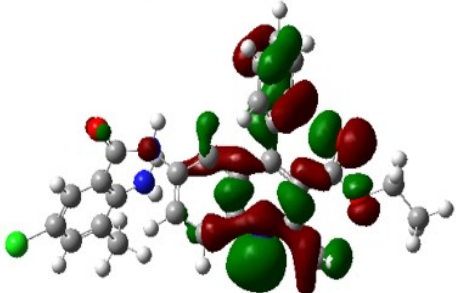
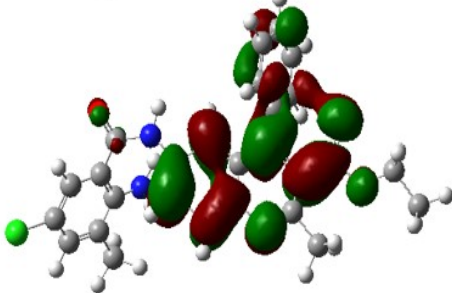
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
26	6aj	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-1</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

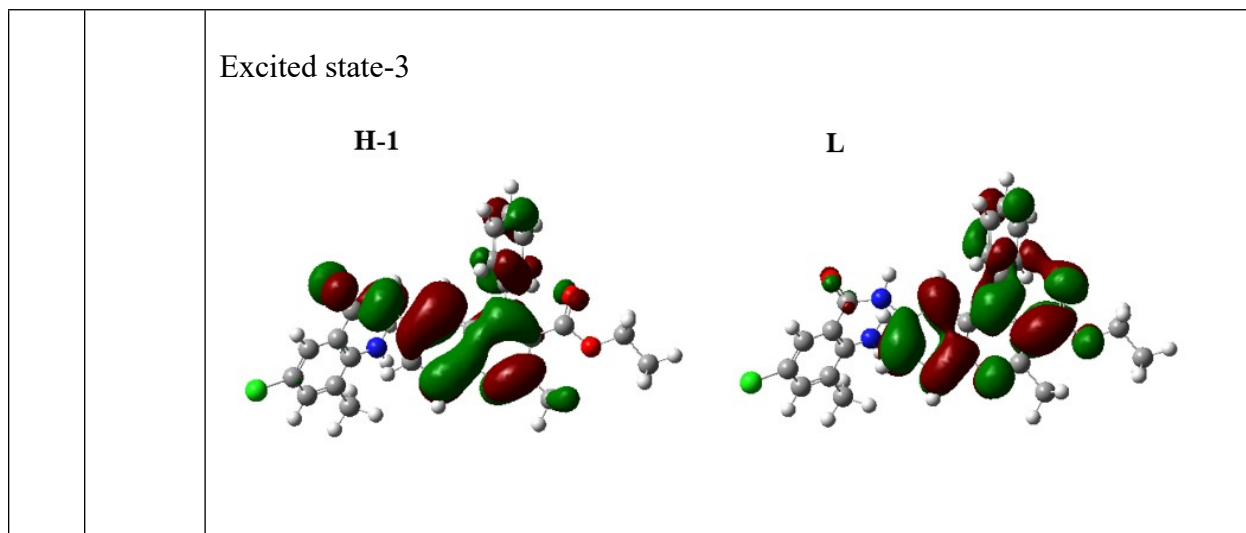
		<p>Excited state-3</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H-2</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>
27	6ak	<p>Excited state-1</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div> <p>Excited state-2</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><b>H</b></p>  </div> <div style="text-align: center;"> <p><b>L</b></p>  </div> </div>

		<p>Excited state-3</p> <p><b>H-2</b></p>  <p><b>L</b></p> 
28	6al	<p>Excited state-1</p> <p><b>H-1</b></p>  <p><b>L</b></p>  <p>Excited state-2</p> <p><b>H</b></p>  <p><b>L</b></p> 

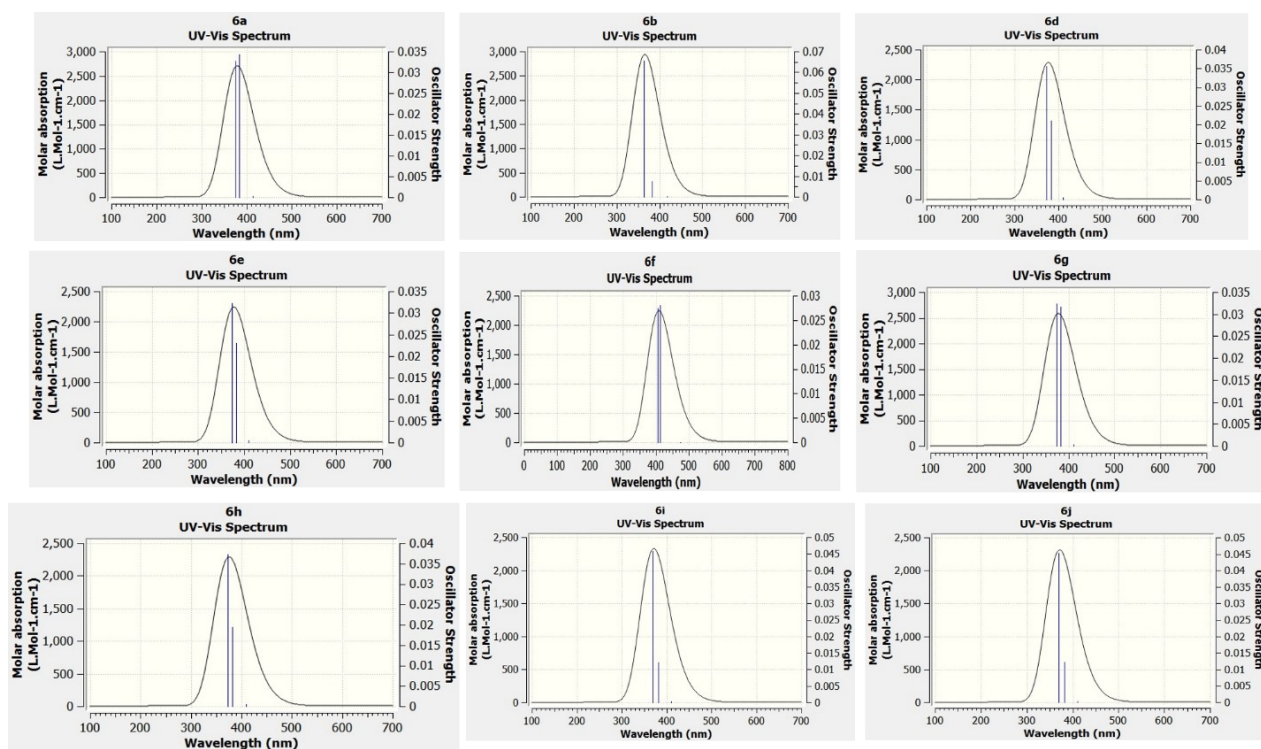
		<p>Excited state-3</p> <p style="text-align: center;"><b>H-3</b></p>  <p style="text-align: center;"><b>L</b></p> 
29	6am	<p>Excited state-1</p> <p style="text-align: center;"><b>H-1</b></p>  <p style="text-align: center;"><b>L</b></p>  <p>Excited state-2</p> <p style="text-align: center;"><b>H</b></p>  <p style="text-align: center;"><b>L</b></p> 

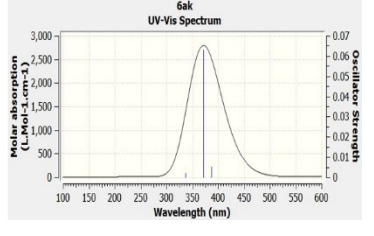
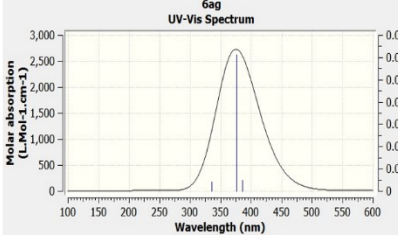
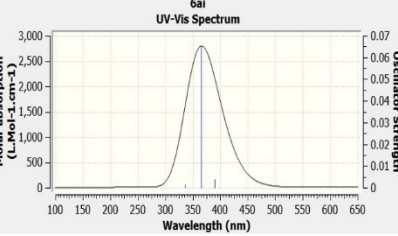
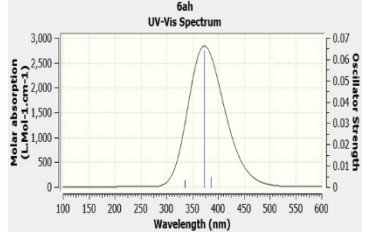
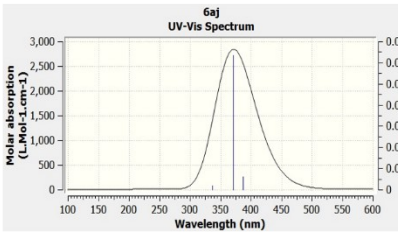
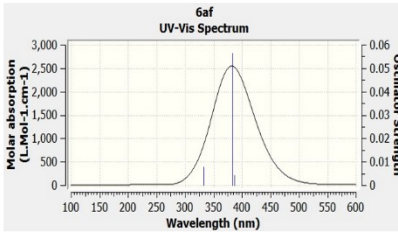
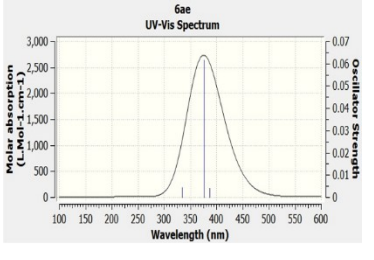
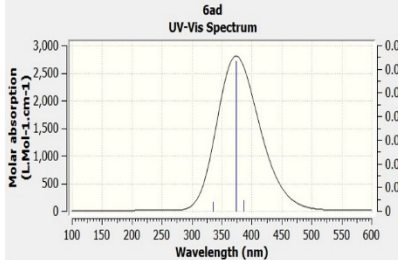
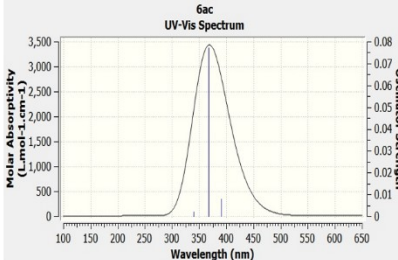
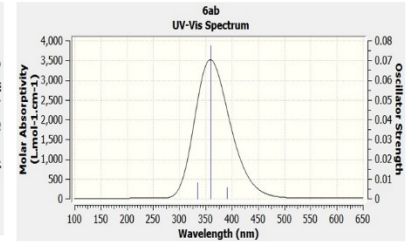
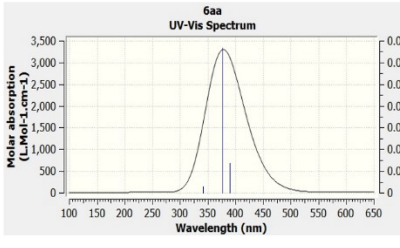
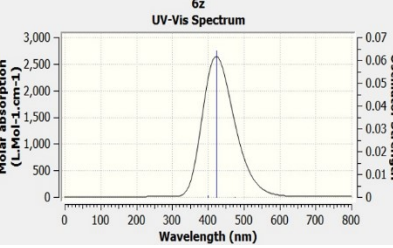
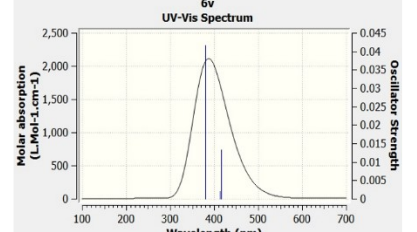
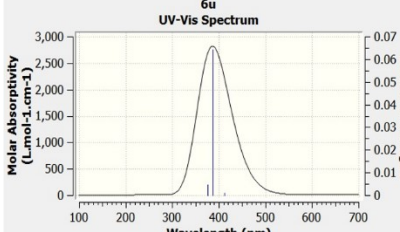
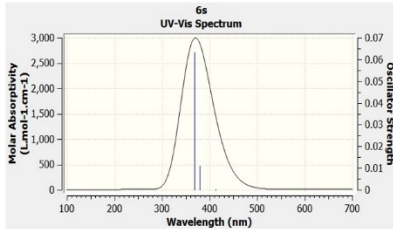
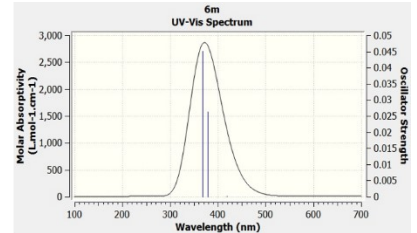
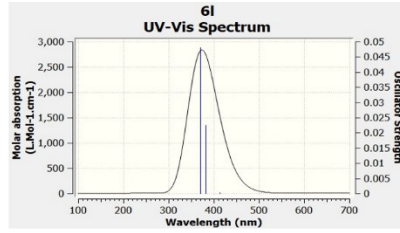
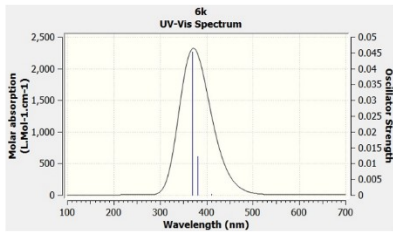


		<p>Excited state-3</p> <p><b>H-1</b></p>  <p><b>L</b></p> 
31	6ap	<p>Excited state-1</p> <p><b>H</b></p>  <p><b>L</b></p>  <p>Excited state-2</p> <p><b>H-2</b></p>  <p><b>L</b></p> 

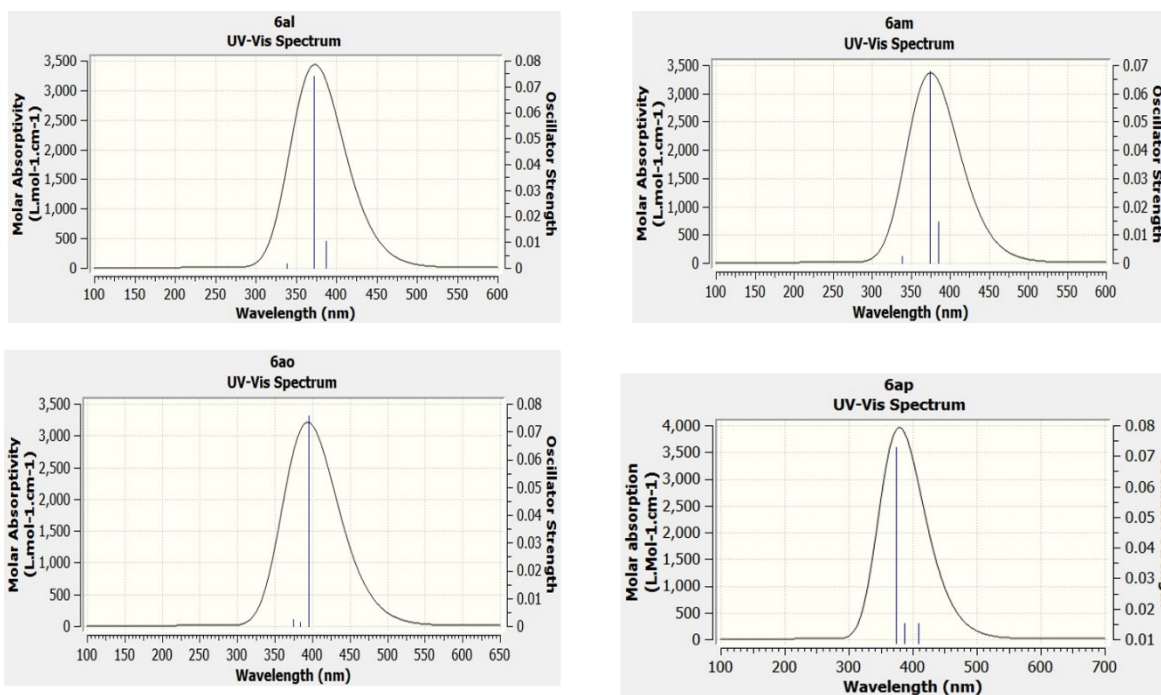


**Figure S9:** Theoretical UV-Vis spectra of compounds by TD-DFT at level using the the B3LYP/6-31G'(d,p).









## 5. Photophysical characteristics Study and Fluorescent Spectra.

The structural quinoline and extended  $\pi$  conjugation induced by the aromatic- system and amide functional group encouraged us to investigate the photophysical properties of compounds. Thus, absorption and emission spectra were recorded for 31 compound the compounds (fig 9(1) – 9(31)) in methanol. In the absorption spectra of compounds 31 compounds, a higher energy band in the range of 250 to 320 nm begins with  $\pi$ - $\pi^*$  electronic transition [intramolecular charge transfer (ICT)] and other bands with lower energy  $n$ - $\pi^*$  electronic transition in the region 320 to 380 nm were observed. The corresponding emission band was observed in the 410–520 nm region. In the emission spectra, it was observed that with the increase in the size of the aromatic ring connected by the pivotal bond to the quinoline core, the emission band has been shifted to higher wavelengths. All fluorescent spectra below Fig S9.1 to Fig S9.34.

All the compounds exhibited Absorbance, Emission and Stoke's shift values (Table 2, entries 1–31).

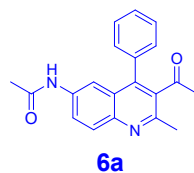
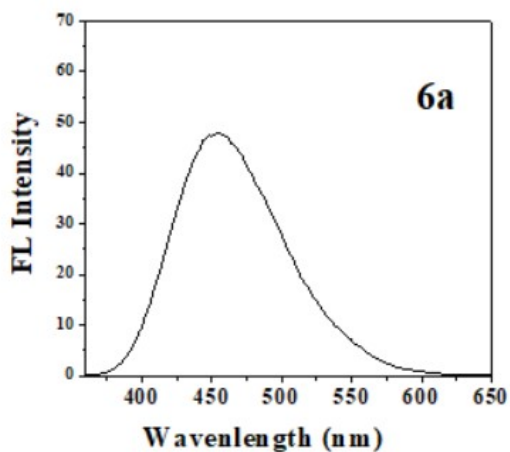
## Photophysical Data (Table – S3)

Entry	Compound code	$\lambda_{\text{Absorption}}$ (nm)	$\lambda_{\text{Emission}}$ (nm)	Stokes shift $\Delta \times 10^4$	Molar extinction Coefficient $\times 10^4$	Quantum Yield ( $\phi$ )
1	6a	341.12	455.19	0.7347		
2	6b	338.22	440.15	0.6858	6.2125	0.0020
3	6d	340.38	462.33	0.7766	4.6795	0.0014
4	6e	342.76	452.81	0.7116	5.1485	0.0019
5	6f	341.45	457.39	0.7444	5.0510	0.0022
6	6g	343.51	450.43	0.6932	3.0205	0.0057
7	6h	340.28	451.36	0.7239	5.3315	0.0020
8	6i	344.68	448.98	0.6748	4.8225	0.0037
9	6j	341.09	450.16	0.7103	4.2445	0.0038
10	6k	340.29	450.38	0.7189	4.8250	0.0015
11	6l	338.87	441.77	0.691	4.4505	0.0030
12	6m	337.12	446.06	0.7252	3.6155	0.0050
13	6s	352.83	452.8	0.6286	5.3030	0.0035
14	6u	352.63	434.54	0.5368	6.2180	0.0005
15	6v	347.33	450.28	0.5959	3.6155	0.00012
16	6z	309.18	457.29	1.0411	7.9805	0.0012
17	6aa	338.87	442.94	0.6961	6.4730	0.0013
18	6ab	372.65	501.58	0.6921	6.5455	0.0021
19	6ac	339.11	411.03	0.5168	5.3670	0.0171
20	6ad	342.78	417.73	0.5259	8.2825	0.0096
21	6ae	341.95	423.86	0.5685	8.3715	0.0103
22	6af	340.42	420.21	0.5602	7.1585	0.0156
23	6ag	342.67	420.73	0.543	8.3370	0.0110
24	6ah	340.22	418.34	0.5488	8.8605	0.0124
25	6ai	340.43	423.52	0.5771	9.5080	0.0062
26	6aj	339.17	422.27	0.5802	8.3370	0.0150
27	6ak	340.54	417.61	0.5431	7.9785	0.0188
28	6al	337.72	416.98	0.5635	9.0055	0.0179
29	6am	338.16	416.04	0.5547	8.1260	0.0053
30	6ao	370.32	502.67	0.7107	9.1775	0.0082
31	6ap	350.27	454.16	0.6545	6.9935	0.0154

### 4.1 Fluorescent Spectra

Fig S9.1 to S9.34

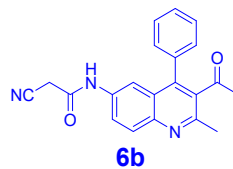
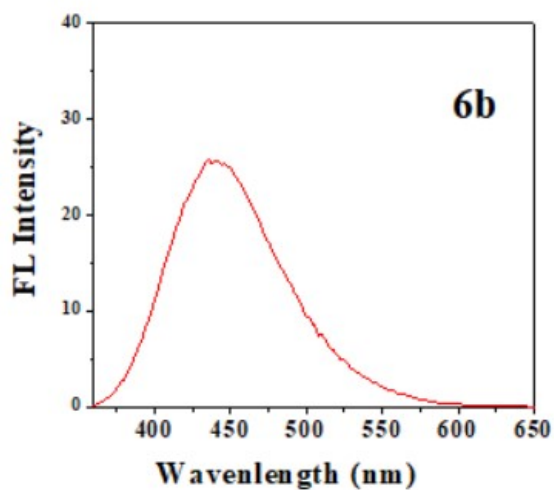
S9.1: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl) acetamide (6a).



10<sup>-5</sup> M solution in Methanol

- Maximum absorption: 341 nm
- Maximum emission: 455 nm
- Stokes Shift: 0.7347×10<sup>-4</sup>

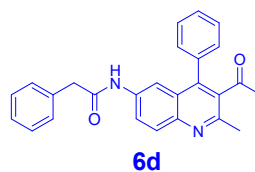
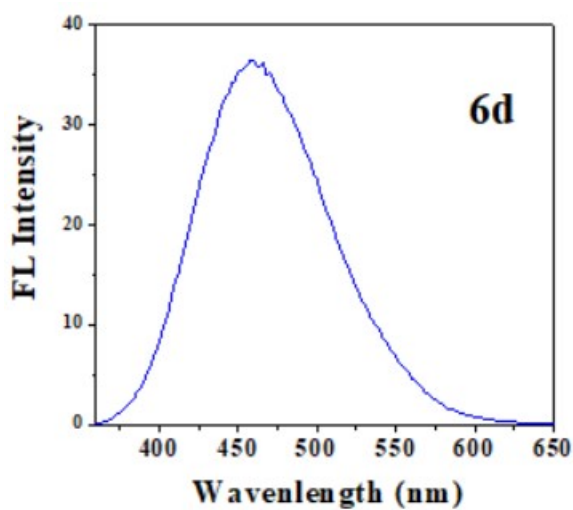
### S9.2 (3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).



10<sup>-5</sup> M solution in Methanol

- Maximum absorption: 338 nm
- Maximum emission: 440 nm
- Stokes Shift: 0.6858×10<sup>-4</sup>

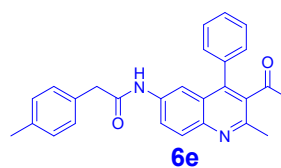
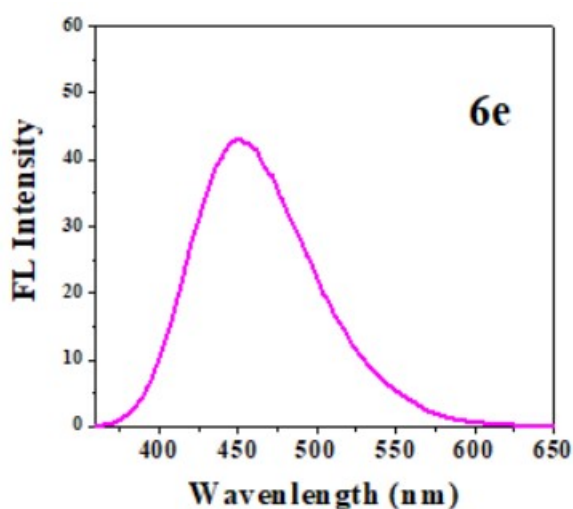
### S9.3: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).



10<sup>-5</sup> M solution in Methanol

- Maximum absorption: 340 nm
- Maximum emission: 462 nm
- Stokes Shift: 0.7766×10<sup>-4</sup>

S9.4: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl) acetamide (6e).



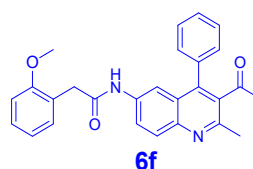
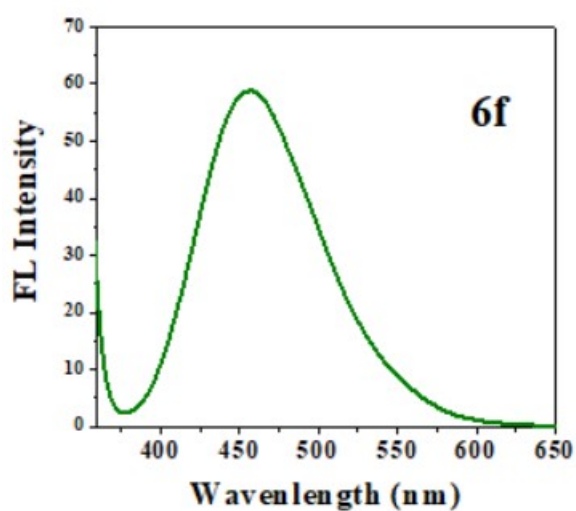
$10^{-5}$  M solution in Methanol

Maximum absorption: 342 nm

Maximum emission: 452 nm

Stokes Shift: $0.7116 \times 10^{-4}$

S9.5: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl) acetamide (6f).



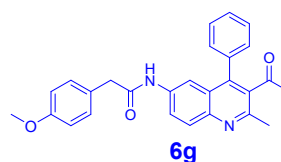
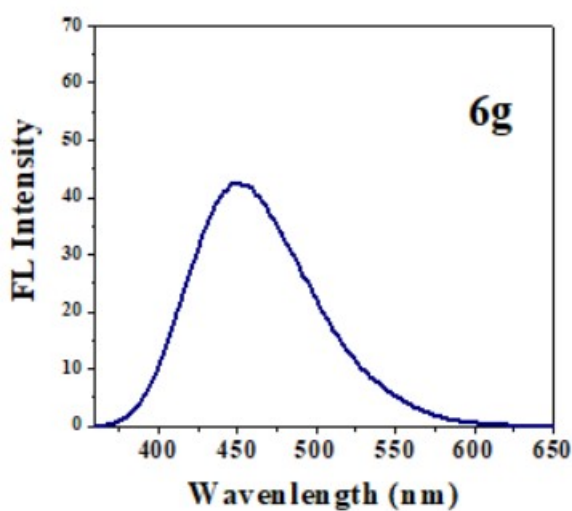
$10^{-5}$  M solution in Methanol

Maximum absorption: 341 nm

Maximum emission: 457 nm

Stokes Shift: $0.7444 \times 10^{-4}$

S9. 6: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl) acetamide (6g).



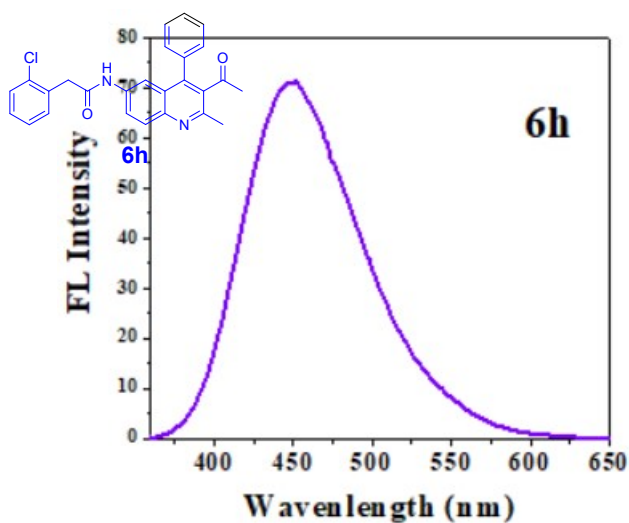
$10^{-5}$  M solution in Methanol

➤ Maximum absorption: 343 nm

➤ Maximum emission: 450 nm

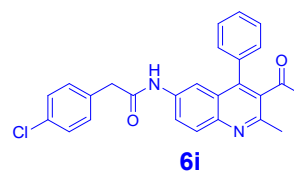
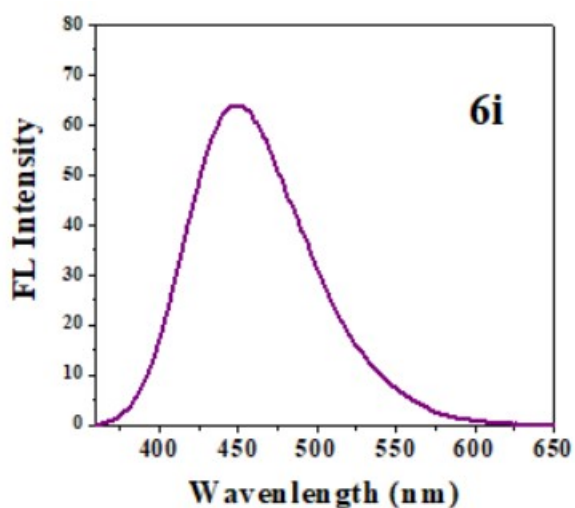
➤ Stokes Shift: $0.6932 \times 10^{-4}$

**S9.7: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl) acetamide (6h).**



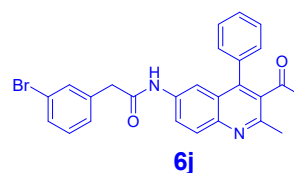
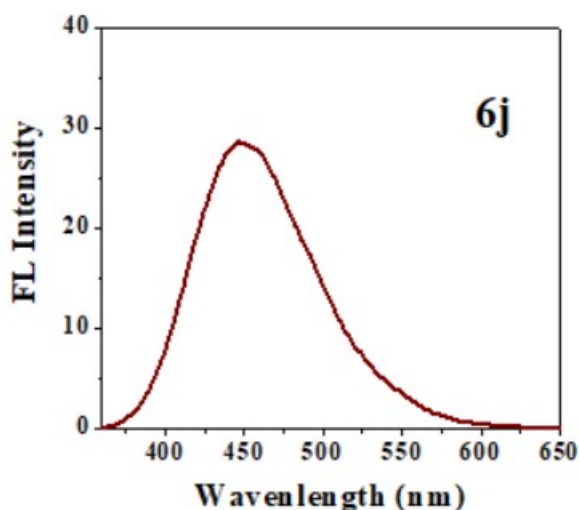
- $10^{-5}$  M solution in Methanol
- Maximum absorption: 340 nm
- Maximum emission: 451 nm
- Stokes Shift:  $0.7239 \times 10^{-4}$

**S9.8: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl) acetamide (6i).**



- $10^{-5}$  M solution in Methanol
- Maximum absorption: 344 nm
- Maximum emission: 448 nm
- Stokes Shift:  $0.6748 \times 10^{-4}$

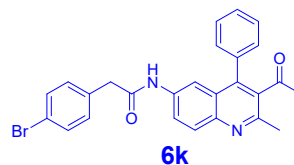
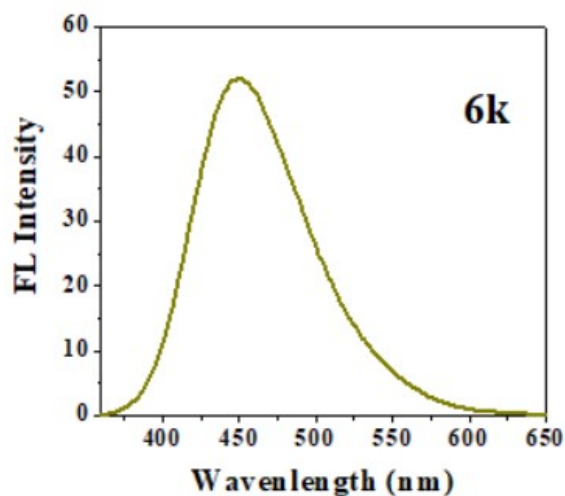
**S9.9: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl) acetamide (6j).**



- $10^{-5}$  M solution in Methanol
- Maximum absorption: 341 nm
- Maximum emission: 450 nm

➤ Stokes Shift:  $0.7103 \times 10^{-4}$

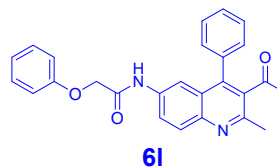
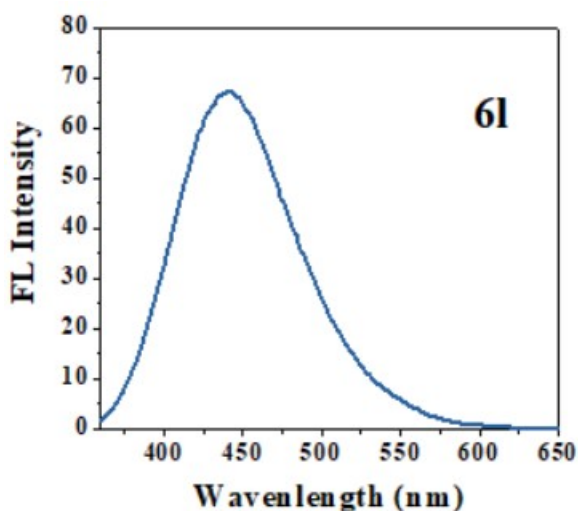
**S9.10: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-bromophenyl) acetamide (6k).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 340 nm
- Maximum emission: 450 nm
- Stokes Shift:  $0.7189 \times 10^{-4}$

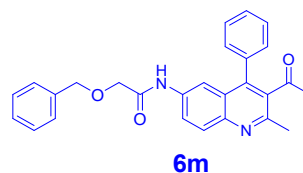
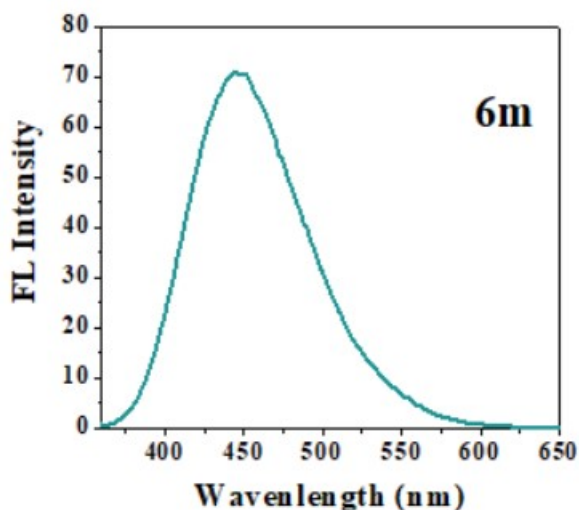
**S9.11: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxy acetamide (6l).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 338 nm
- Maximum emission: 441 nm
- Stokes Shift:  $0.6910 \times 10^{-4}$

**S9.12: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy) acetamide (6m)**

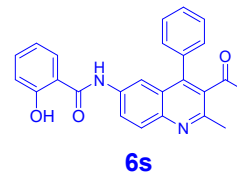
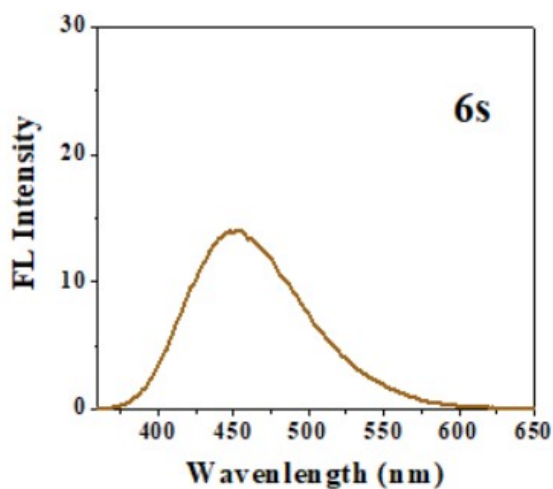


$10^{-5}$  M solution in Methanol

- Maximum absorption: 337 nm
- Maximum emission: 446 nm

➤ Stokes Shift:  $0.7252 \times 10^{-4}$

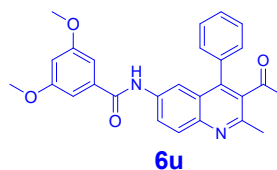
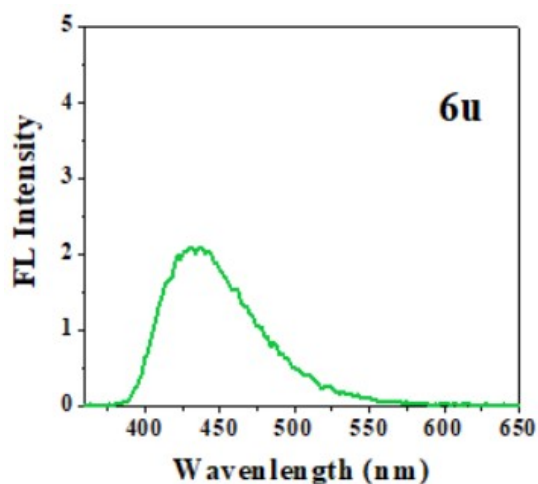
**S9.13: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 352 nm
- Maximum emission: 452 nm
- Stokes Shift:  $0.6286 \times 10^{-4}$

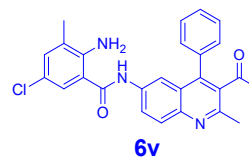
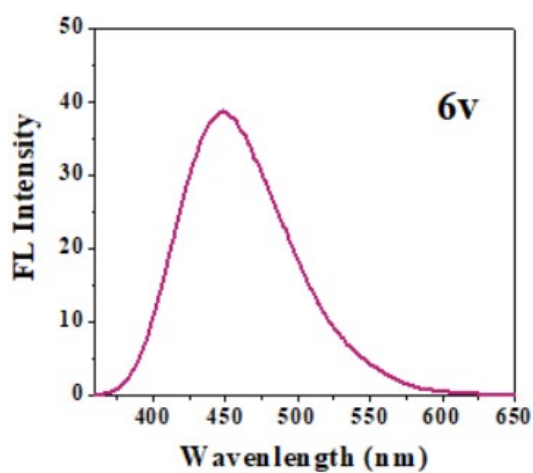
**S9.14: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 352 nm
- Maximum emission: 434 nm
- Stokes Shift:  $0.5368 \times 10^{-4}$

**S9.15: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).**



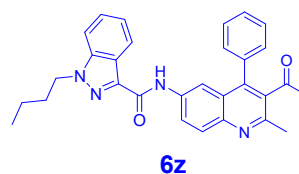
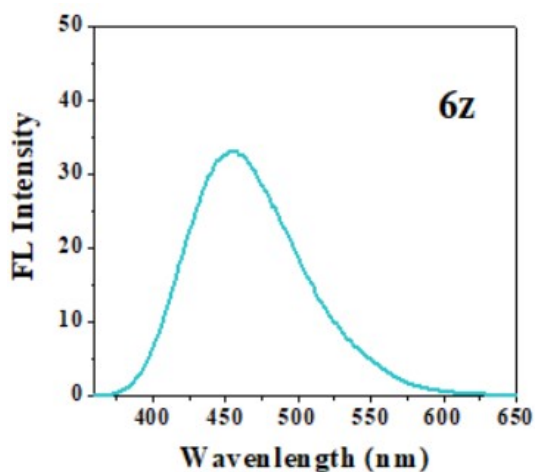
$10^{-5}$  M solution in Methanol

- Maximum absorption: 347 nm

- Maximum emission: 450 nm
- Stokes Shift:  $0.5929 \times 10^{-4}$

**S9.16: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-1-butyl-1H-indazole-3-carboxamide**

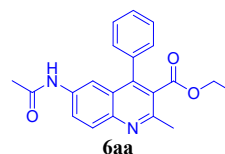
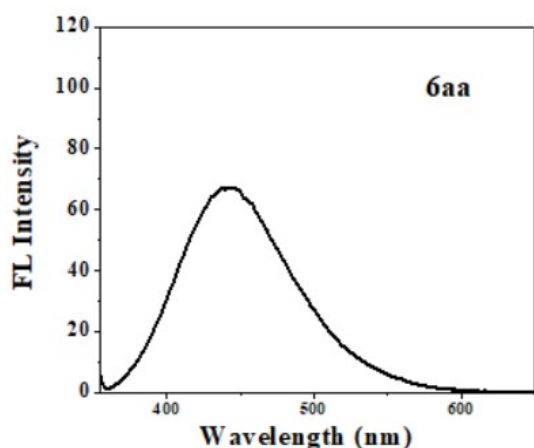
(6z).



$10^{-5}$  M solution in Methanol

- Maximum absorption: 309 nm
- Maximum emission: 457 nm
- Stokes Shift:  $1.0481 \times 10^{-4}$

**S9.17: Ethyl 6-acetamido-2-methyl-4-phenylquinoline-3-carboxylate (6aa).**

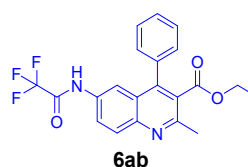
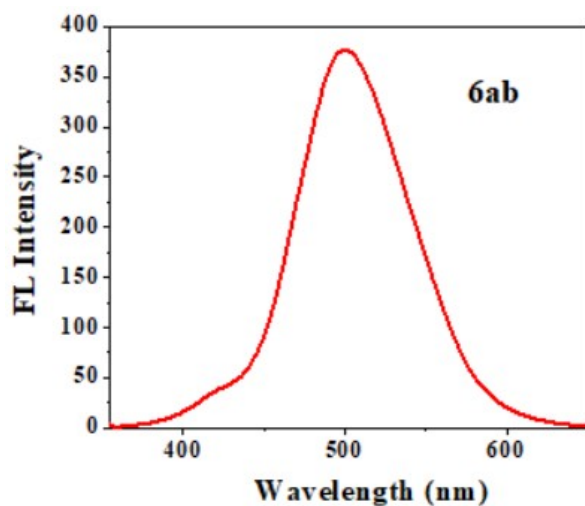


$10^{-5}$  M solution in Methanol

- Maximum absorption: 338 nm
- Maximum emission: 442 nm
- Stokes Shift:  $0.6961 \times 10^{-4}$

**S9.18: Ethyl 2-methyl-4-phenyl-6-(2,2,2-trifluoroacetamido) quinoline-3-carboxylate**

(6ab).

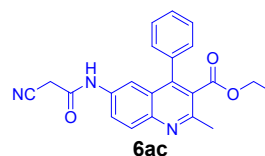
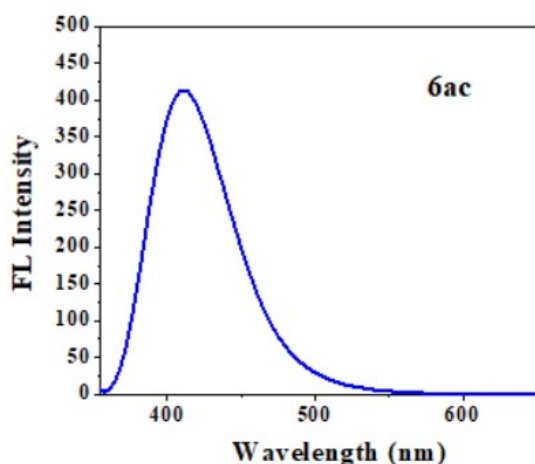


$10^{-5}$  M solution in Methanol



- Maximum absorption: 372 nm
- Maximum emission: 501 nm
- Stokes Shift:  $0.6921 \times 10^{-4}$

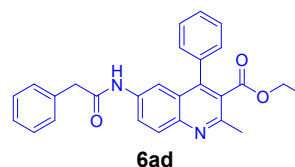
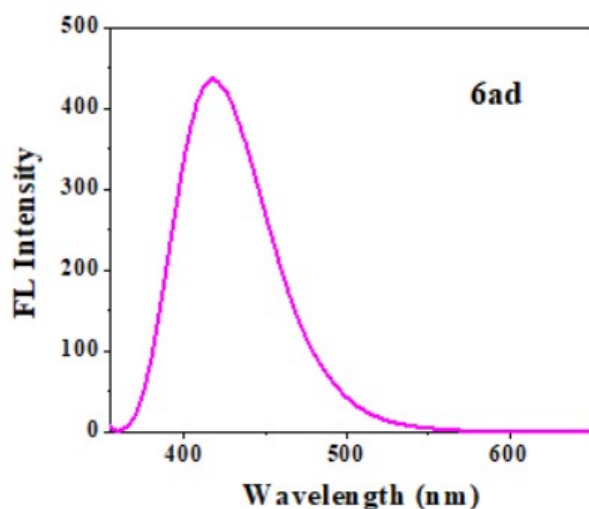
**S9.19: Ethyl 6-(2-cyanoacetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ac).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 339 nm
- Maximum emission: 411 nm
- Stokes Shift:  $0.5168 \times 10^{-4}$

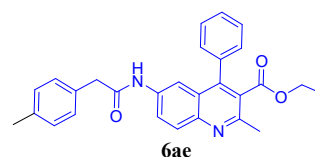
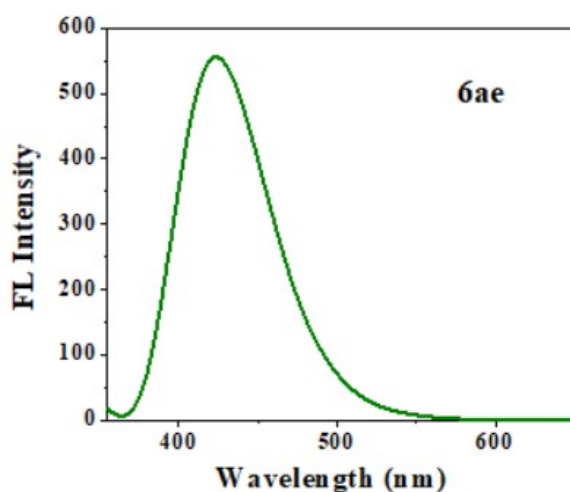
**S9.20: Ethyl 2-methyl-4-phenyl-6-(2-phenylacetamido) quinoline-3-carboxylate (6ad).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 342 nm
- Maximum emission: 417 nm
- Stokes Shift:  $0.5259 \times 10^{-4}$

**S9.21: Ethyl 2-methyl-4-phenyl-6-(2-(p-tolyl) acetamido) quinoline-3-carboxylate (6ae).**



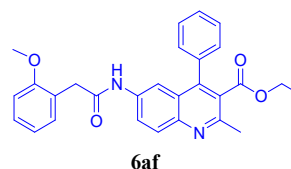
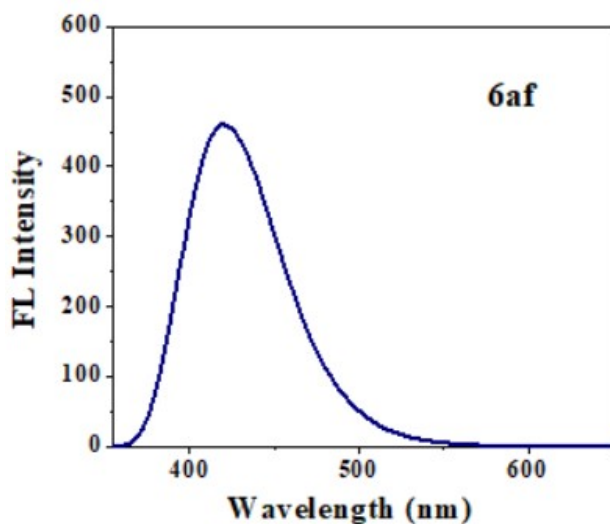
$10^{-5}$  M solution in Methanol

- Maximum absorption: 341 nm
- Maximum emission: 423 nm

- Stokes Shift:  $0.5685 \times 10^{-4}$

**S9.22: Ethyl 6-(2-(2-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate**

(6af).

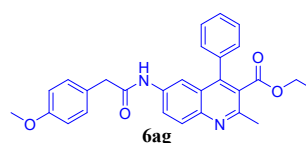
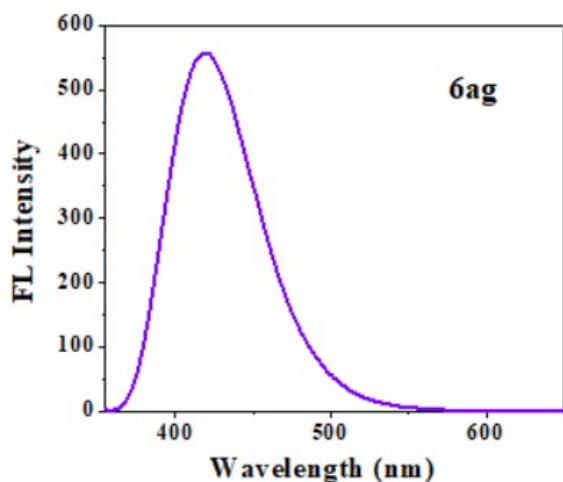


$10^{-5}$  M solution in Methanol

- Maximum absorption: 340 nm
- Maximum emission: 420 nm
- Stokes Shift:  $0.5602 \times 10^{-4}$

**S9.23: Ethyl 6-(2-(4-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate**

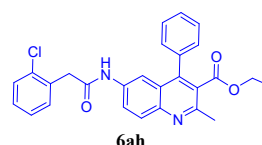
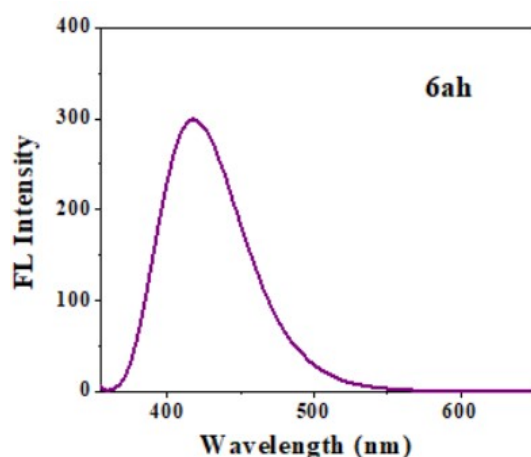
(6ag).



$10^{-5}$  M solution in Methanol

- Maximum absorption: 342 nm
- Maximum emission: 420 nm
- Stokes Shift:  $0.5430 \times 10^{-4}$

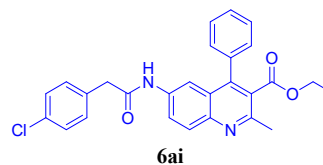
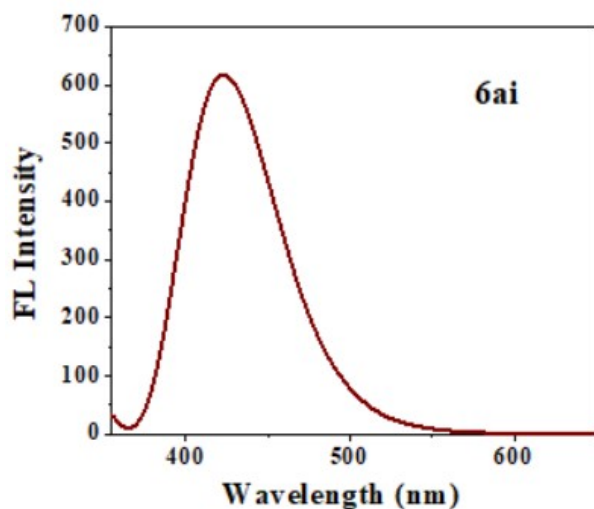
**S9.24: Ethyl 6-(2-(2-chlorophenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ah).**



$10^{-5}$  M solution in Methanol

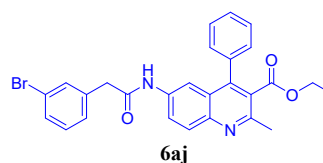
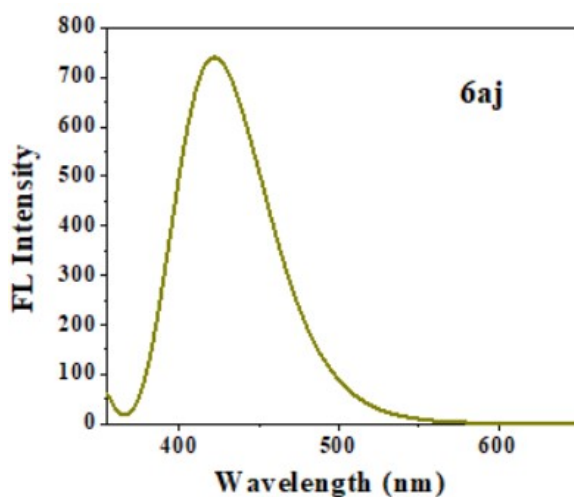
- Maximum absorption: 340 nm
- Maximum emission: 418 nm
- Stokes Shift:  $0.5488 \times 10^{-4}$

**S9.25: Ethyl 6-(2-(4-chlorophenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ai).**



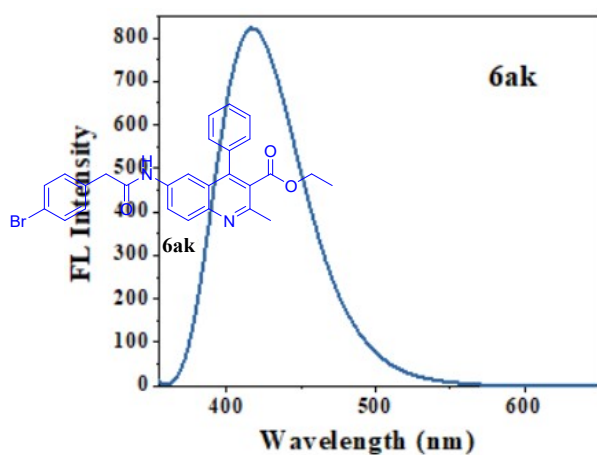
- 10<sup>-5</sup> M solution in Methanol
- Maximum absorption: 340 nm
  - Maximum emission: 423 nm
  - Stokes Shift: 0.5771 × 10<sup>-4</sup>

**S9.26: Ethyl 6-(2-(3-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aj).**



- 10<sup>-5</sup> M solution in Methanol
- Maximum absorption: 339 nm
  - Maximum emission: 423 nm
  - Stokes Shift: 0.5802 × 10<sup>-4</sup>

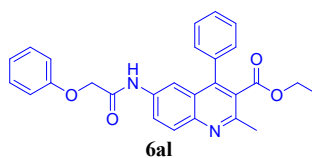
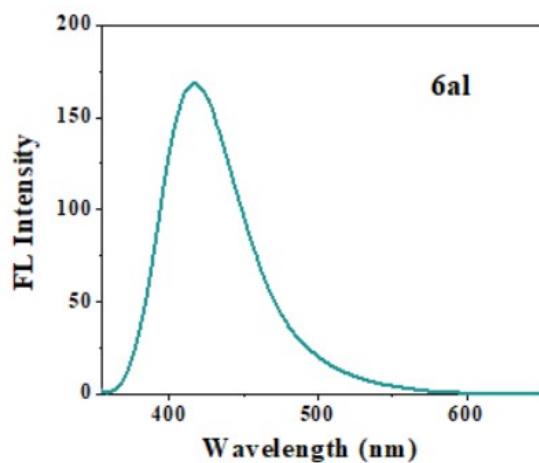
**S9.27: Ethyl 6-(2-(4-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ak)**



- 10<sup>-5</sup> M solution in Methanol
- Maximum absorption: 340 nm

- Maximum emission: 417 nm
- Stokes Shift:  $0.5439 \times 10^{-4}$

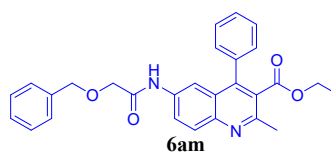
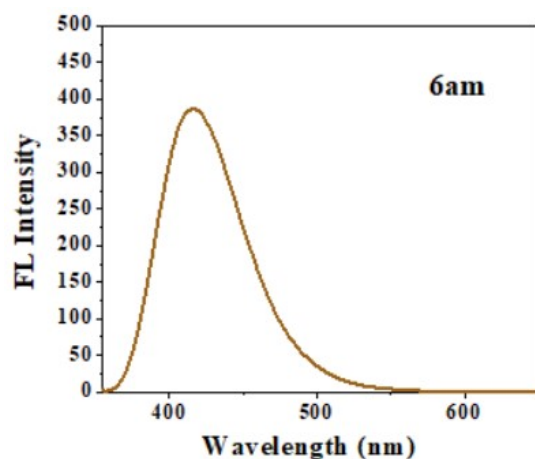
**S9.28: Ethyl 2-methyl-6-(2-phenoxyacetamido)-4-phenylquinoline-3-carboxylate (6al).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 337 nm
- Maximum emission: 416 nm
- Stokes Shift:  $0.5635 \times 10^{-4}$

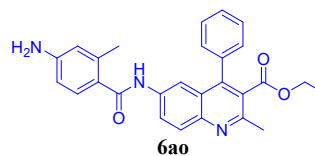
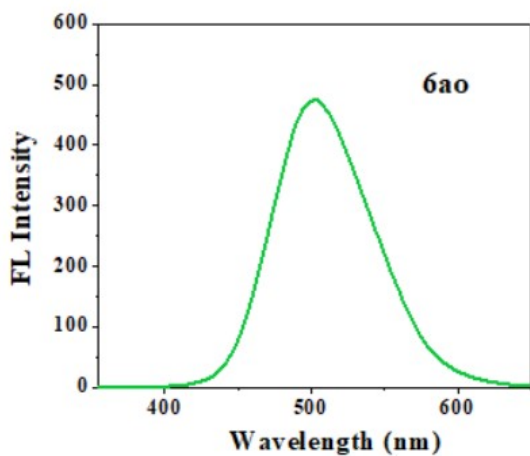
**S9.29: Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).**



$10^{-5}$  M solution in Methanol

- Maximum absorption: 338 nm
- Maximum emission: 416 nm
- Stokes Shift:  $0.5547 \times 10^{-4}$

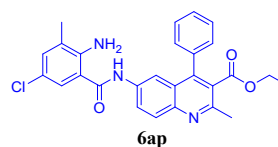
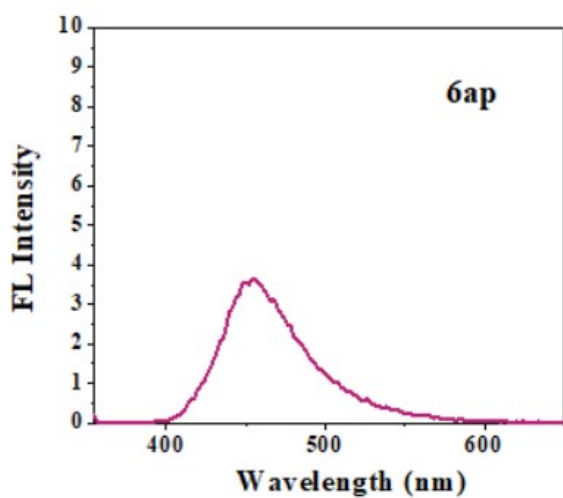
**S9.30: Ethyl 6-(4-amino-2-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ao).**



10<sup>-5</sup> M solution in Methanol

- Maximum absorption: 370 nm
- Maximum emission: 502 nm
- Stokes Shift: 0.7107 × 10<sup>-4</sup>

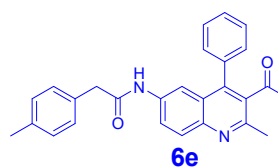
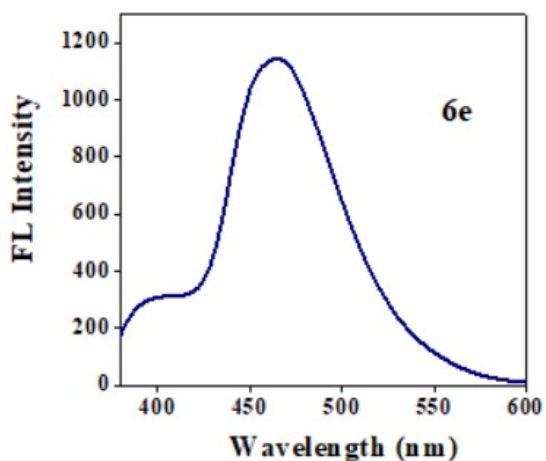
**S9.31: Ethyl 6-(2-amino-5-chloro-3-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ap).**



10<sup>-5</sup> M solution in Methanol

- Maximum absorption: 350 nm
- Maximum emission: 454 nm
- Stokes Shift: 0.6545 × 10<sup>-4</sup>

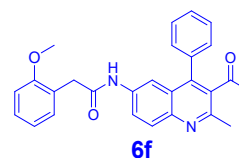
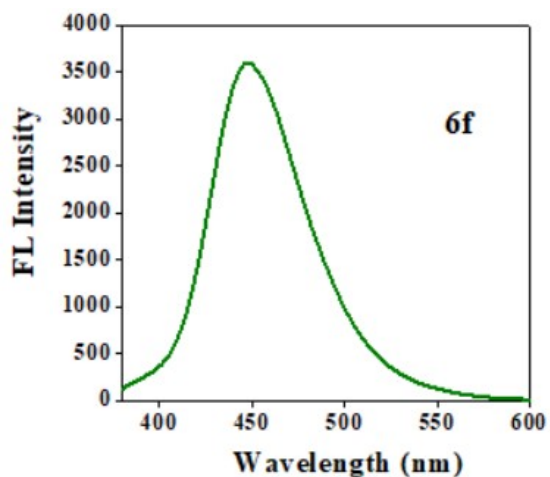
S9.32: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl) acetamide (6e).



**Solid State**

- Maximum absorption: 360 nm
- Maximum emission: 464 nm
- Stokes Shift:  $0.6226 \times 10^{-4}$

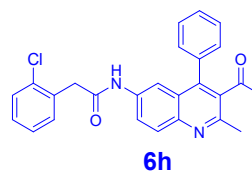
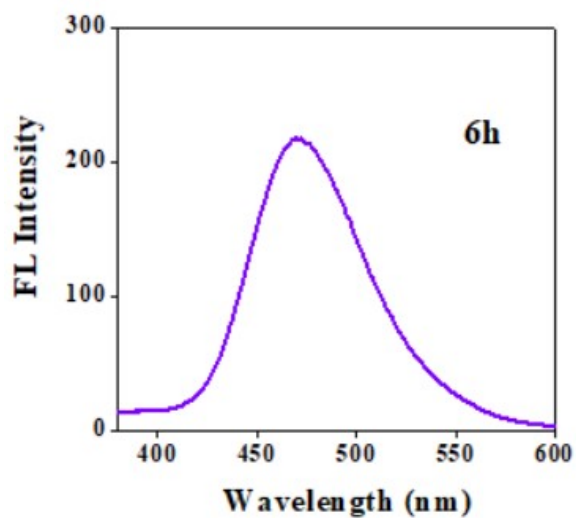
S9.33: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl) acetamide (6f).



**Solid State**

- Maximum absorption: 363 nm
- Maximum emission: 448 nm
- Stokes Shift:  $0.5226 \times 10^{-4}$

S9.34: N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl) acetamide (6h).



**Solid State**

- Maximum absorption: 347 nm
- Maximum emission: 471 nm
- Stokes Shift:  $0.7587 \times 10^{-4}$



VM-029

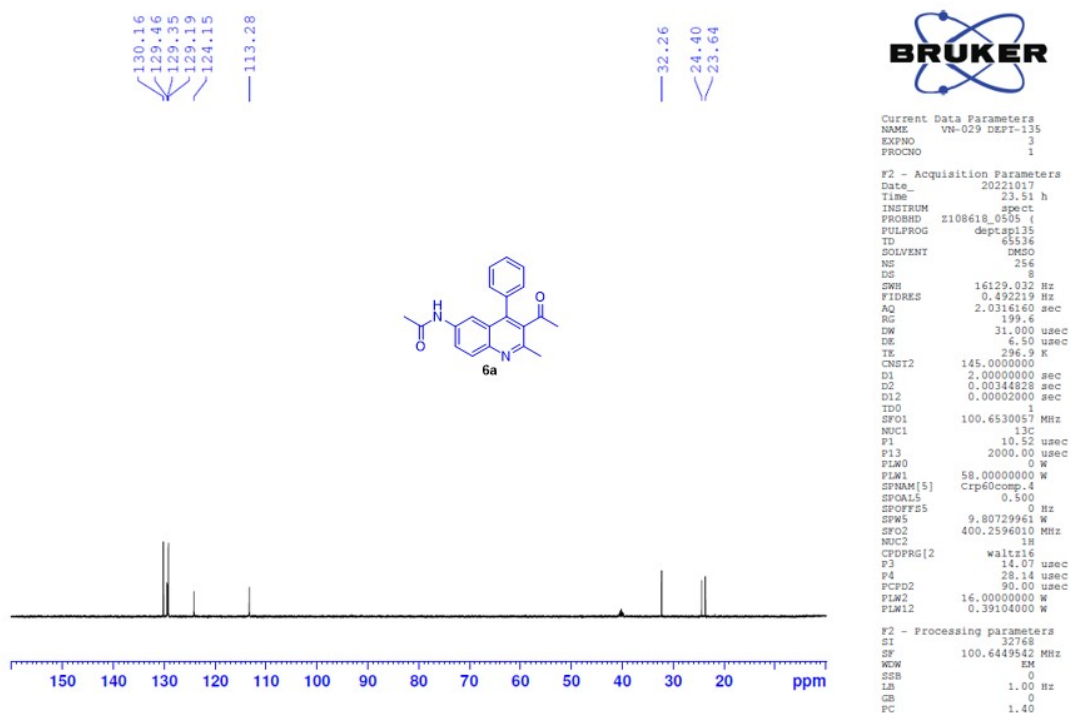


Fig.S12 DEPT-DEPT-135 of NMR of N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).

Signature SIF VIT VELLORE  
 VN-029

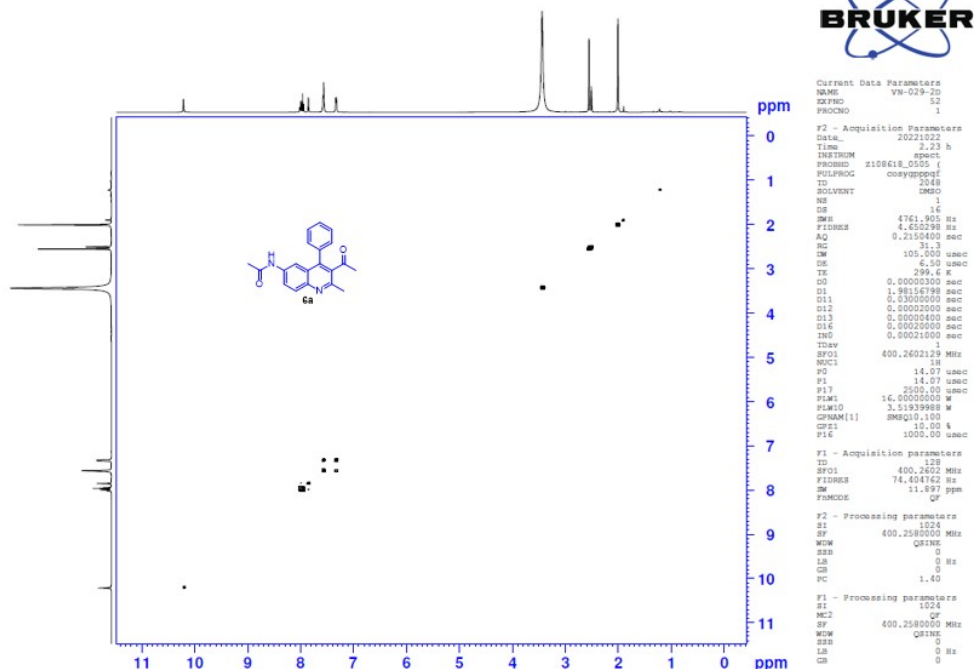


Fig.S13 H-H COSY NMR of N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).



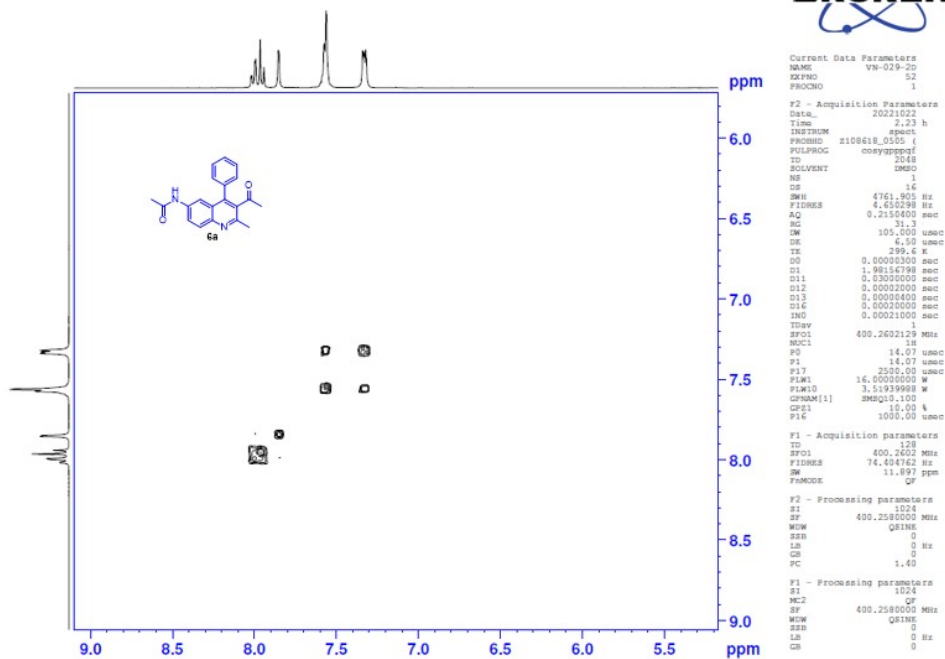


Fig.S14 Enlarged H-H COSY NMR of N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).

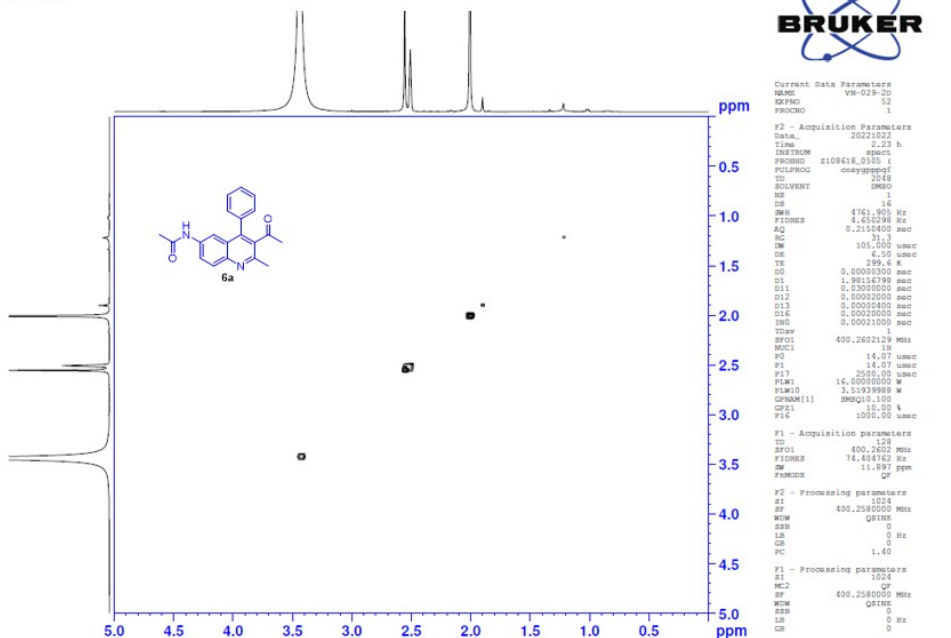


Fig.S15 Enlarged H-H COSY NMR of N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).



Signature SIF VIT VELLORE  
VN-029

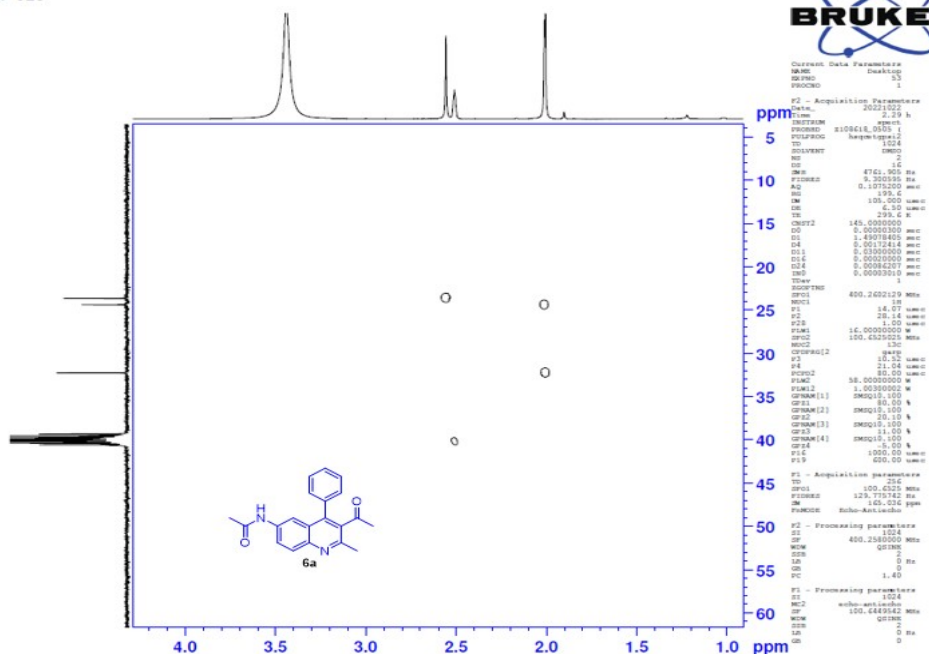


Fig.S18 Enlarged HSQC NMR of N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).

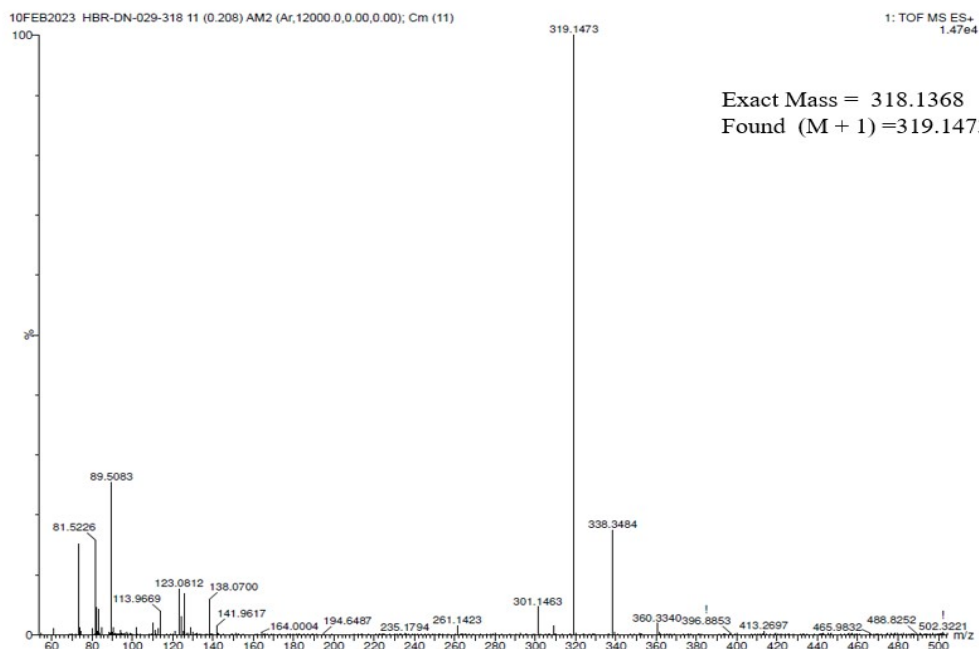
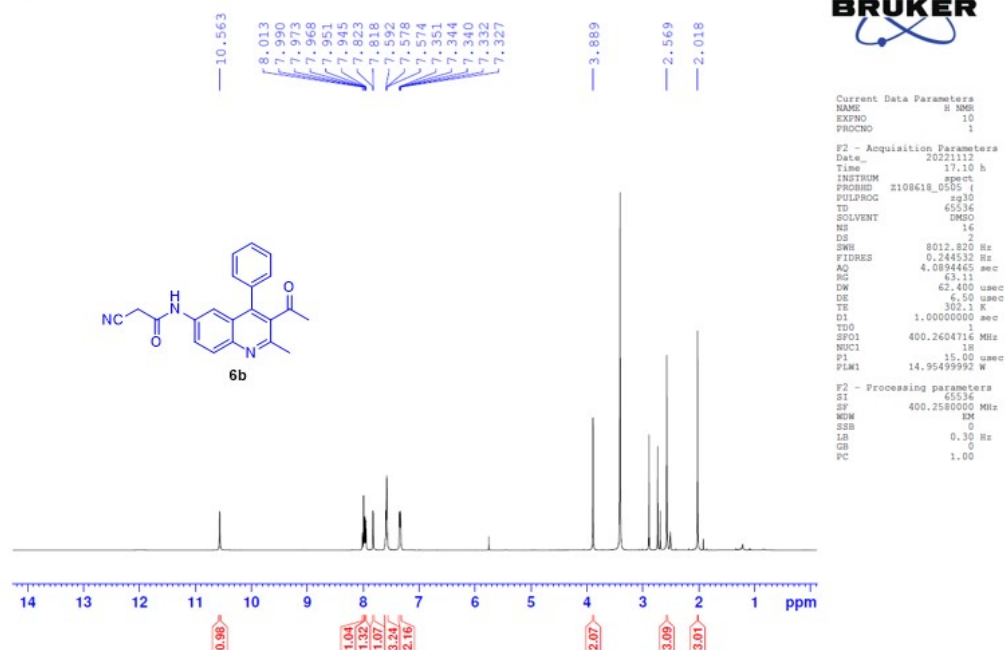
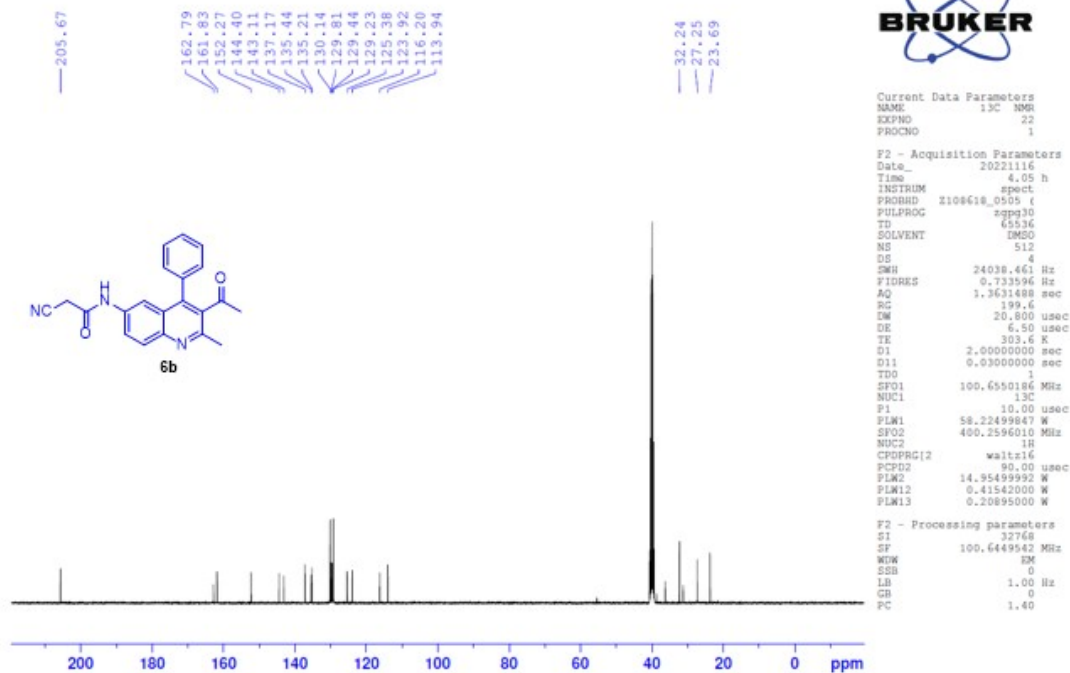


Fig.S19 HRMS of N-(3-Acetyl-2-methyl-4-phenylquinolin-6-yl)acetamide (6a).

VN-037

Fig.S20 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (**6b**).Signature SIF VIT VELLORE  
VN-037Fig.S21 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (**6b**).

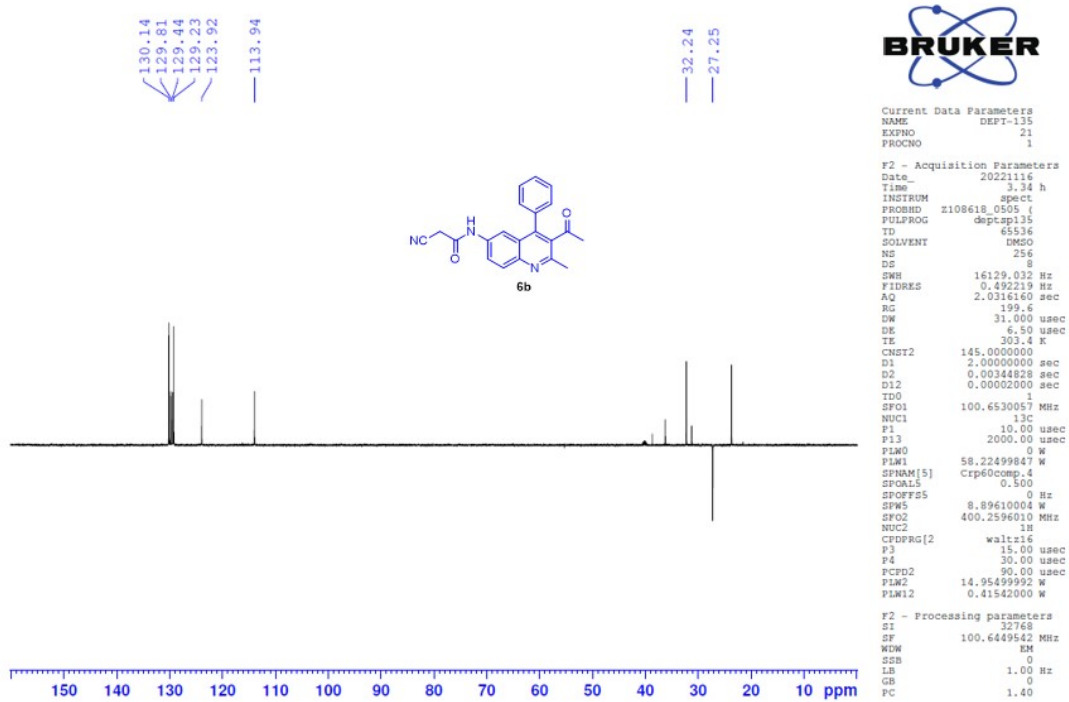


Fig.S22 DEPT-135 NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).

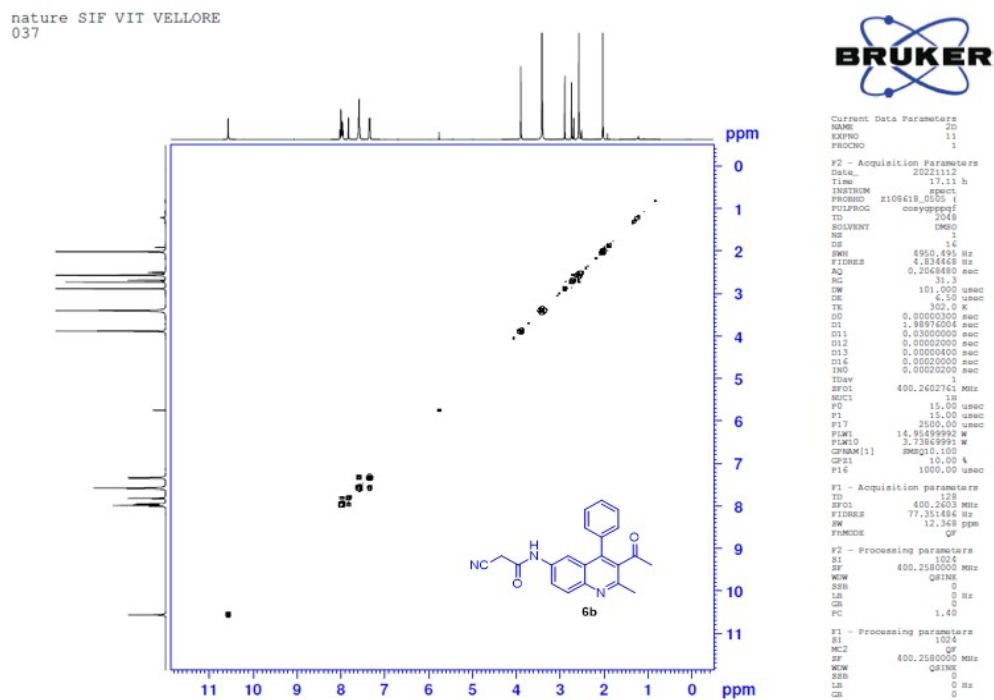


Fig.S23 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).

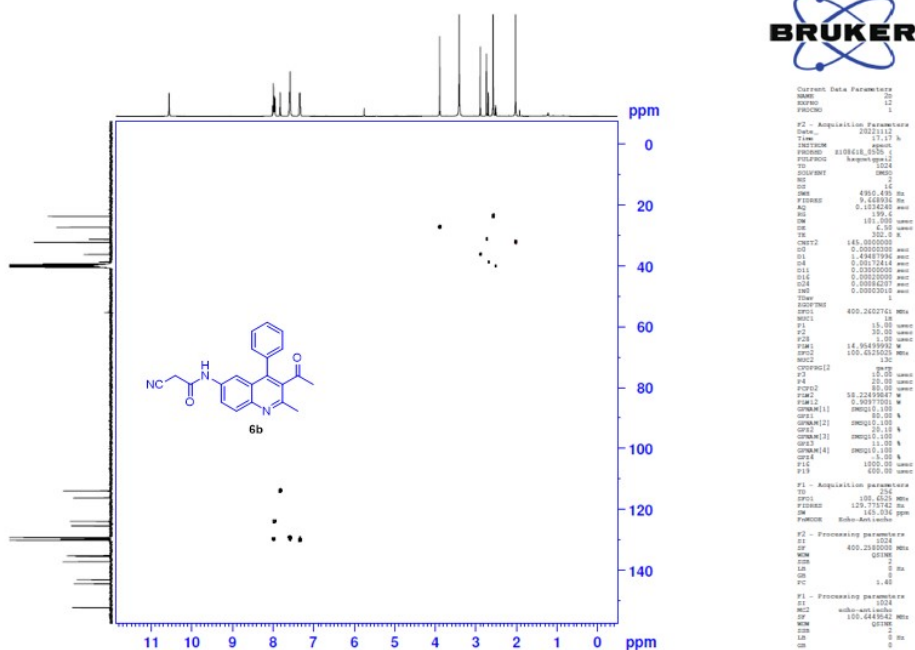


Fig.S24 HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).

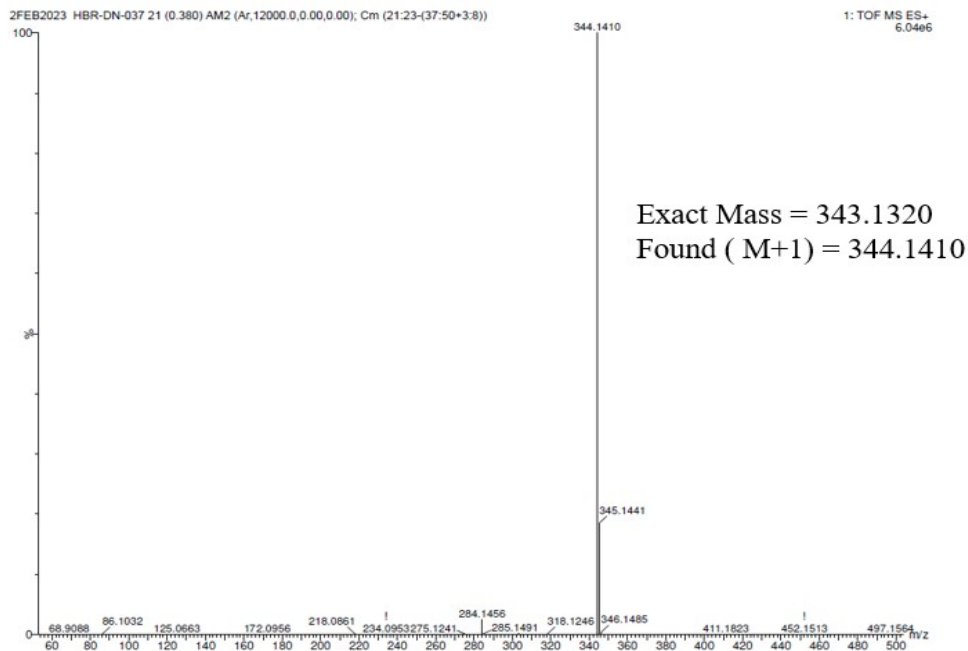


Fig.S25 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).

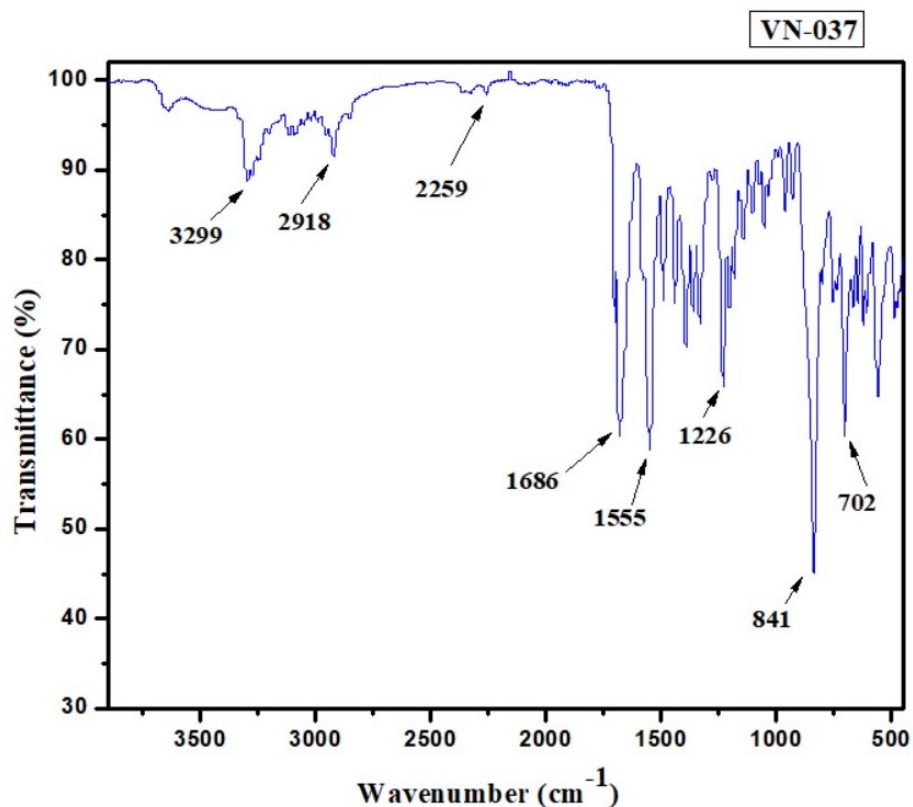


Fig.S26 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-cyanoacetamide (6b).

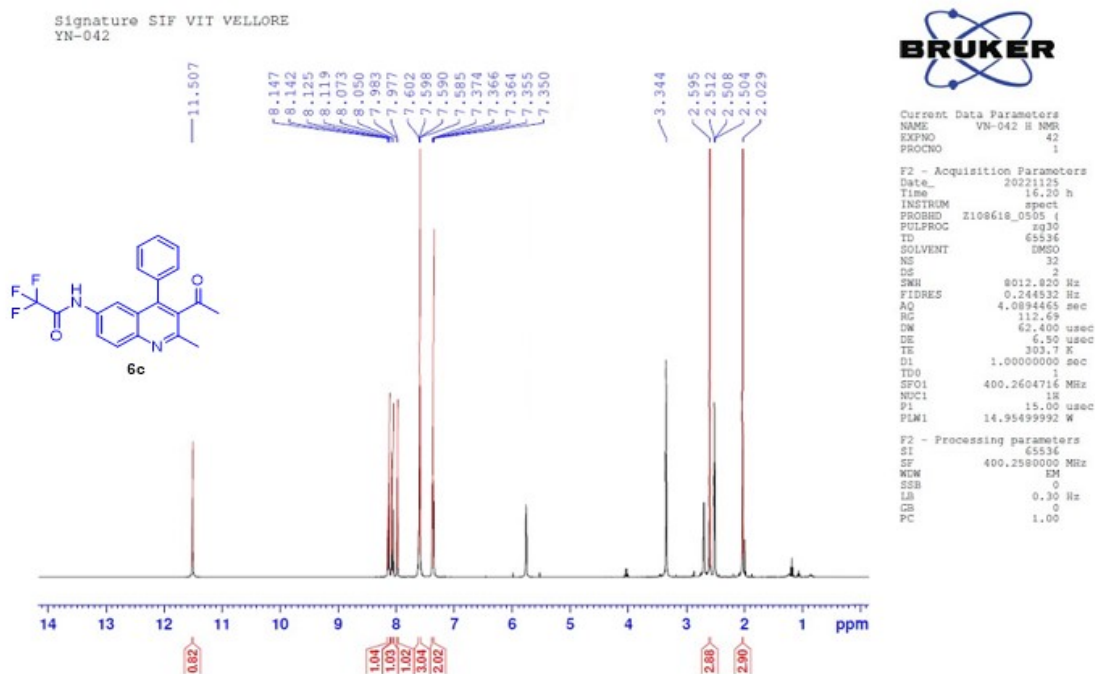
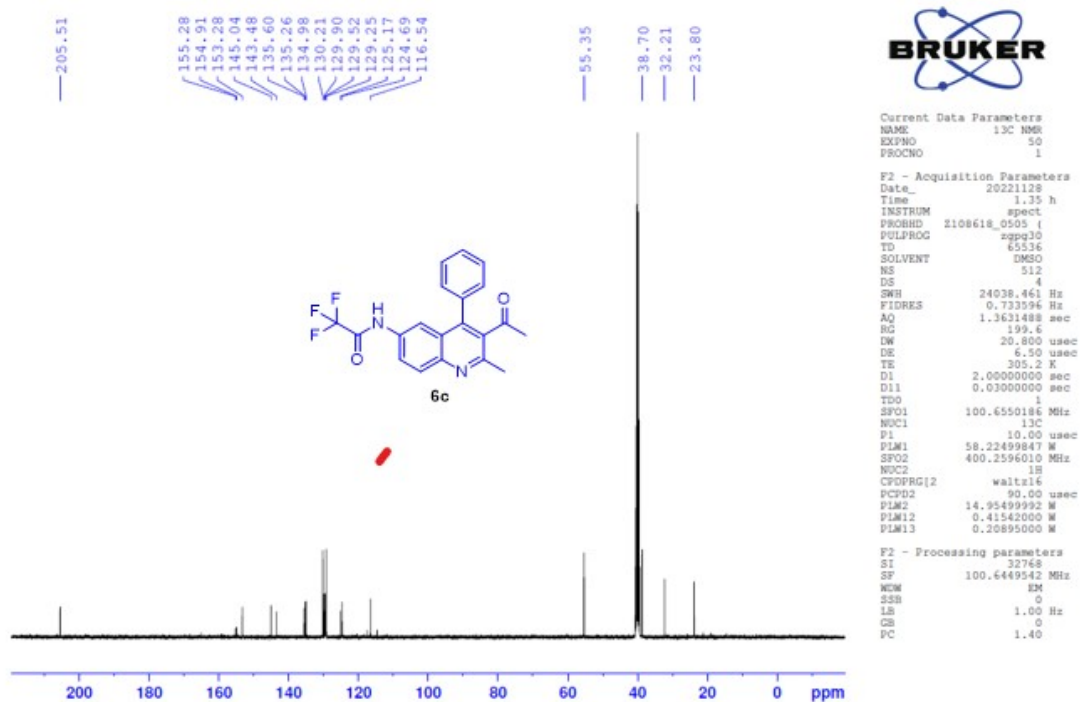
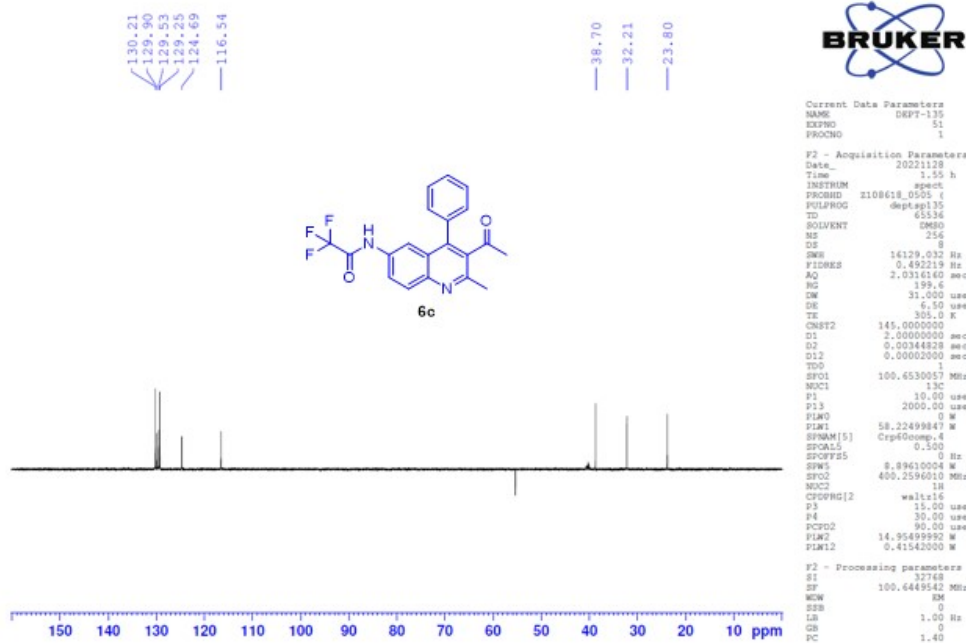


Fig.S27  $^1\text{H}$  NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (6c).

YN-042

Fig.S28 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (**6c**).

YN-042

Fig.S29 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (**6c**).



Signature SIF VIT VELLORE  
YN-042

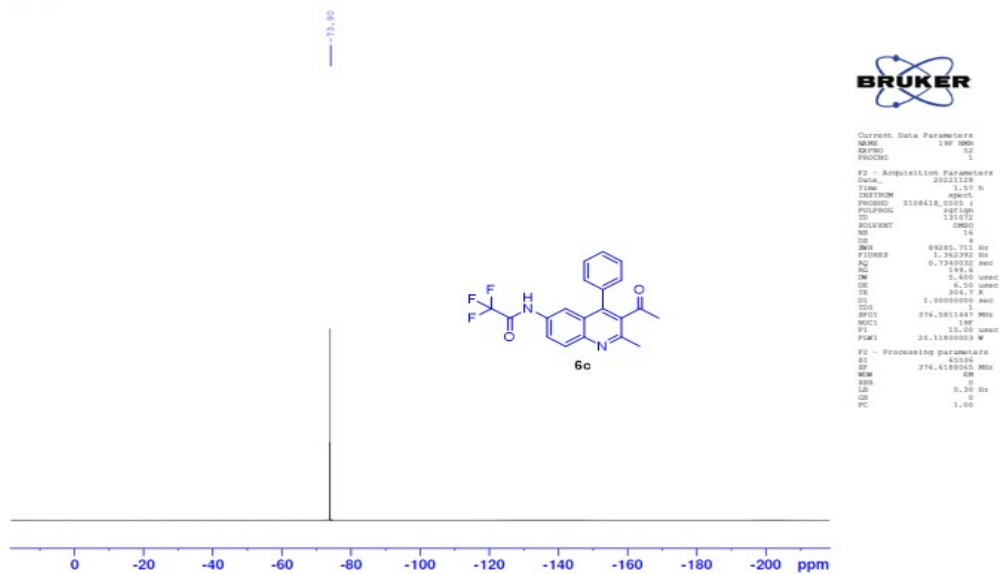


Fig.S30 <sup>19</sup>F NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (6c).

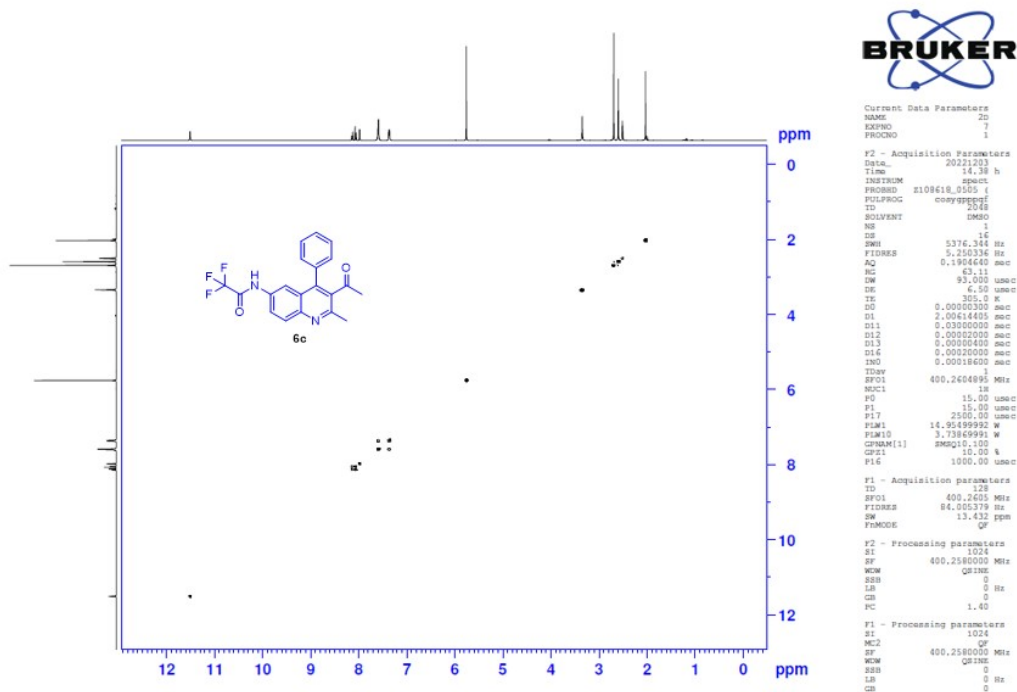


Fig.S31 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (6c).

Signature SIF VIT VELLORE  
VN-042

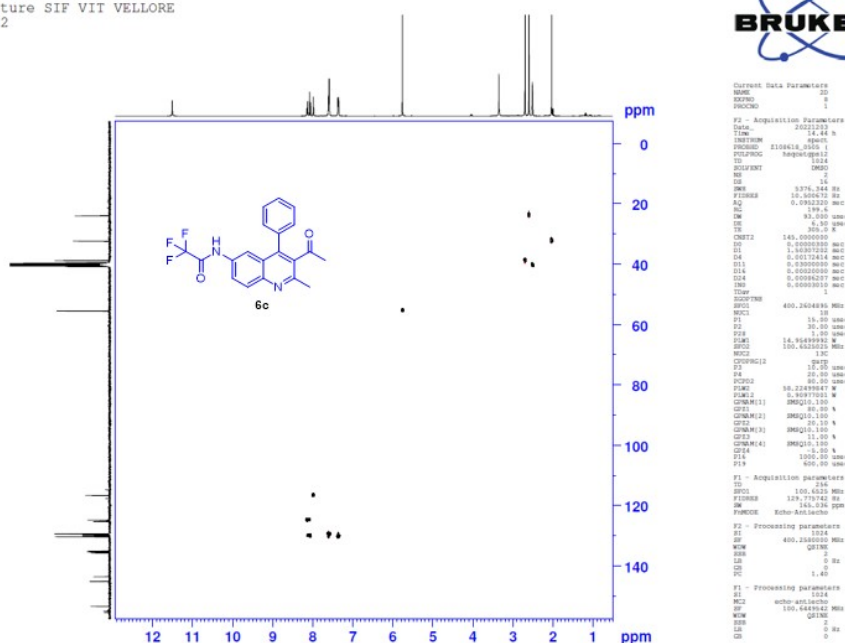


Fig.S32 HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (6c).

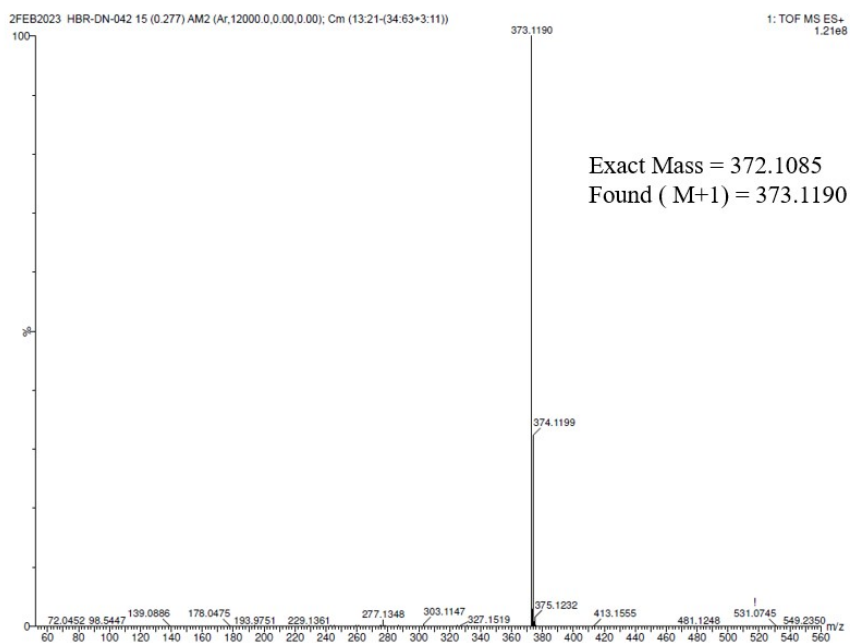
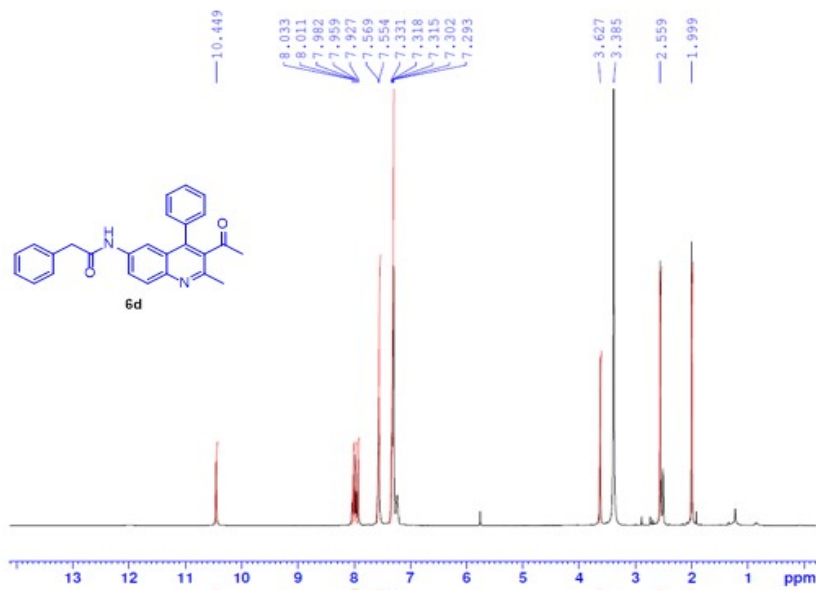


Fig.S33 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,2,2-trifluoroacetamide (6c).

Signature SIF VIL VELLORE  
VN-084



```

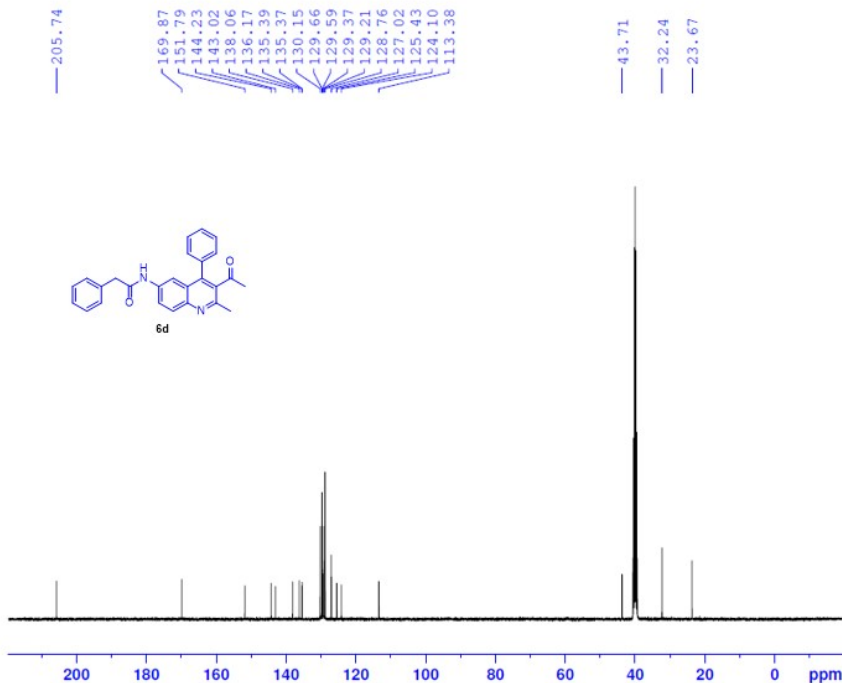
Current Data Parameters
NAME      034 H NMR
EXPNO     9
PROCNO    1

F2 - Acquisition Parameters
Date_     20221112
Time      12.23 h
INSTRUM   spect
PROBHD    Z108618_0505
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         32
DS         2
SWH        8015.820 Hz
FIDRES     0.244533 Hz
AQ         4.0894465 sec
RG         79.73
DM         62.400 usec
DE         6.50 usec
TE         302.4 K
D1         1.0000000 sec
TDO        400.2604714 MHz
SFO1       400.1463700 MHz
NUC1       1H
P1          15.00 usec
PLW1       14.95499992 W

F2 - Processing parameters
SI          65536
SF          400.2580000 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
  
```

Fig.S34 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).

VN-034



```

Current Data Parameters
NAME      Desktop
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20230504
Time      6.53 h
INSTRUM   spect
PROBHD    Z108618_0505
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         512
DS         4
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         1.3631488 sec
RG         199.6
DM         20.800 usec
DE         6.50 usec
TE         303.9 K
D1         2.0000000 sec
D11        0.0300000 sec
TDO        100.6550186 MHz
SFO1       100.6261262 MHz
NUC1       13C
P1          10.00 usec
PLW1       58.22499847 W
SFO2       400.2596010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     90.00 usec
PLW2       14.95499992 W
PLW12     0.41542000 W
PLW13     0.20895000 W

F2 - Processing parameters
SI          32768
SF          100.6449542 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```

Fig.S35 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).

VN-034

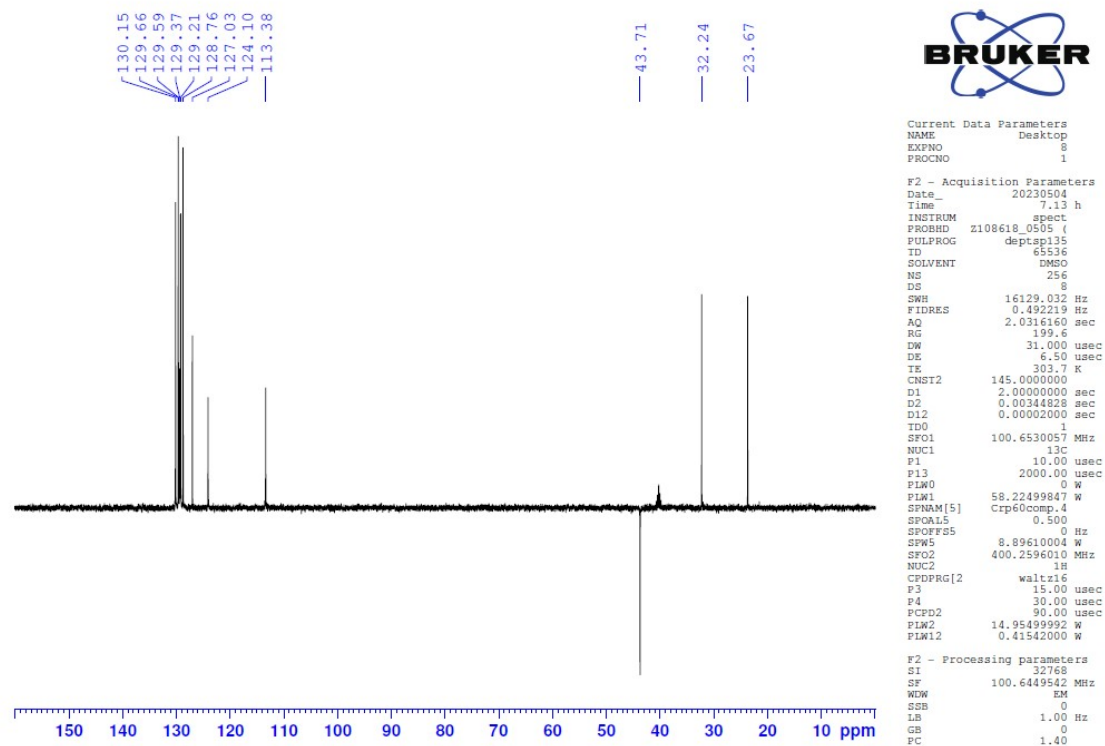


Fig.S36 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).

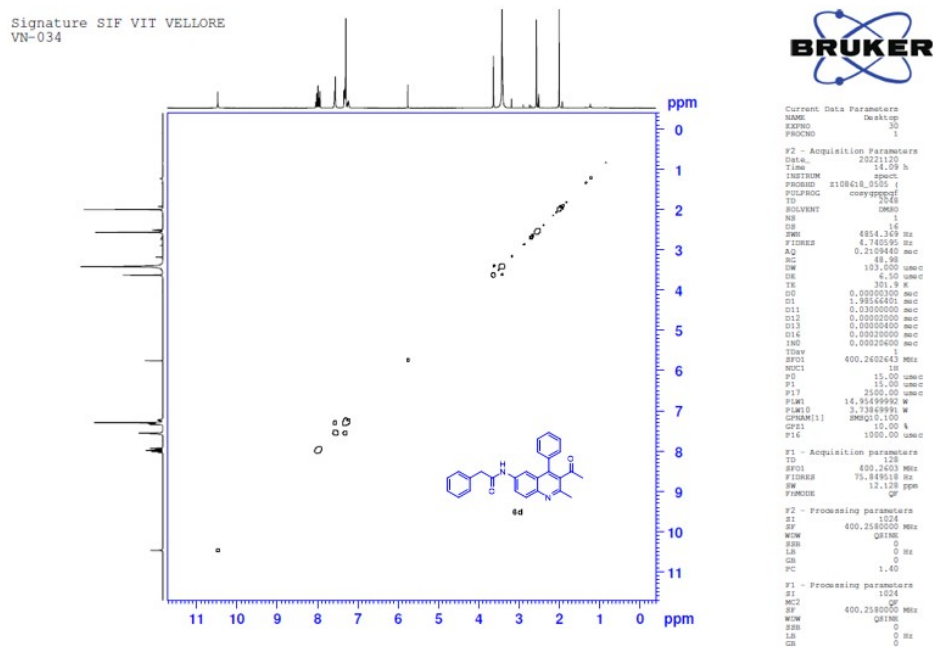


Fig.S37 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).

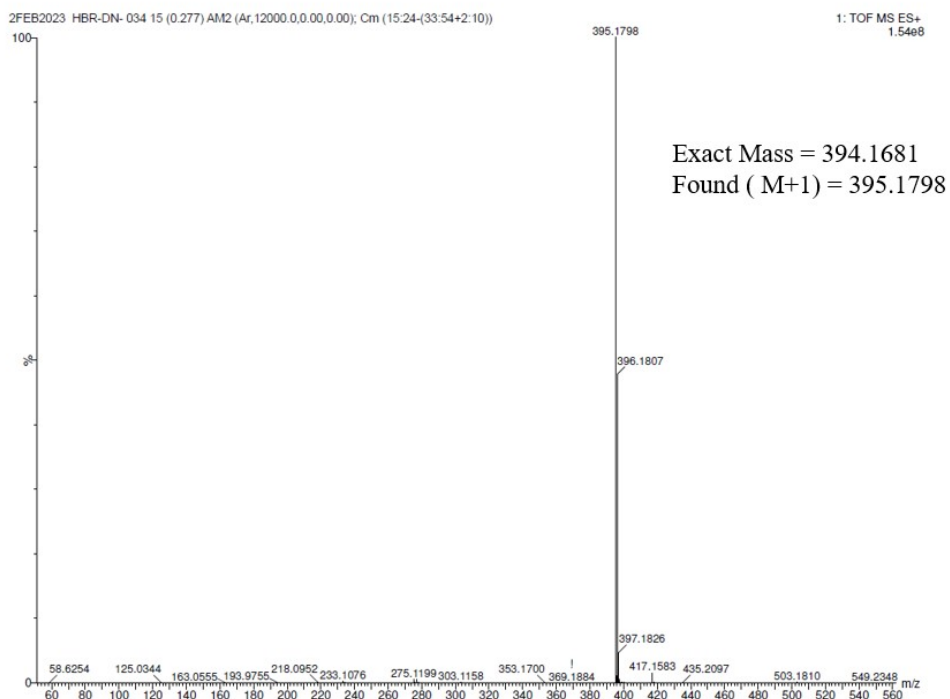


Fig.S38 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).

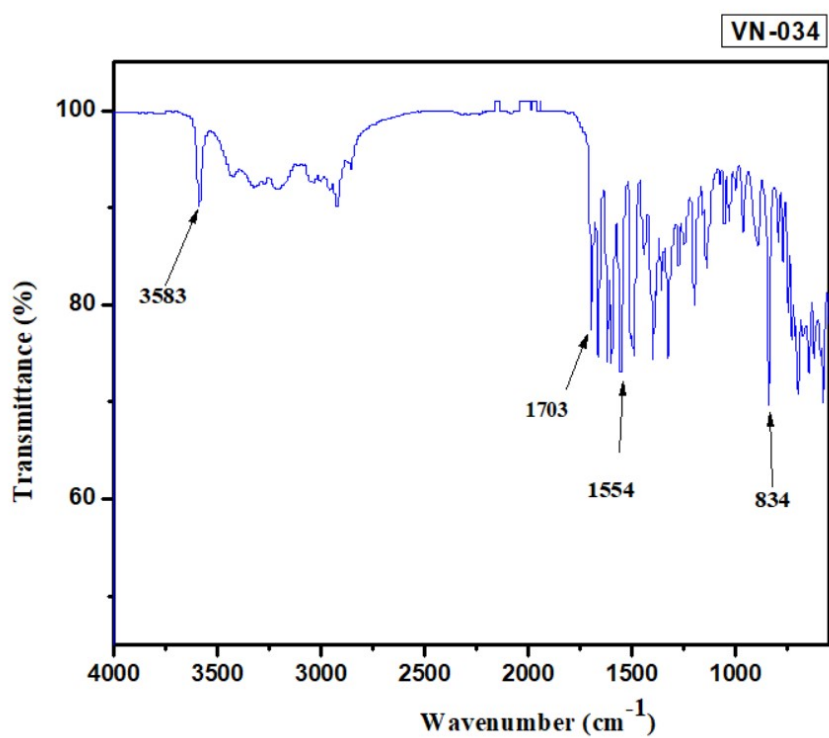


Fig.S39 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenylacetamide (6d).

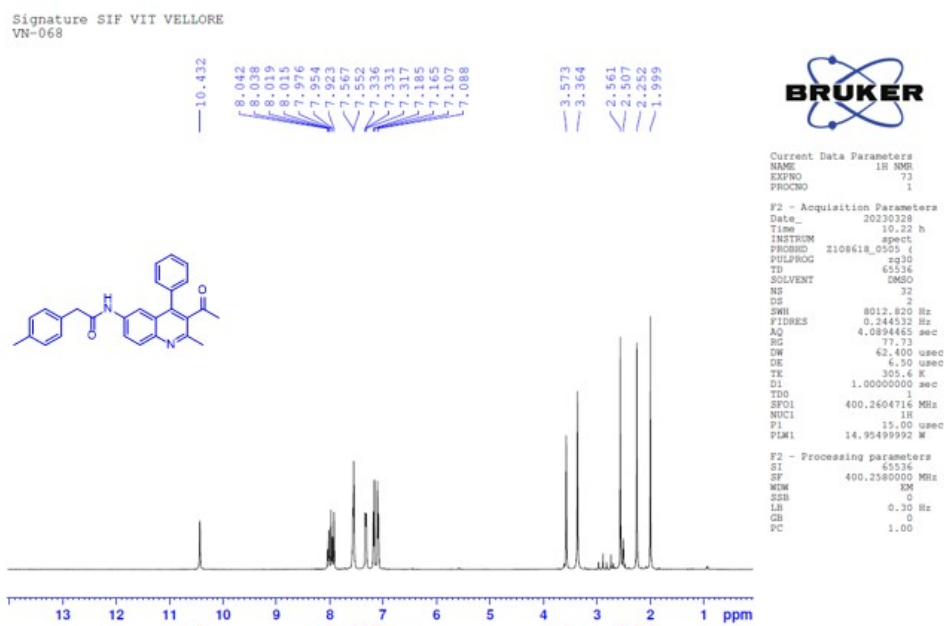


Fig.S40 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl)acetamide (6e).

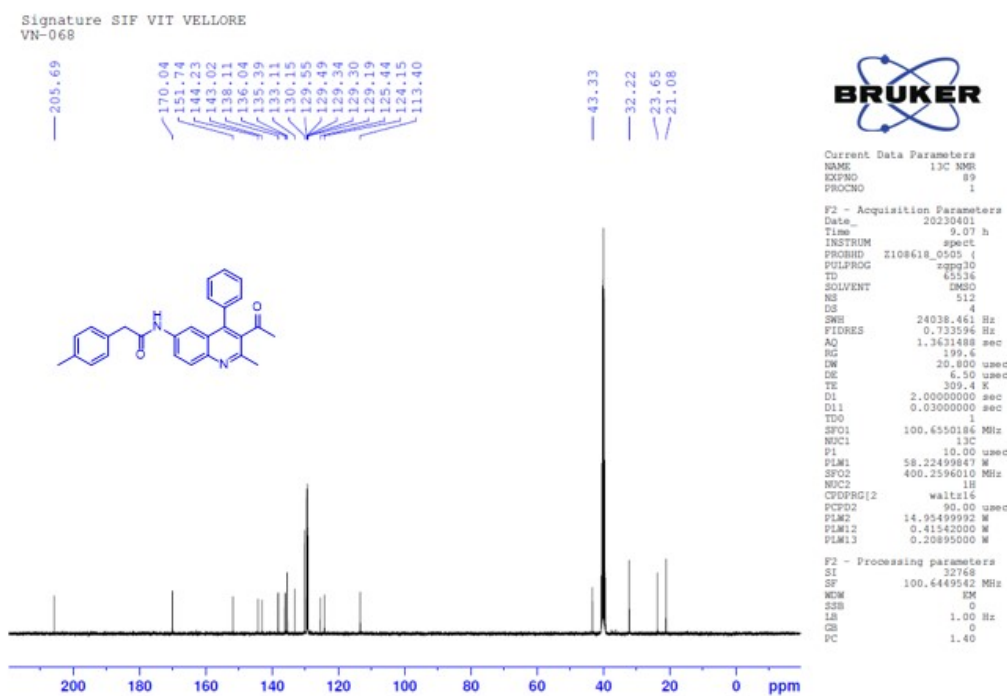


Fig.S41 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl)acetamide (6e).

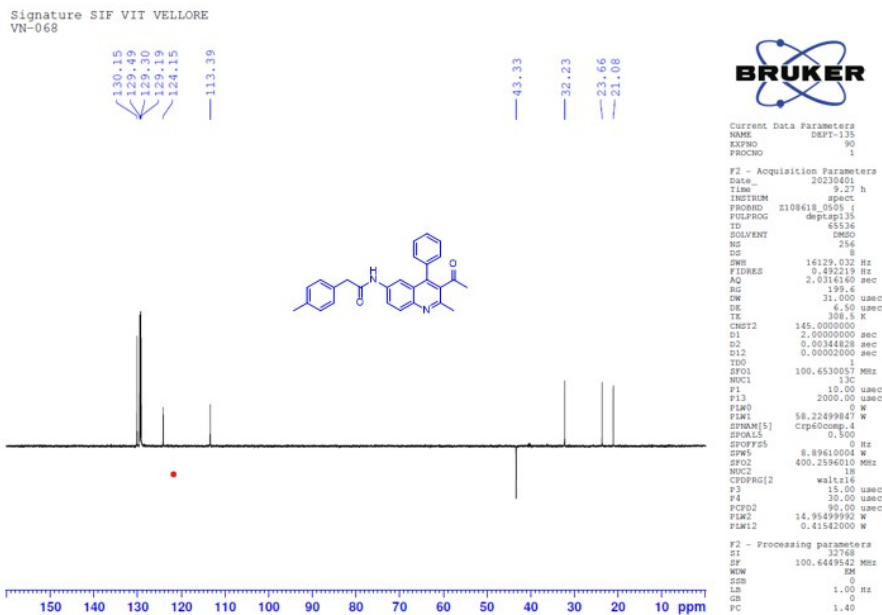


Fig.S42 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl)acetamide (6e).

Thermo Scientific Orbitrap Exploris 120  
Analysed by G SAIKRISHNA

#BR-DN-068 #3-21 RT: 0.01-0.11 AV: 10 SB: 80 0.32-1.20 NL: 9.37E8  
T: FTMS + p ESI Full ms [50.0000-2000.0000]

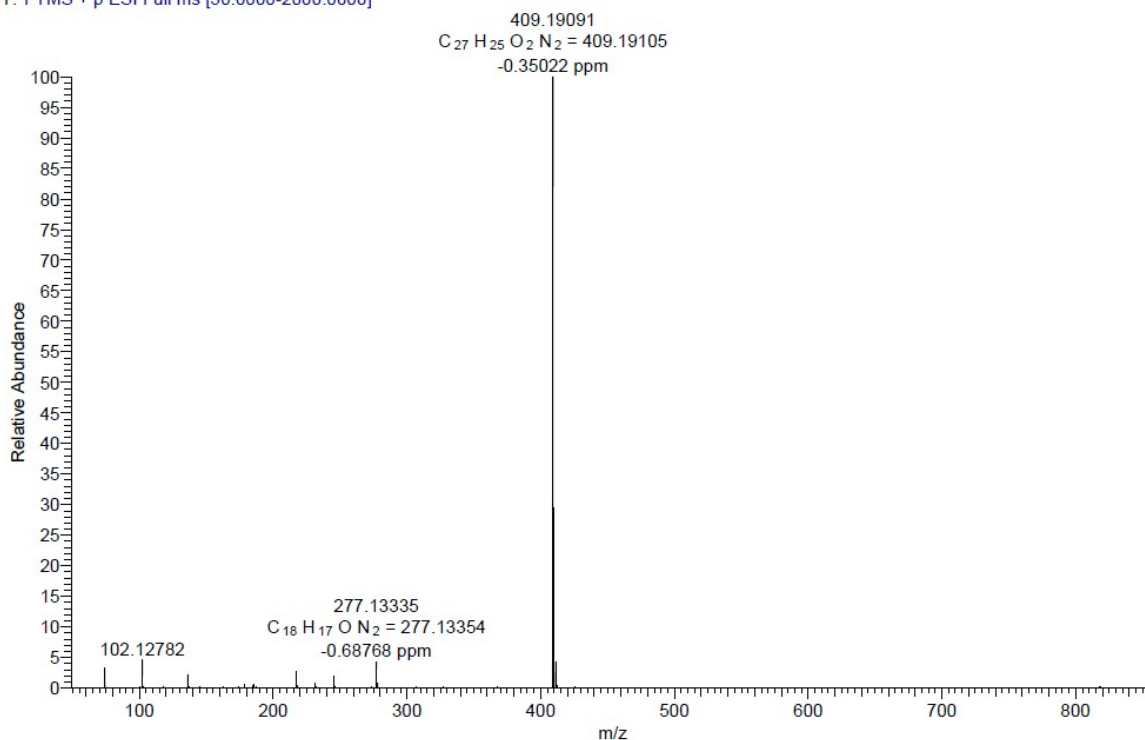


Fig.S43 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl)acetamide (6e).

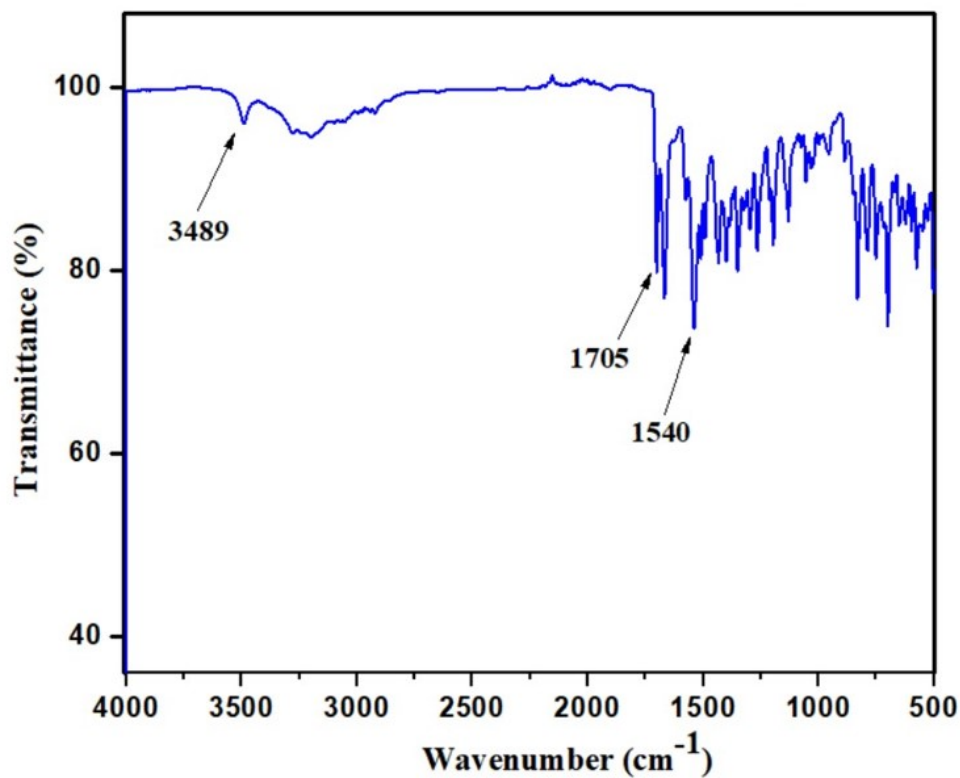


Fig.S44 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(p-tolyl)acetamide (6e).

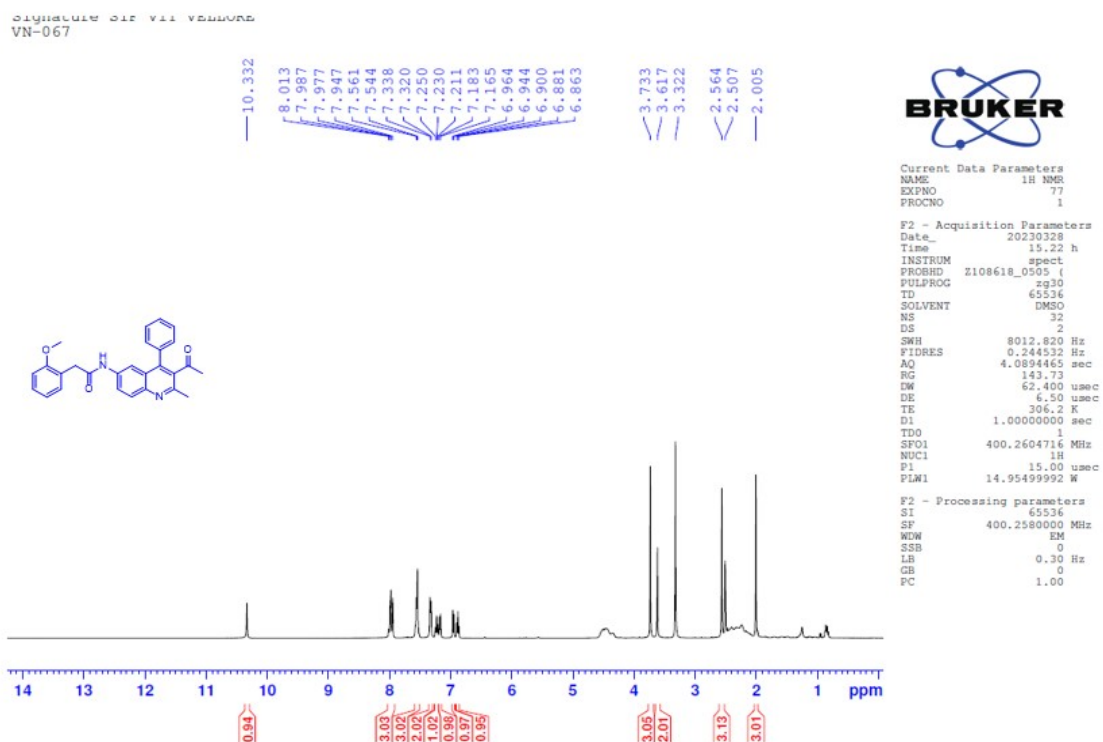


Fig.S45 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl)acetamide

(6f).



Signature SIF VIT VELLORE  
VN-067

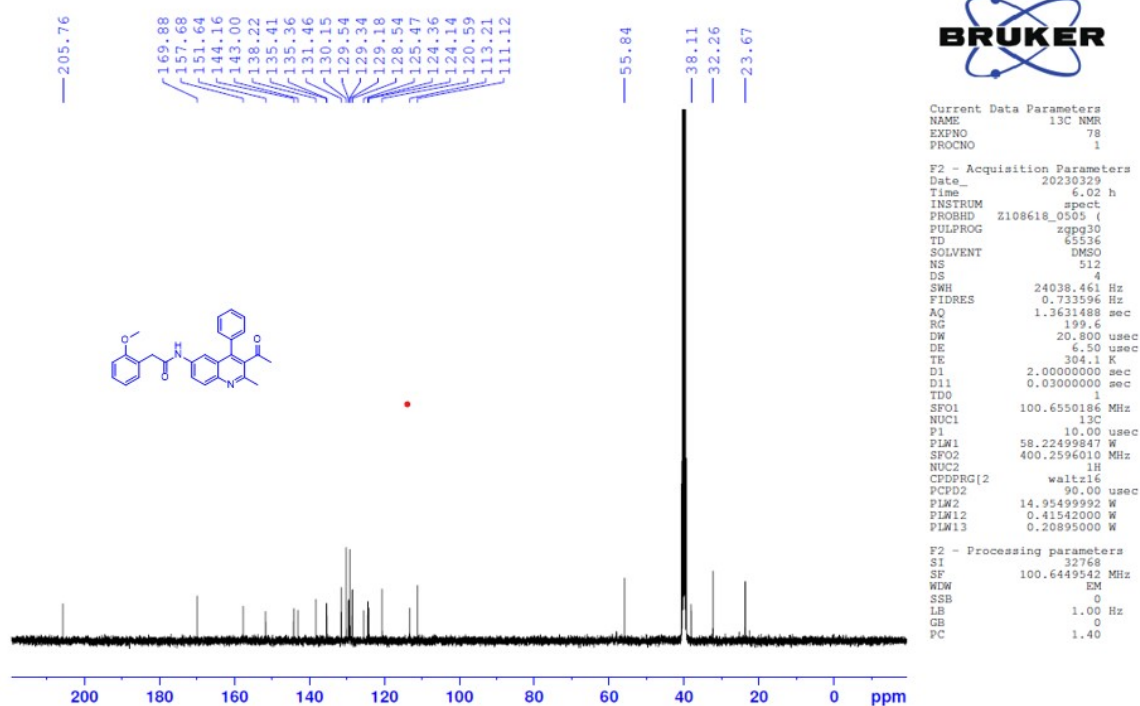


Fig.S46  $^{13}\text{C}$  NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl)acetamide (6f).

VN-067

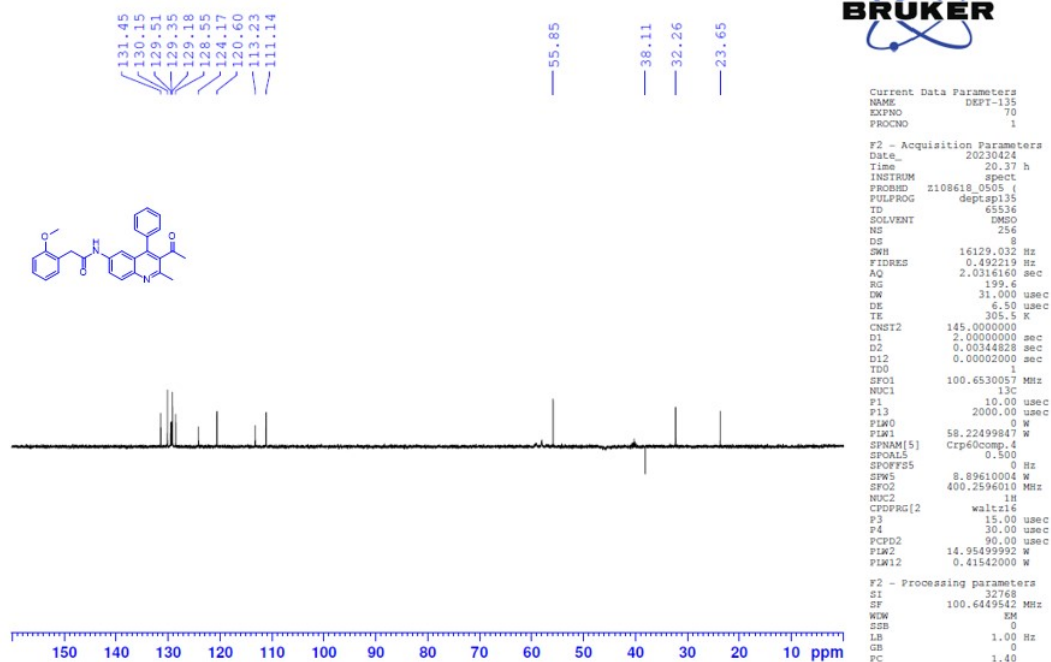


Fig.S47 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl)acetamide

(6f).

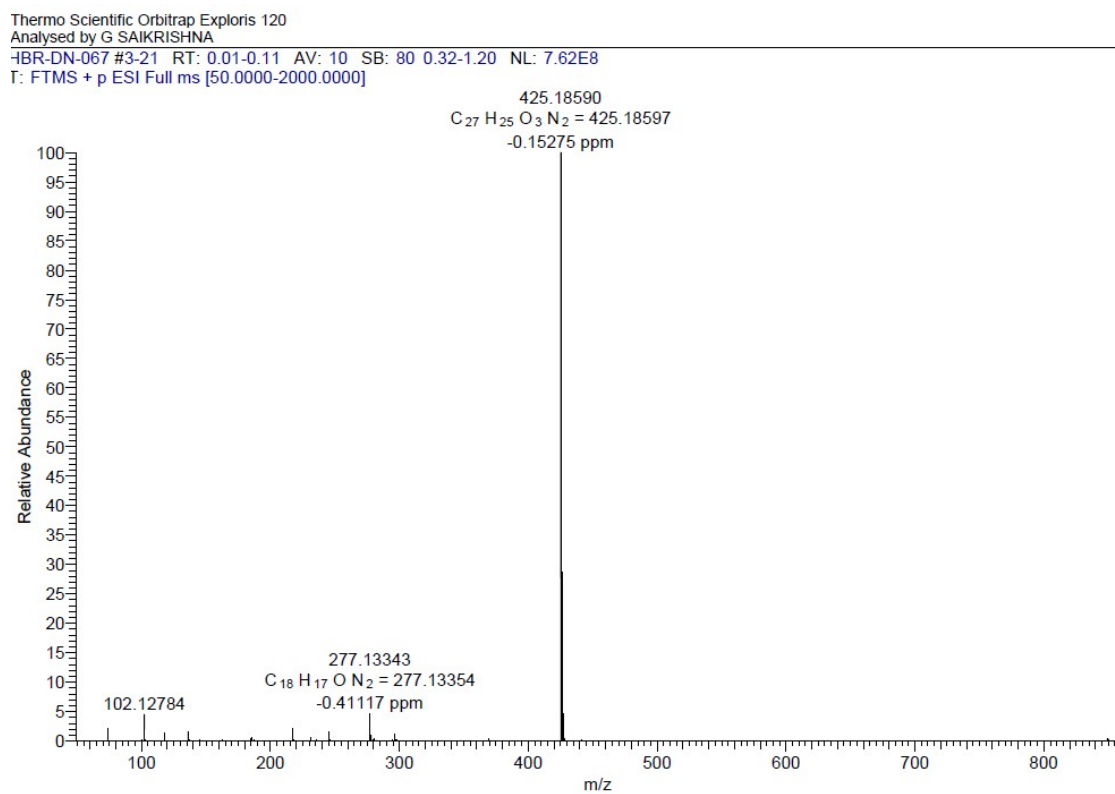


Fig.S48 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl)acetamide (6f).

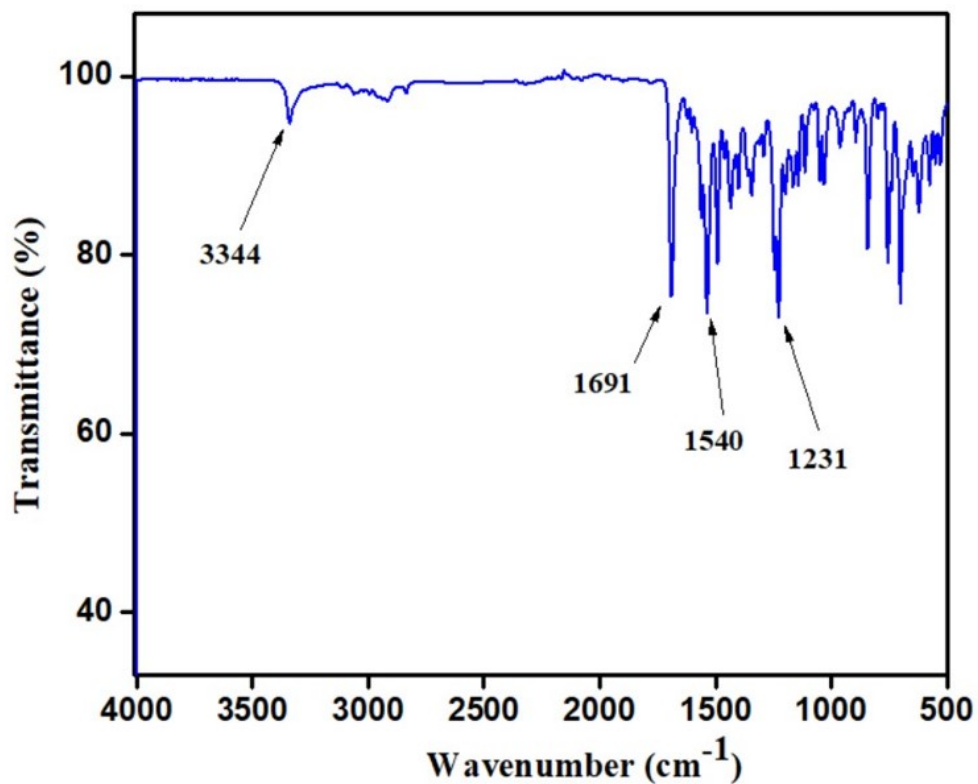


Fig.S49 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-methoxyphenyl)acetamide (6f).

Signature SIF VIT VELLORE  
VN-056

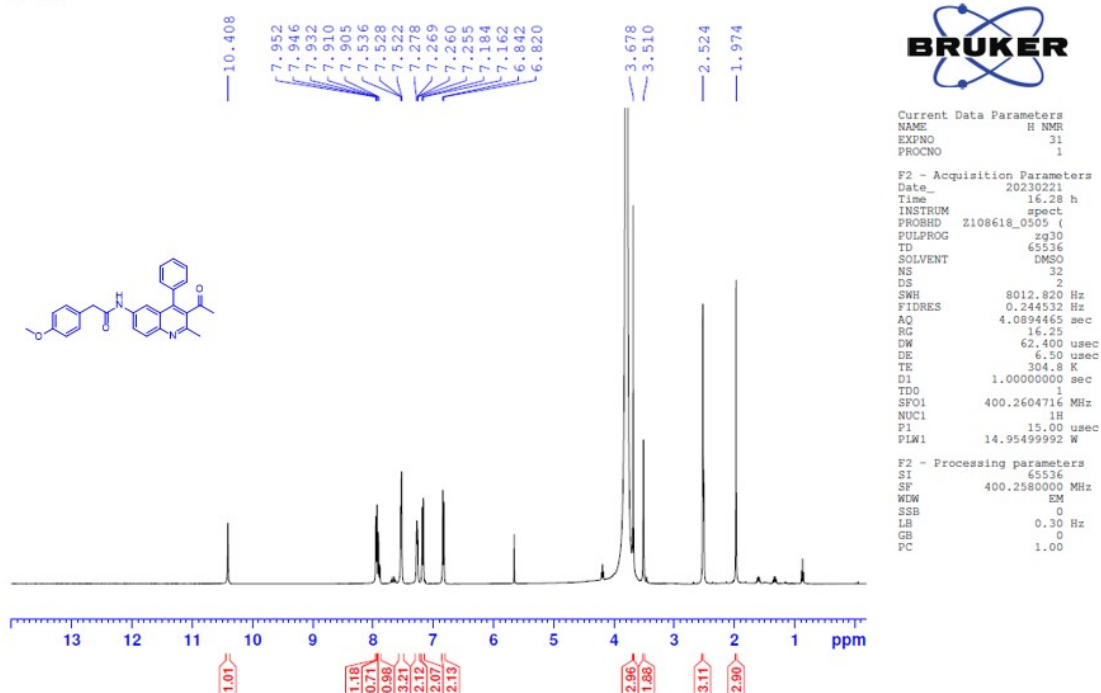


Fig.S50 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-methoxyphenyl)acetamide (6g).

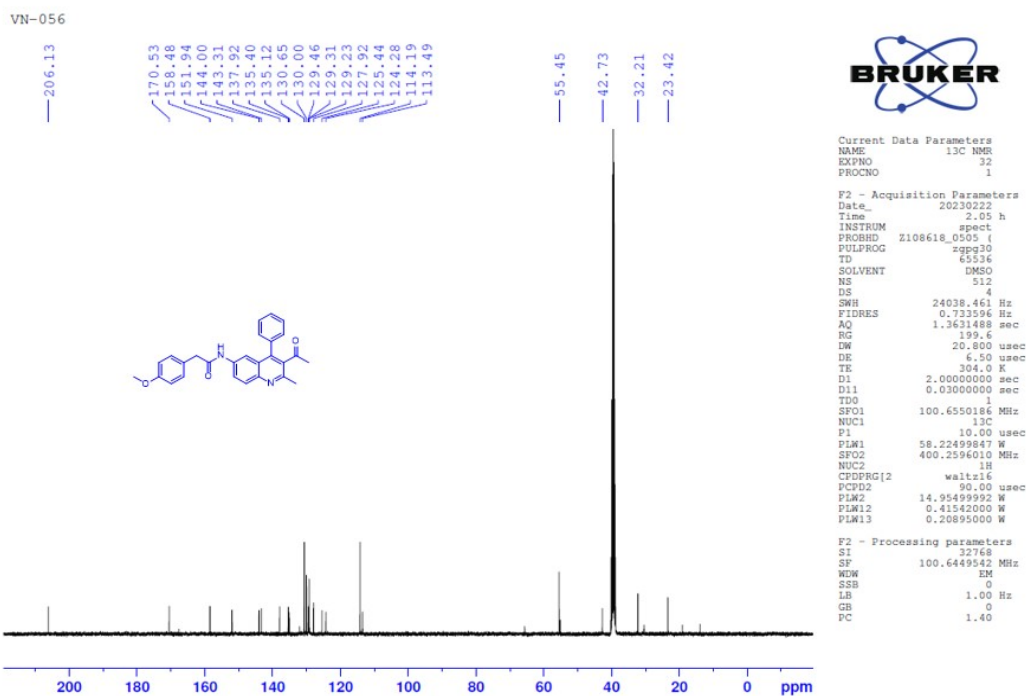


Fig.S51 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-methoxyphenyl)acetamide (6g).

Signature SIF VIT VELLORE  
VN-056

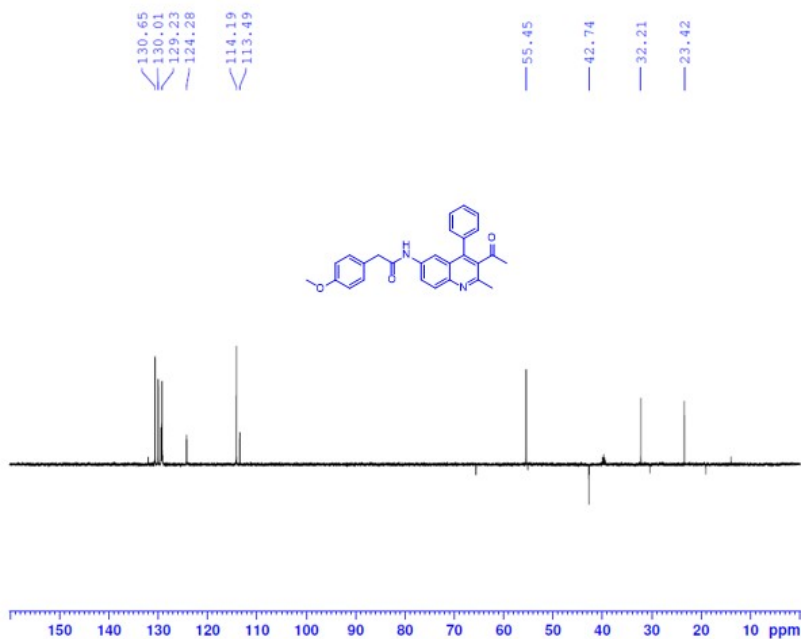


Fig.S52 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-methoxyphenyl)acetamide

(6g).

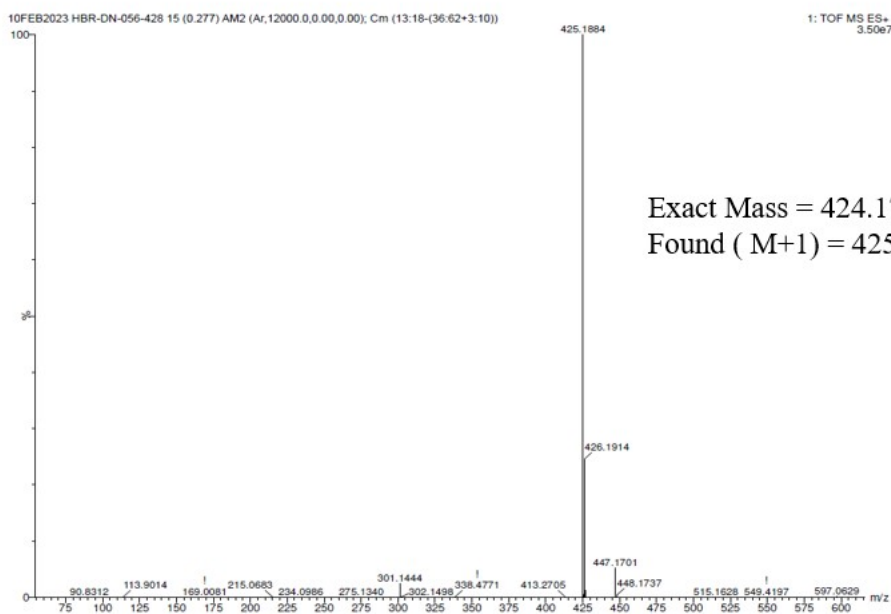


Fig.S53 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-methoxyphenyl)acetamide (6g).

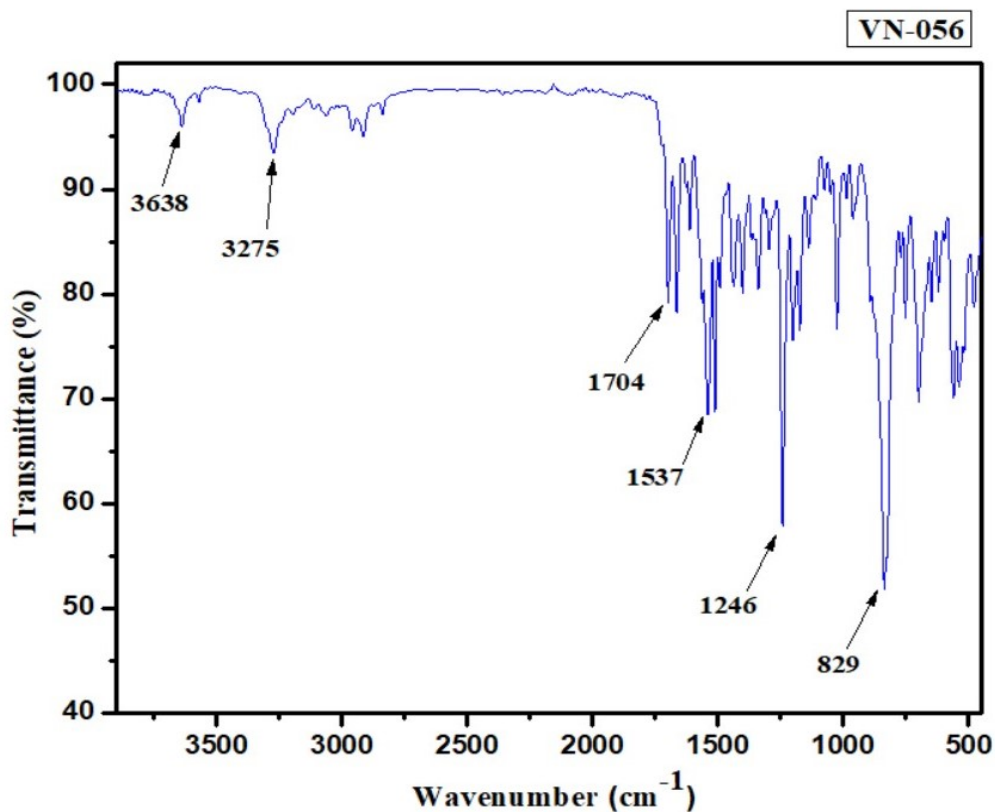


Fig.S54 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-methoxyphenyl)acetamide (6g).

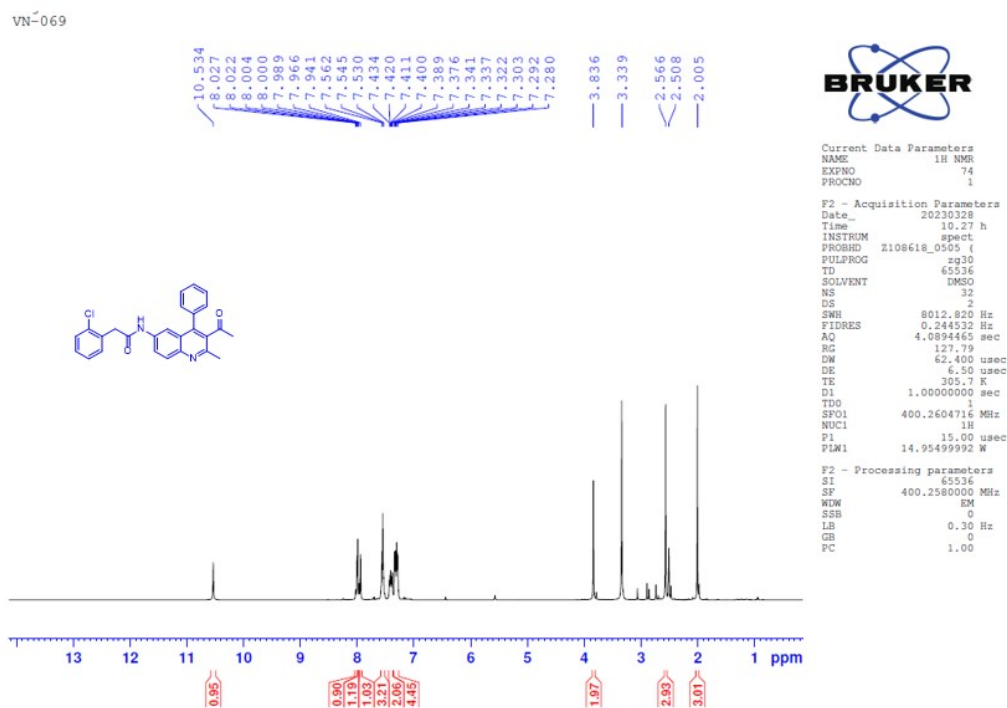


Fig.S55 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl)acetamide (6h).

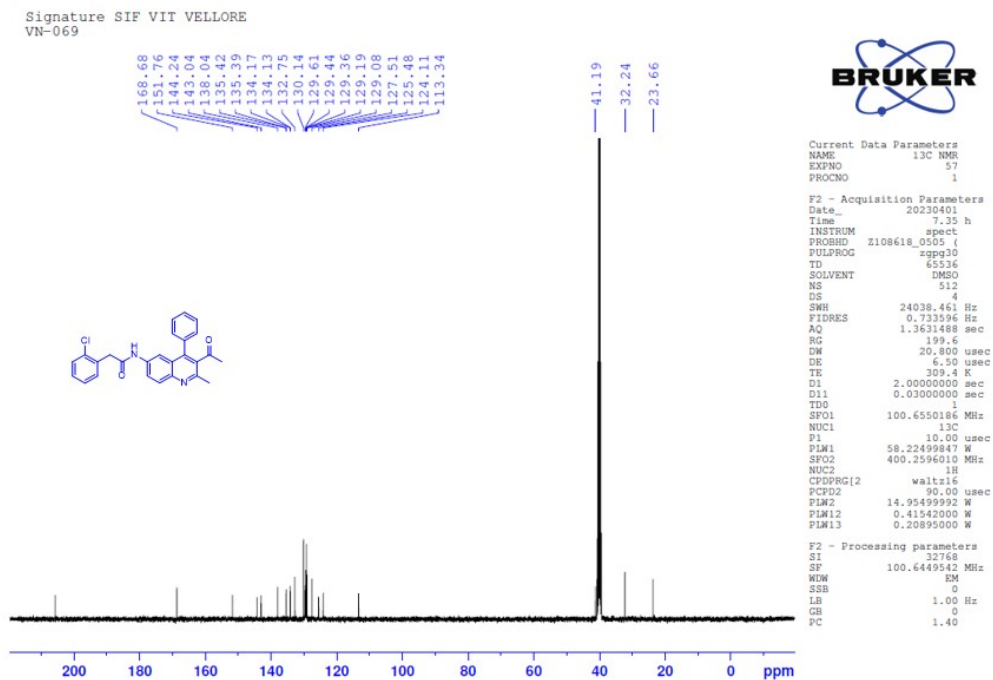


Fig.S56  $^{13}\text{C}$  NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl)acetamide (6h).

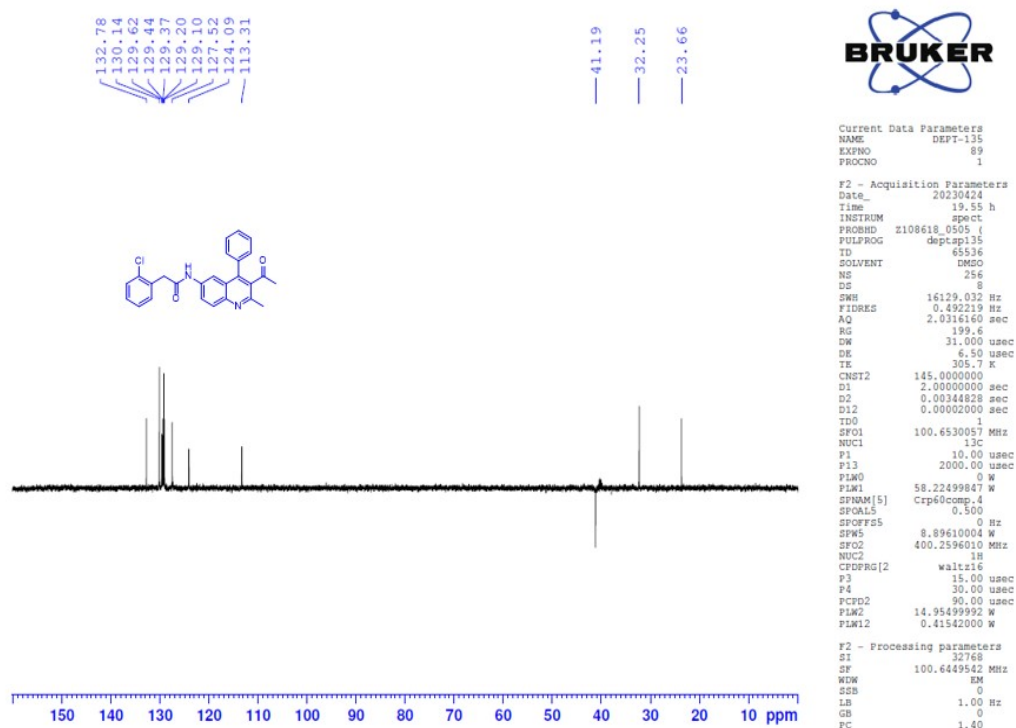


Fig.S57 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl)acetamide (6h).

Thermo Scientific Orbitrap Exploris 120  
Analysed by G SAIKRISHNA  
-IBR-DN-069 #2-18 RT: 0.01-0.09 AV: 8 SB: 80 0.32-1.20 NL: 1.14E9  
T: FTMS + p ESI Full ms [50.0000-2000.0000]

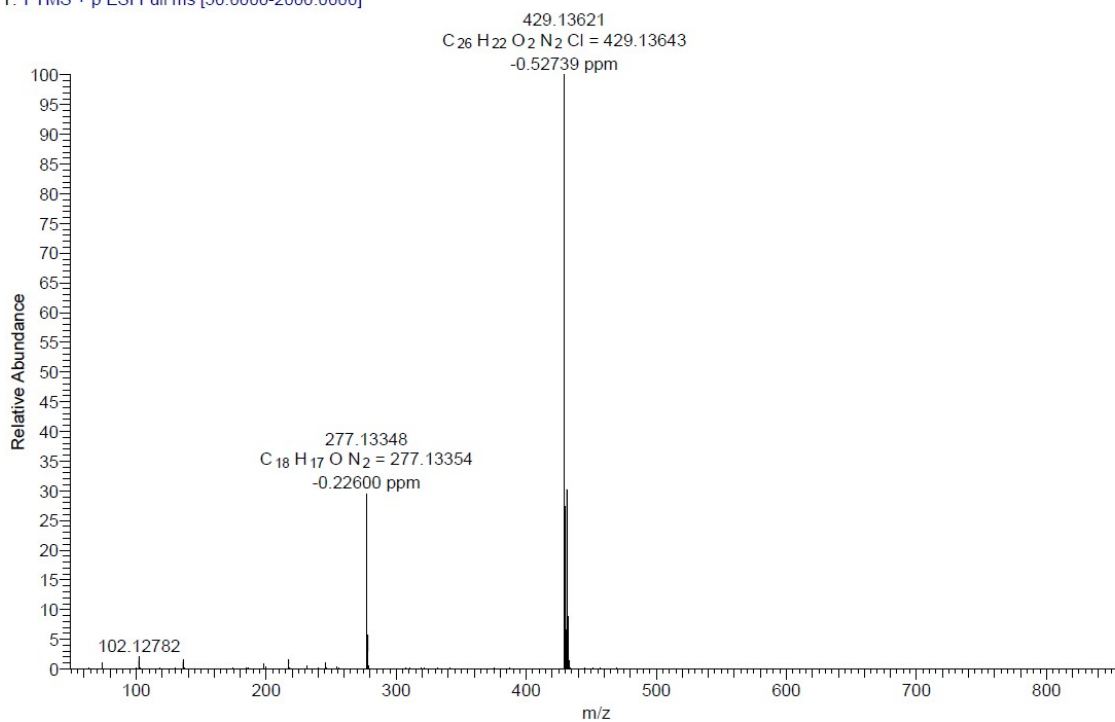


Fig.S58 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl)acetamide (6h).

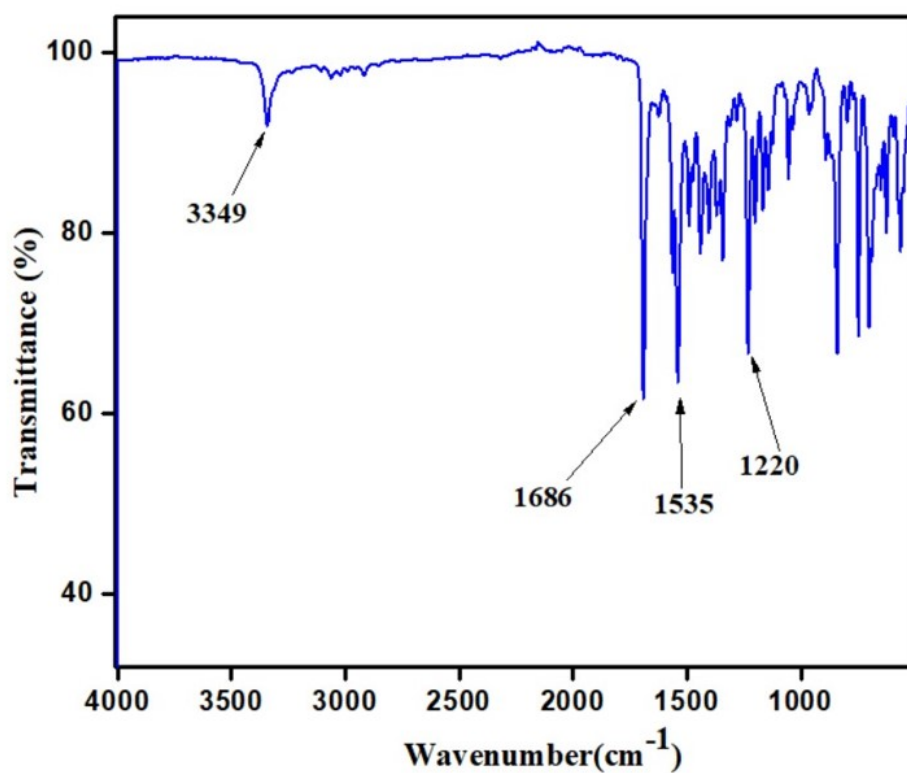


Fig.S59 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(2-chlorophenyl)acetamide (6h).

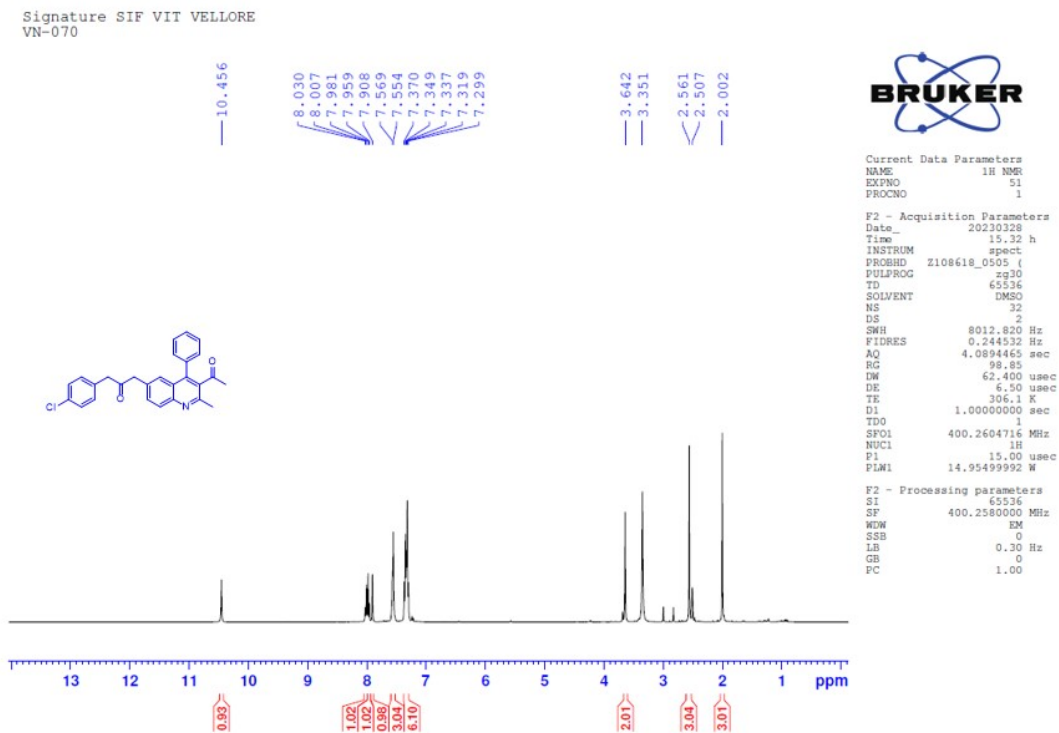


Fig.S60 <sup>1</sup>H NMR of 1-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-chlorophenyl)propan-2-one (6i).

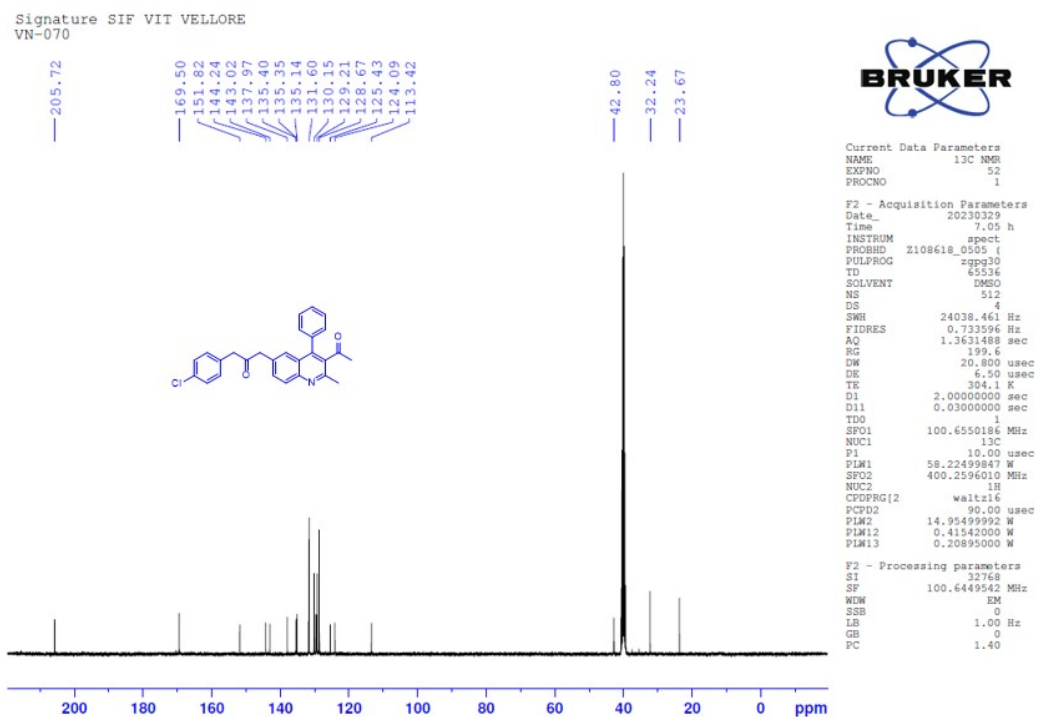


Fig.S61 <sup>13</sup>C NMR of 1-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-chlorophenyl)propan-2-one (6i).



Signature SIF VIT VELLORE  
VN-070

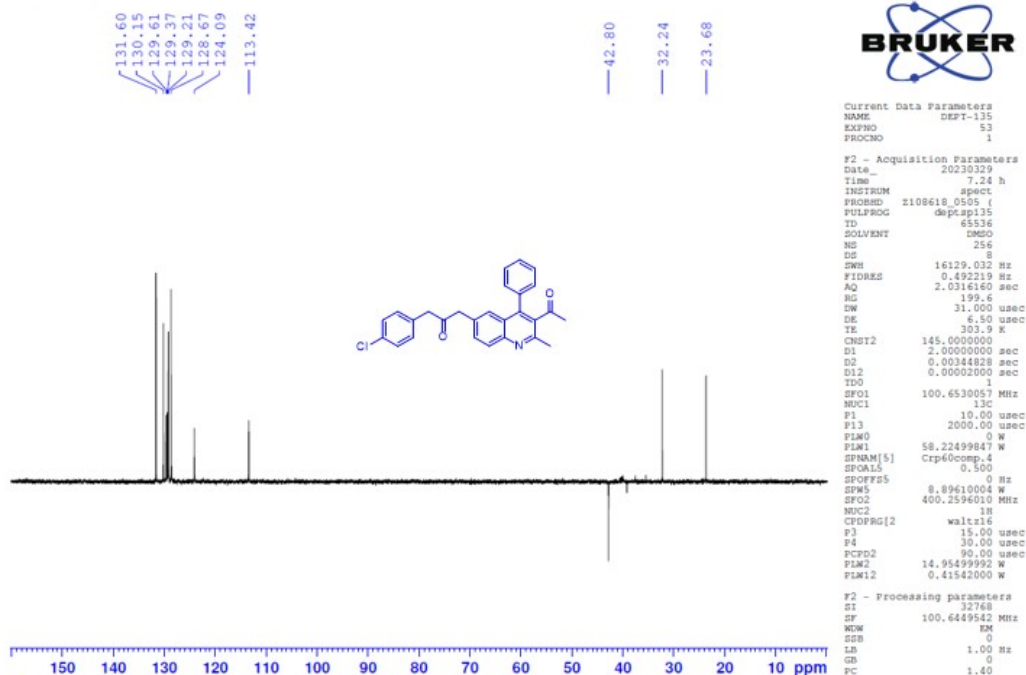


Fig.S62 DEPT-135 of 1-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-chlorophenyl)propan-2-one 1

(6i).

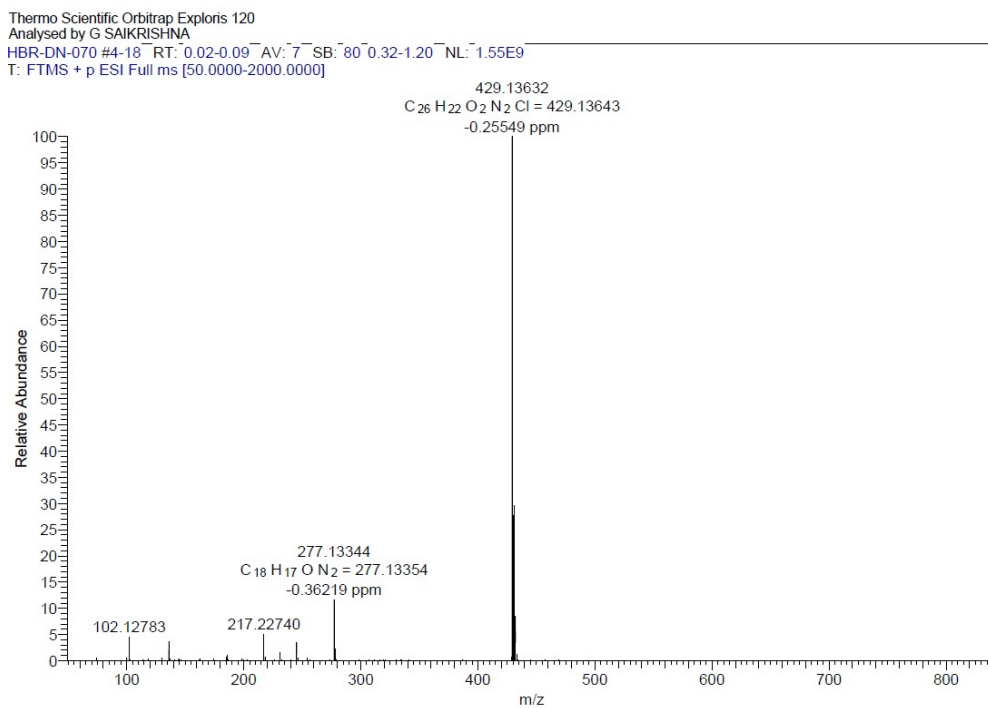


Fig.S63 HRMS of 1-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-chlorophenyl)propan-2-one 1

(6i).

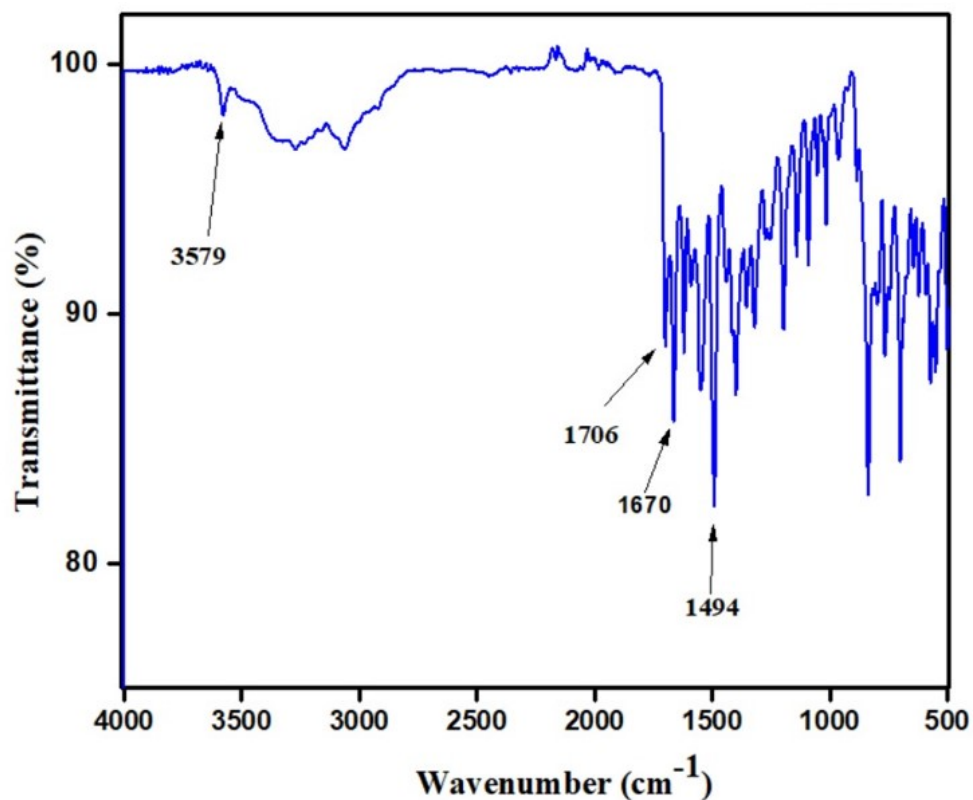


Fig.S64 FT-IR of 1-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-chlorophenyl)propan-2-one1 (6i).

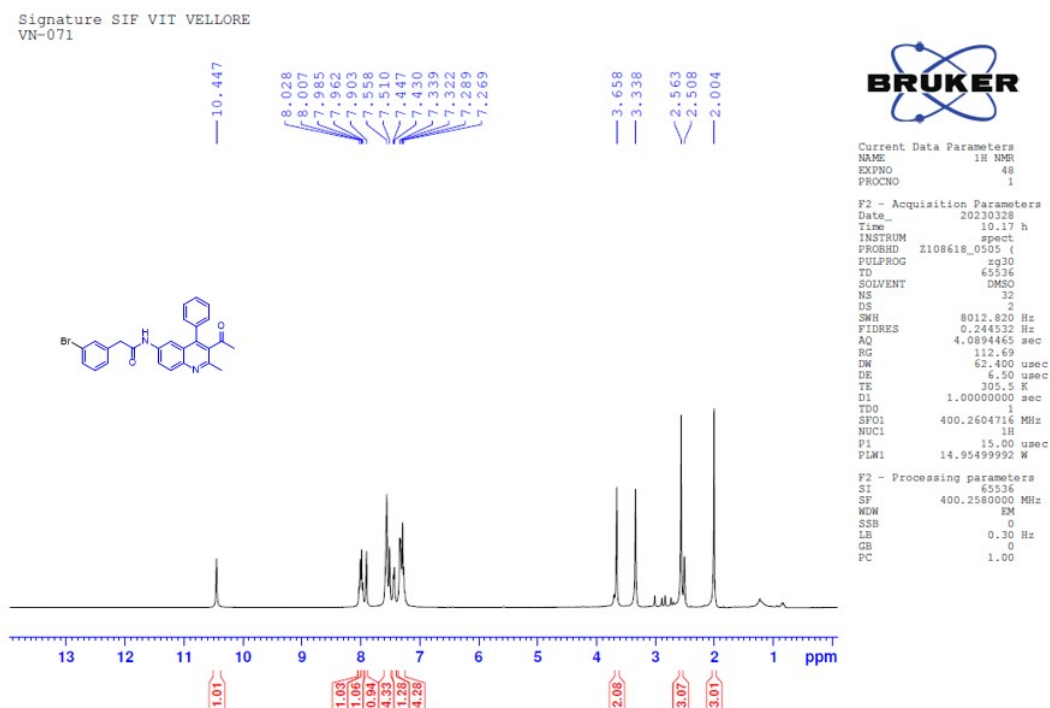


Fig.S65 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl)acetamide (6j).

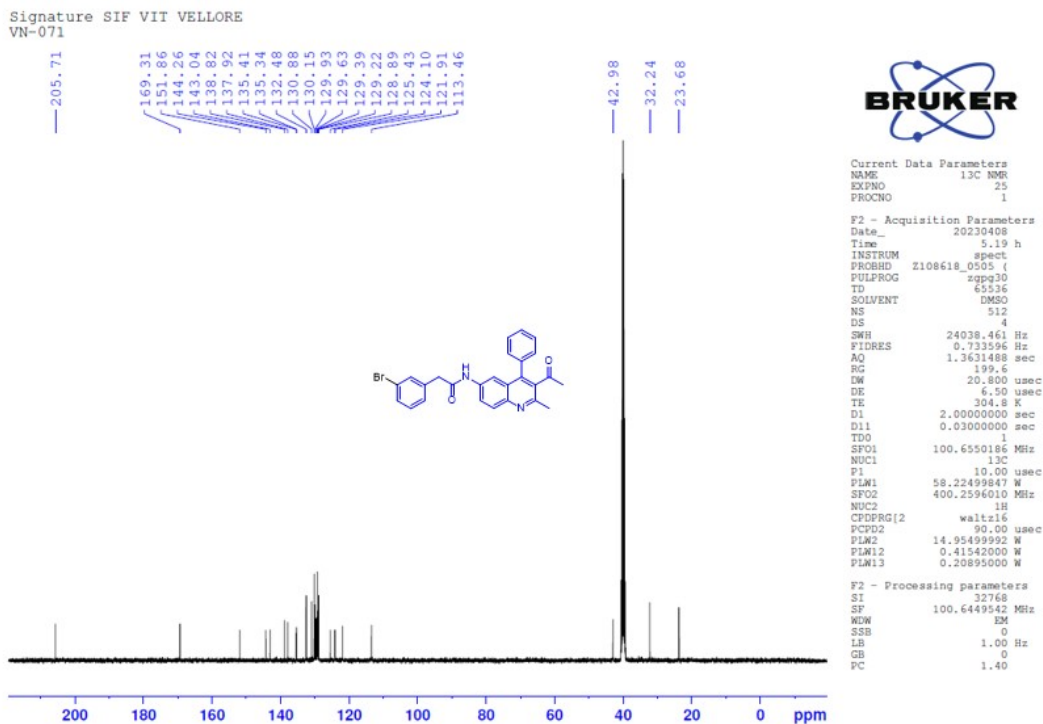


Fig.S66  $^{13}\text{C}$  NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl)acetamide (6j).

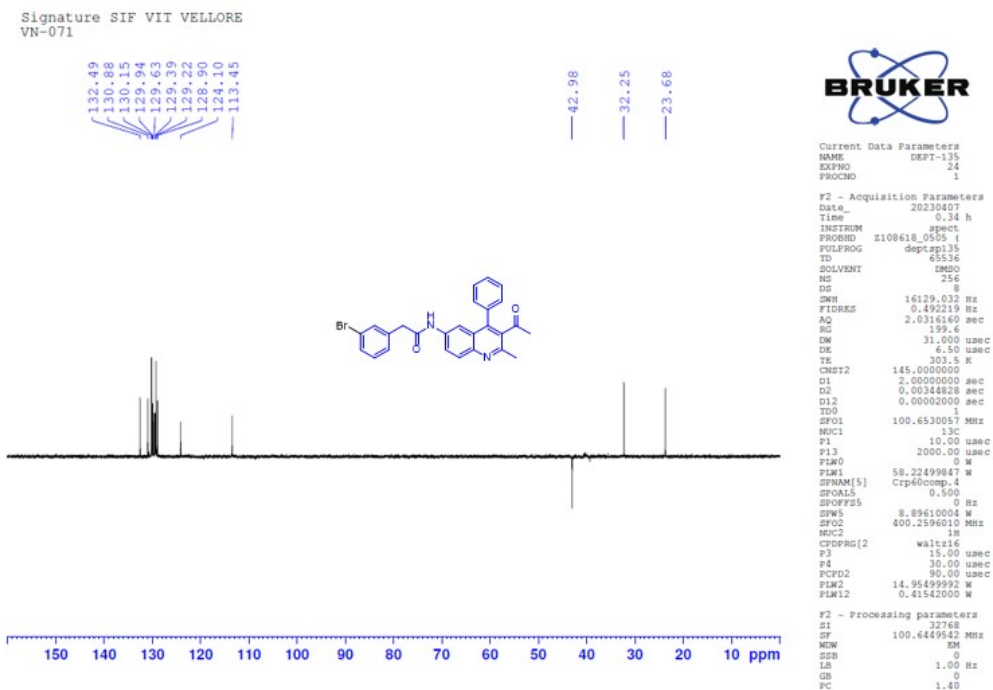


Fig.S67 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl)acetamide

(6j).

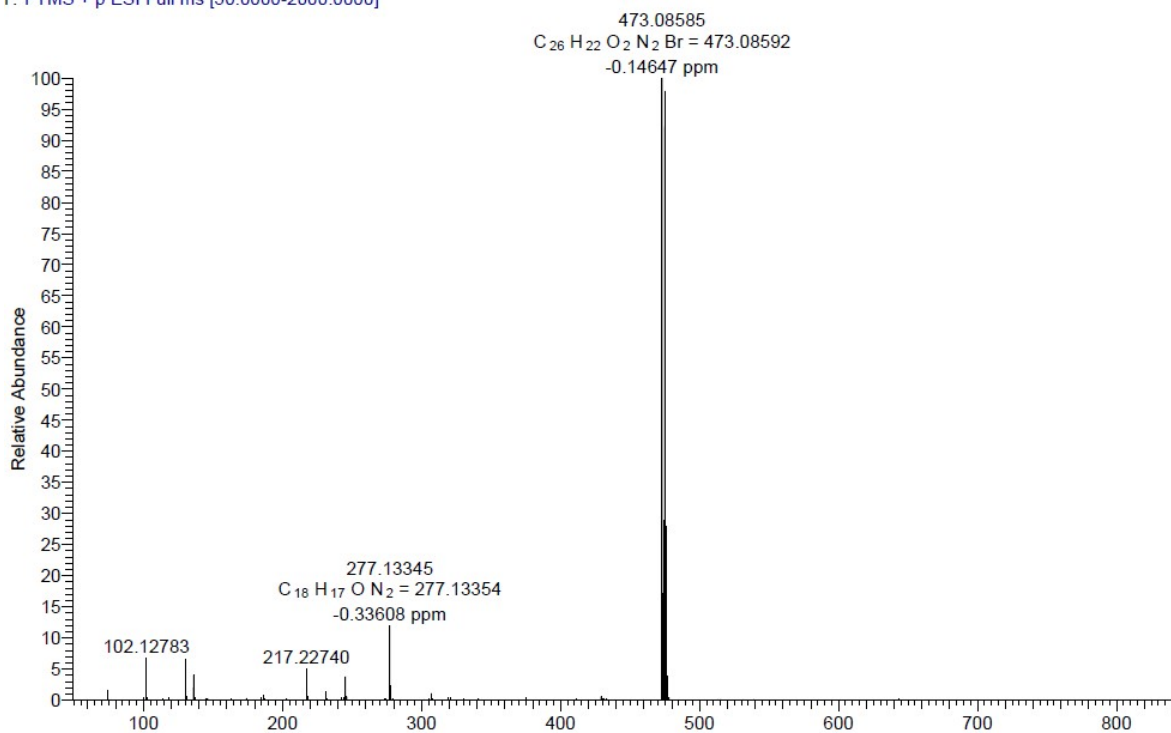


Fig.S68 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl)acetamide (6j).

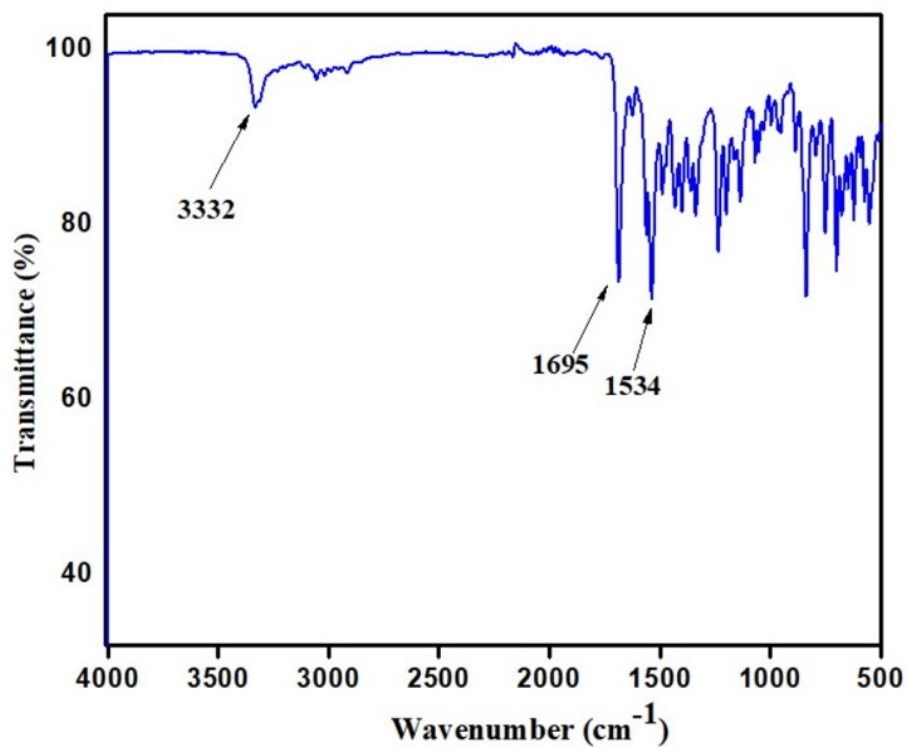


Fig.S69 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(3-bromophenyl)acetamide (6j).



Signature SIF VIT VELLORE  
VN-072

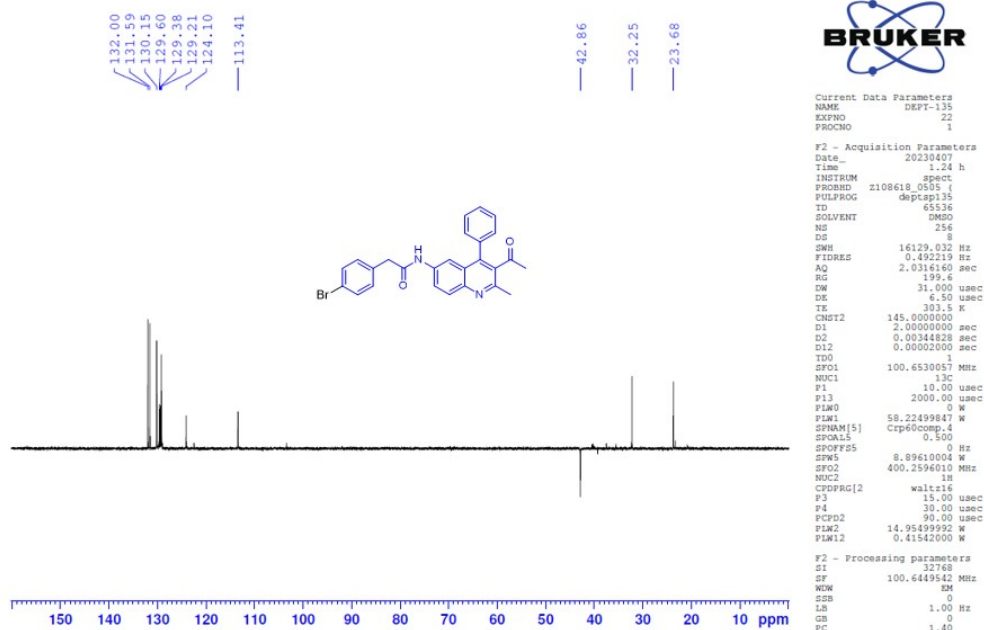


Fig.S72 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-bromophenyl)acetamide (6k).

Thermo Scientific Orbitrap Exploris 120  
Analysed by G SAIKRISHNA

HBR-DN-072 #6-15 RT: 0.03-0.08 AV: 5 SB: 80 0.32-1.20 NL: 5.86E8  
T: FTMS + p ESI Full ms [50.0000-2000.0000]

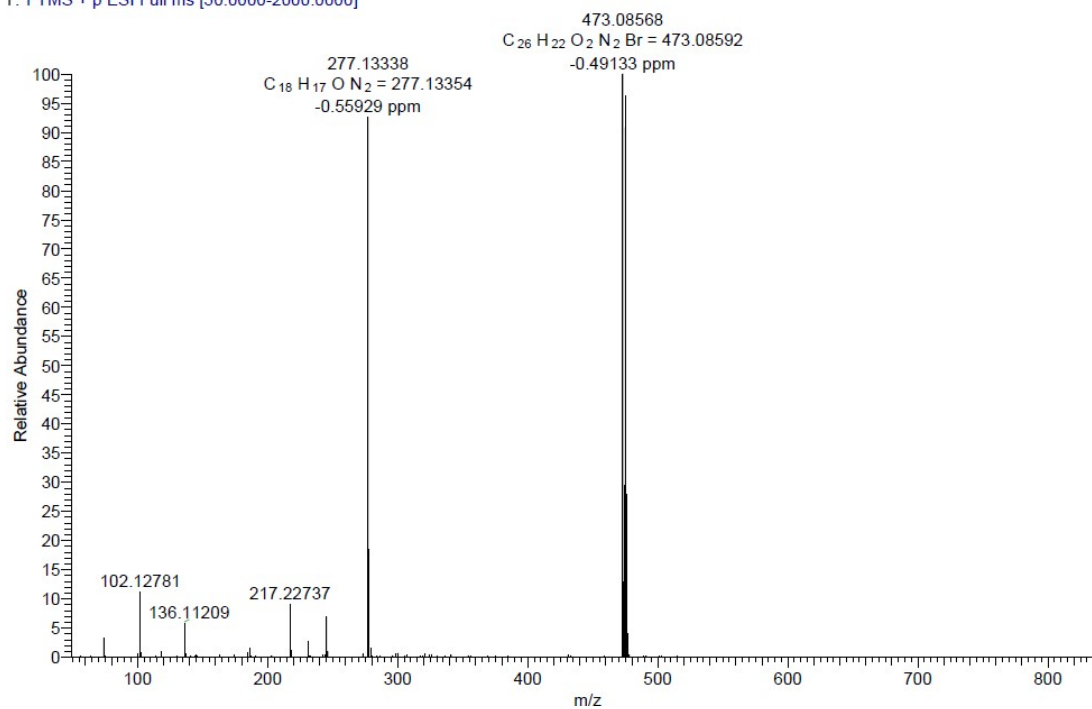


Fig.S73 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-bromophenyl)acetamide (6k)

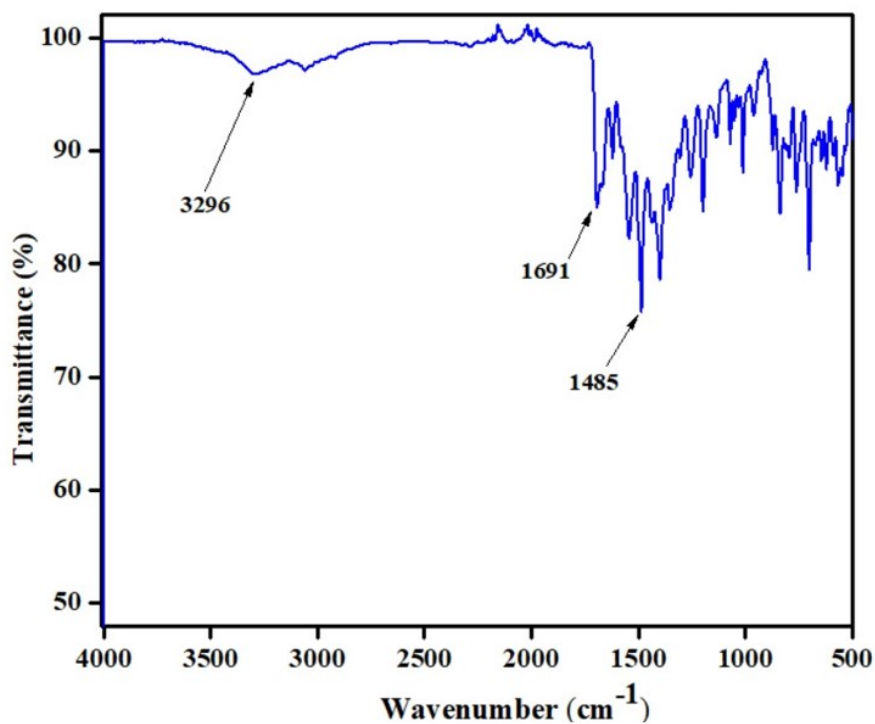


Fig.S74 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(4-bromophenyl)acetamide (6k).

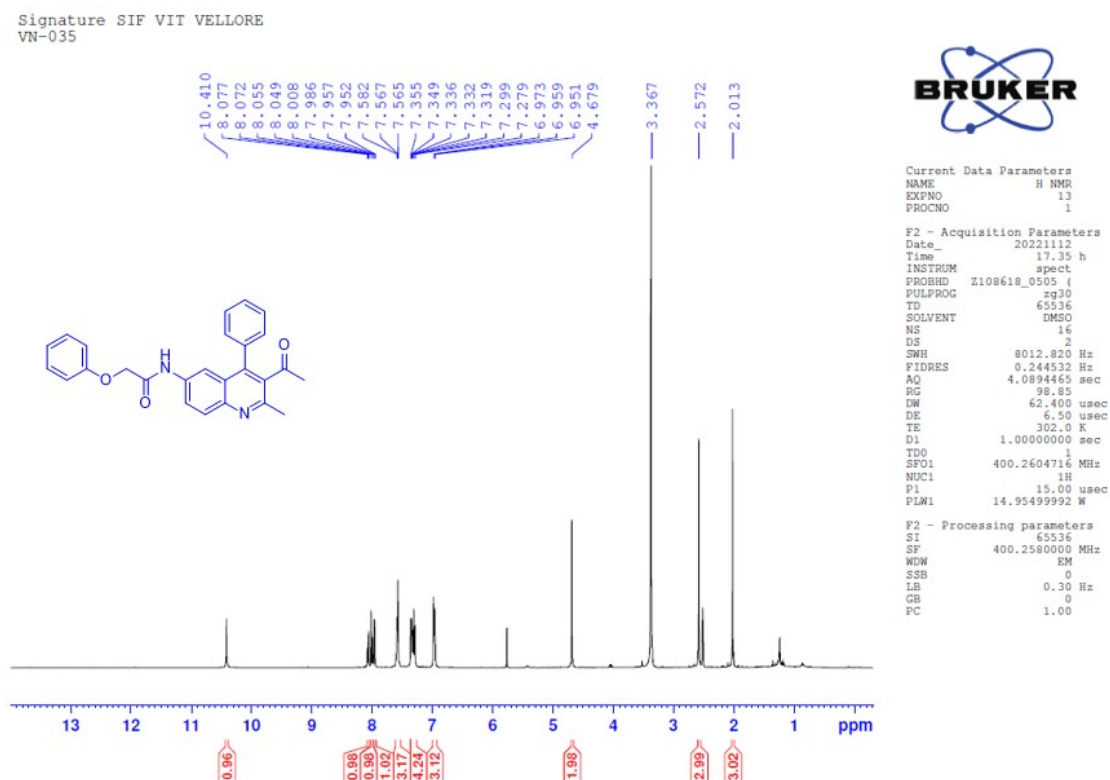
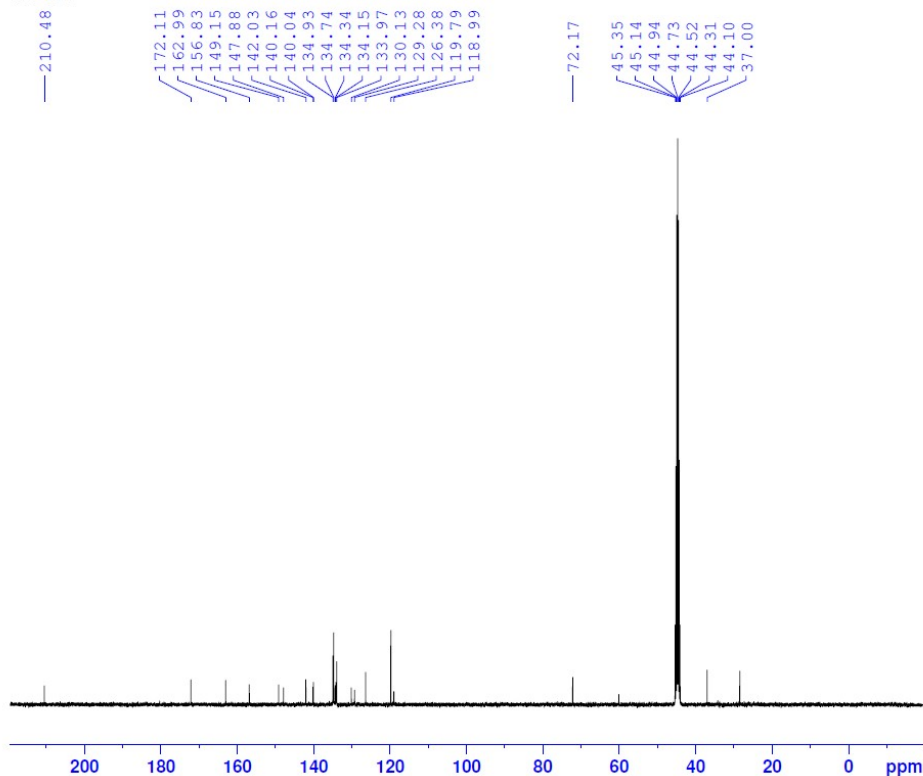


Fig.S75 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (6l).

Signature SIF VIT VELLORE  
VN-035



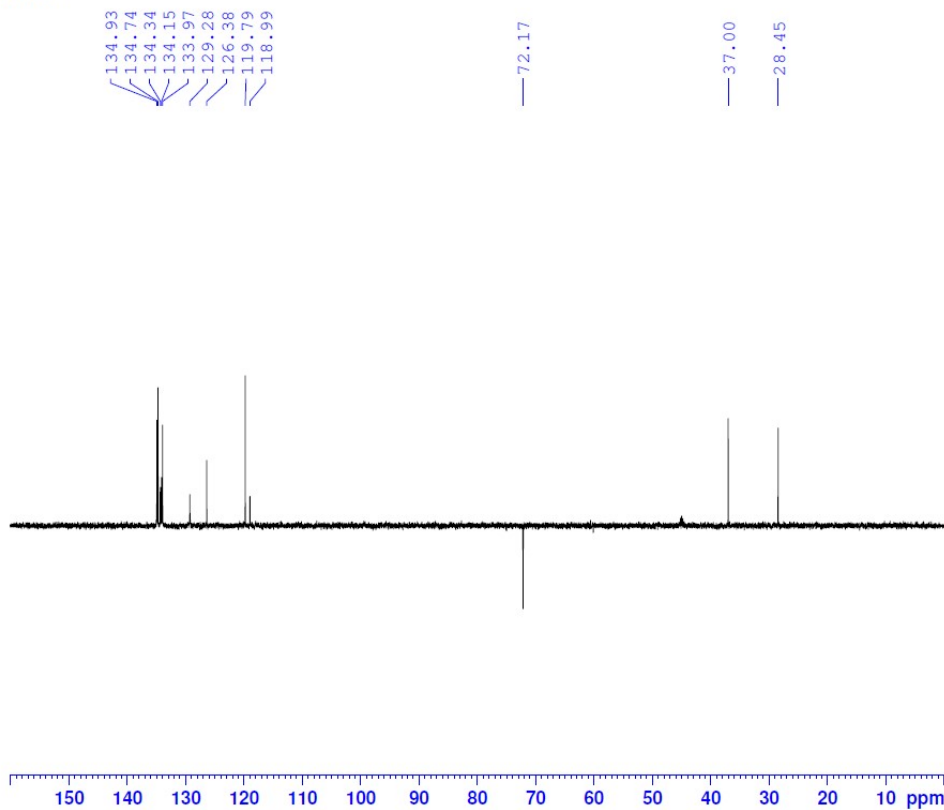
Current Data Parameters  
NAME 13C NMR  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221115  
Time\_ 2.07 h  
INSTRUM spect  
PROBHD Z108618\_0505 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 199.6  
DW 20.800 usec  
DE 6.50 usec  
TE 303.4 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6550186 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 58.22499847 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W  
PLW13 0.20895000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S76 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (6l).

Signature SIF VIT VELLORE  
VN-035



Current Data Parameters  
NAME DEPT-135  
EXPNO 17  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221115  
Time\_ 2.26 h  
INSTRUM spect  
PROBHD Z108618\_0505 (  
PULPROG deptsp135  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 8  
SWH 16129.032 Hz  
FIDRES 0.492219 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DE 6.50 usec  
TE 303.2 K  
CNST2 145.000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1  
SFO1 100.6530057 MHz  
NUC1 13C  
P1 10.00 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 58.22499847 W  
SPNAM[5] Crp60comp.4  
SPOALS 0.500  
SPOFFS5 0 Hz  
SPW5 8.89610004 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
P3 15.00 usec  
P4 30.00 usec  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S77 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (6l).



Signature SIF VIT VELLORE  
VN-035

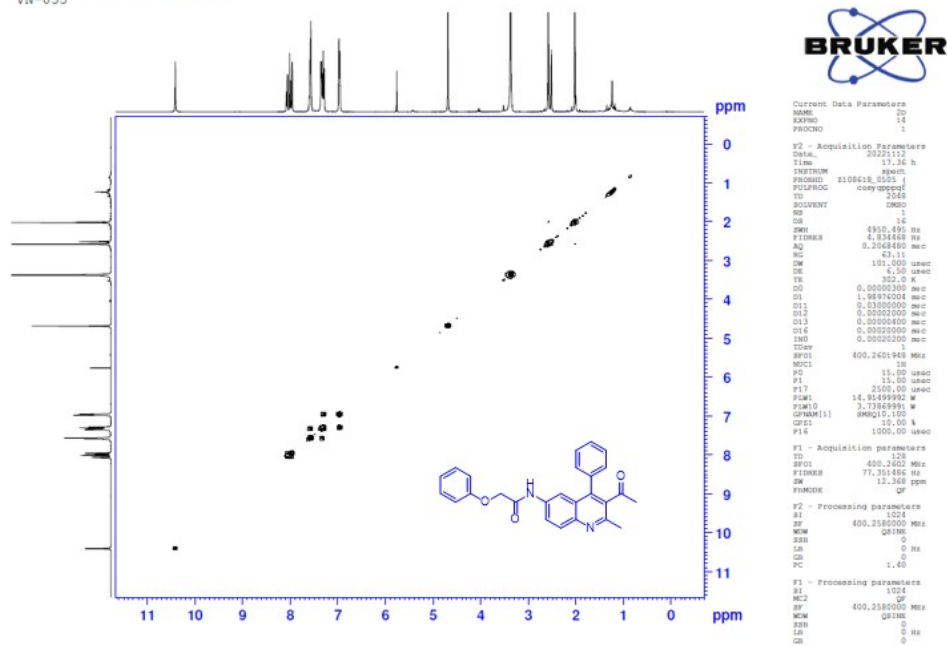


Fig.S78 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (61).

Signature SIF VIT VELLORE  
VN-035

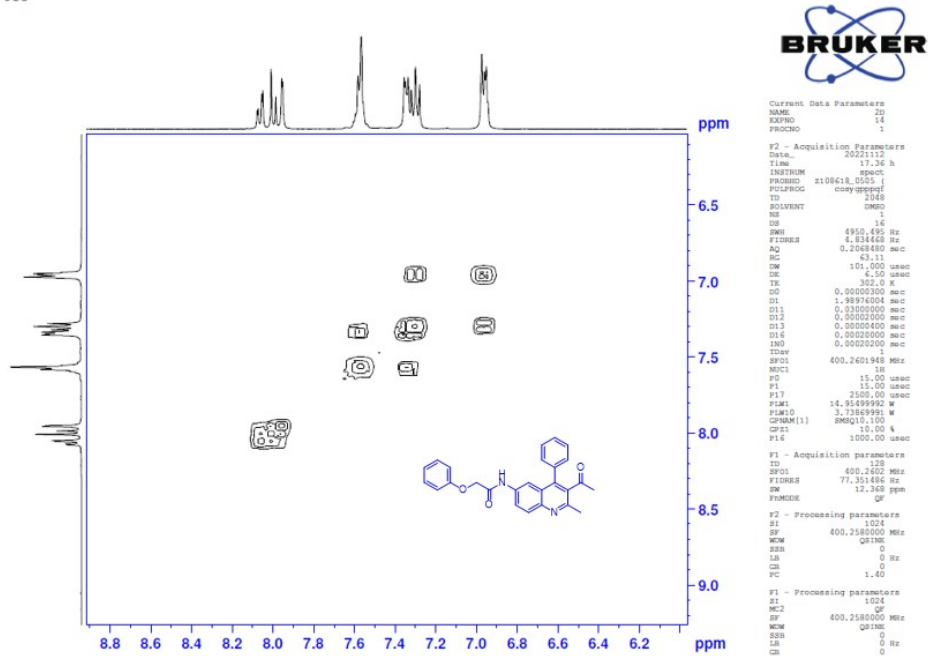


Fig.S79 Enlarged H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide

(61).

Signature SIF VIT VELLORE  
VN-035

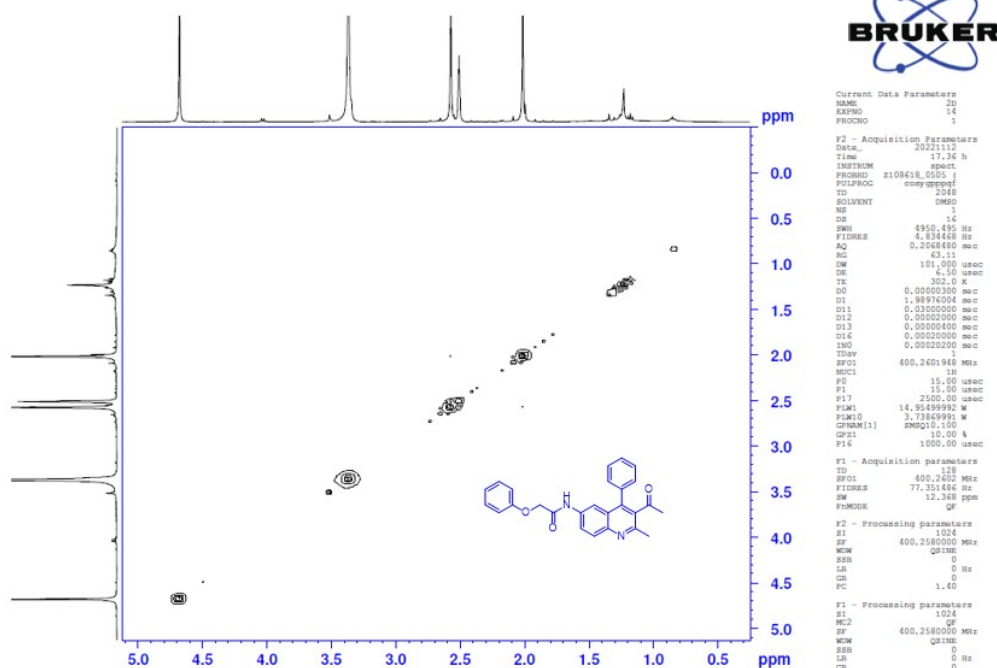


Fig.S80 Enlarged H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (61).

Signature SIF VIT VELLORE  
VN-035

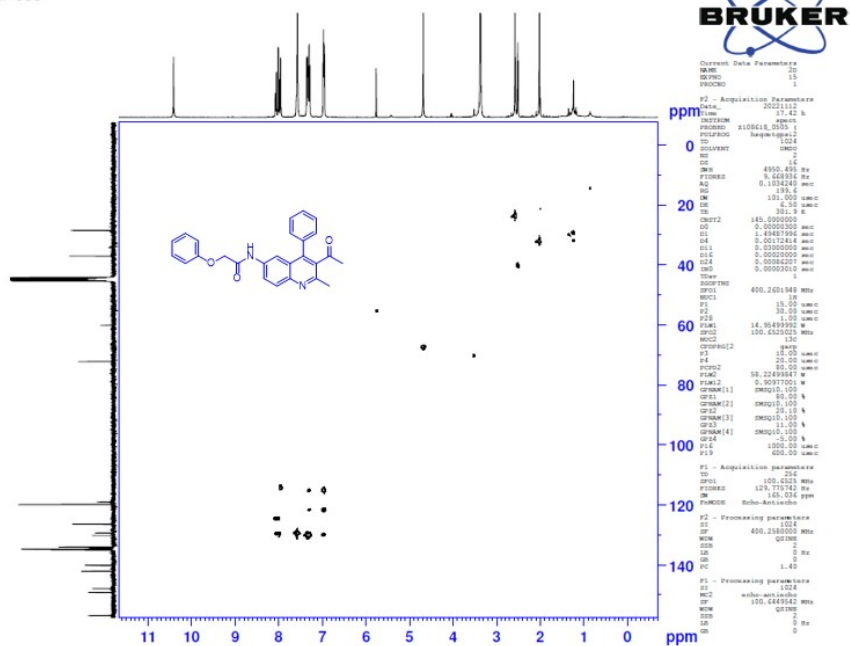


Fig.S81 HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (61).

Signature SIF VIT VELLORE  
VN-035

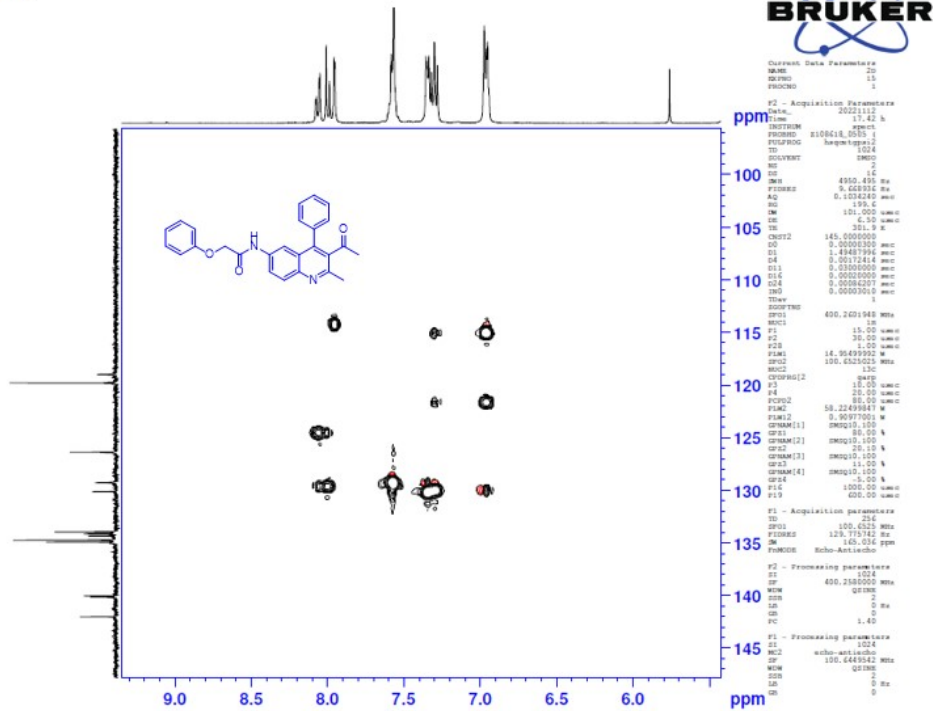


Fig.S82 Enlarged HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (61).

Signature SIF VIT VELLORE  
VN-035

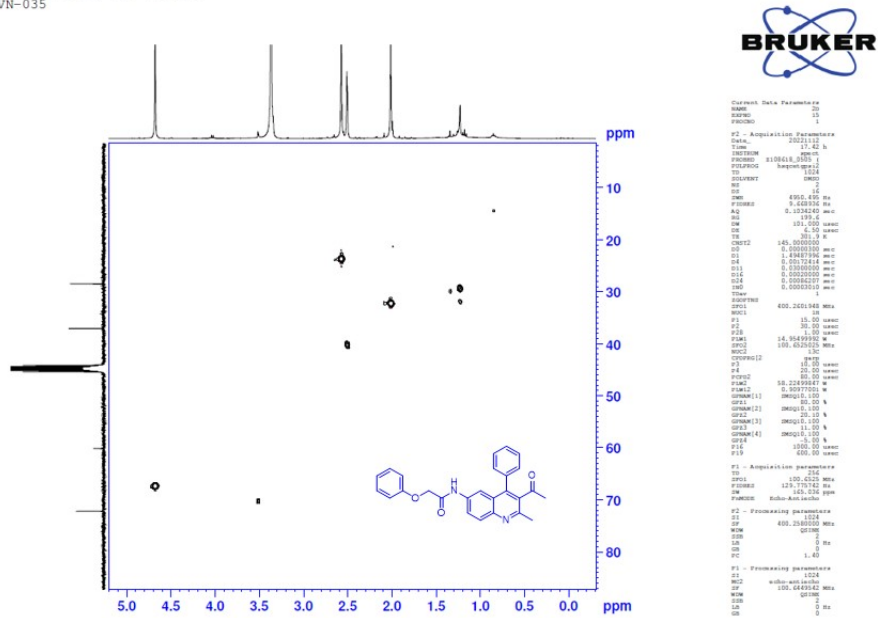


Fig.S83 Enlarged HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (61).

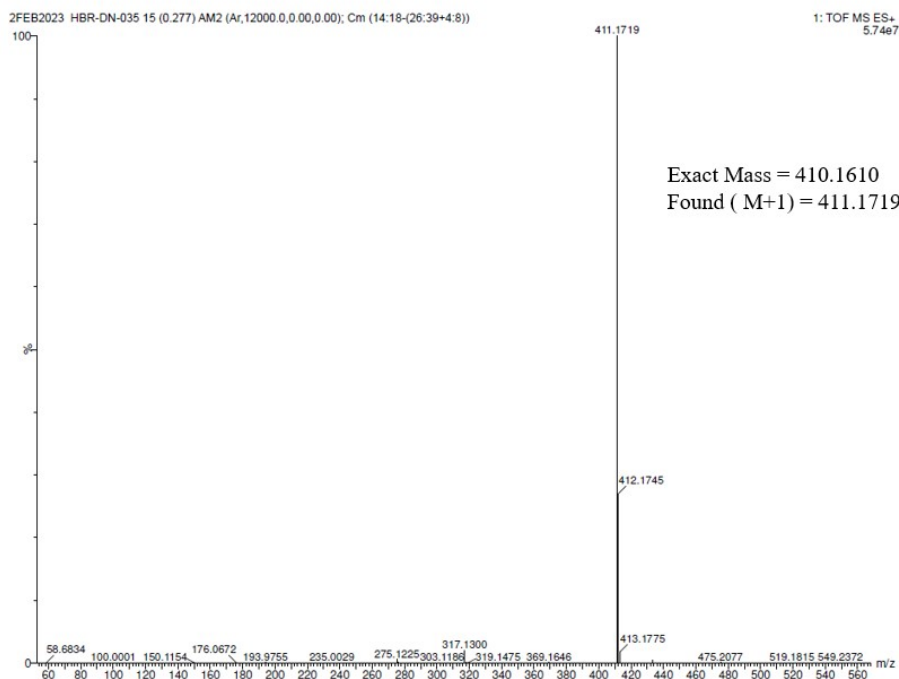


Fig.S84 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (6l).

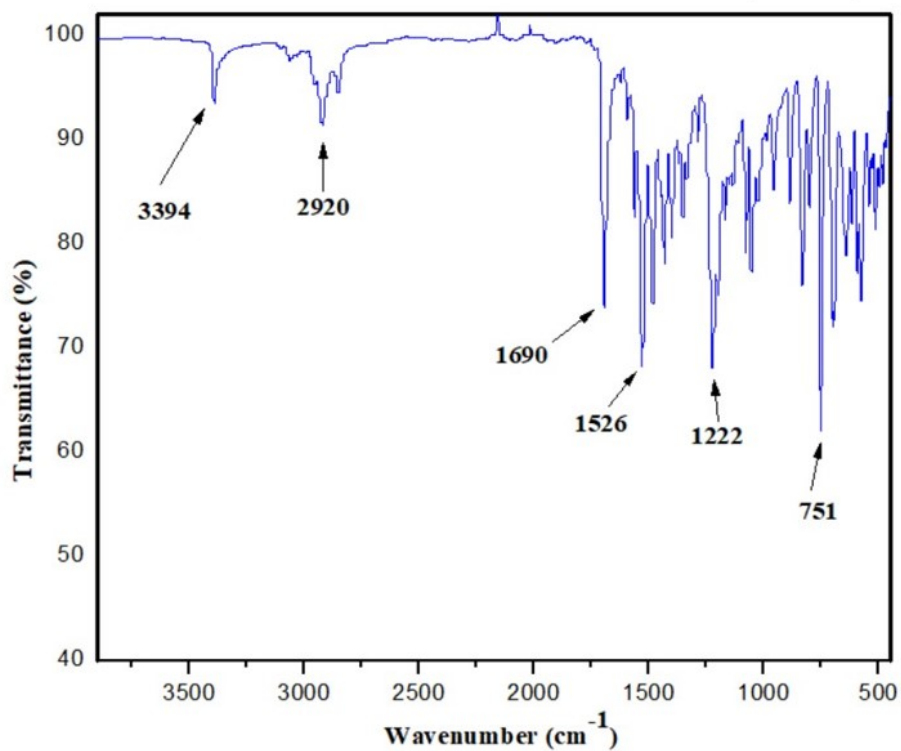
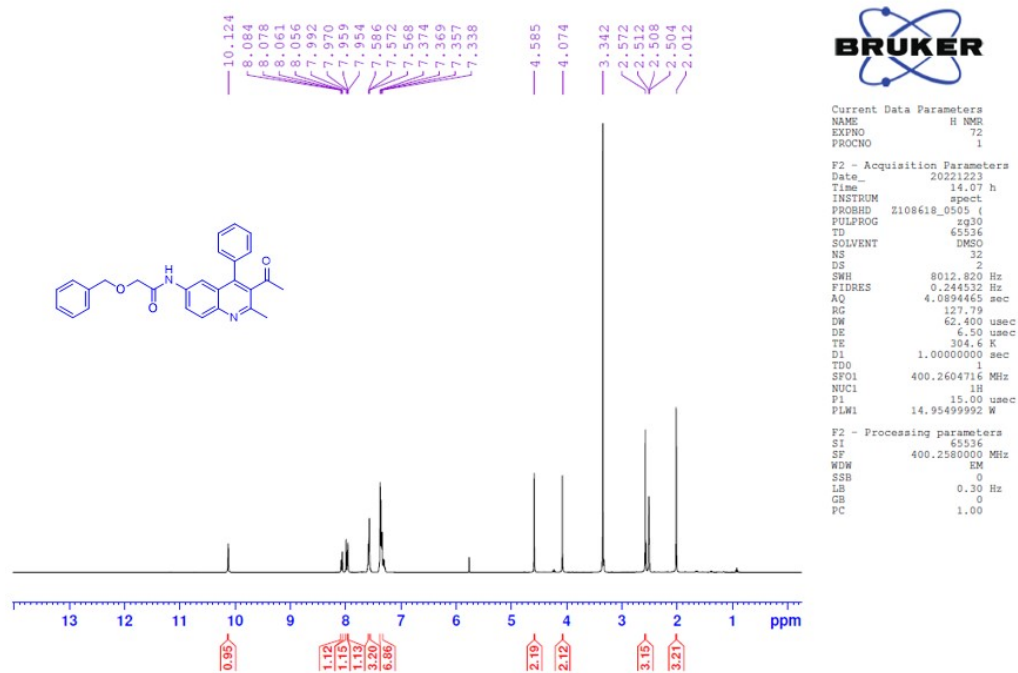
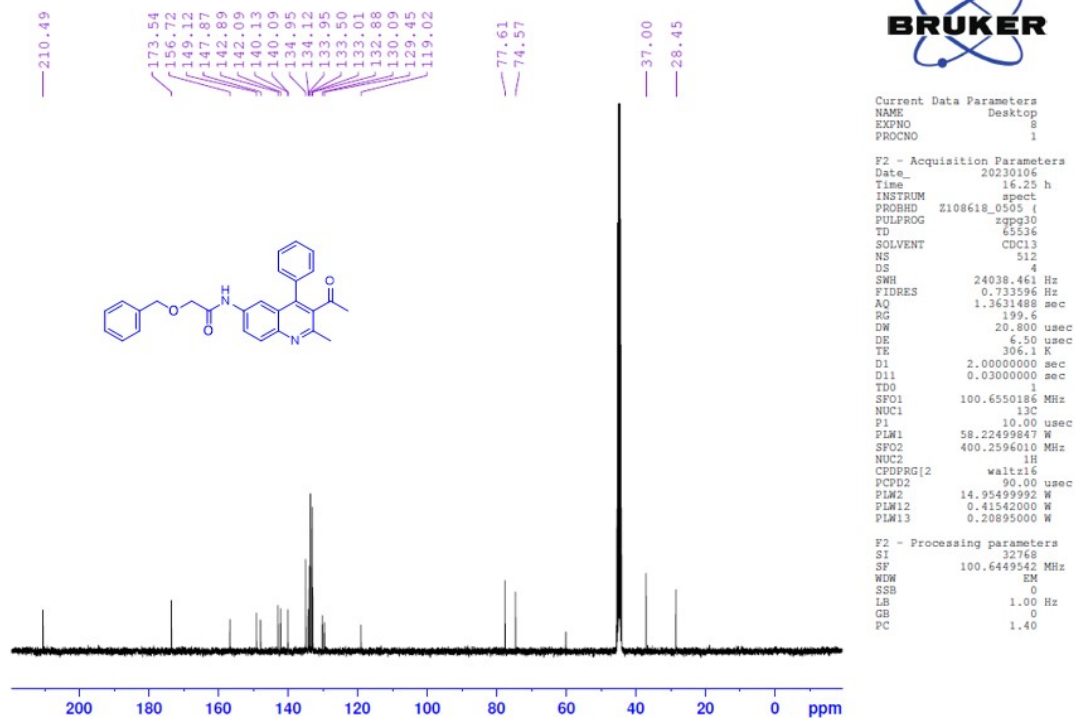


Fig.S85 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-phenoxyacetamide (6l).

VN-055

Fig.S86 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).Signature SIF VIT VELLORE  
VN-055Fig.S87 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).

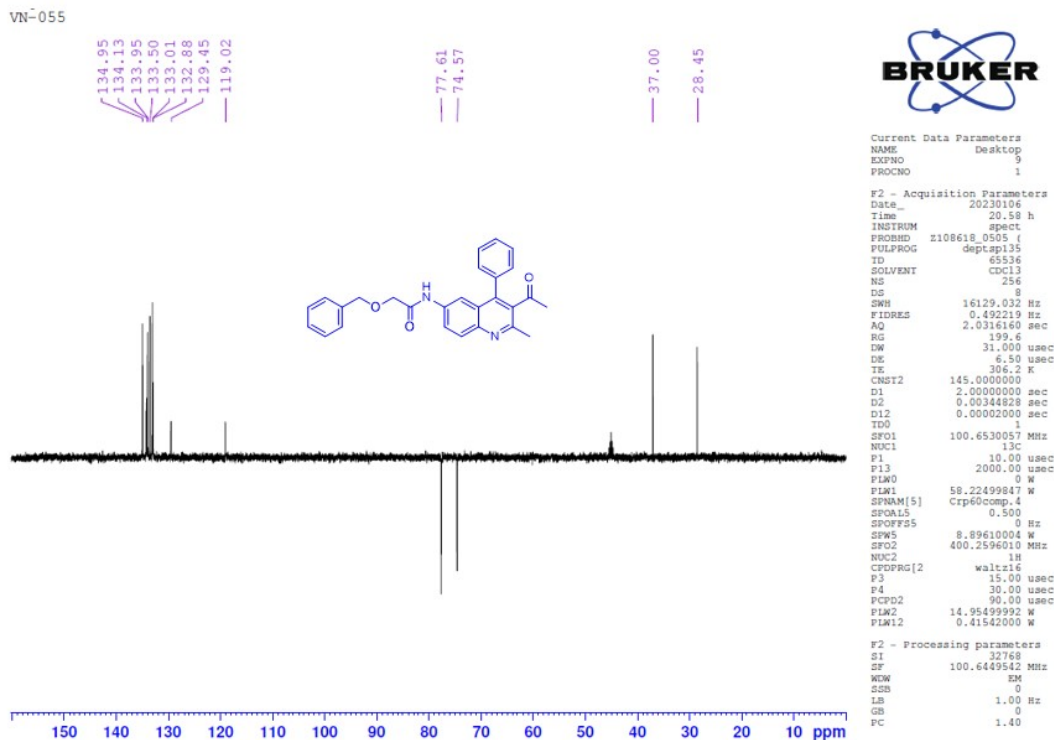


Fig.S88 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).

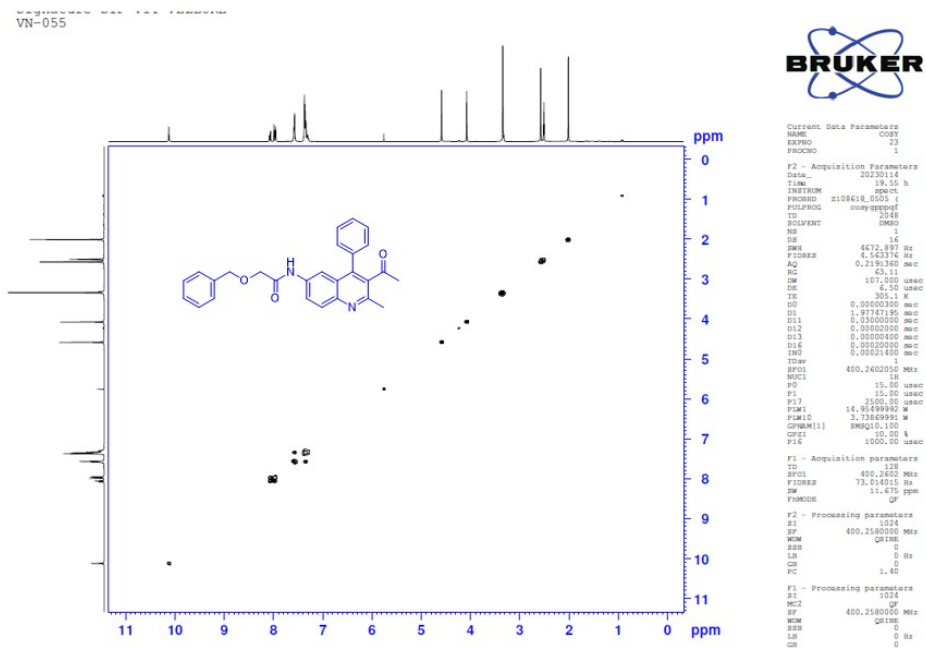


Fig.S89 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).

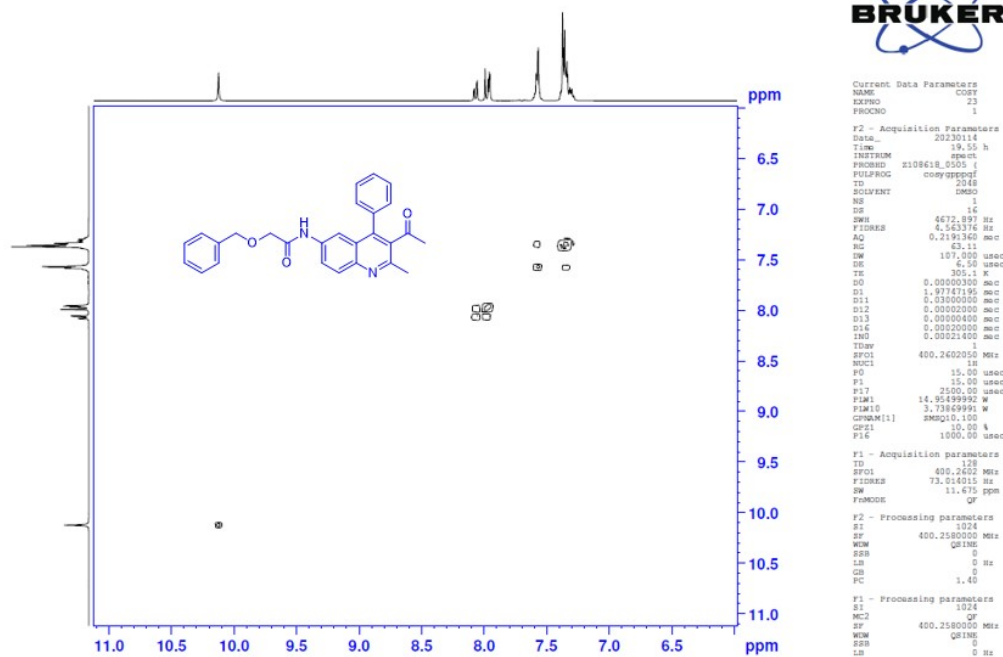


Fig.S90 Enlarged H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).

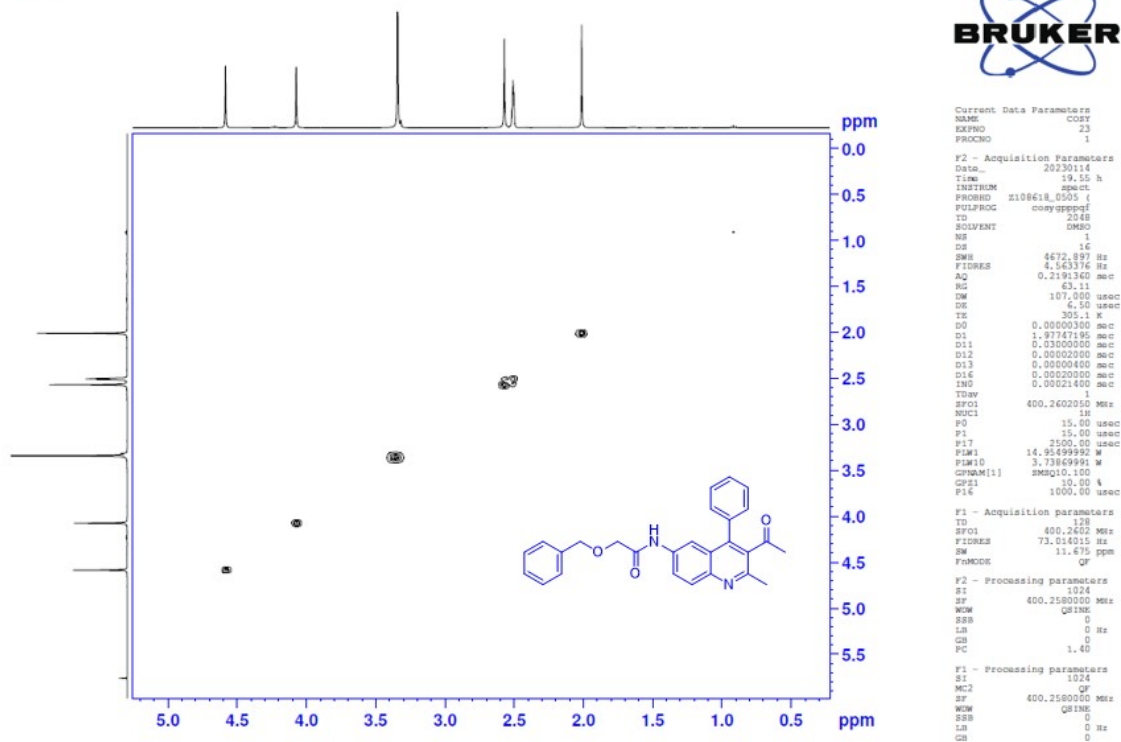


Fig.S91 Enlarged H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).

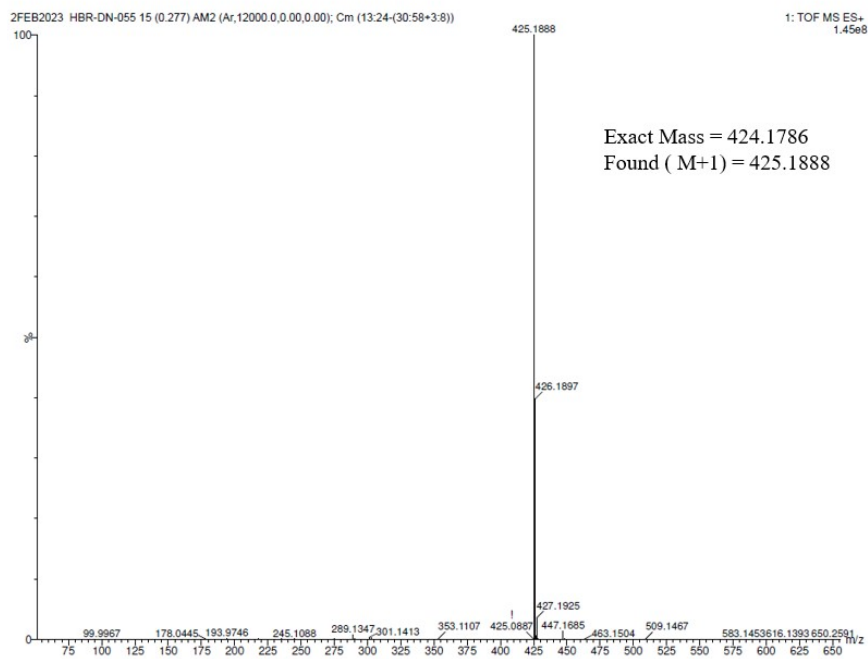


Fig.S92 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).

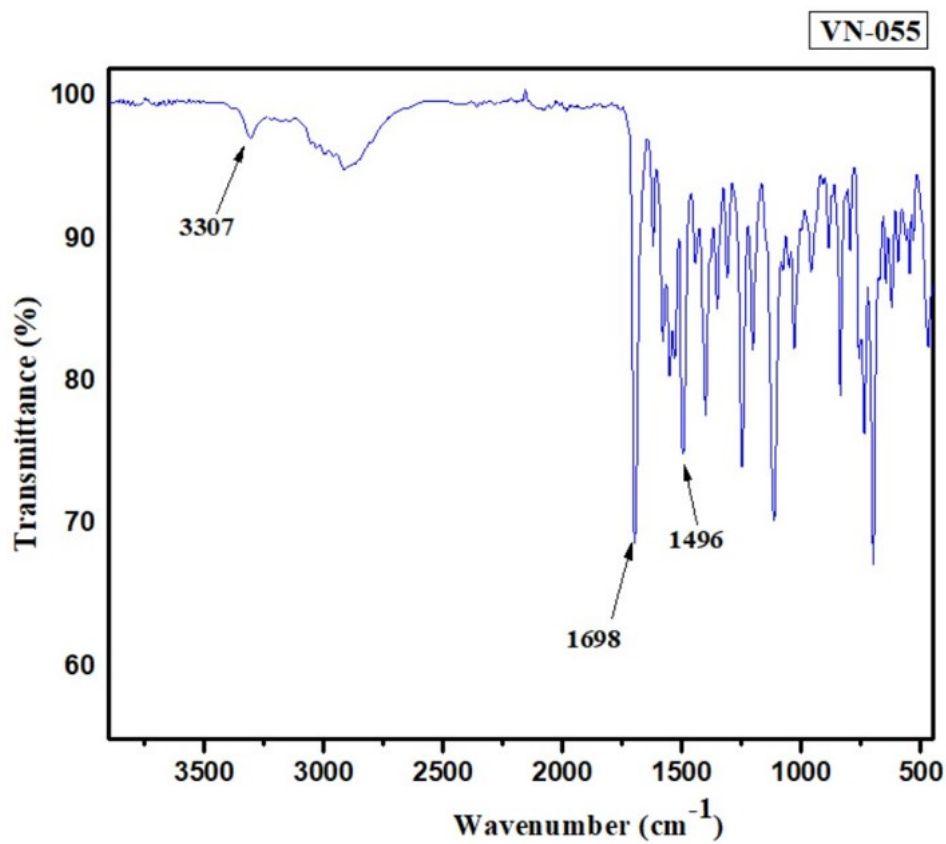


Fig.S93 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(benzyloxy)acetamide (6m).



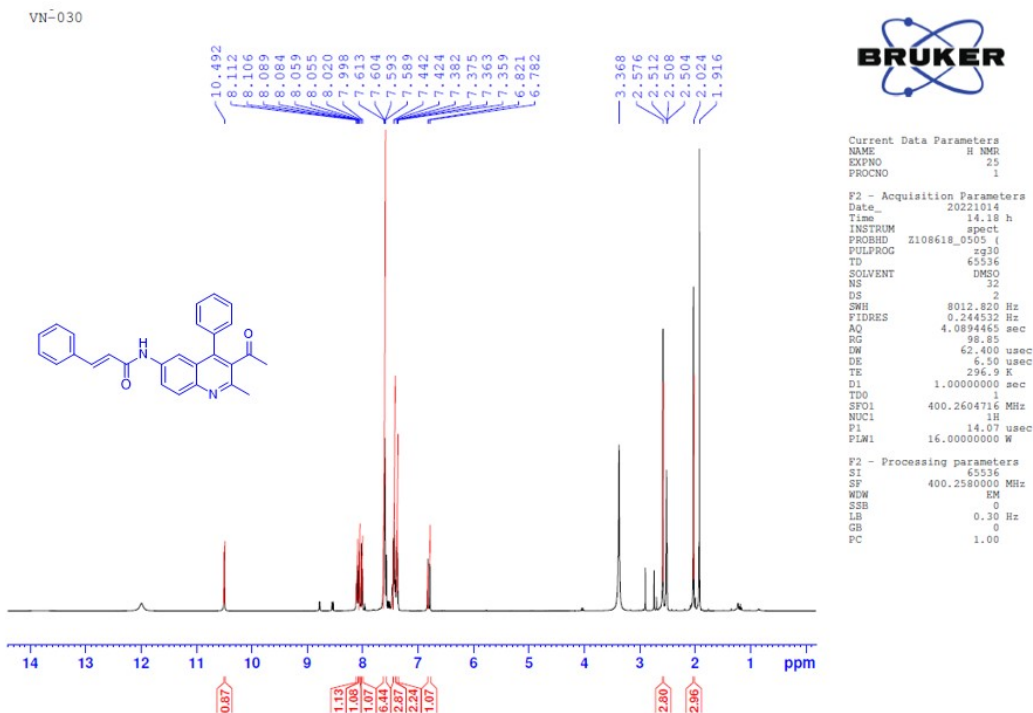


Fig.S94 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)cinnamamide (6n).

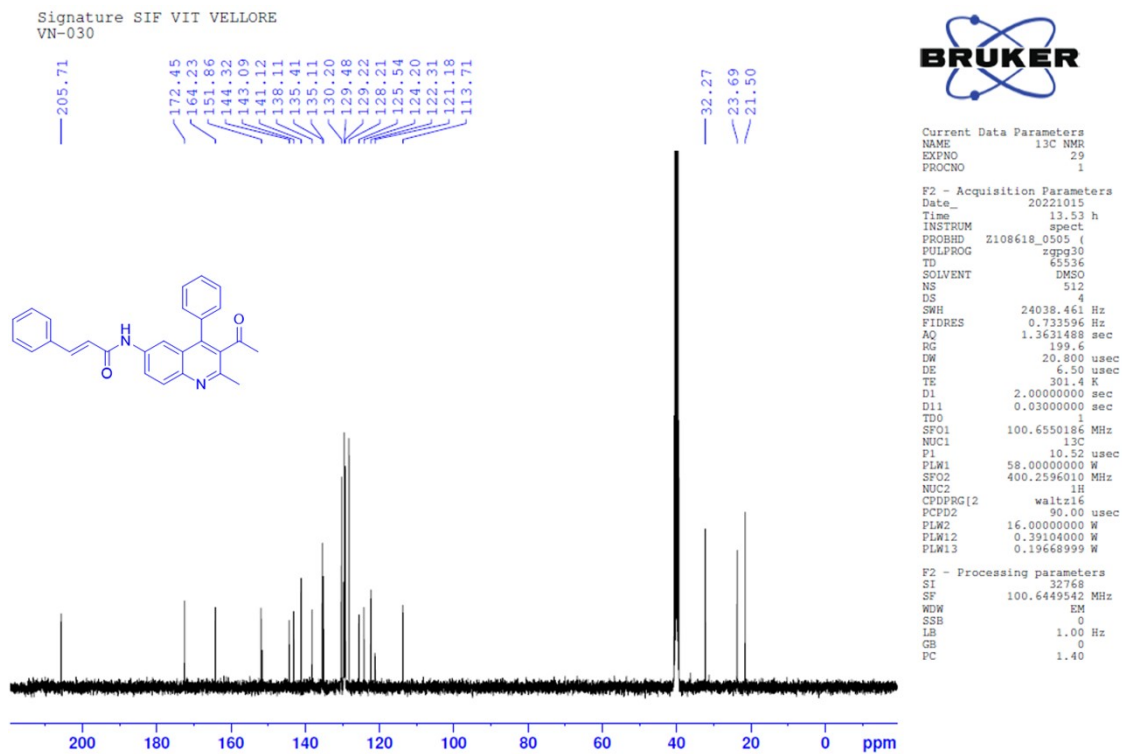
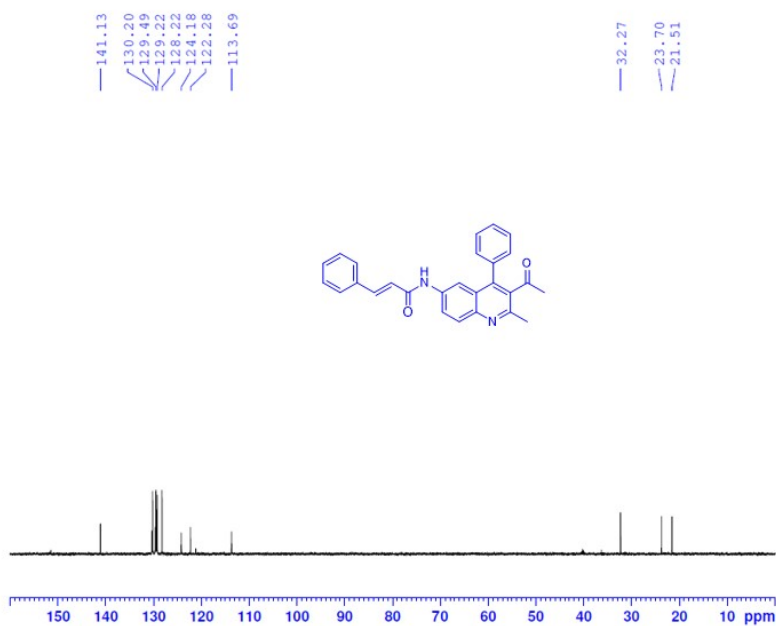


Fig.S95 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)cinnamamide (6n).

Signature SIF VIT VELLORE  
VN-030



Current Data Parameters  
 NAME DEPT-135  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230405  
 Time 4.33 h  
 INSTRUM spect  
 PROBHD Z108618\_0505 ( )  
 PULPROG deptapl135  
 TD 65536  
 SOLVENT DMSO  
 NS 256  
 DS 8  
 SWH 16129.032 Hz  
 FIDRES 0.492219 Hz  
 AQ 2.0316160 sec  
 RG 199.6  
 DW 31.000 usec  
 DE 6.50 usec  
 TE 303.7 K  
 CNST2 145.0000000  
 D1 2.0000000 sec  
 D2 0.0034828 sec  
 D12 0.00002000 sec  
 ID0 1  
 SFO1 100.6530057 MHz  
 NUCL1 13C  
 P1 10.00 usec  
 F13 2000.00 usec  
 PLW0 0 W  
 PLW1 58.22499847 W  
 SFOAL5 Ccp60comp.4  
 SFOAL5 0.500  
 SFOAL5 0 Hz  
 SPW5 8.89610004 W  
 SFO2 400.2596010 MHz  
 NUCL2 1H  
 CPDPRG2 waltz16  
 P3 15.00 usec  
 P4 30.00 usec  
 PCPD2 90.00 usec  
 PLW2 14.95499952 W  
 PLW12 0.41542000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6449542 MHz  
 NUX 64  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Fig.S96 DEPT-135 of NMR OF N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)cinnamamide (6n).

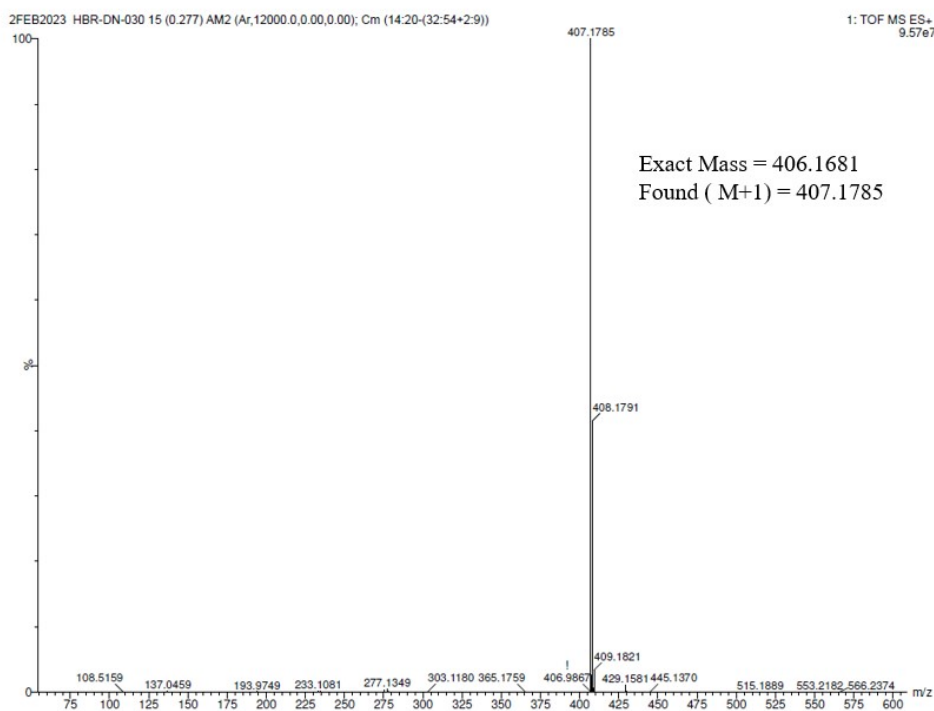


Fig.S97 HRMS OF NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)cinnamamide (6n).

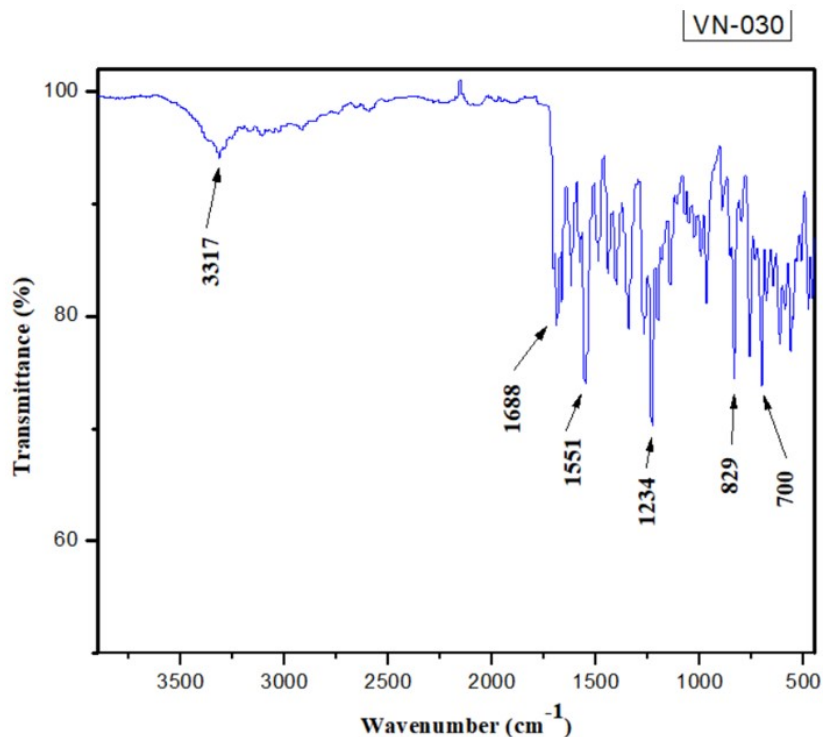


Fig.S98 FT-IR OF NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)cinnamamide (6n).

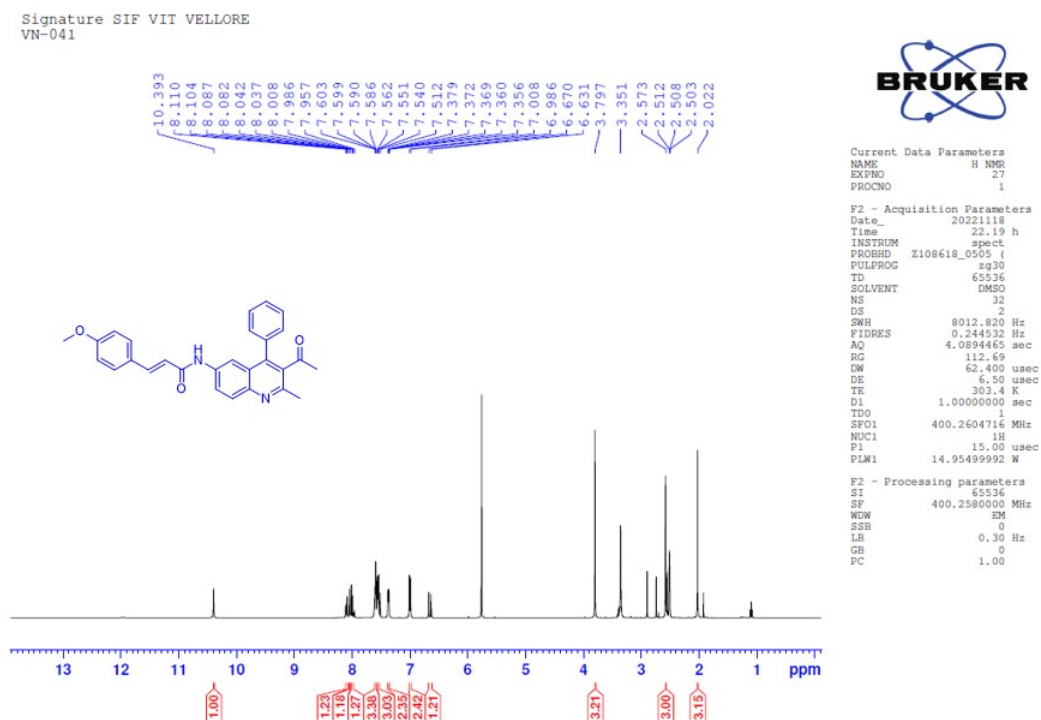
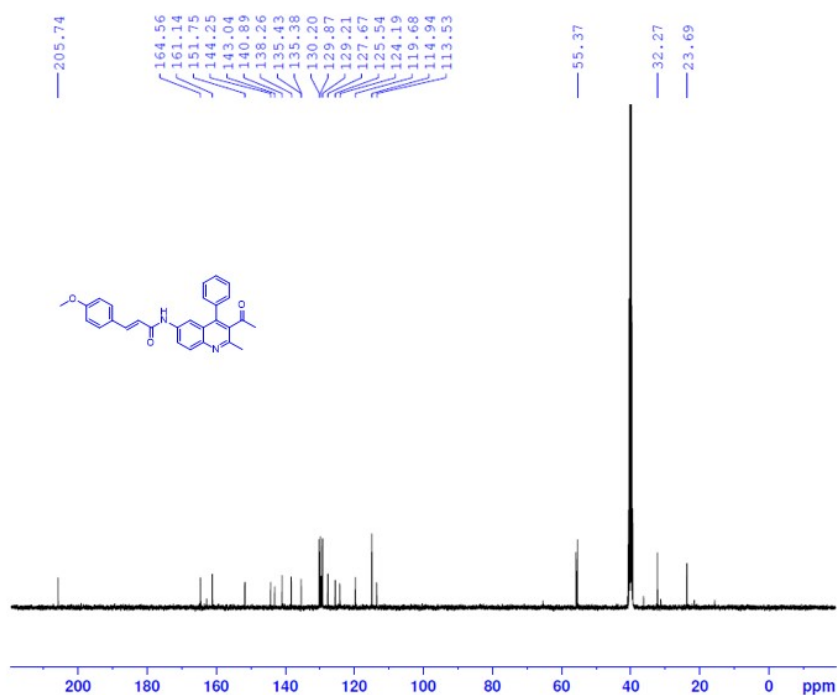


Fig.S99  $^1\text{H}$  NMR of (E)-N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-methoxyphenyl)acrylamide (6o).

Signature SIF VIT VELLORE  
VN-041



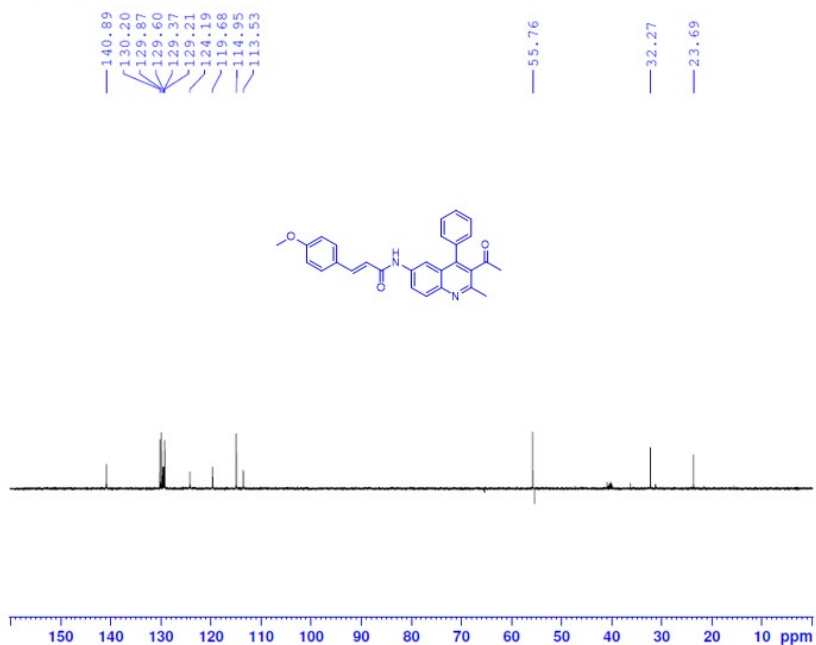
Current Data Parameters  
NAME 13 C NMR  
EXPNO 28  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221118  
Time 22.49 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.363188 sec  
RG 199.6  
DW 20.800 usec  
DE 6.50 usec  
TE 303.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6550186 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 58.22499847 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W  
PLW13 0.20895000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S100 <sup>13</sup>C NMR of (E)-N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-methoxyphenyl)acrylamide (6o).

Signature SIF VIT VELLORE  
VN-041



Current Data Parameters  
NAME DEPT-135  
EXPNO 29  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221118  
Time 23.09 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG deptsp135  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 8  
SWH 16129.032 Hz  
FIDRES 0.492219 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DE 6.50 usec  
TE 303.7 K  
CNST2 145.0000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1  
SFO1 100.6530057 MHz  
NUC1 13C  
P1 10.00 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 58.22499847 W  
SPNAM[5] Crp60comp.4  
SFOAL5 0.500  
SFOFSS5 0 Hz  
SPW5 8.89610004 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
P3 15.00 usec  
P4 30.00 usec  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S101 DEPT-135 of (E)-N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-methoxyphenyl)acrylamide (6o).

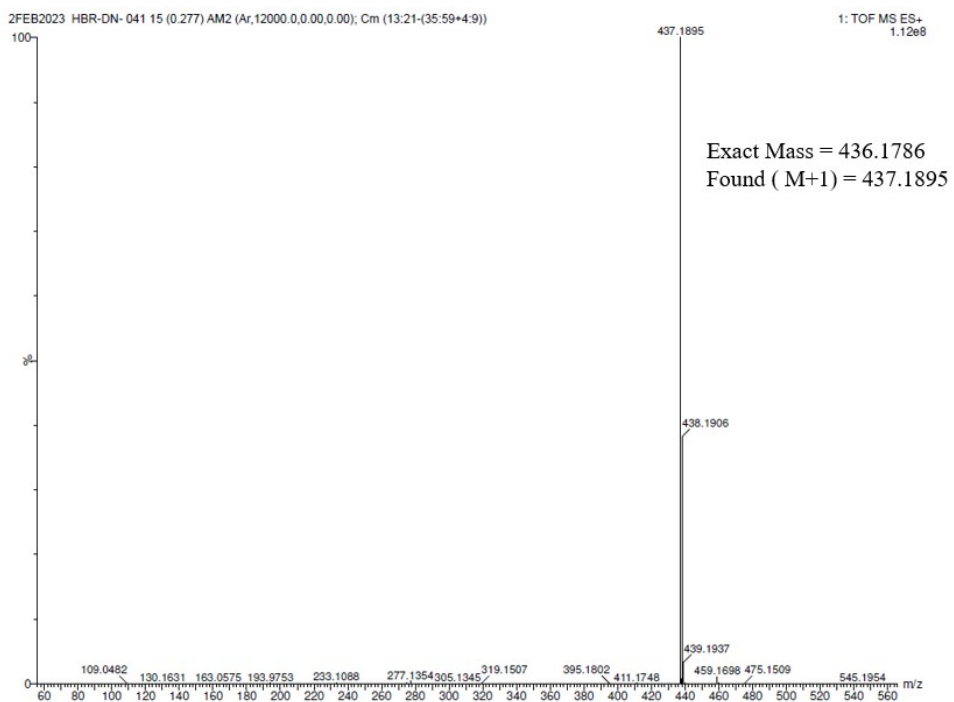


Fig.S102 HRMS of (E)-N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-methoxyphenyl)acrylamide (6o).

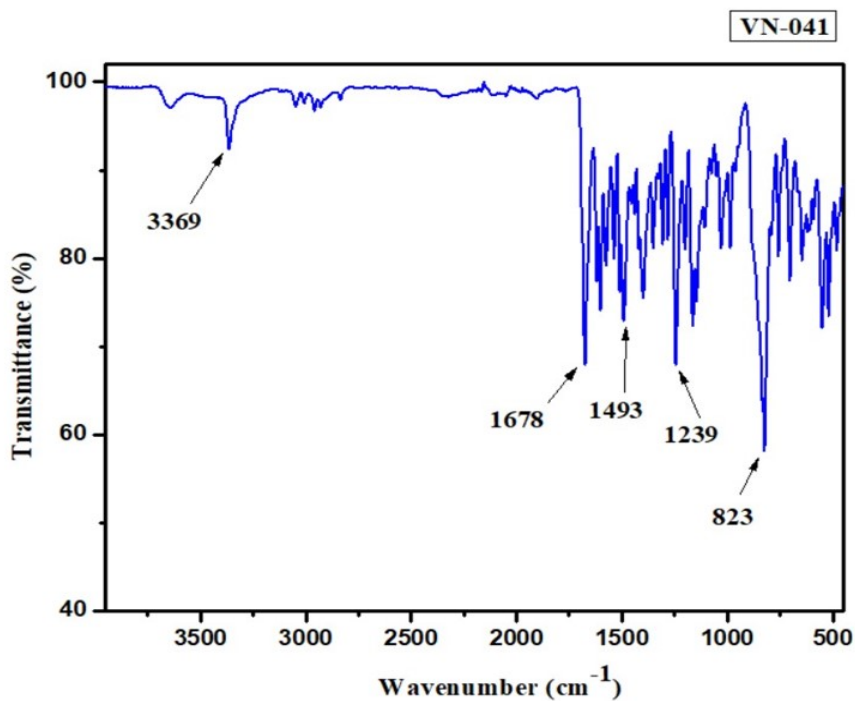
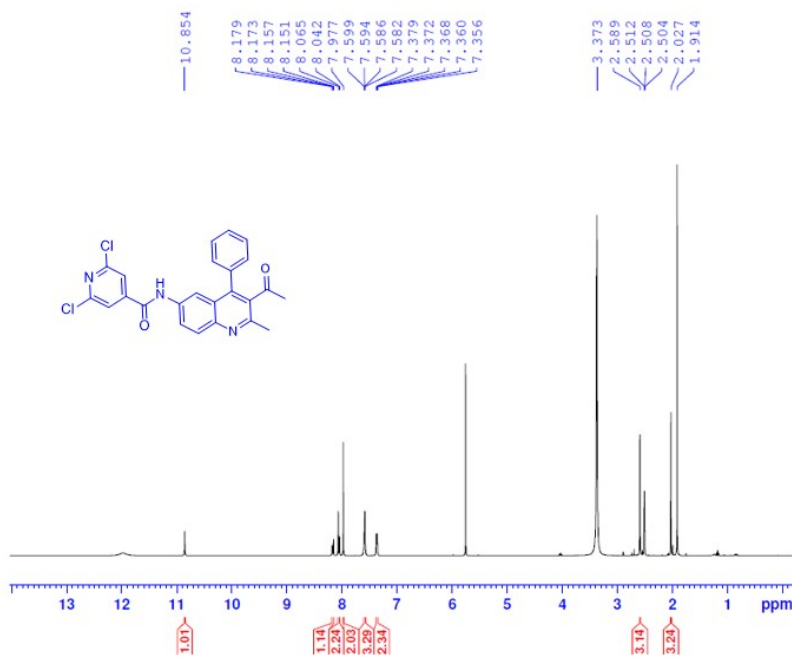


Fig.S103 FT-IR of (E)-N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-(4-methoxyphenyl)acrylamide (6o).

Signature SIF VIT VELLORE  
VN-039



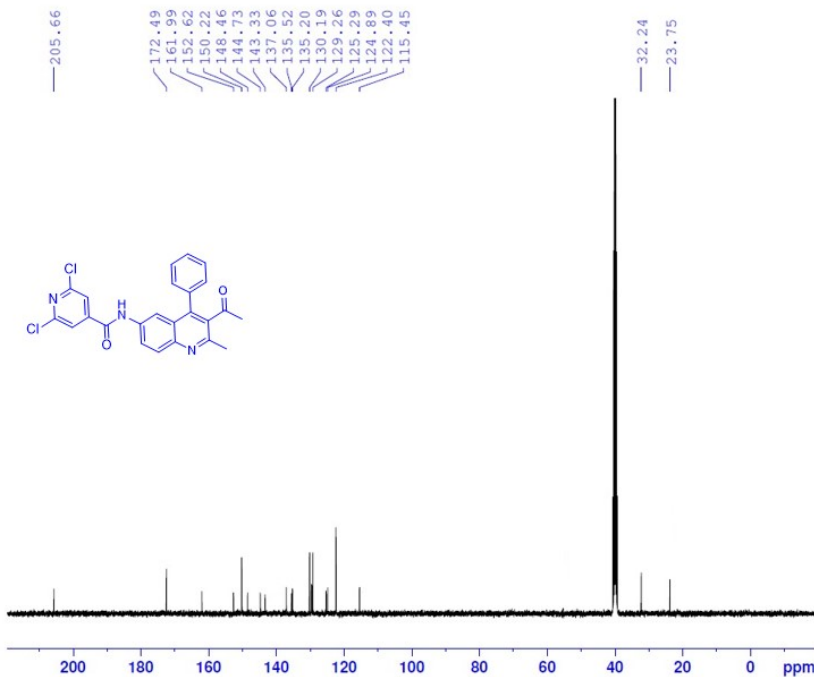
Current Data Parameters  
NAME H NMR  
EXPNO 18  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221115  
Time 16.56 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 98.85  
DW 62.400 usec  
DE 6.50 usec  
TE 302.7 K  
D1 1.00000000 sec  
TDO 1  
SFO1 400.2604716 MHz  
NUC1 1H  
P1 15.00 usec  
PLW1 14.95499992 W

F2 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Fig.S104 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).

Signature SIF VIT VELLORE  
VN-039



Current Data Parameters  
NAME 13 C NMR  
EXPNO 19  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221116  
Time 8.37 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 199.6  
DW 20.800 usec  
DE 6.50 usec  
TE 303.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1  
SFO1 100.6550186 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 58.22499847 W  
SFO2 400.2596010 MHz  
NUC2 1H  
PCPDG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W  
PLW13 0.20895000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S105 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).

Signature SIF VIT VELLORE  
VN-039

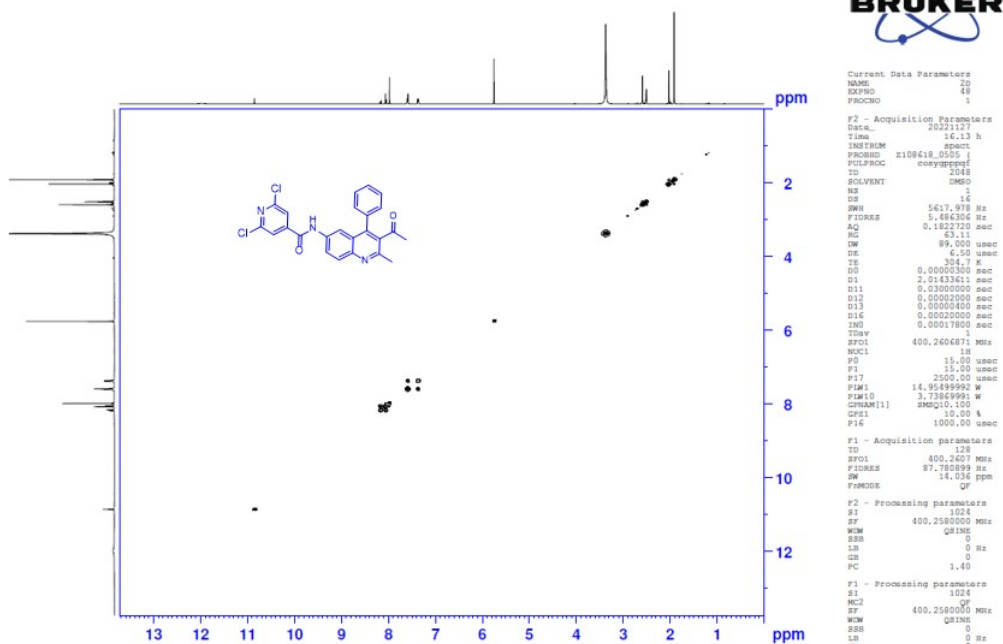


Fig.S106 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).

Signature SIF VIT VELLORE  
VN-039

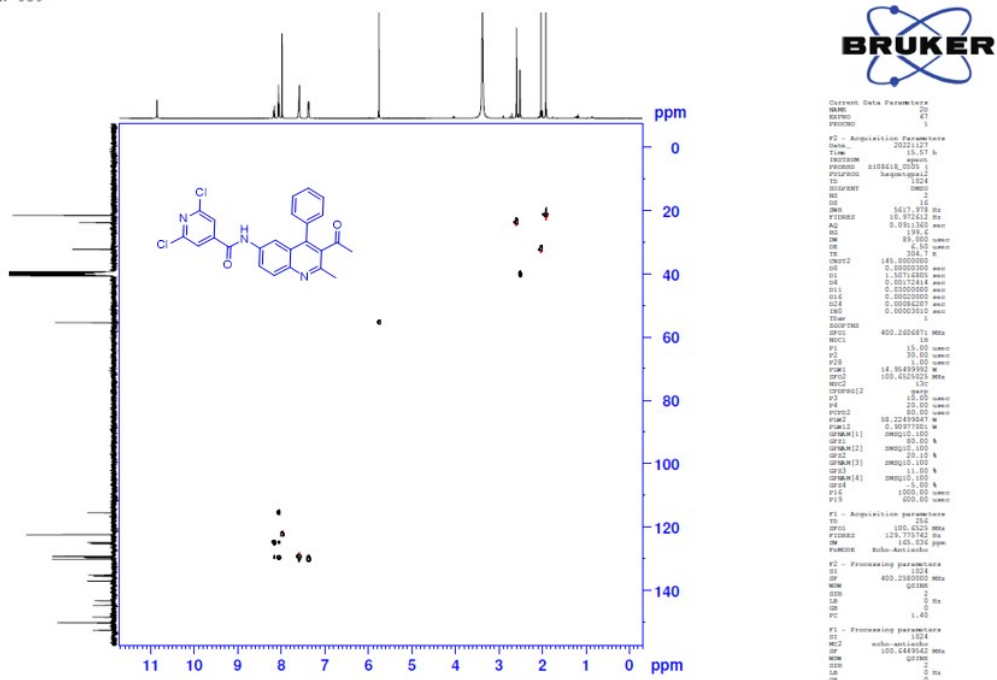


Fig.S107 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).

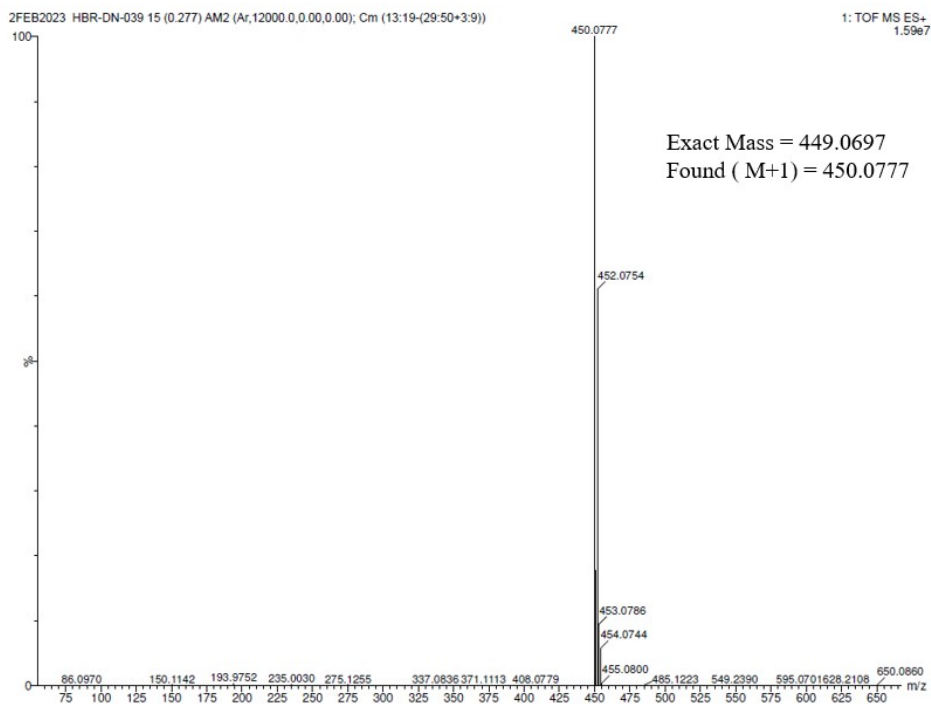


Fig.S108 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).

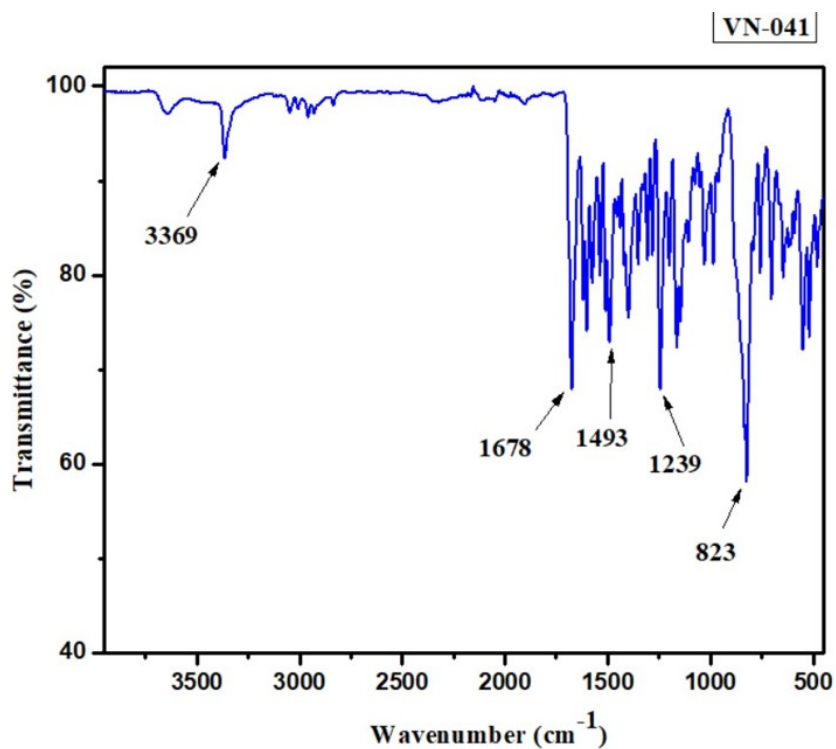


Fig.S109 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2,6-dichloroisonicotinamide (6p).



Signature SIF VIT VELLORE  
VN-046

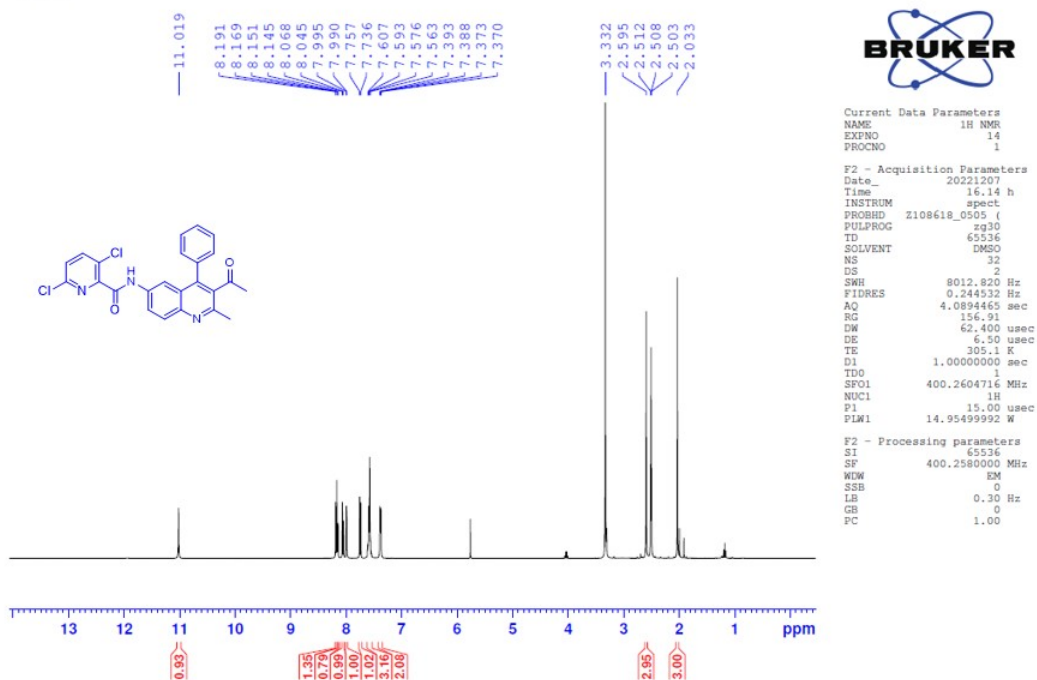


Fig.S110 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,6-dichloropicolinamide (6q).

Signature SIF VIT VELLORE  
VN-046

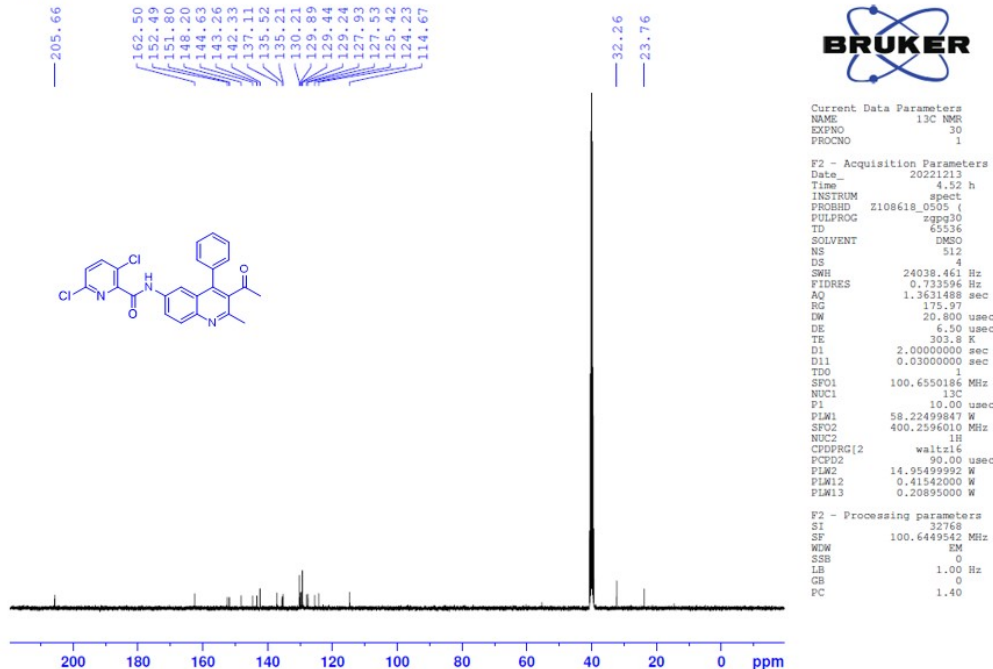
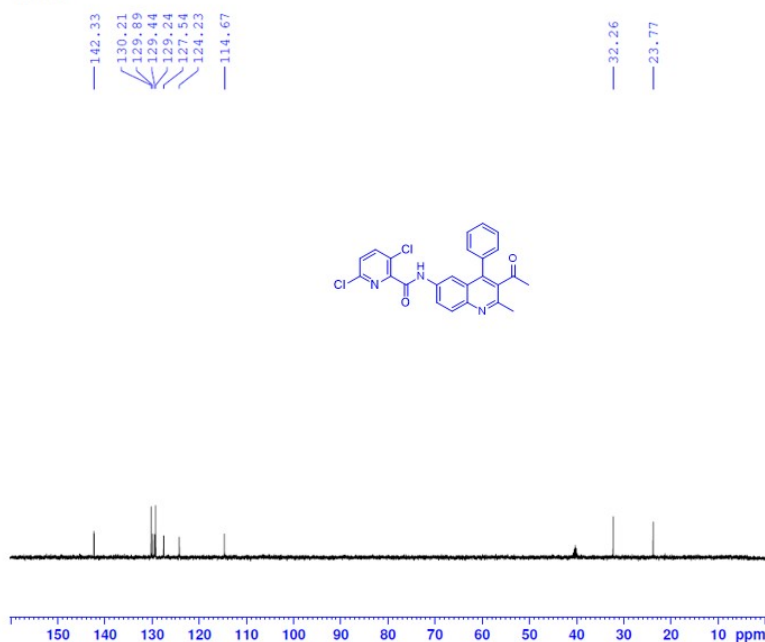


Fig.S111 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,6-dichloropicolinamide (6q).

Signature SIF VIT VELLORE  
VN-046



Current Data Parameters  
NAME DEPT-135  
EXFNO 31  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221213  
Time\_ 5.12 h  
INSTRUM spect  
PROBHD z108618\_0505 (   
PULPROG deptsp135  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 8  
SWH 16129.032 Hz  
FIDRES 0.49219 Hz  
AQ 2.0316160 sec  
RG 199.6  
DM 31.000 usec  
DE 6.50 usec  
TE 303.4 K  
CNST2 145.0000000  
D1 2.0000000 sec  
D2 0.00348028 sec  
D12 0.00002000 sec  
TD0 1  
SFO1 100.6530057 MHz  
NUC1 13C  
P1 10.00 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 58.22499847 W  
SPNAM[5] Crp60comp.4  
SFOAL5 0.500  
SFOFF5 0 Hz  
SFW5 8.89610004 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
P3 15.00 usec  
P4 30.00 usec  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SGB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S112 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,6-dichloropicolinamide (6q).

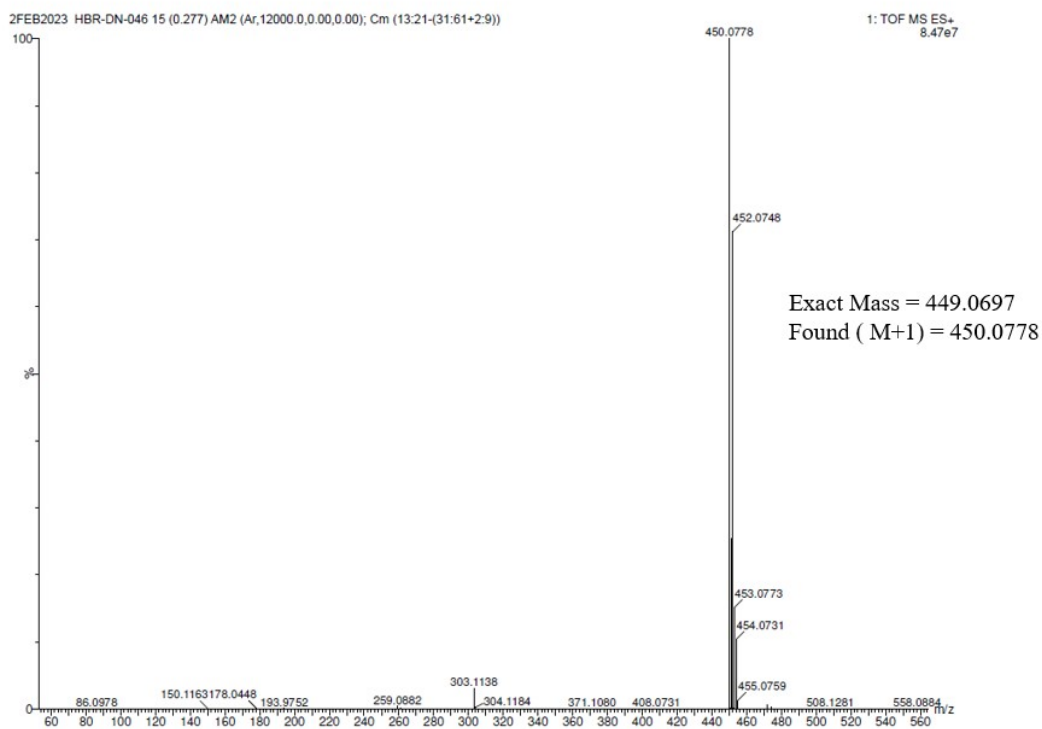


Fig.S113 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,6-dichloropicolinamide (6q).

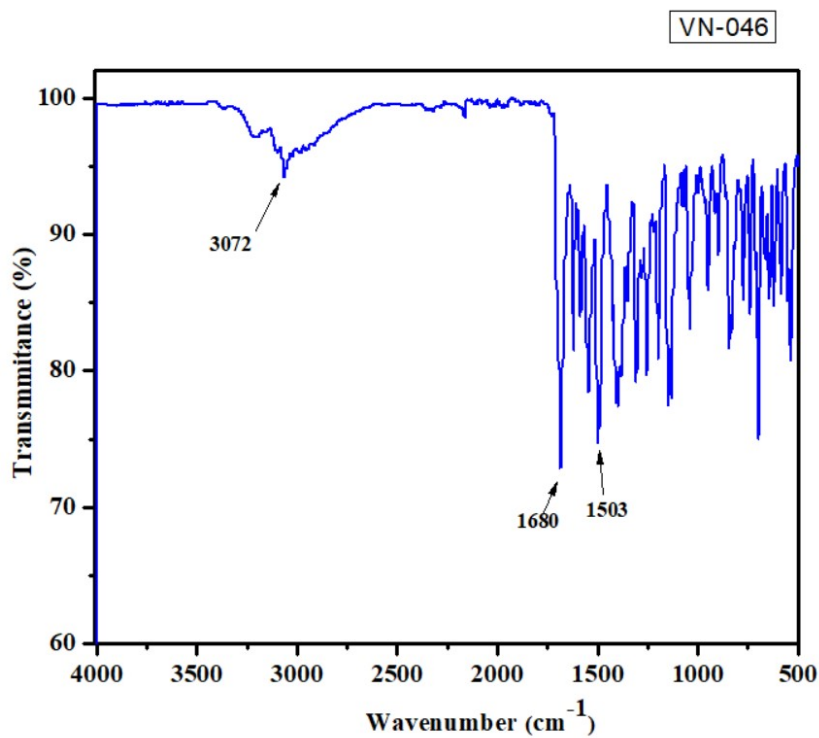


Fig.S114 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,6-dichloropicolinamide (6q).

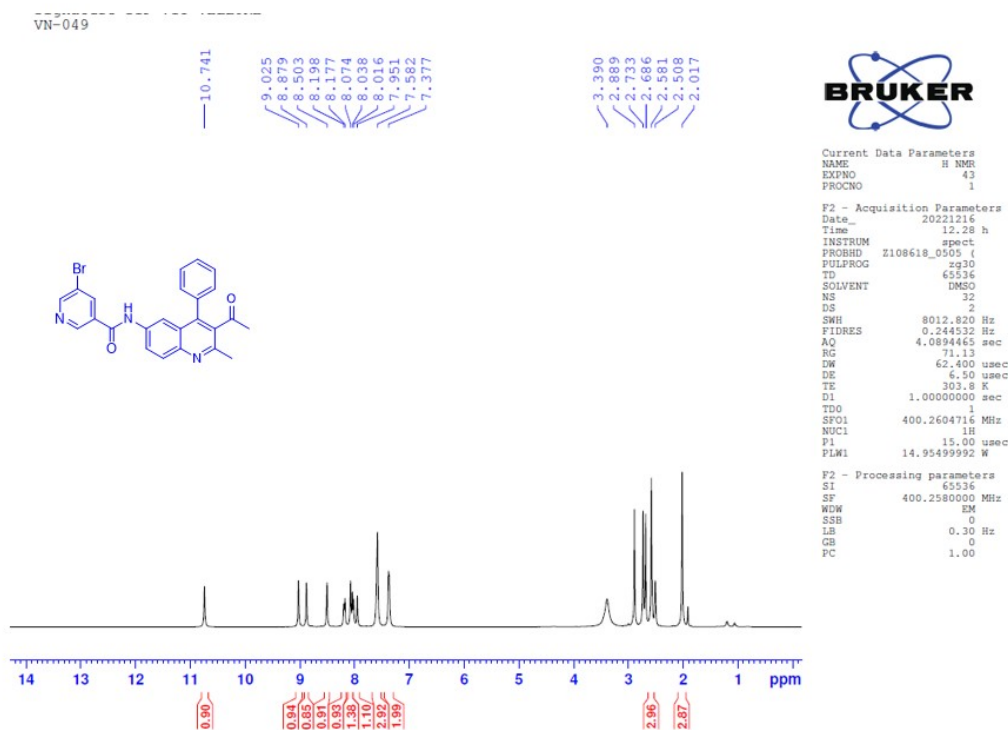


Fig.S115 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-bromonicotinamide (6r).

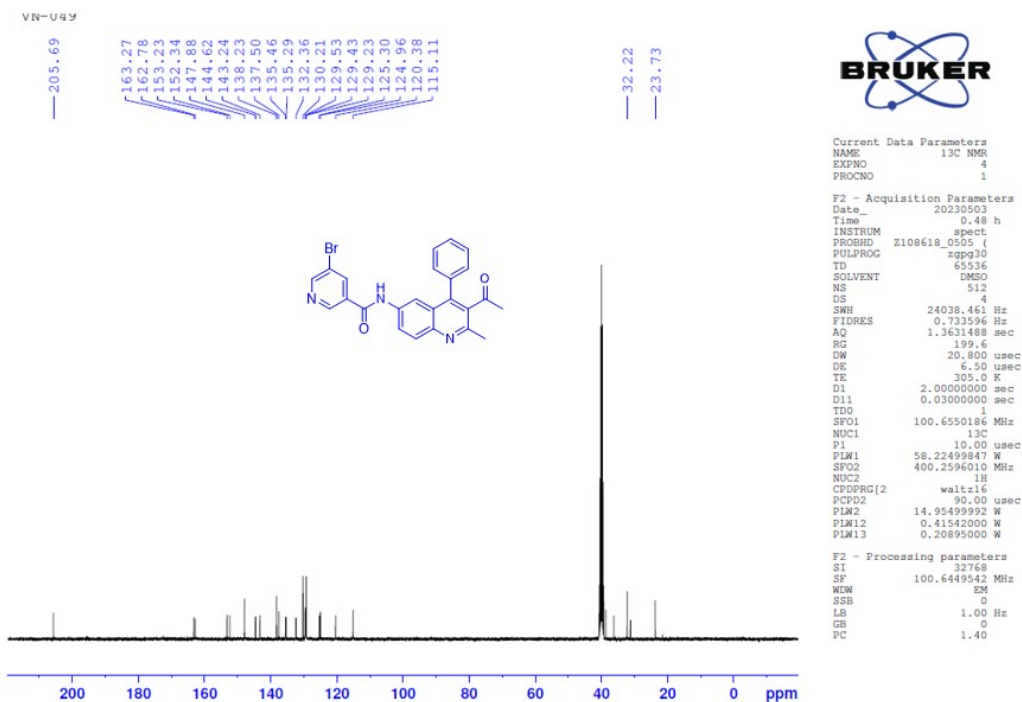


Fig.S116  $^{13}\text{C}$  NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-bromonicotinamide (6r).

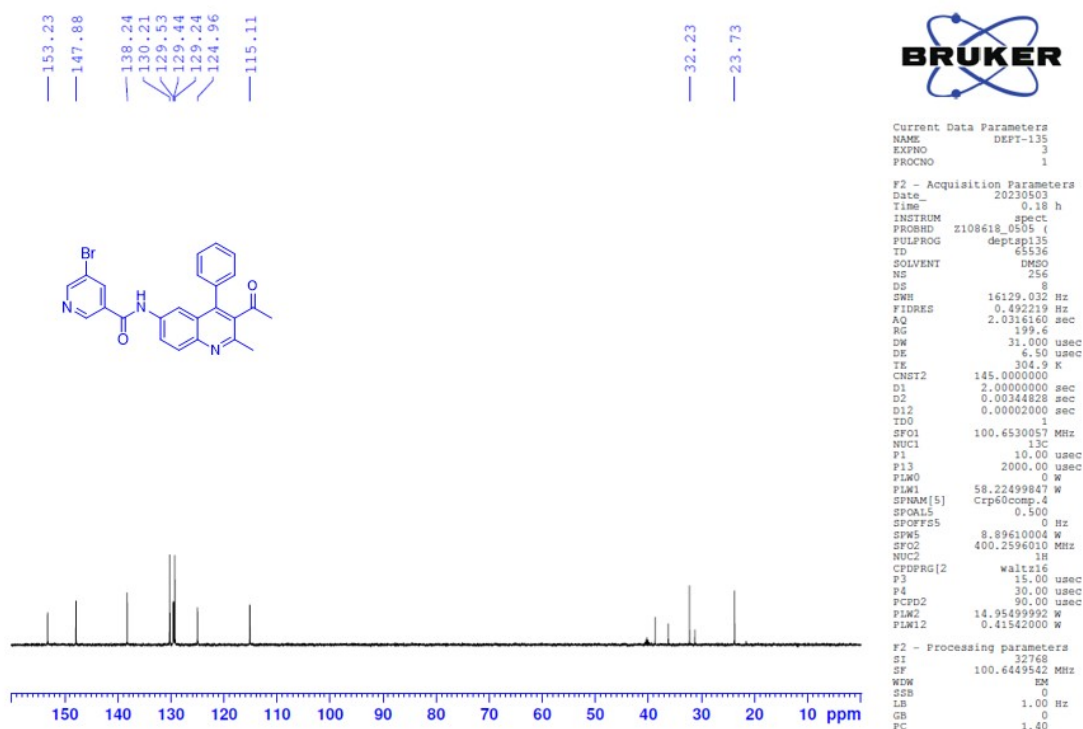


Fig.S117 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-bromonicotinamide (6r).

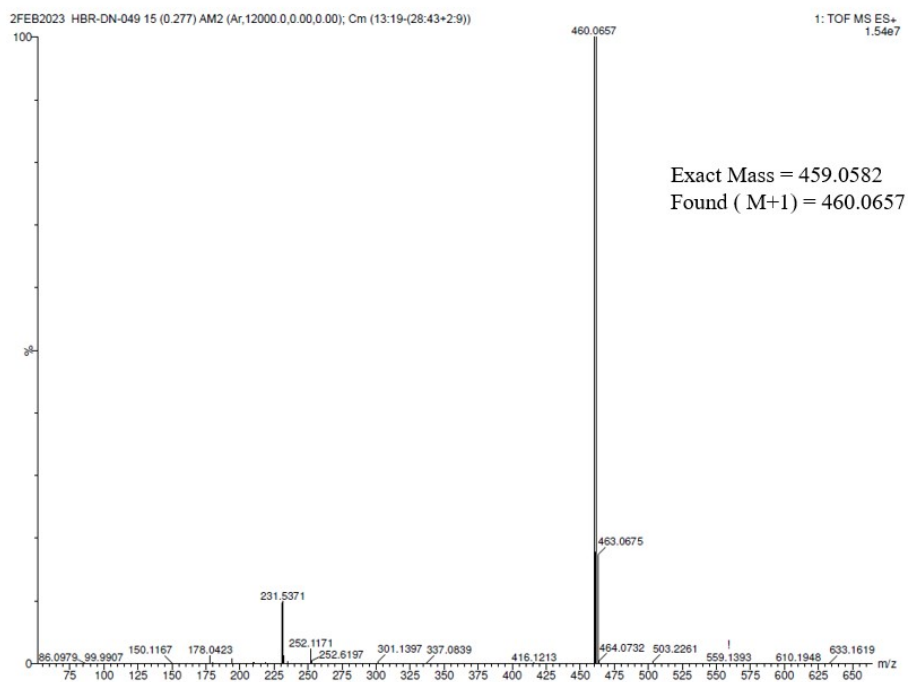


Fig.S118 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-bromonicotinamide (6r).

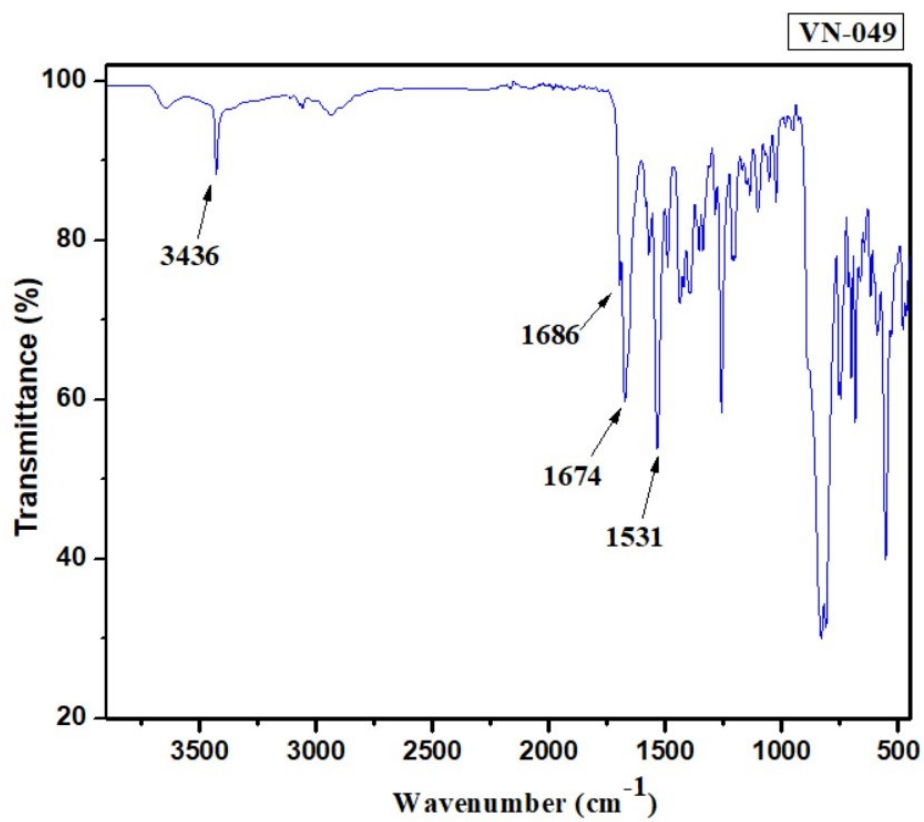


Fig.S119 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-bromonicotinamide (6r).

Signature SIF VIT VELLORE  
VN-031

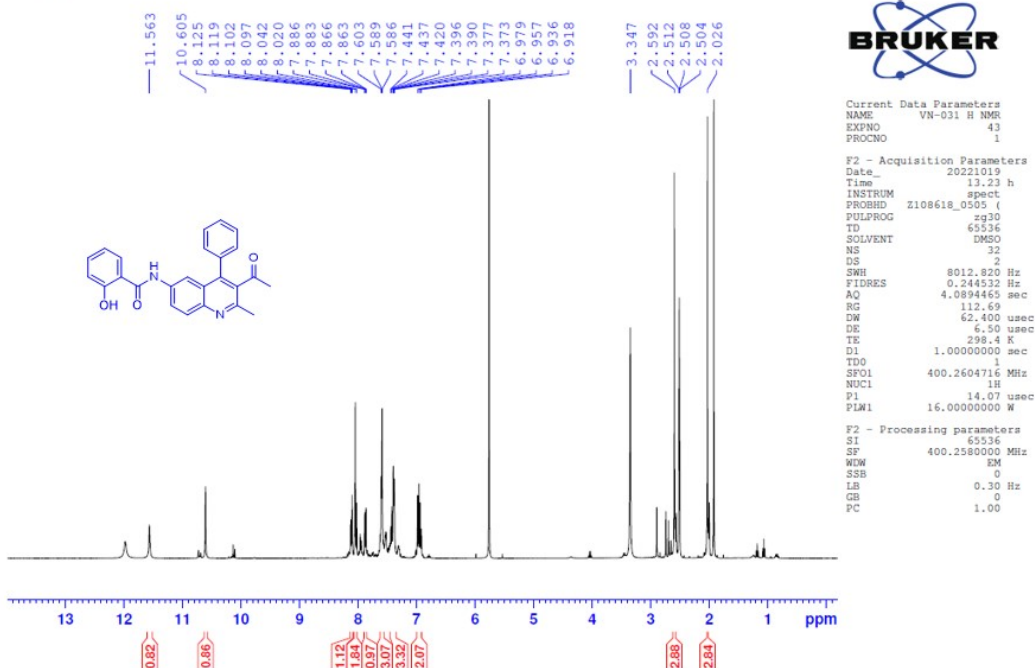


Fig.S120 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).

Signature SIF VIT VELLORE  
VN-031

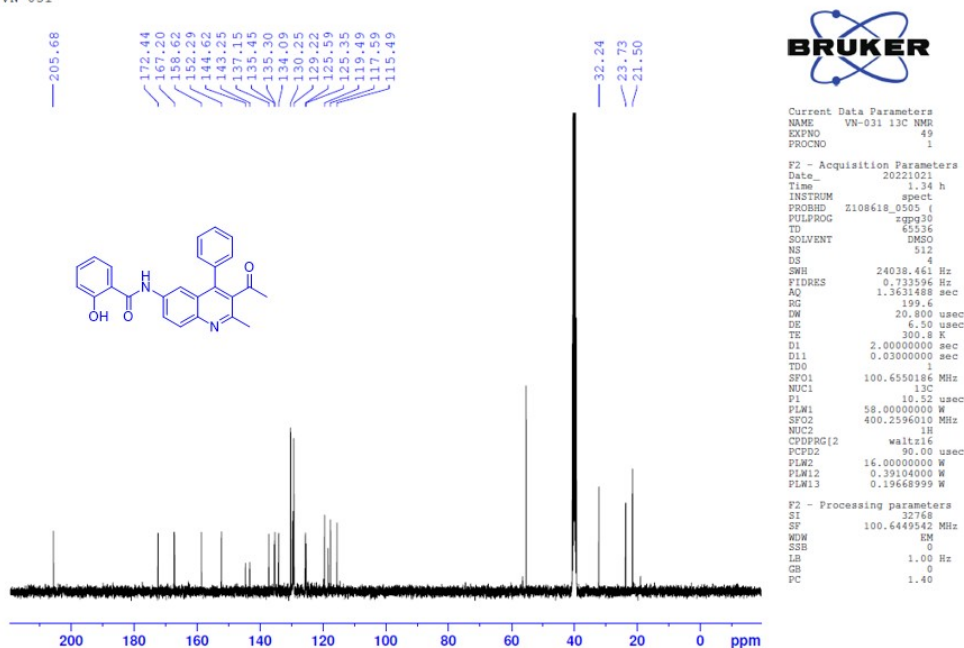
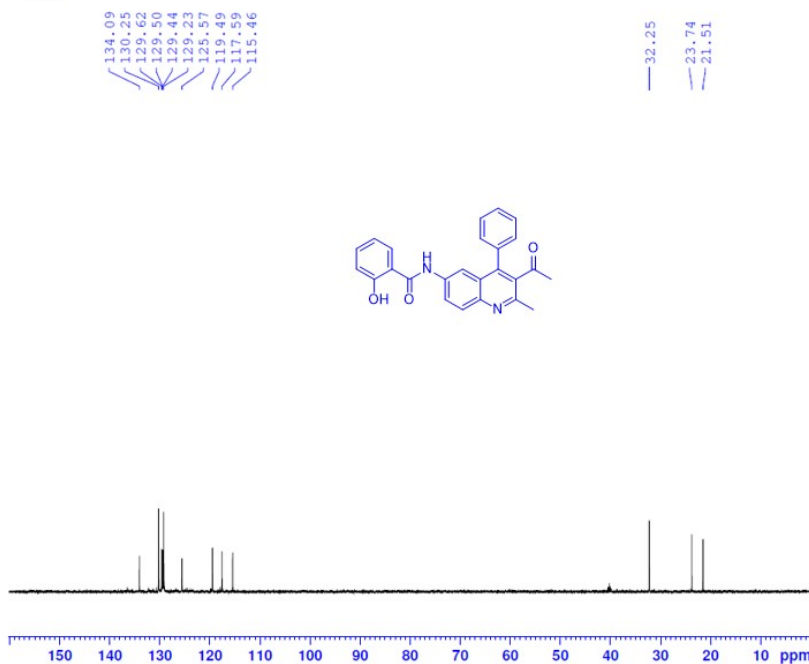


Fig.S121 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).

Signature SIF VIT VELLORE  
VN-031



Current Data Parameters  
NAME DEPT-135  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230406  
Time 16.18 h  
INSTRUM spect  
PROBHD z108618\_0505 f  
PULPROG deptspl35  
ID 65536  
SOLVENT DMSO  
NS 256  
DS 8  
SWH 16129.032 Hz  
FIDRES 0.492219 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DK 6.50 usec  
TE 304.0 K  
CNST2 145.0000000  
D1 2.00000000 sec  
D2 0.0034828 sec  
D12 0.00002000 sec  
TD0 1  
SFO1 100.6530057 MHz  
NUC1 13C  
P1 10.00 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 58.22499847 W  
SPNAM[5] Ccp60comp.4  
SFO15 0.500  
SPOFF55 0 Hz  
SPW5 8.89610004 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPOPRG[2] waltz16  
P3 15.00 usec  
P4 30.00 usec  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W

F2 - Processing parameters  
SI 32768  
SF 100.6448942 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S122 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).

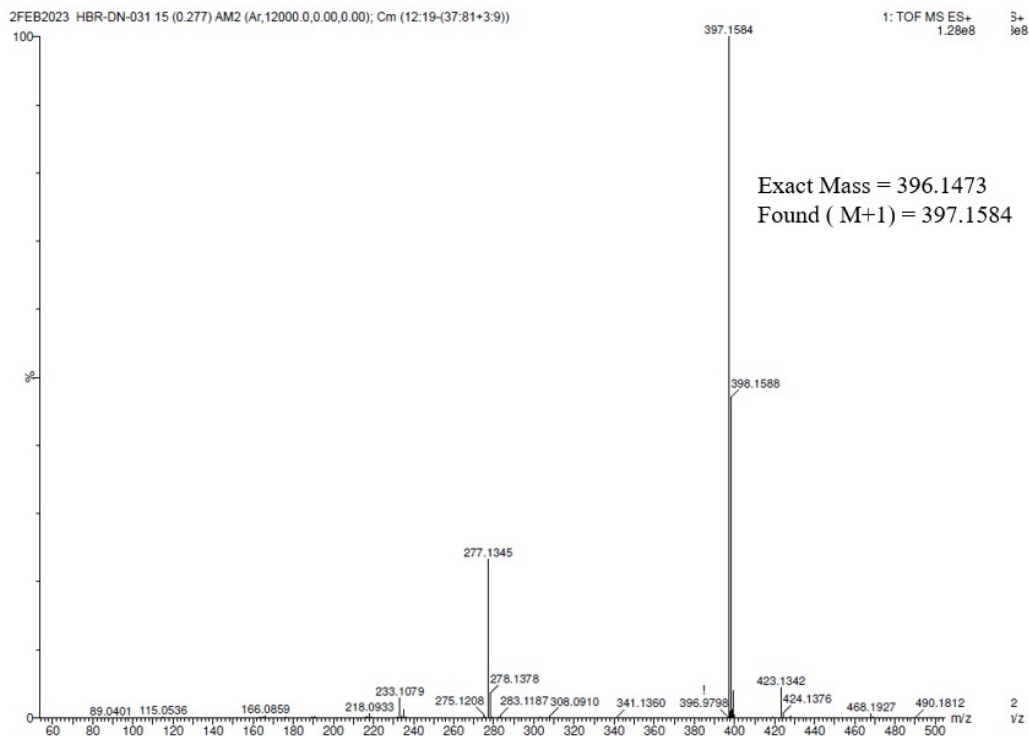


Fig.S123 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).

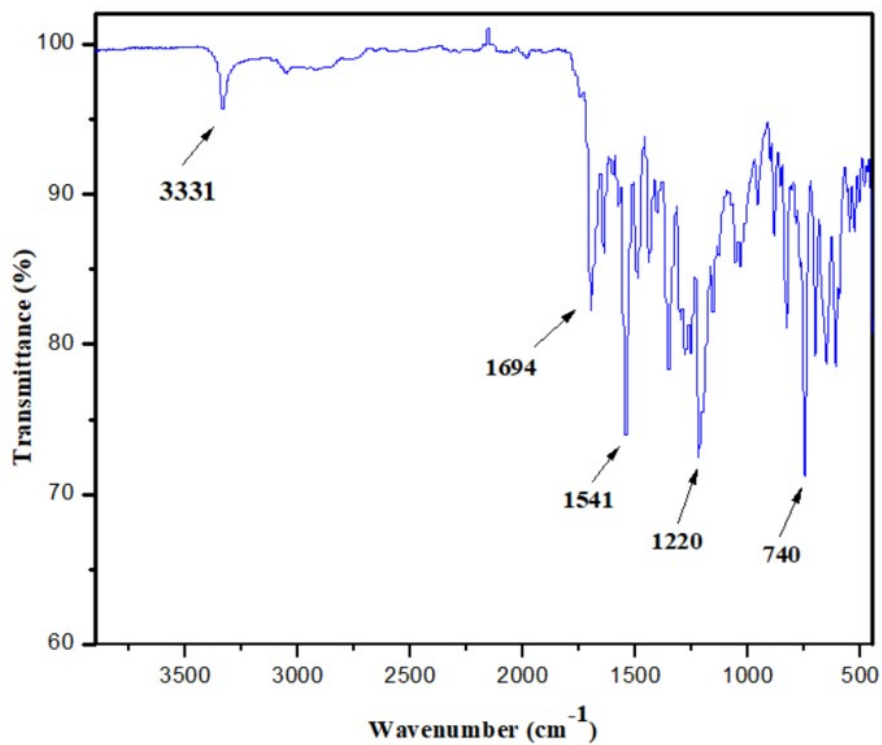


Fig.S124 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-hydroxybenzamide (6s).

Signature SIF VIT VELLORE  
VN-040

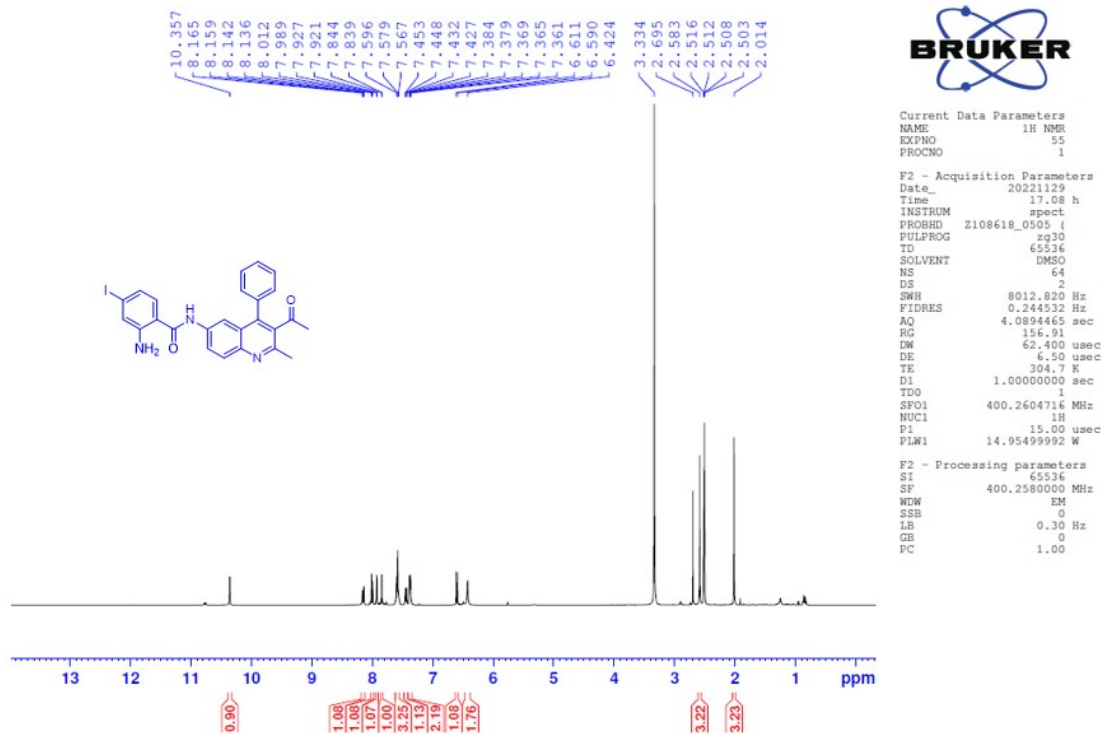


Fig.S125 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).



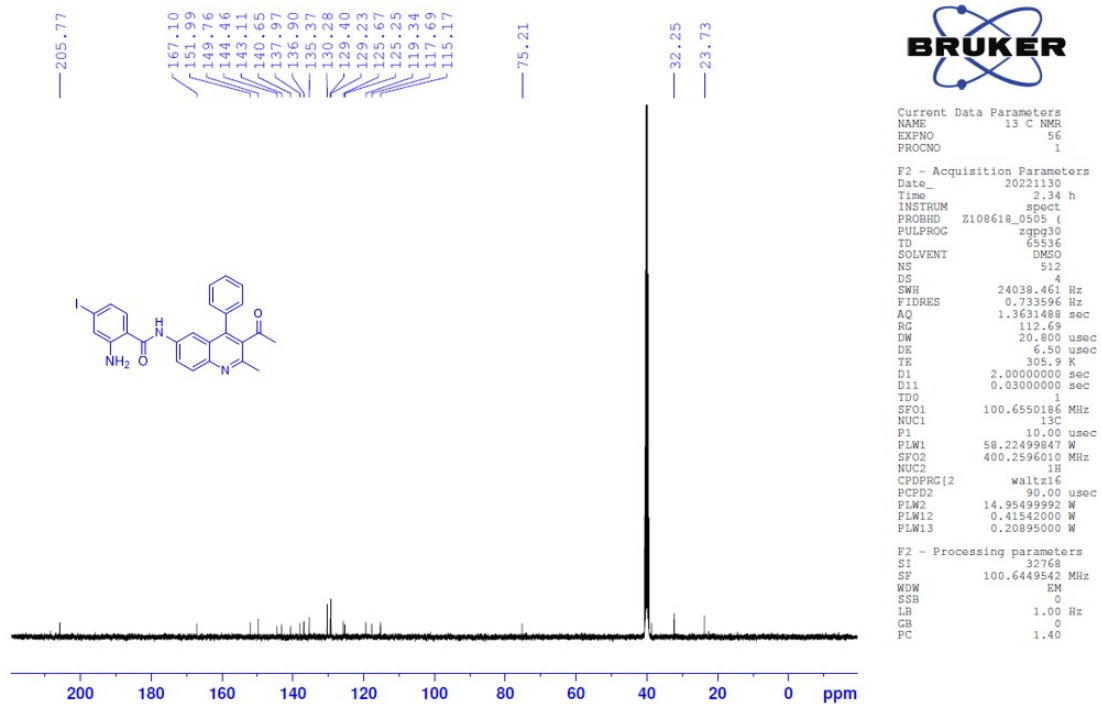


Fig.S126 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

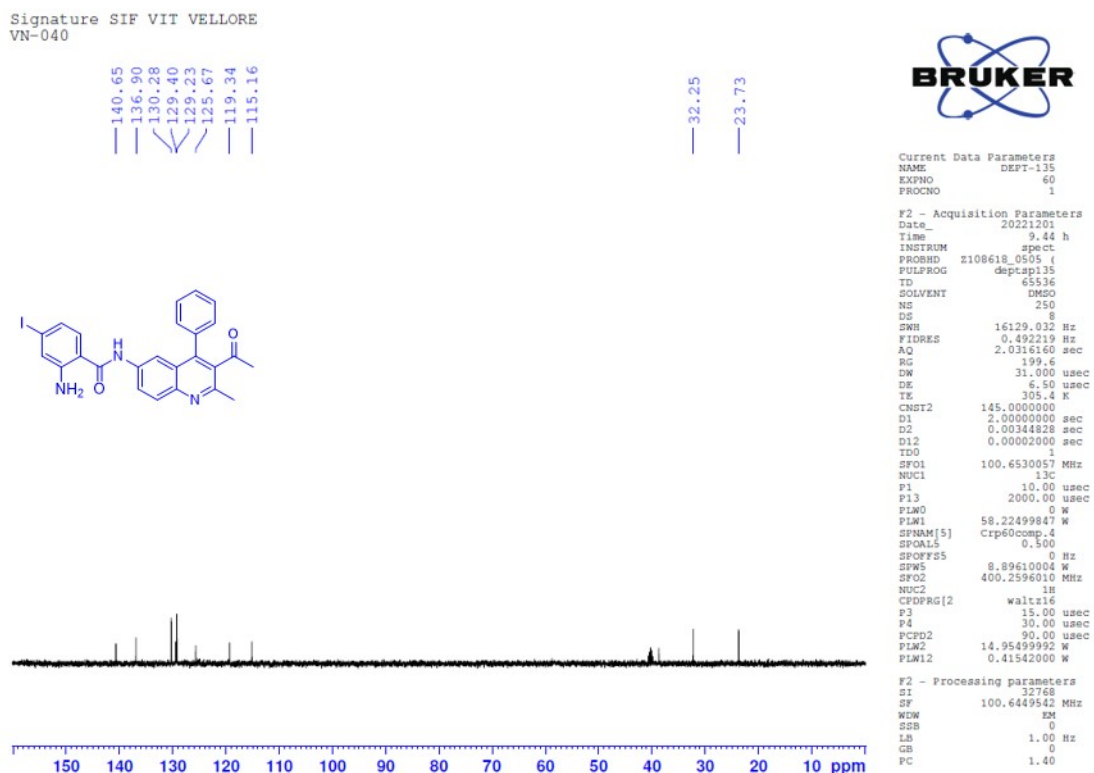


Fig.S127 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

Signature SIF VIT VELLORE  
VN-040

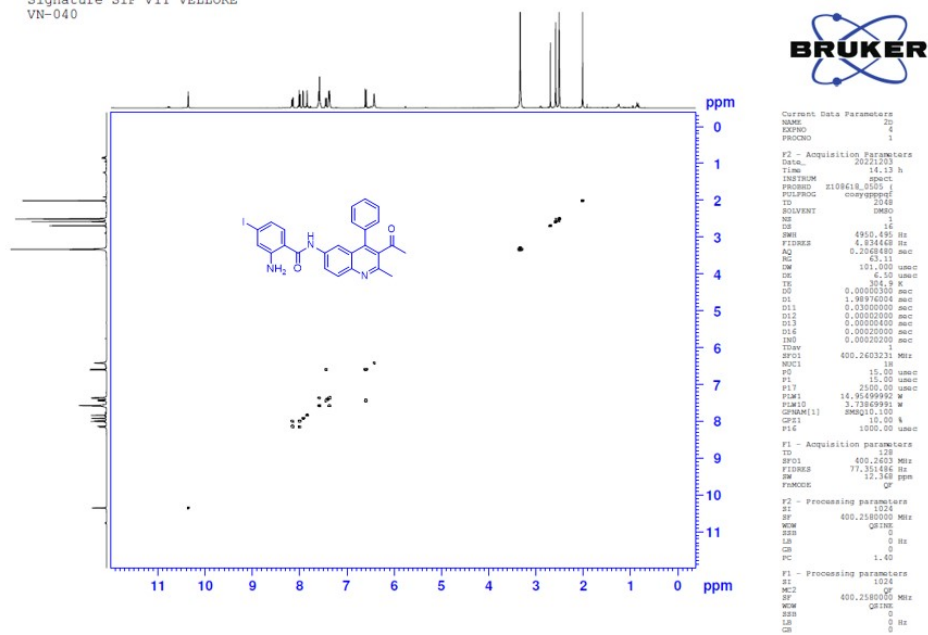


Fig.S128 H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

Signature SIF VIT VELLORE  
VN-040

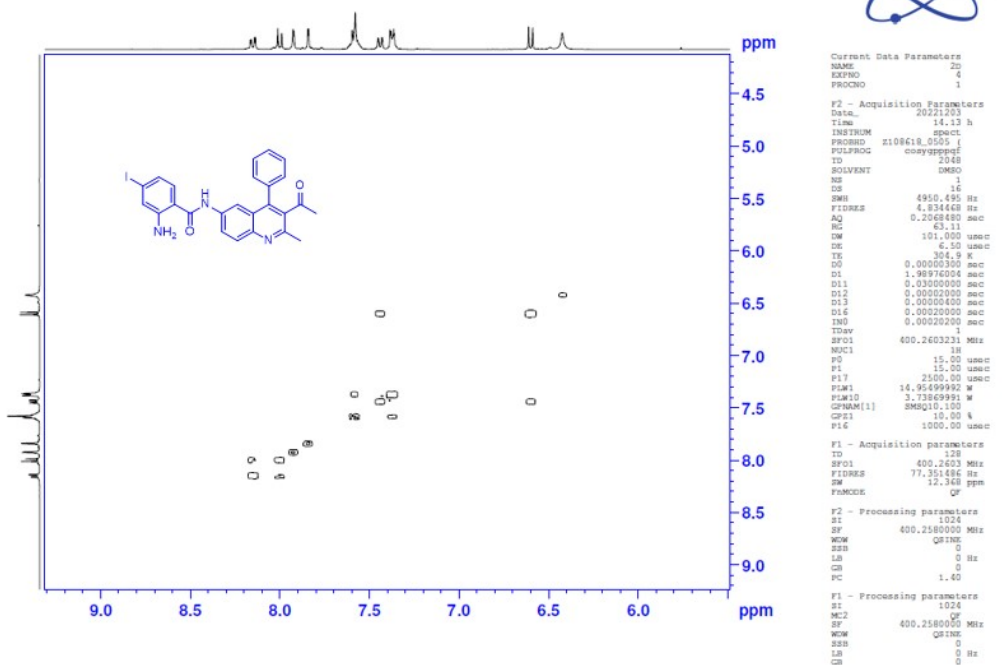
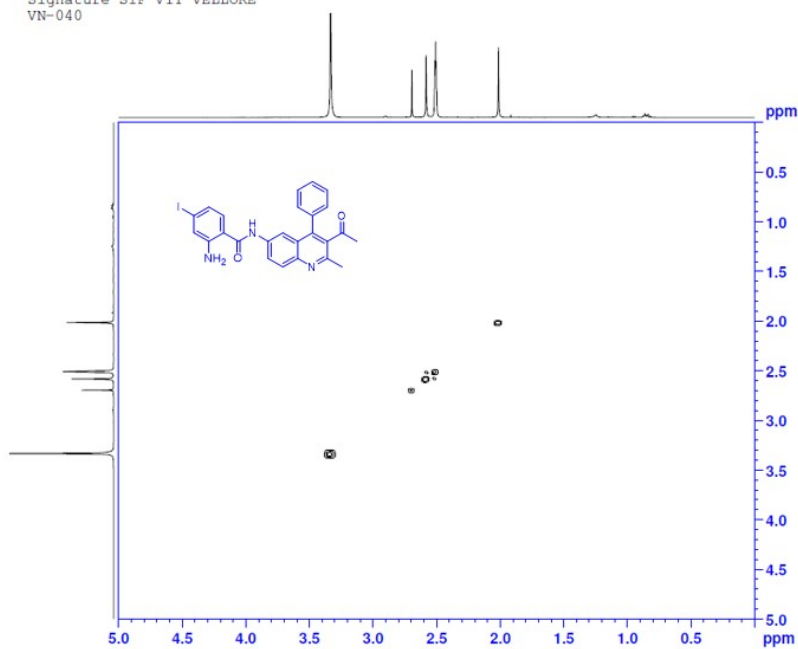


Fig.S129 Enlarged H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

Signature SIF VIT VELLORE  
VN-040



```

Current Data Parameters
NAME      20
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20221203
Time     14.13 h
INSTRUM  spect
PROBHD   z106c13_0305 (
PULPROG  zgpg30
SOLVENT  dmso
NS        1
DS        1
SWH       4950.495 Hz
FIDRES   4.824408 Hz
AQ        0.2068480 sec
RG        63.11
DM        101.000 usec
DE        6.50 usec
TE        301.2 K
D0        0.0000000 sec
D1        1.36976000 sec
D11       0.03000000 sec
D12       0.00000000 sec
D13       0.00000400 sec
D14       0.00000000 sec
IND0      0.0000000 sec
IND1      1
SFO1     400.2603231 MHz
NUC1      13
PC        15.00 usec
P1        15.00 usec
P18       2300.00 usec
P19       14.95499992 W
P19B1     3.73569991 W
CPHASE1[1] SMSG10.100
CP1       10.00 usec
P16       1000.00 usec

F1 - Acquisition parameters
TD        128
SFO1     400.2603 MHz
FIDRES   77.351486 Hz
SW        12.148 ppm
FAMODES  QF

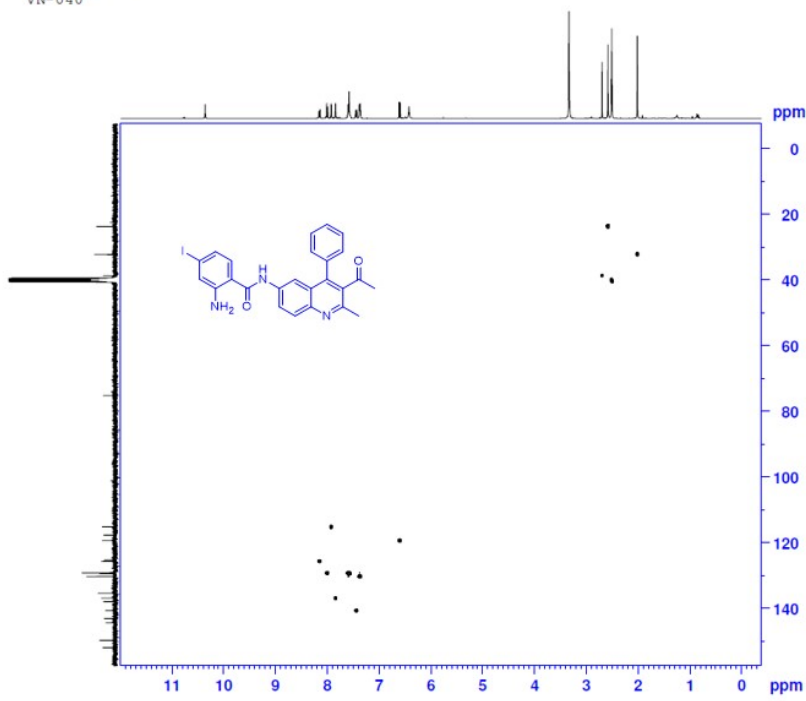
F2 - Processing parameters
SI        1324
SF        400.2580000 MHz
WDW       QFHM
SSB        0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI        1324
MC2       QF
SF        400.2580000 MHz
WDW       QFHM
SSB        0
LB         0 Hz
GB         0
PC         1.40

```

Fig.S130 Enlarged H-H COSY of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

VN-040



```

Current Data Parameters
NAME      20
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20221203
Time     14.13 h
INSTRUM  spect
PROBHD   z106c13_0305 (
PULPROG  zgpg30
SOLVENT  dmso
NS        1
DS        1
SWH       4950.495 Hz
FIDRES   9.682016 Hz
AQ        0.1034240 sec
RG        63.11
DM        101.000 usec
DE        6.50 usec
TE        301.2 K
D0        0.0000000 sec
D1        1.4497284 sec
D11       0.0312484 sec
D12       0.00000000 sec
D13       0.00000000 sec
D14       0.00000000 sec
IND0      0.0004207 sec
IND1      1
SFO1     400.2603231 MHz
NUC1      13
PC        15.00 usec
P1        15.00 usec
P18       2300.00 usec
P19       14.95499992 W
P19B1     3.73569991 W
CPHASE1[1] SMSG10.100
CP1       10.00 usec
P16       1000.00 usec

F1 - Acquisition parameters
TD        128
SFO1     100.62619 MHz
FIDRES   129.776182 Hz
SW        126.024 ppm
FAMODES  SINE+AQ+EM

F2 - Processing parameters
SI        1324
SF        400.2580000 MHz
WDW       QFHM
SSB        2
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI        1324
MC2       SINE+AQ+EM
SF        100.6448542 MHz
WDW       QFHM
SSB        2
LB         0 Hz
GB         0
PC         1.40

```

Fig.S131 HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

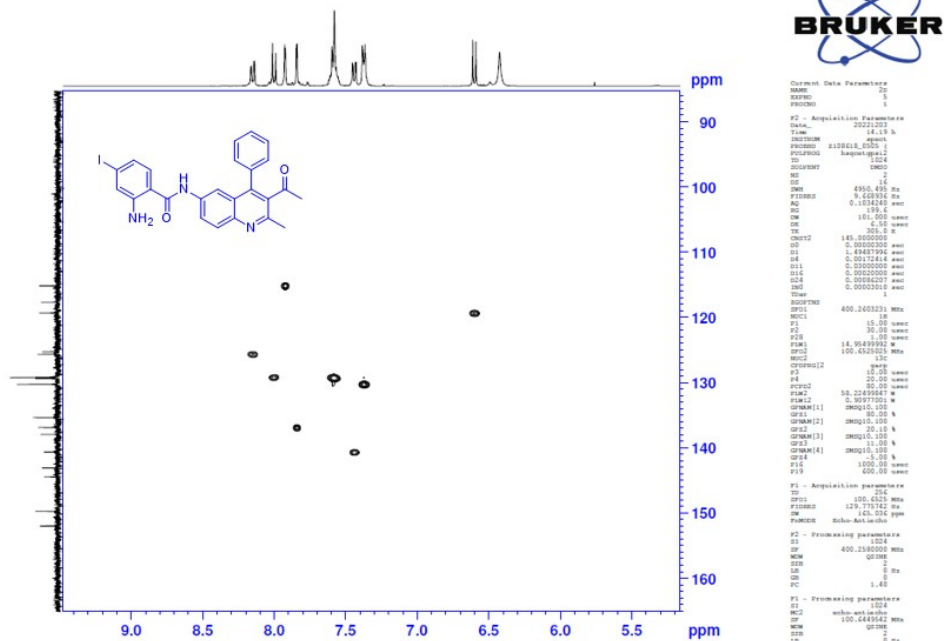


Fig.S132 Enlarged HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

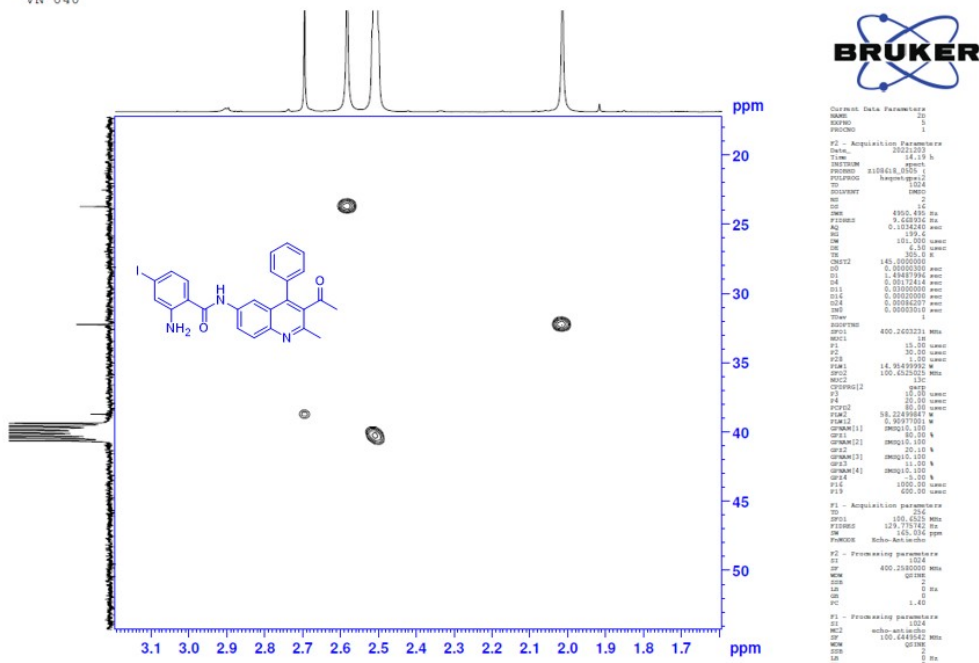


Fig.S133 Enlarged HSQC of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide

(6t).

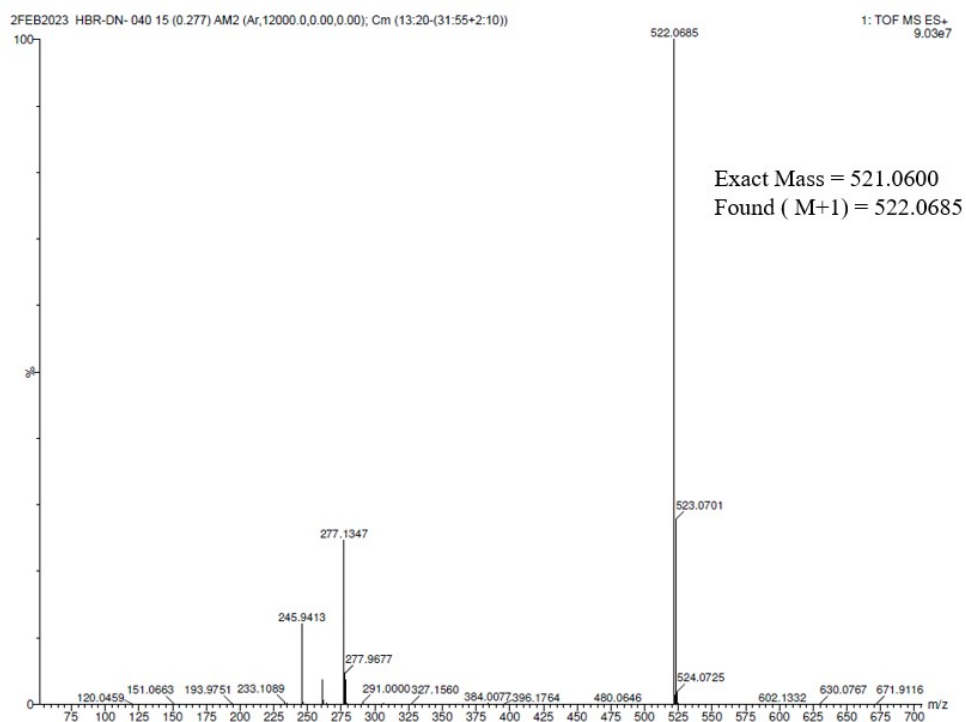


Fig.S134 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

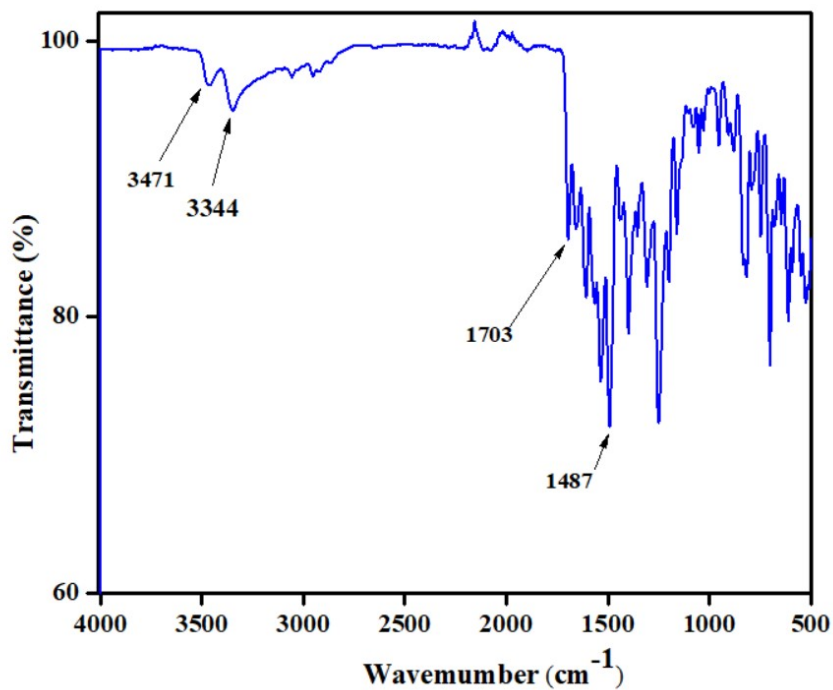


Fig.S135 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-4-iodobenzamide (6t).

Signature SIF VIT VELLORE  
VN-043

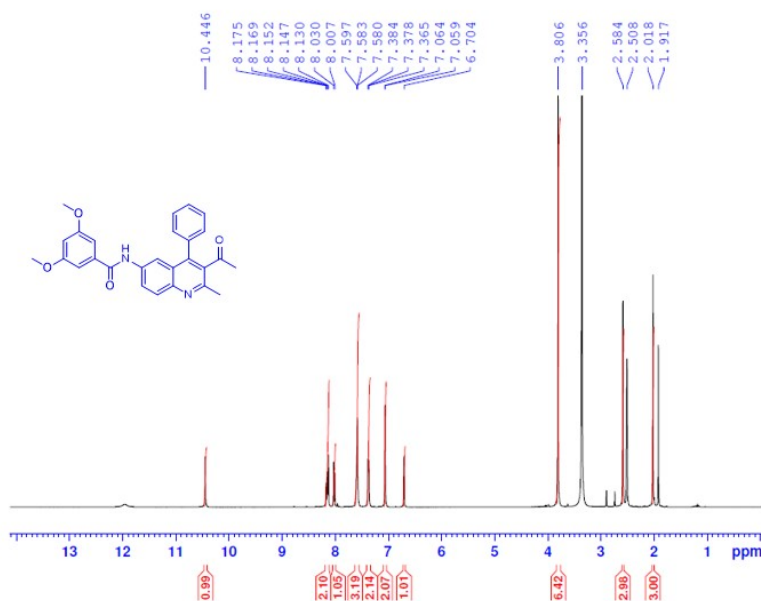


Fig.S136 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).

VN-043

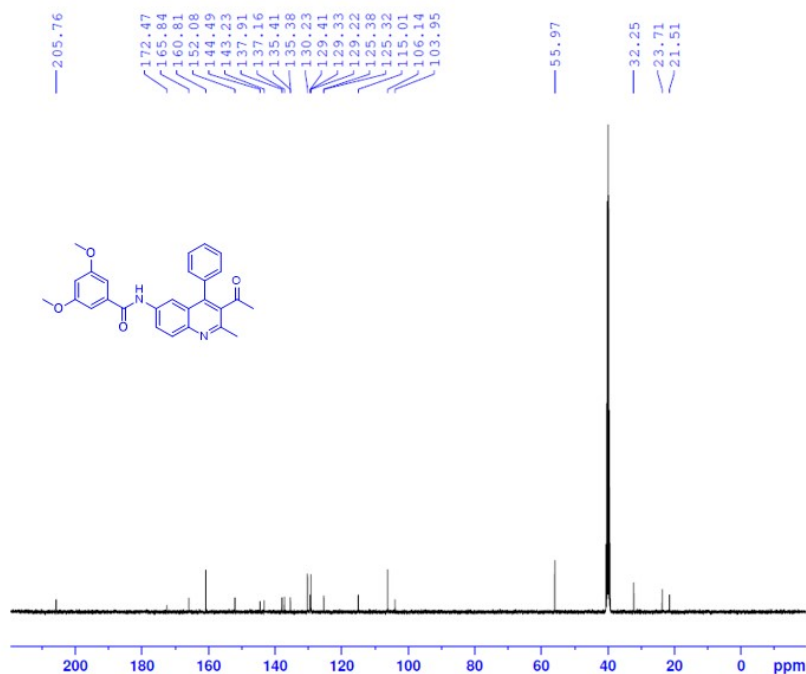


Fig.S137 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).

Signature SIF VIT VELLORE  
VN-043

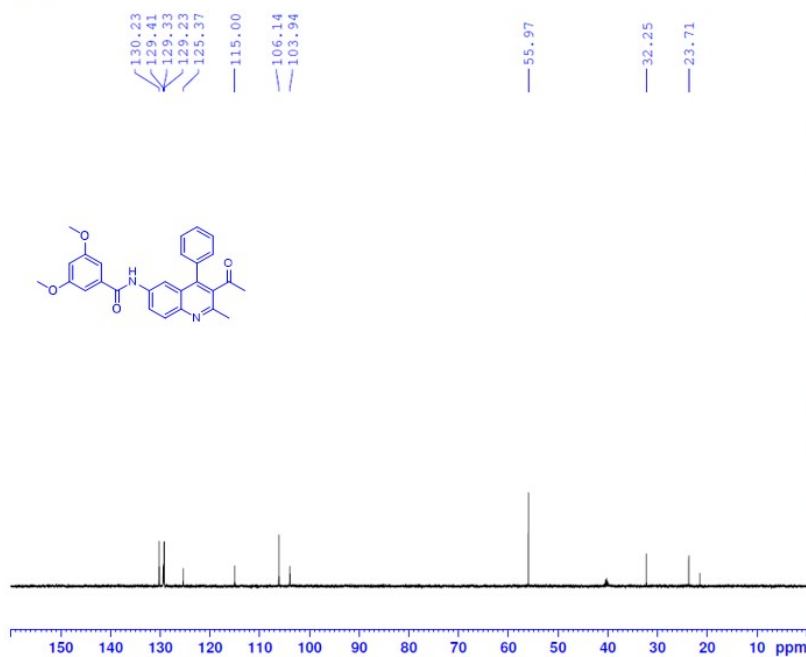


Fig.S138 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).

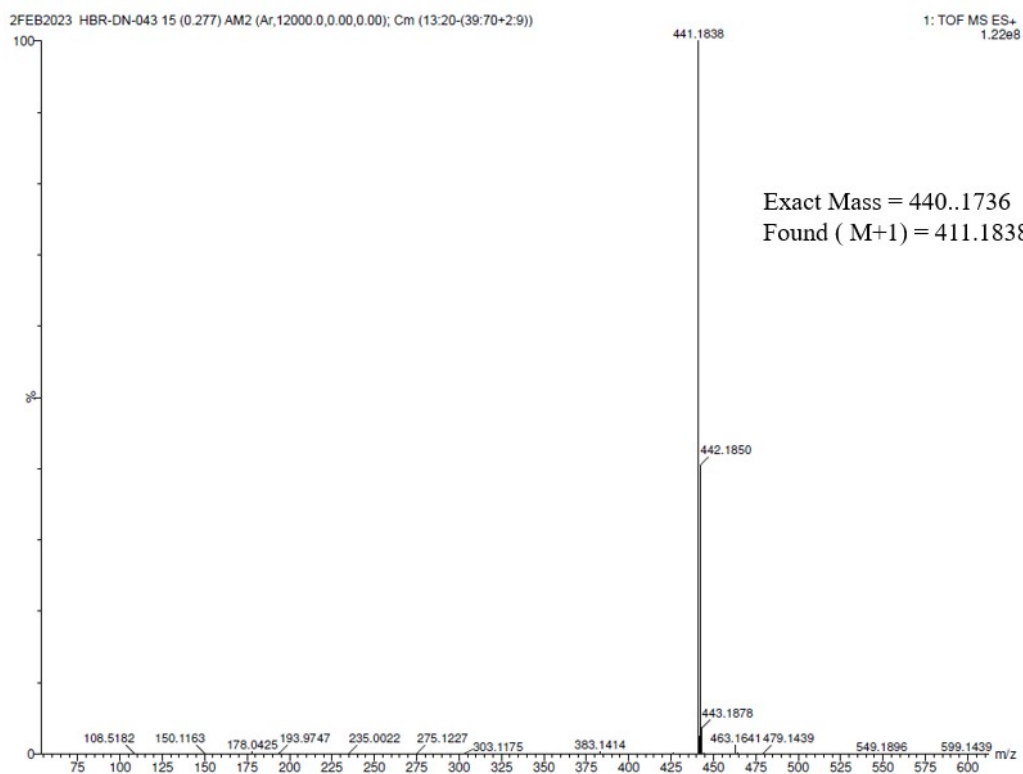


Fig.S139 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).

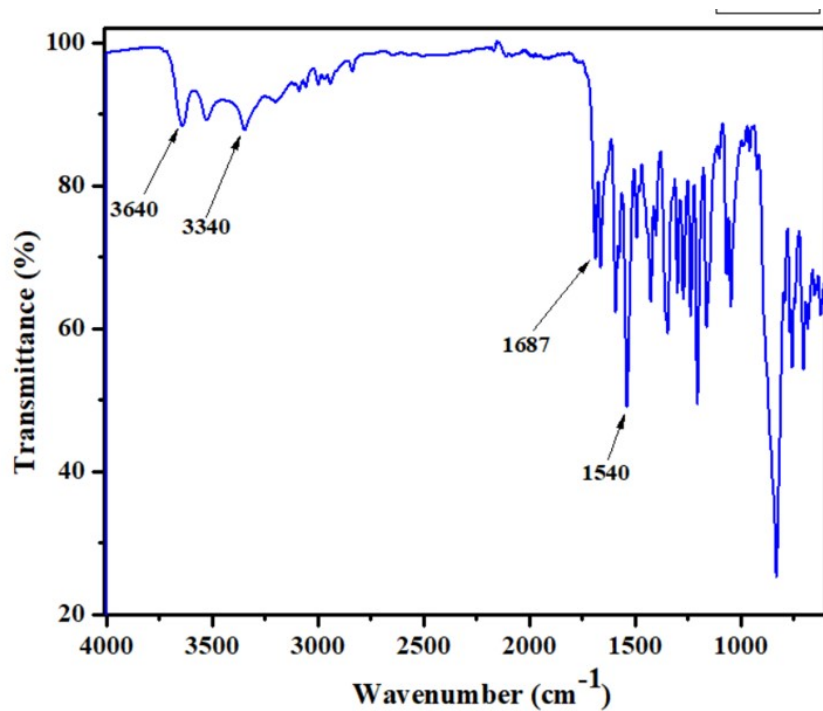


Fig.S140 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3,5-dimethoxybenzamide (6u).

Signature SIF VIT VELLORE  
VN-044

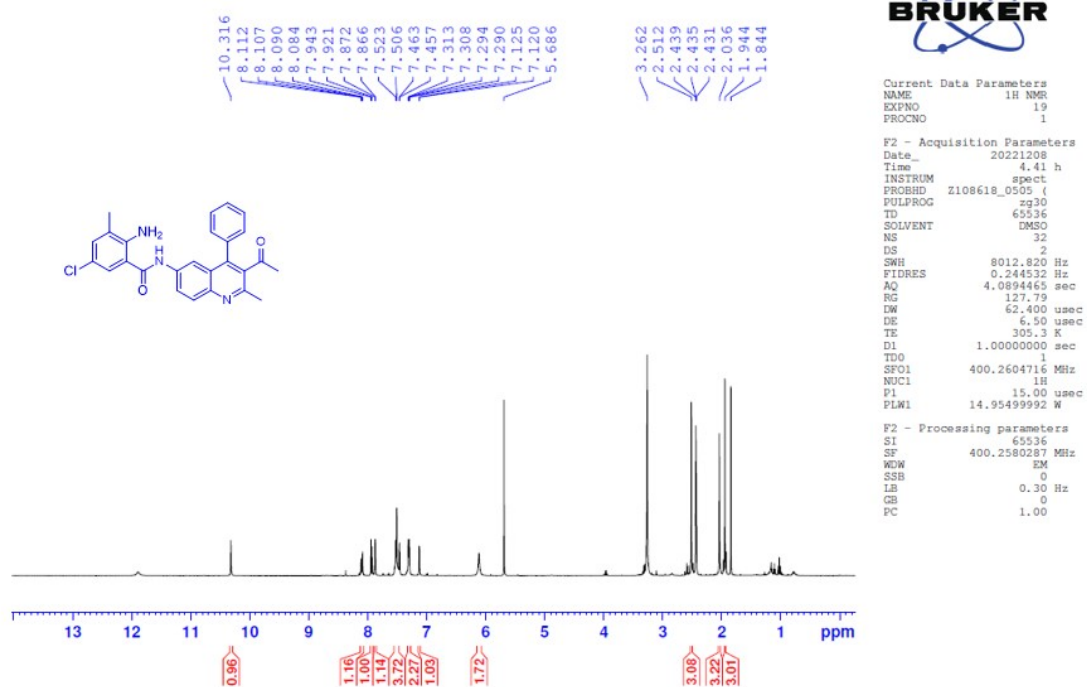


Fig.S141 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).



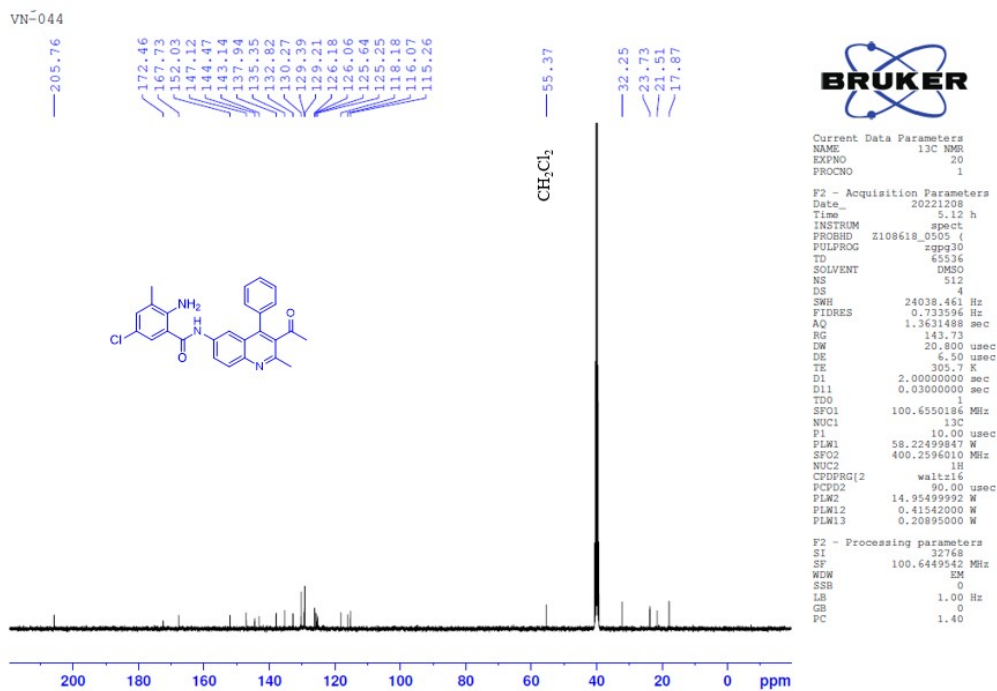


Fig.S142  $^{13}\text{C}$  NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).

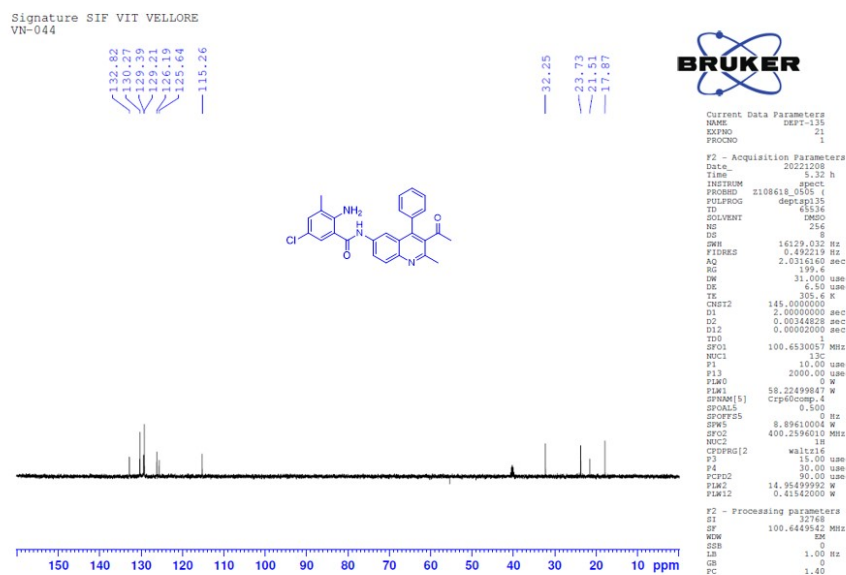


Fig.S143 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).

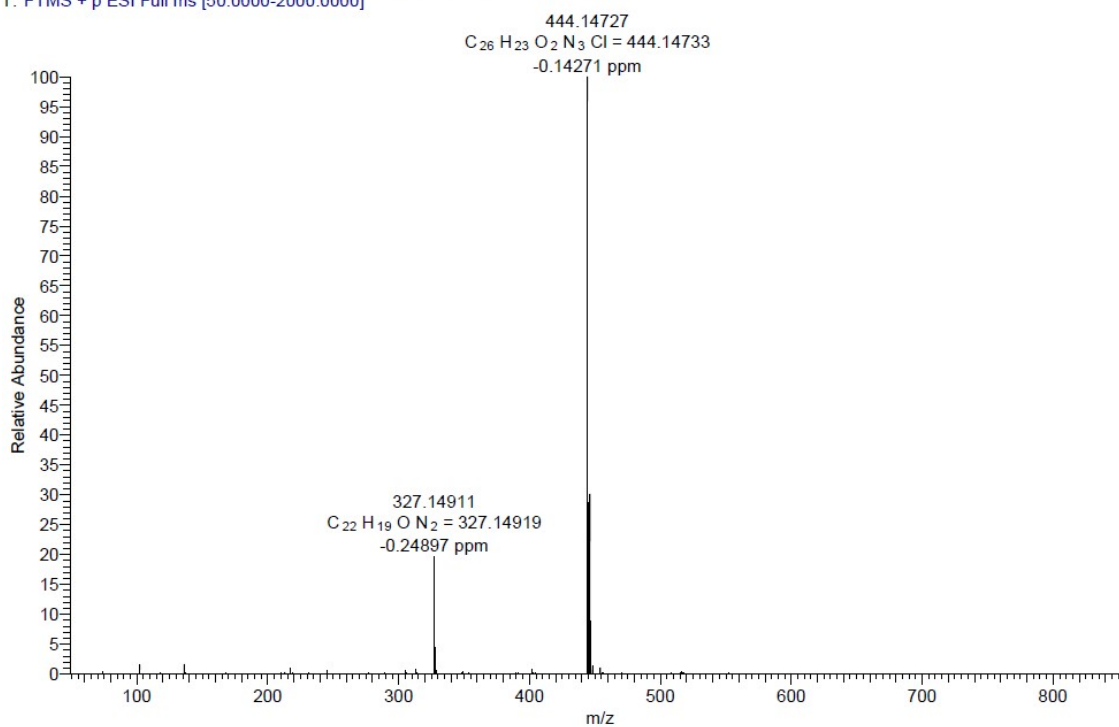


Fig.S144 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).

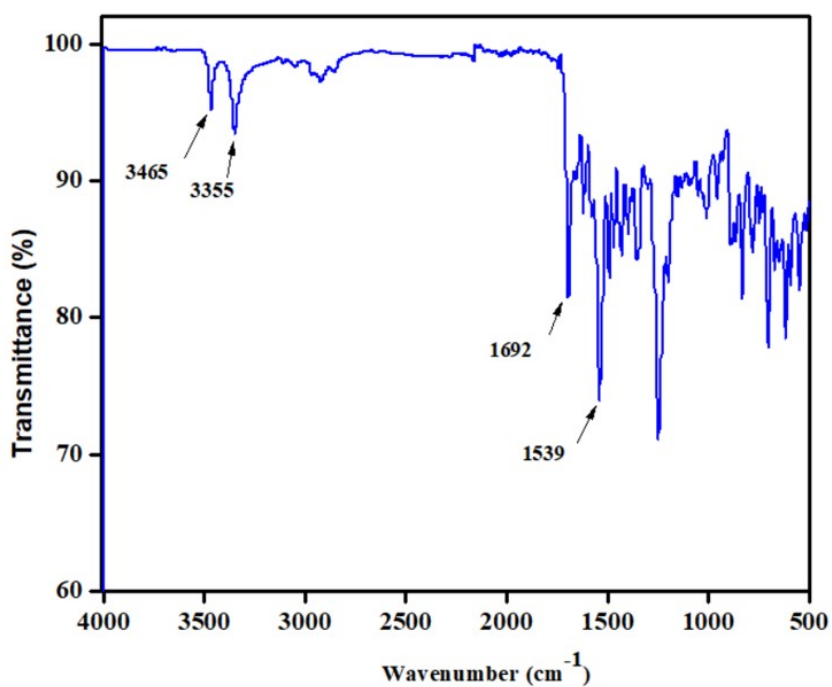
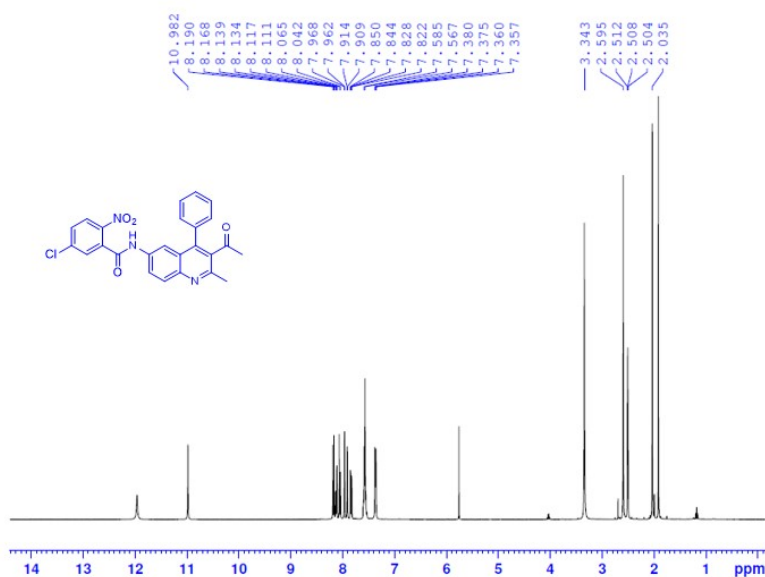


Fig.S145 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-amino-5-chloro-3-methylbenzamide (6v).

Signature SIF VII VELLORE  
VN-047



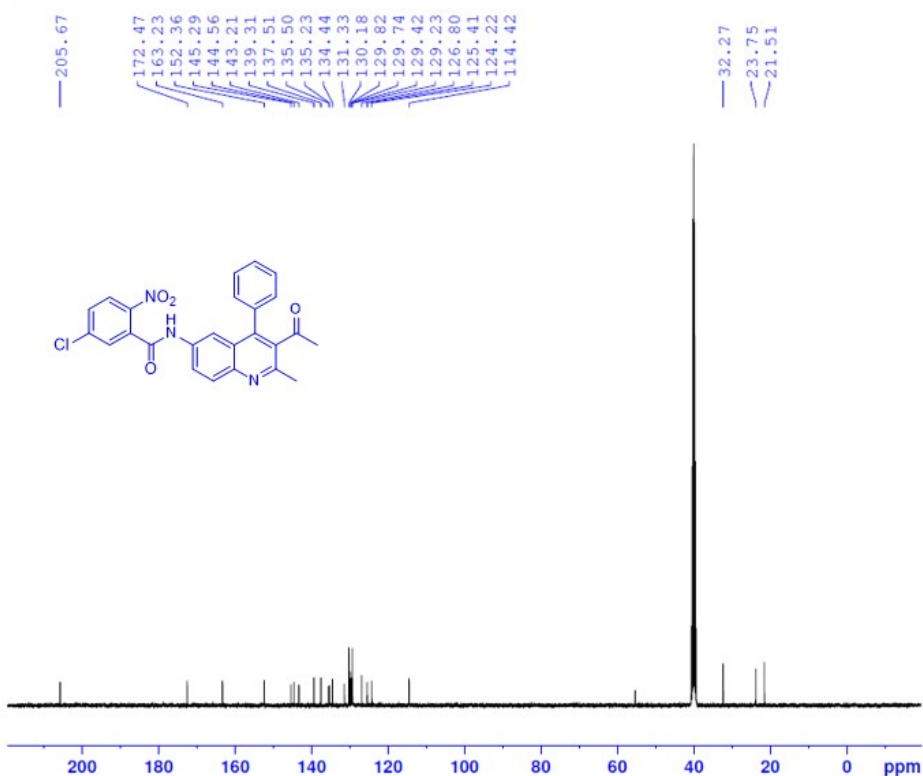
Current Data Parameters  
NAME 1H NMR  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221207  
Time 16.09 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894455 sec  
RG 127.79  
DW 62.400 usec  
DE 6.50 usec  
TE 305.1 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.2604716 MHz  
NUC1 1H  
P1 15.00 usec  
PLM1 14.95499992 W

F2 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Fig.S146 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-chloro-2-nitrobenzamide (6w).

Signature SIF VII VELLORE  
VN-047



Current Data Parameters  
NAME 13C NMR  
EXPNO 26  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221213  
Time 5.43 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 175.97  
DW 20.800 usec  
DE 6.50 usec  
TE 303.8 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6550186 MHz  
NUC1 13C  
P1 10.00 usec  
PLM1 58.22499847 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLM2 14.95499992 W  
PLM12 0.41542000 W  
PLM13 0.20895000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S147 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-chloro-2-nitrobenzamide (6w).

VN-047

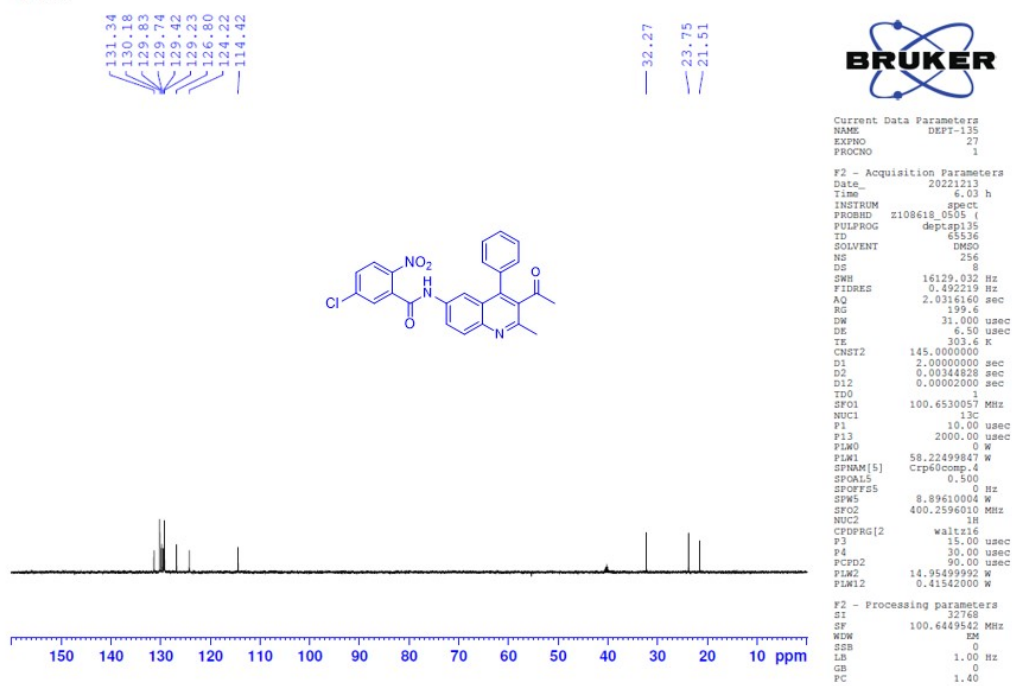


Fig.S148 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-chloro-2-nitrobenzamide (6w).

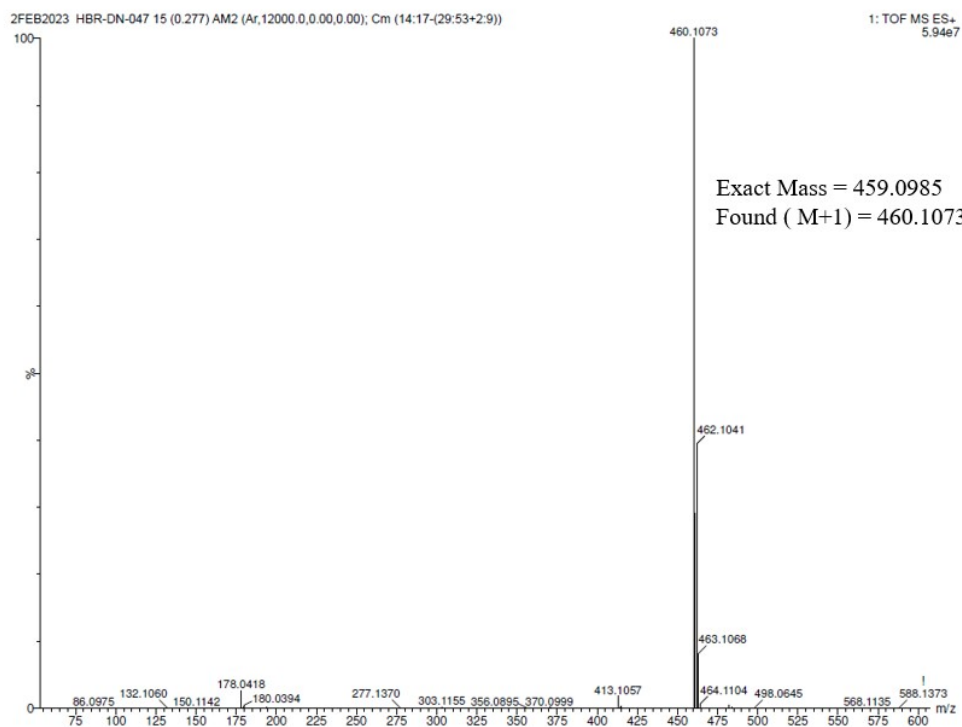


Fig.S149 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-5-chloro-2-nitrobenzamide (6w).

Signature SIF VIT VELLORE  
VN-048

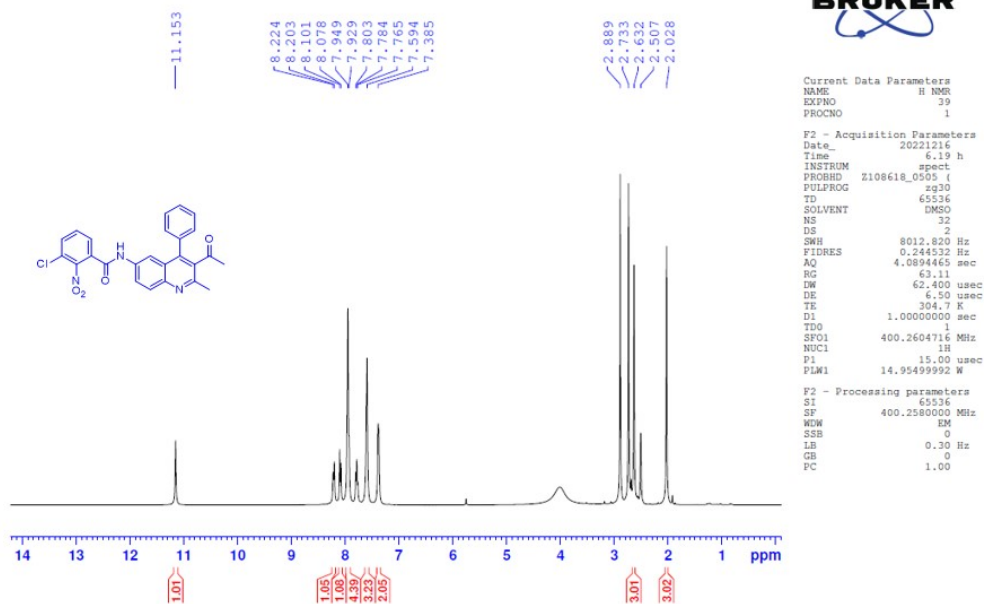


Fig.S150 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-chloro-2-nitrobenzamide (6x).

VN-048

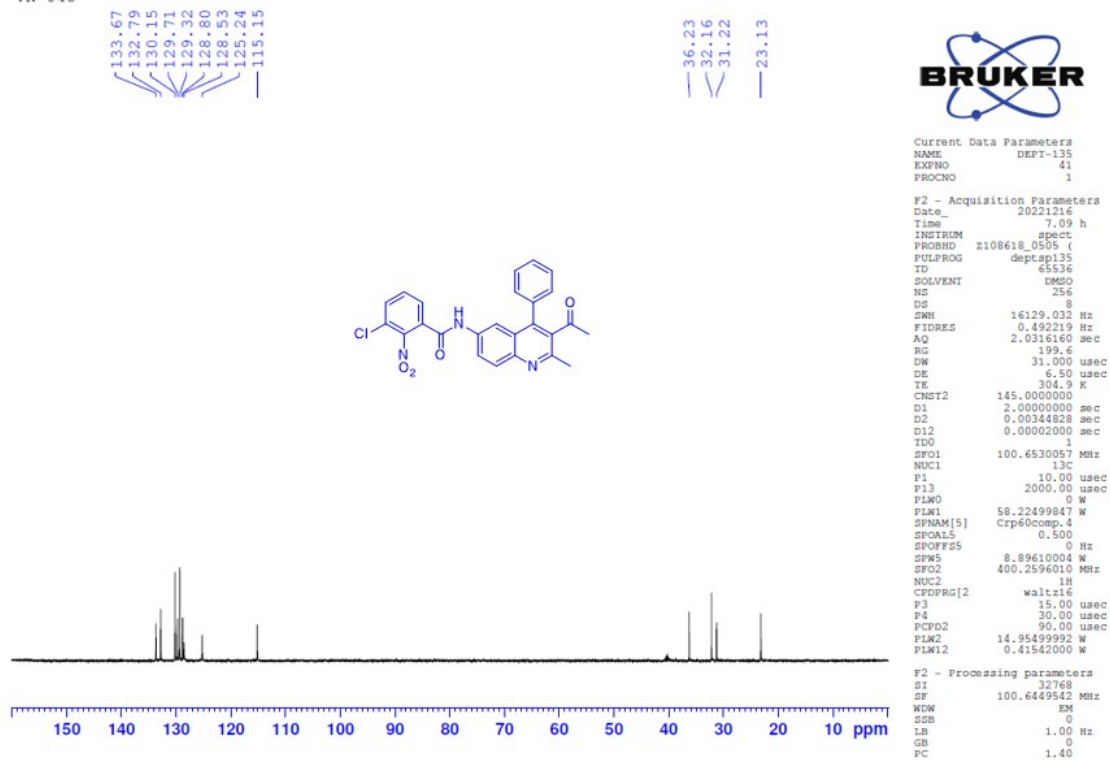


Fig.S151 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-chloro-2-nitrobenzamide (6x).

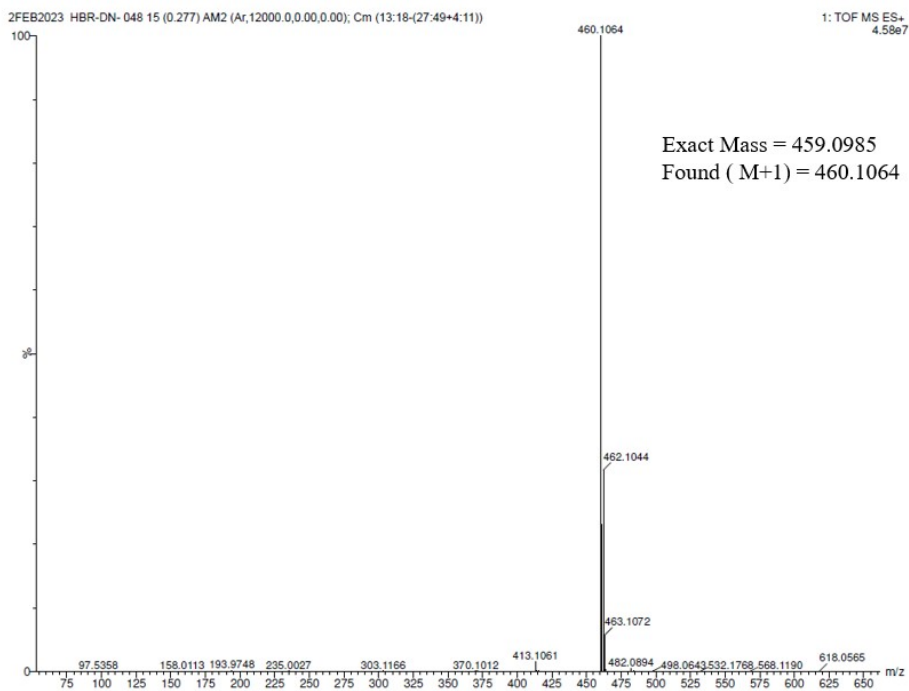


Fig.S152 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-chloro-2-nitrobenzamide (6x).

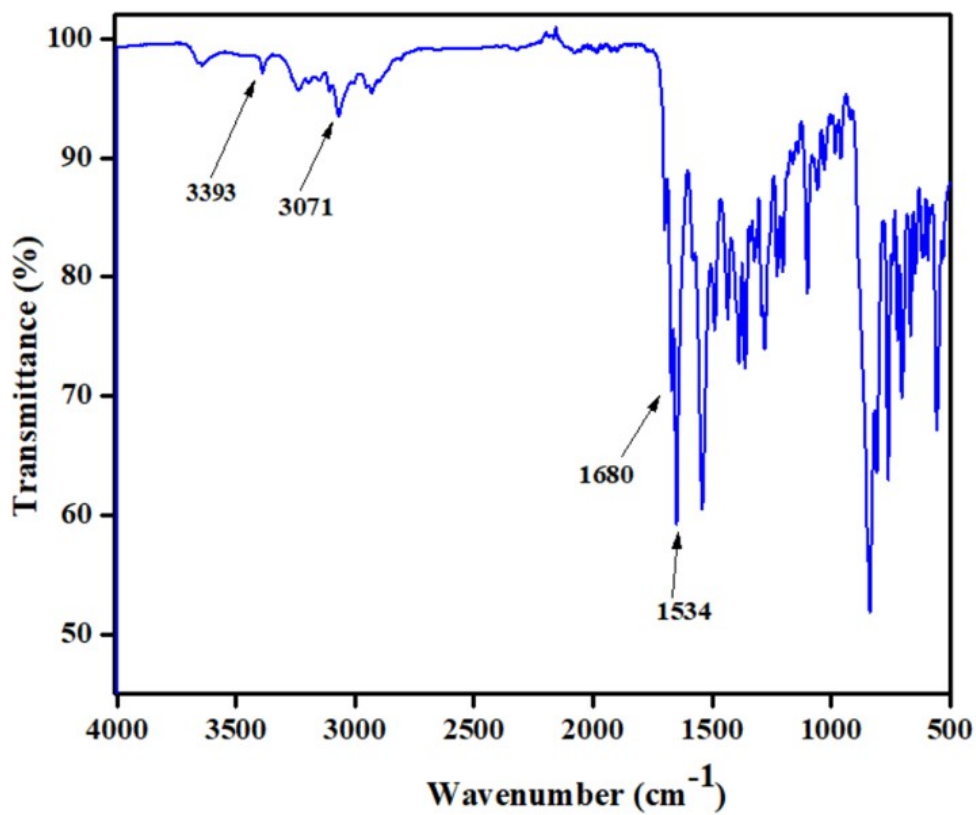


Fig.S153 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-3-chloro-2-nitrobenzamide (6x).

Signature SIF VIT VELLORE  
VN-052

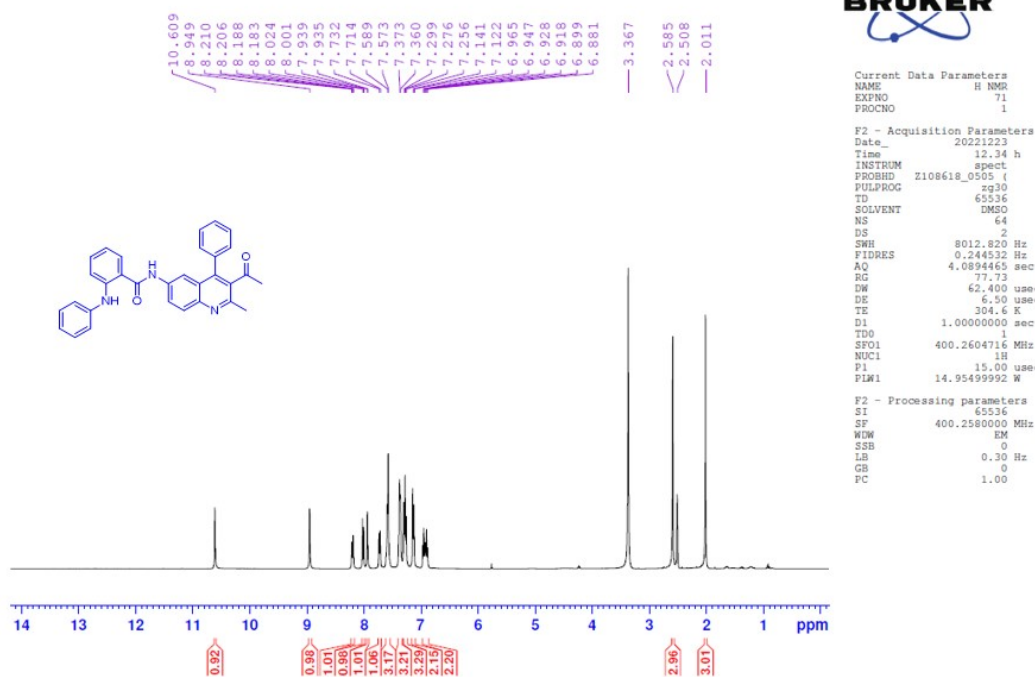


Fig.S154 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(phenylamino)benzamide (6y).

Signature SIF VIT VELLORE  
MN-052

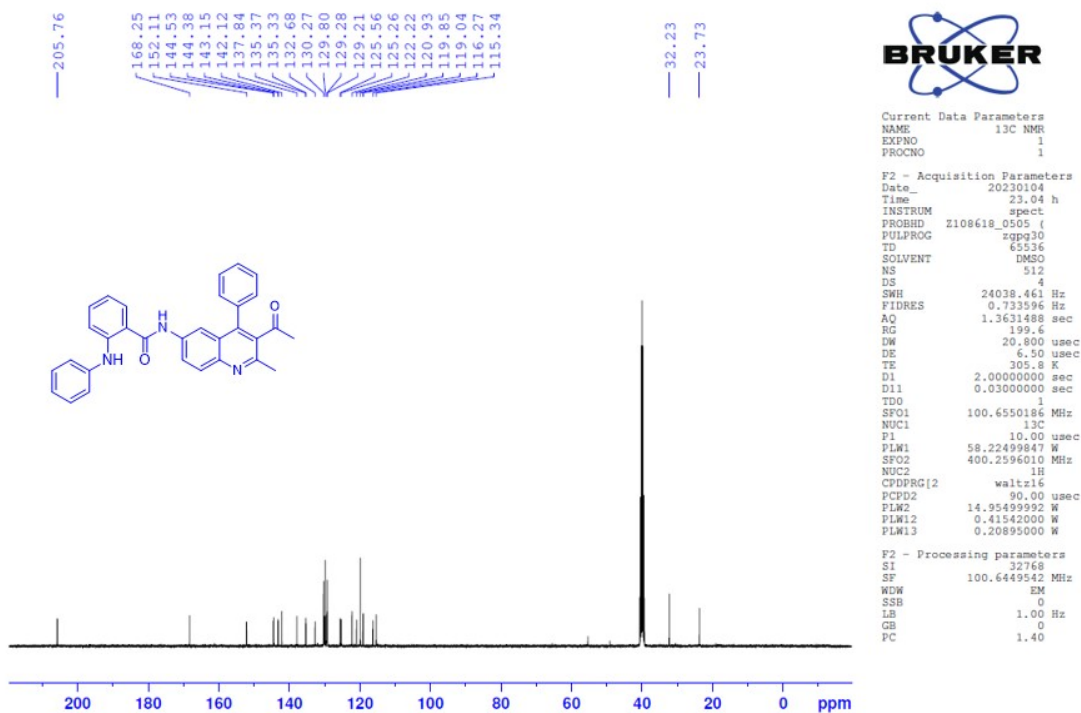


Fig.S155 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(phenylamino)benzamide (6y).

Signature SIF VIT VELLORE  
MN-052

132.68  
130.27  
130.08  
129.80  
129.40  
129.28  
129.21  
125.56  
122.22  
119.85  
119.04  
116.27  
115.34

— 32.23  
— 23.73



Current Data Parameters  
NAME DEPT-135  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230104  
Time 23.23 h  
INSTRUM spect  
PROCNO 2108618\_0505 (deptap135)  
ID 65536  
SOLVENT DMSO  
NS 256  
DS 8  
SWH 16129.032 Hz  
FIDRES 0.492219 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DE 6.50 usec  
TE 305.7 K  
CNST2 145.0000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.0002000 sec  
TD0 1  
SFO1 100.6520057 MHz  
NUC1 13C  
P1 10.00 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 58.22499847 W  
SPNAM[5] Crp60comp.4  
SFOALS 0.500  
SPOFFS5 0 Hz  
SPW5 8.89610004 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
P3 15.00 usec  
P4 30.00 usec  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.43542000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

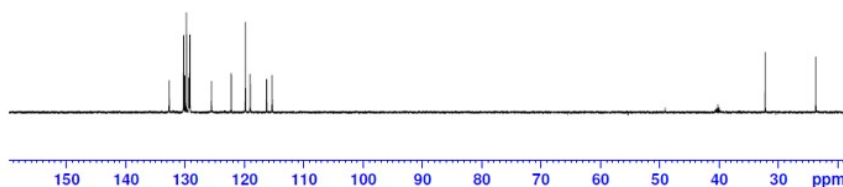
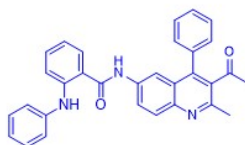


Fig.S156 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(phenylamino)benzamide (6y).

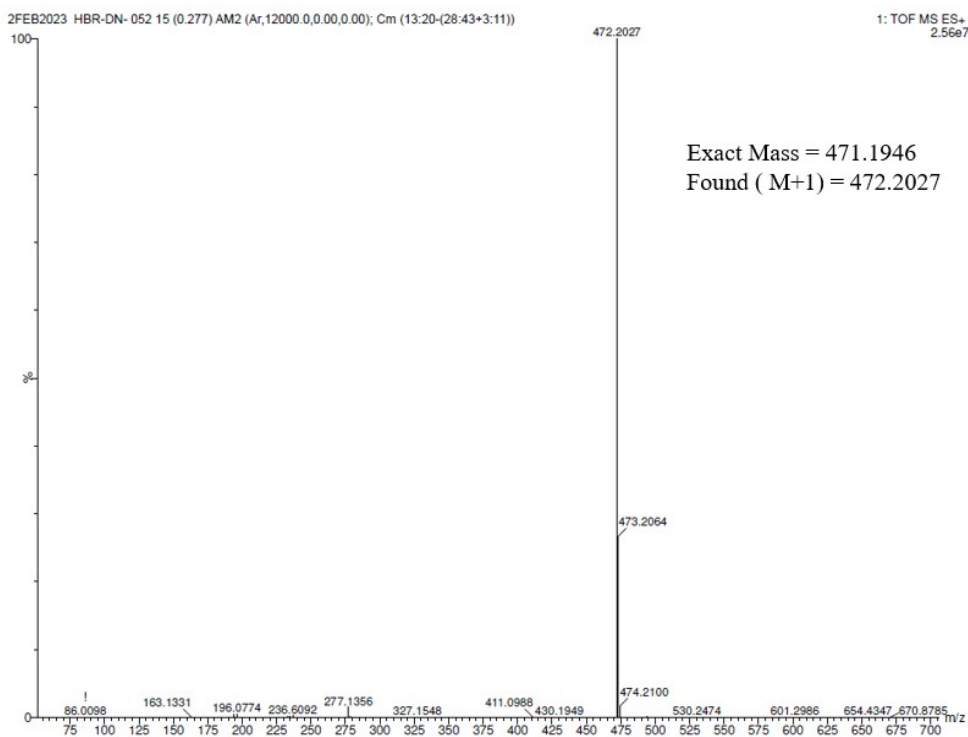


Fig.S157 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(phenylamino)benzamide (6y).



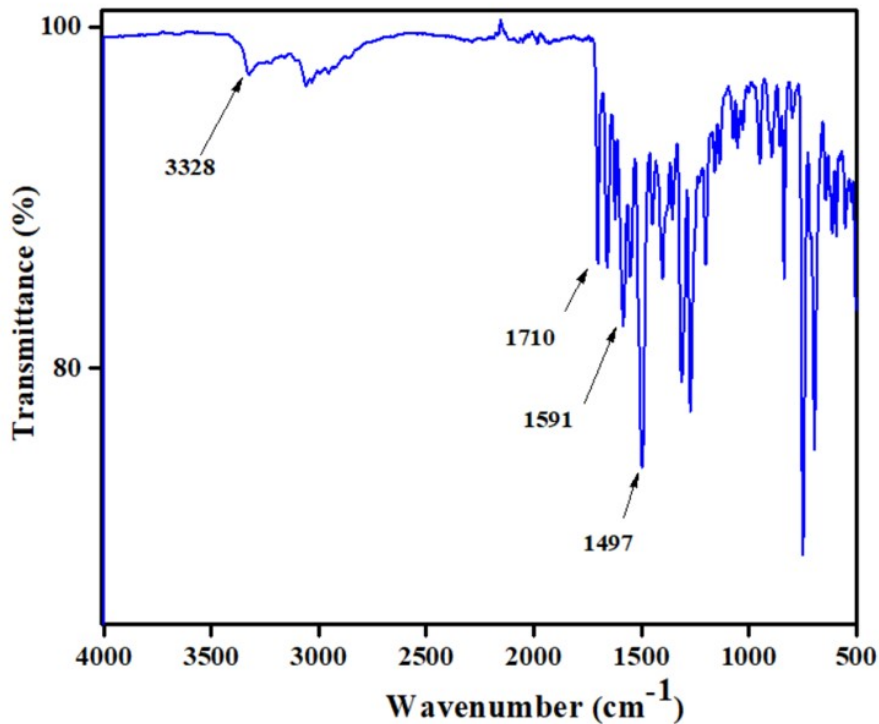


Fig.S158 FT-IR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-2-(phenylamino)benzamide (6y).

Signature SIF VIT VELLORE  
NS-64

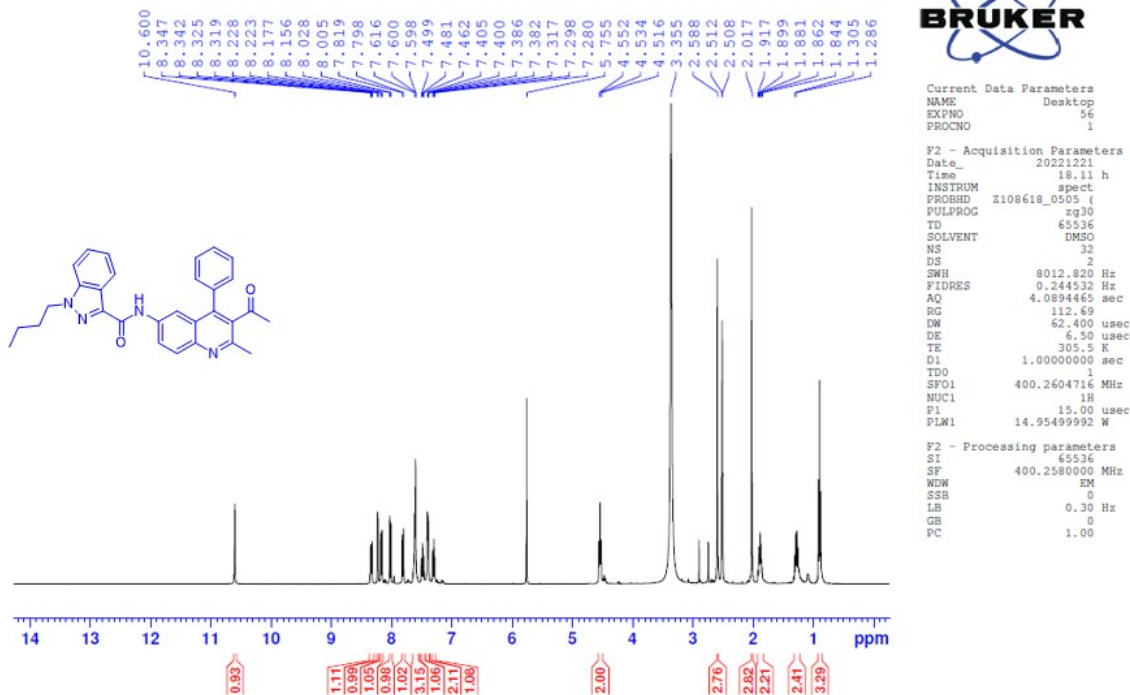


Fig.S159 <sup>1</sup>H NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-1-butyl-1H-indazole-3-carboxamide (6z).

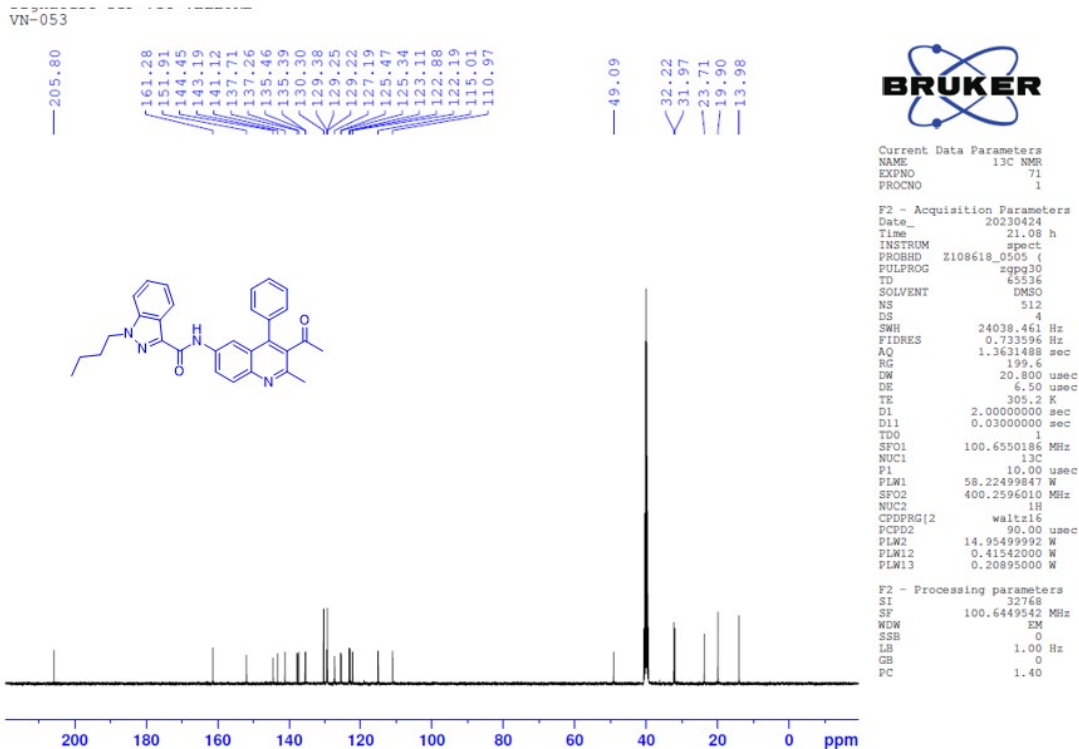


Fig.S160 <sup>13</sup>C NMR of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-1-butyl-1H-indazole-3-carboxamide (6z).

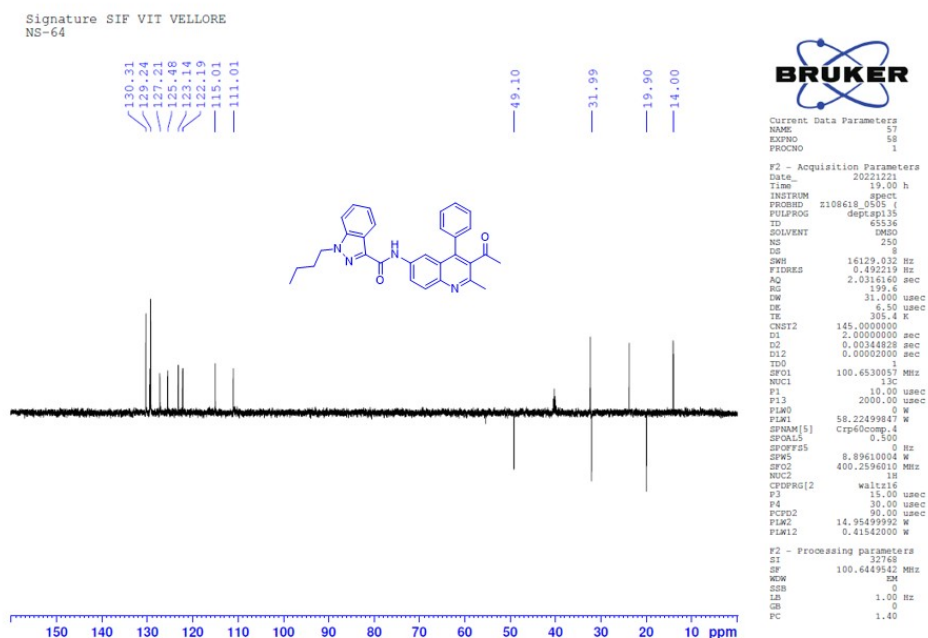


Fig.S161 DEPT-135 of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-1-butyl-1H-indazole-3-carboxamide (6z).

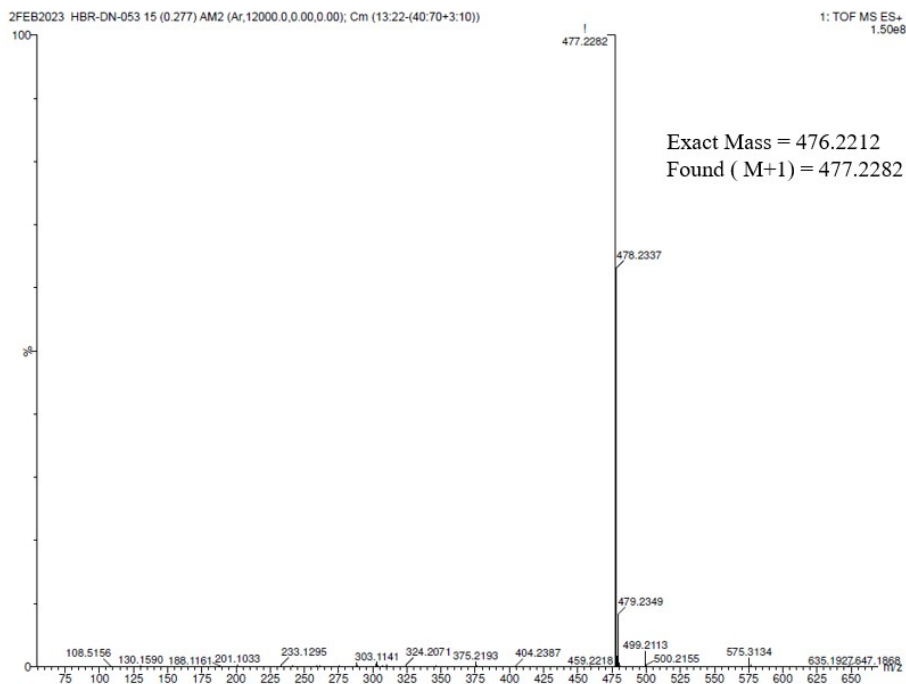


Fig.S162 HRMS of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-1-butyl-1H-indazole-3-carboxamide (6z).

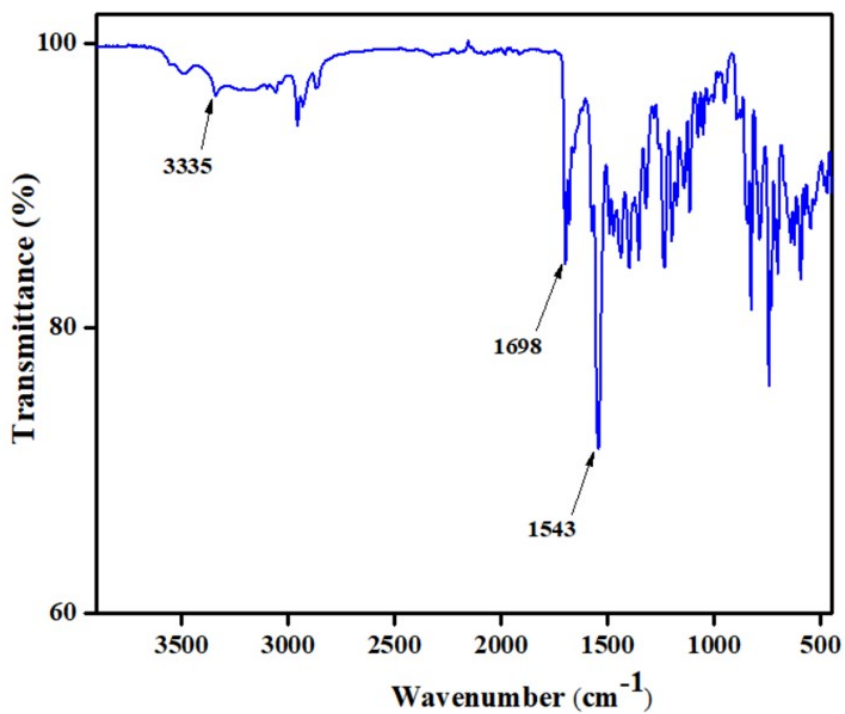


Fig.S163 FT-IR OF N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)-1-butyl-1H-indazole-3-carboxamide (6z).

Signature SIF VIT VELLORE  
VN-076

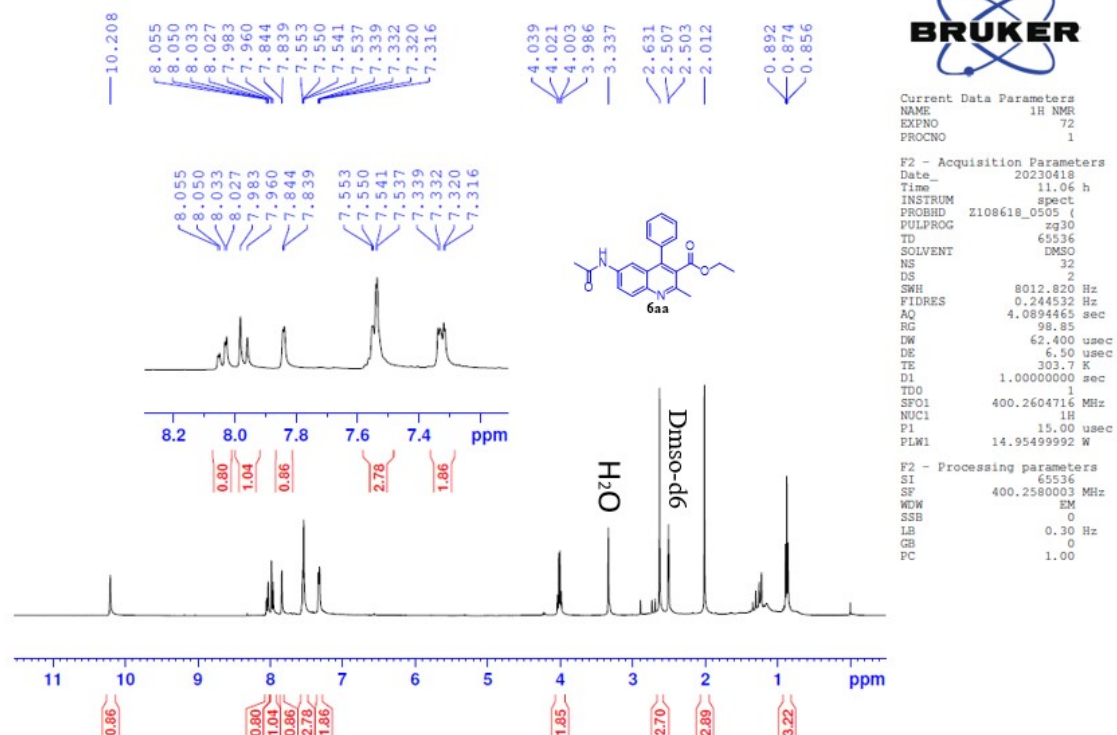


Fig.S164 <sup>1</sup>H NMR of Ethyl 6-acetamido-2-methyl-4-phenyl quinoline-3-carboxylate (6aa)

VN-076

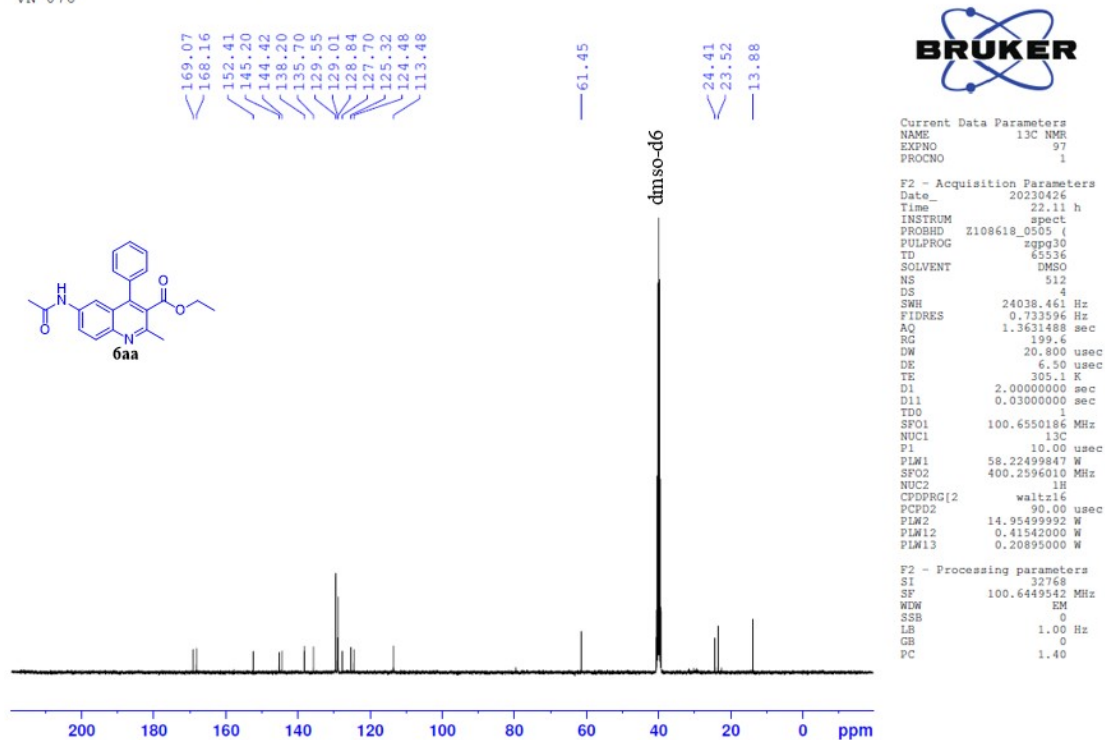


Fig.S165 <sup>13</sup>C NMR of Ethyl 6-acetamido-2-methyl-4-phenyl quinoline-3-carboxylate (6aa).

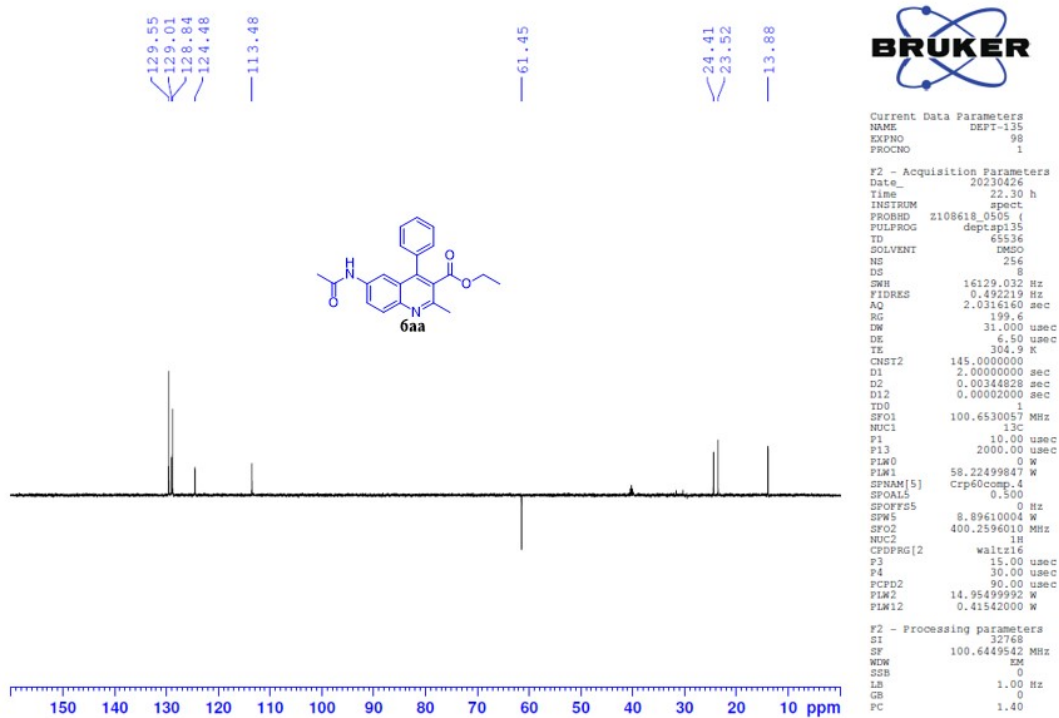


Fig.S166 DEPT-135 of Ethyl 6-acetamido-2-methyl-4-phenyl quinoline-3-carboxylate (6aa).

HBR-DN-86 #3-17 RT: 0.02-0.07 AV: 5 SB: 63 0.32-1.20 NL: 3.42E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

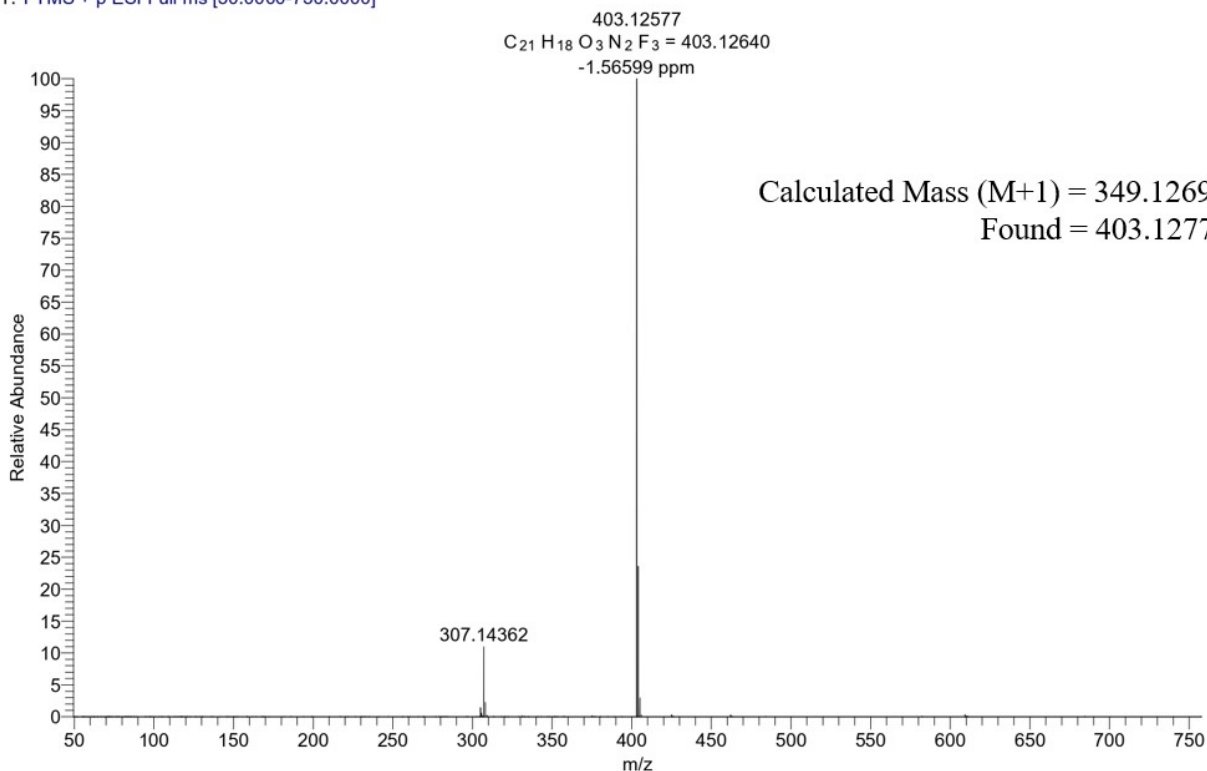


Fig.S167 HRMS of Ethyl 6-acetamido-2-methyl-4-phenyl quinoline-3-carboxylate (6aa).

Signature SIF VIT VELLORE  
VN-086

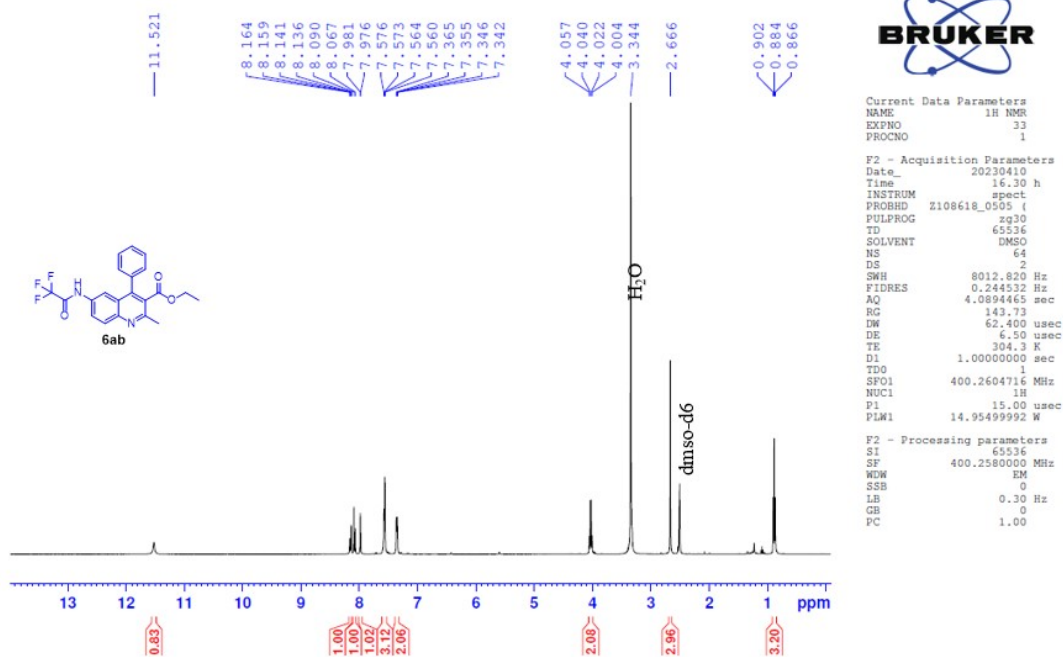


Fig.S168 <sup>1</sup>H NMR of Ethyl 2-methyl-4-phenyl-6-(2,2,2-trifluoroacetamido) quinoline-3-carboxylate (6ab).

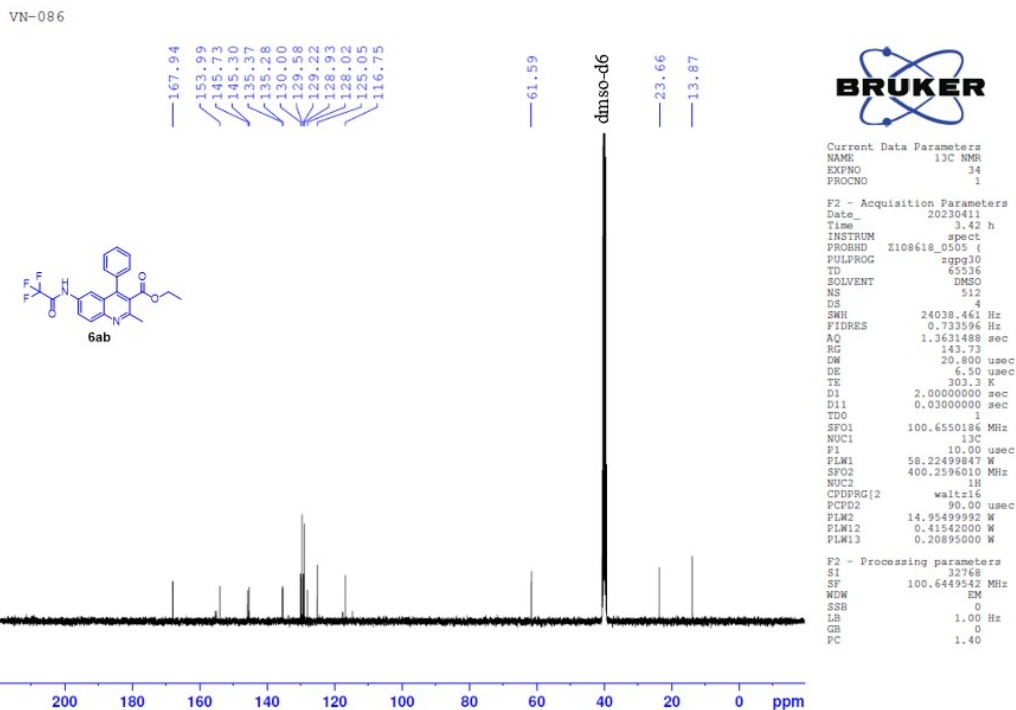


Fig.S169 <sup>13</sup>C NMR of Ethyl 2-methyl-4-phenyl-6-(2,2,2-trifluoroacetamido) quinoline-3-carboxylate (6ab).

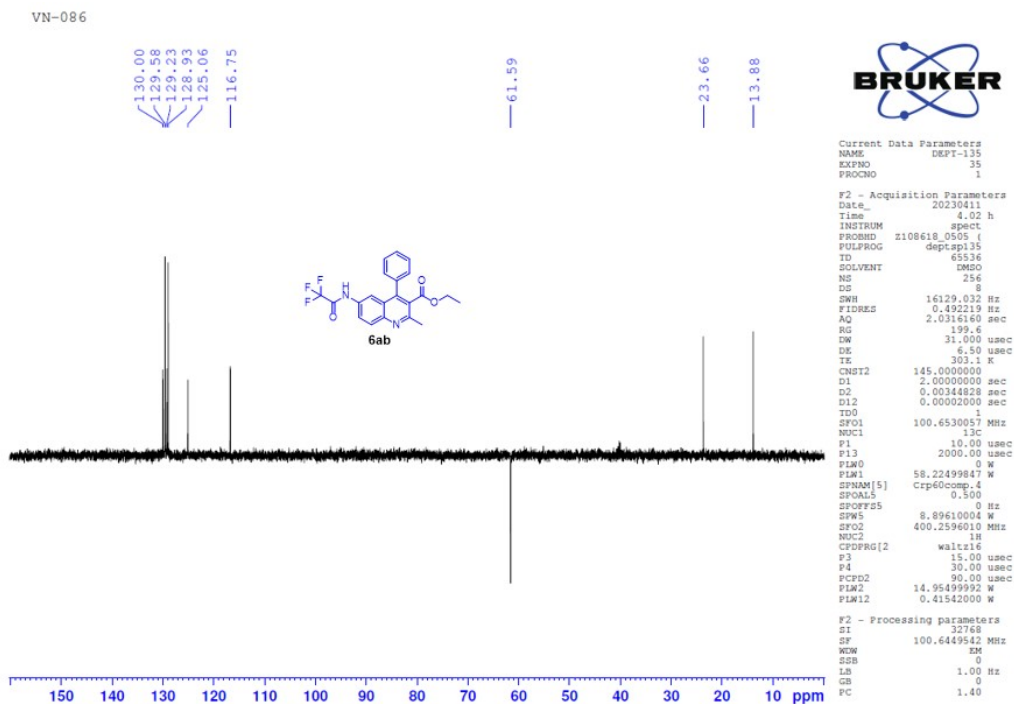


Fig.S170 DEPT-135 of Ethyl 2-methyl-4-phenyl-6-(2,2,2-trifluoroacetamido) quinoline-3-carboxylate (6ab).

HBR-DN-86 #3-17 RT: 0.02-0.07 AV: 5 SB: 63 0.32-1.20 NL: 3.42E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

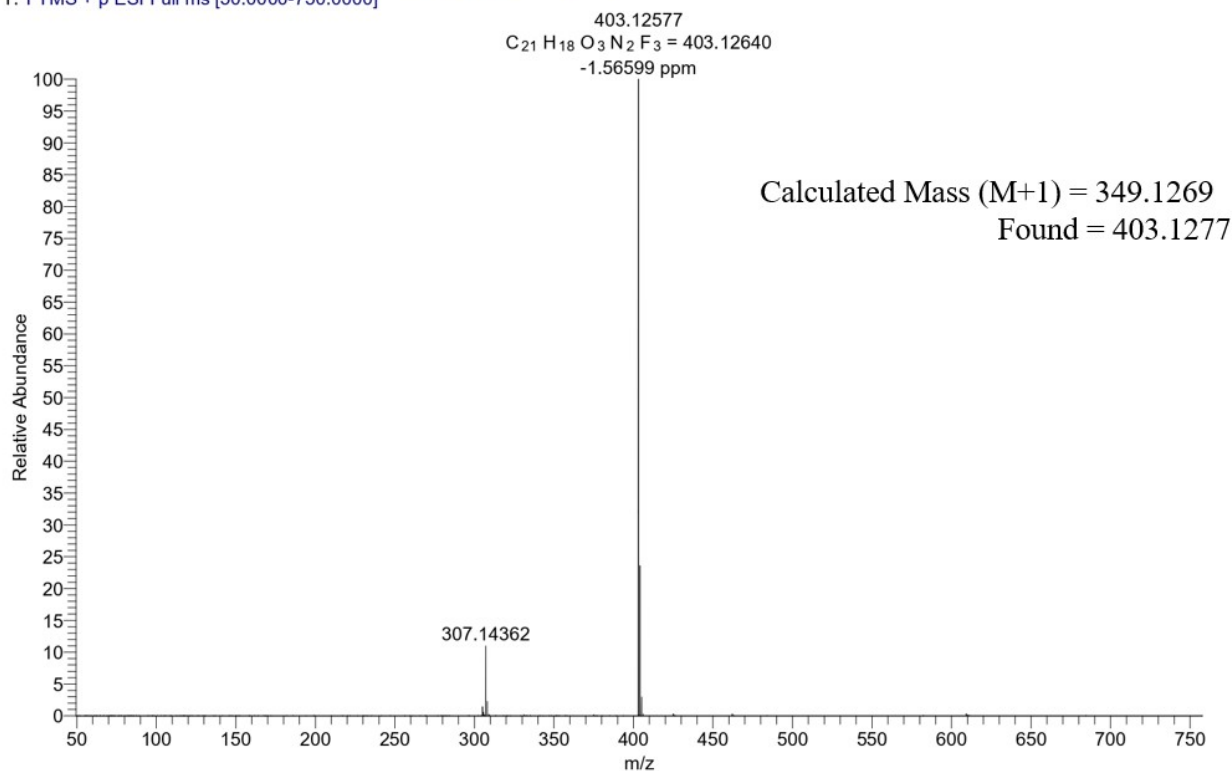


Fig.S171 HRMS of Ethyl 2-methyl-4-phenyl-6-(2,2,2-trifluoroacetamido) quinoline-3-carboxylate (6ab).

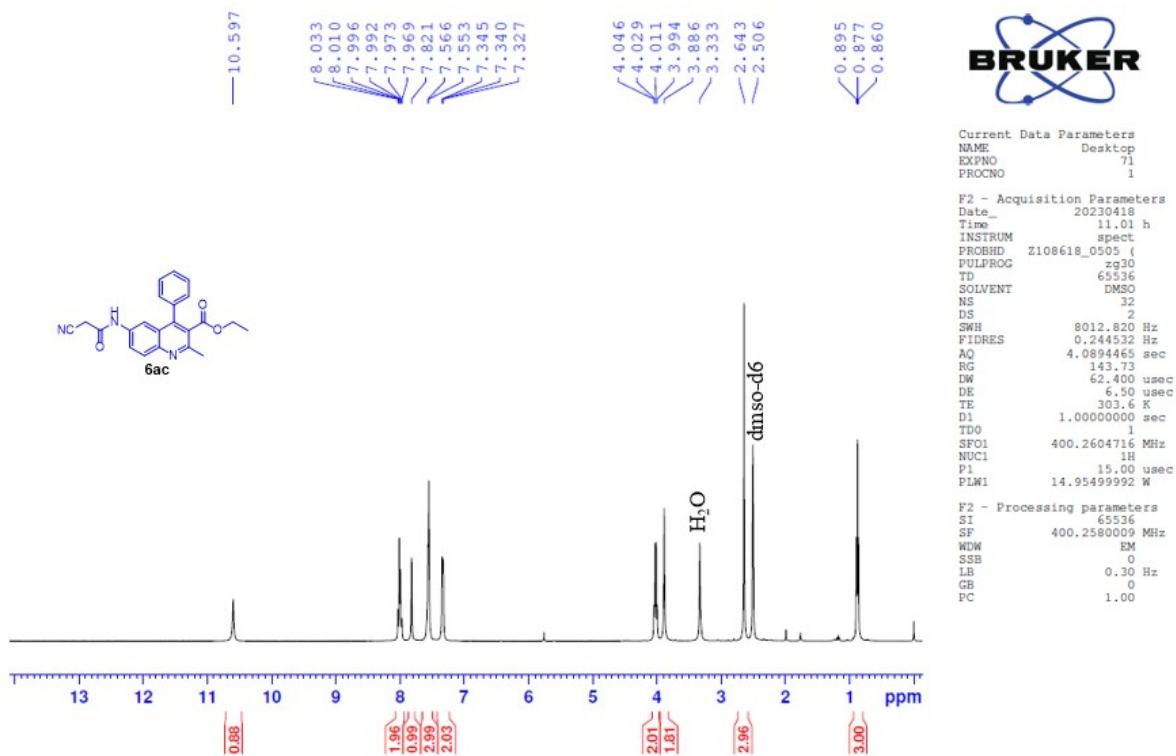


Fig.S172 <sup>1</sup>H NMR of Ethyl 6-(2-cyanoacetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ac).

Signature SIF VIT VELLORE  
 VN-075

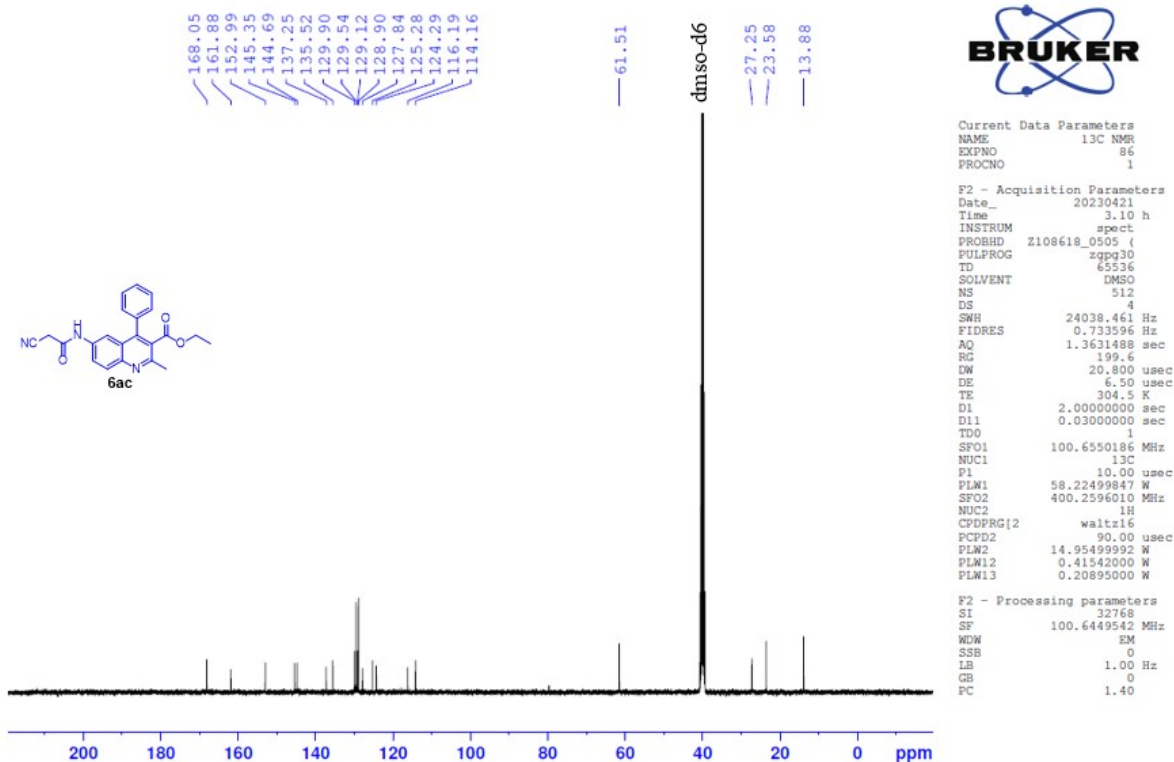


Fig.S173 <sup>13</sup>C NMR of Ethyl 6-(2-cyanoacetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ac).



Signature SIF VIT VELLORE  
VN-075

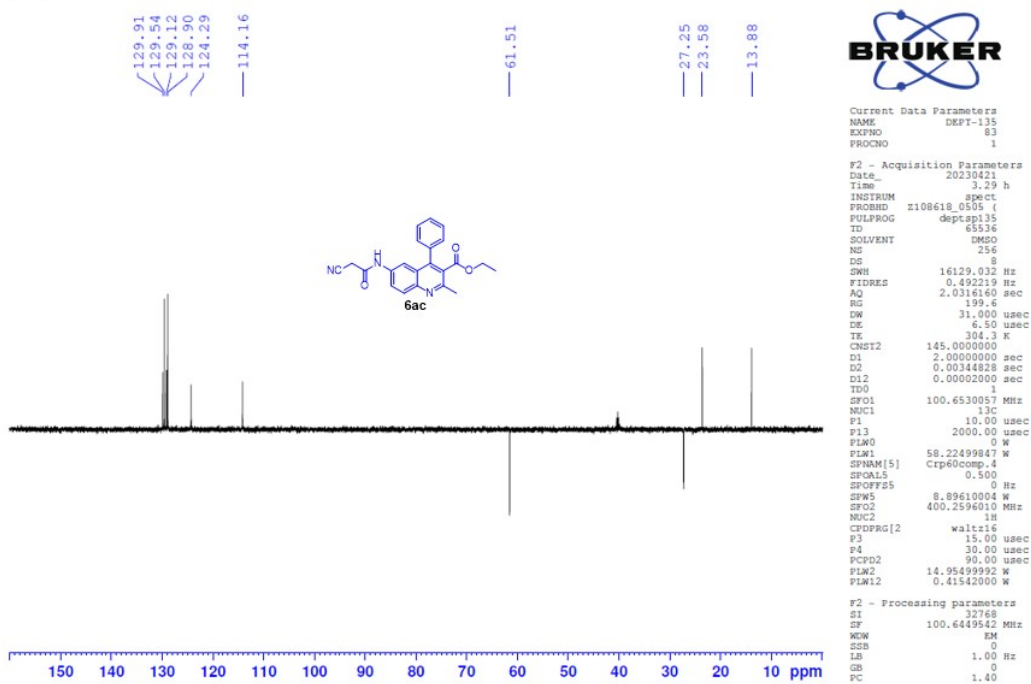


Fig.S174 DEPT-135 of Ethyl 6-(2-cyanoacetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ac).

HBR-DN-075 #1-15 RT: 0.00-0.06 AV: 5 SB: 63 0.32-1.20 NL: 3.53E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

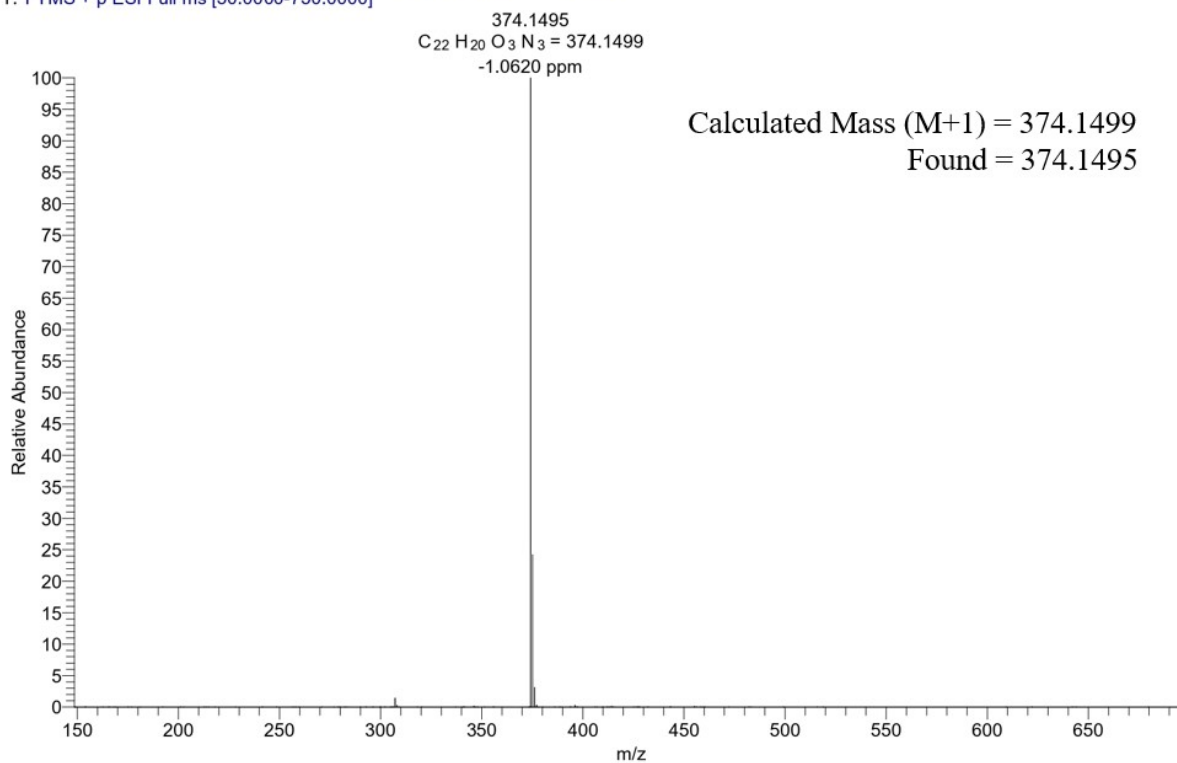


Fig.S175 HRMS of Ethyl 6-(2-cyanoacetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ac).

Signature SIF VIT VELLORE  
VN-066

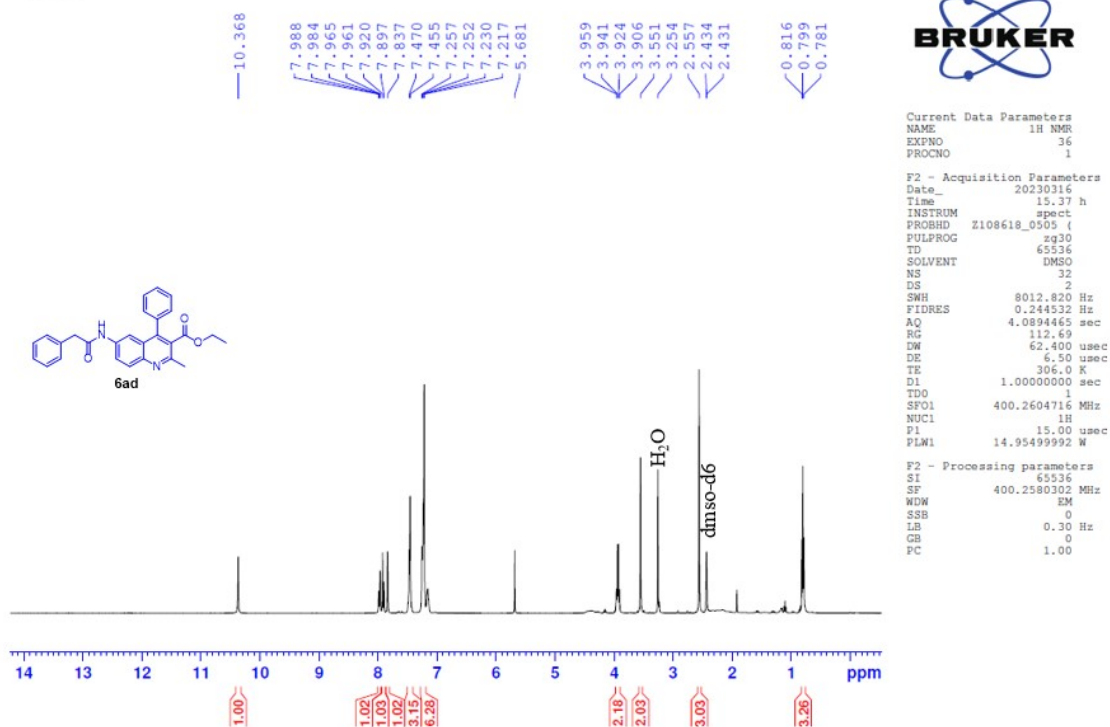


Fig.S176 <sup>1</sup>H NMR of Ethyl 2-methyl-4-phenyl-6-(2-phenylacetamido) quinoline-3-carboxylate(6ad).

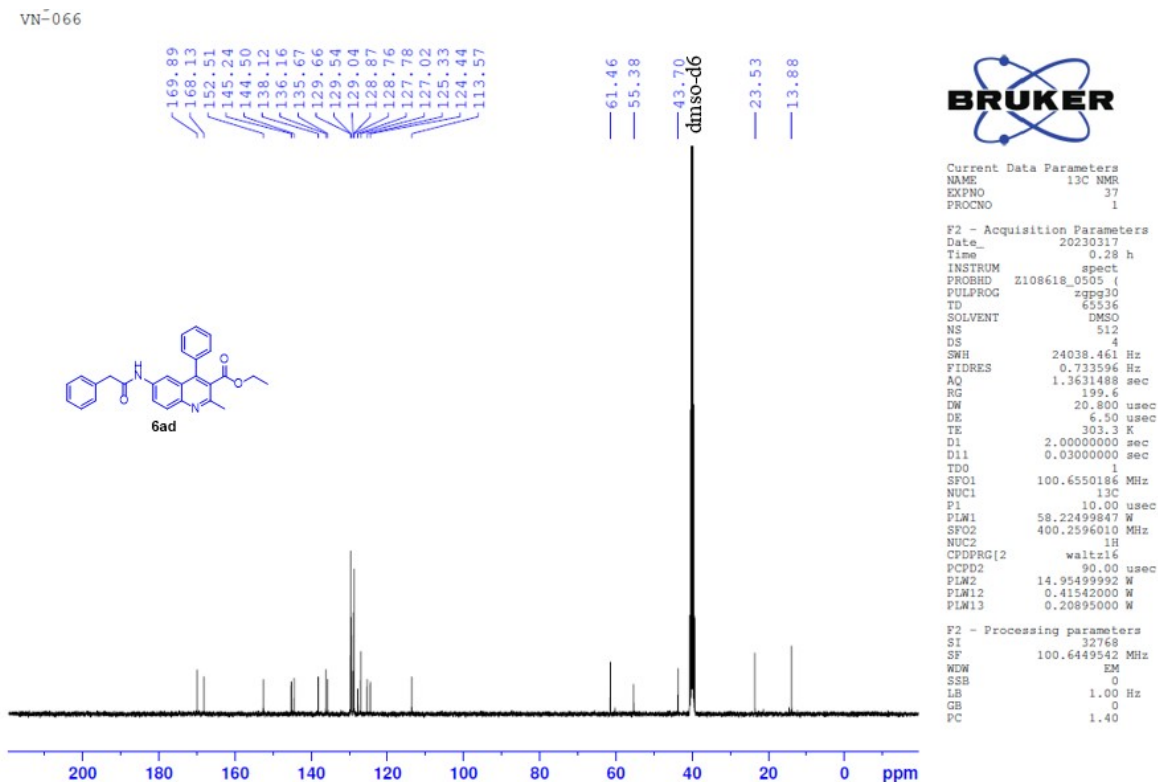


Fig.S177 <sup>13</sup>C NMR of Ethyl 2-methyl-4-phenyl-6-(2-phenylacetamido) quinoline-3-carboxylate(6ad).

Signature SIF VIT VELLORE  
VN-066

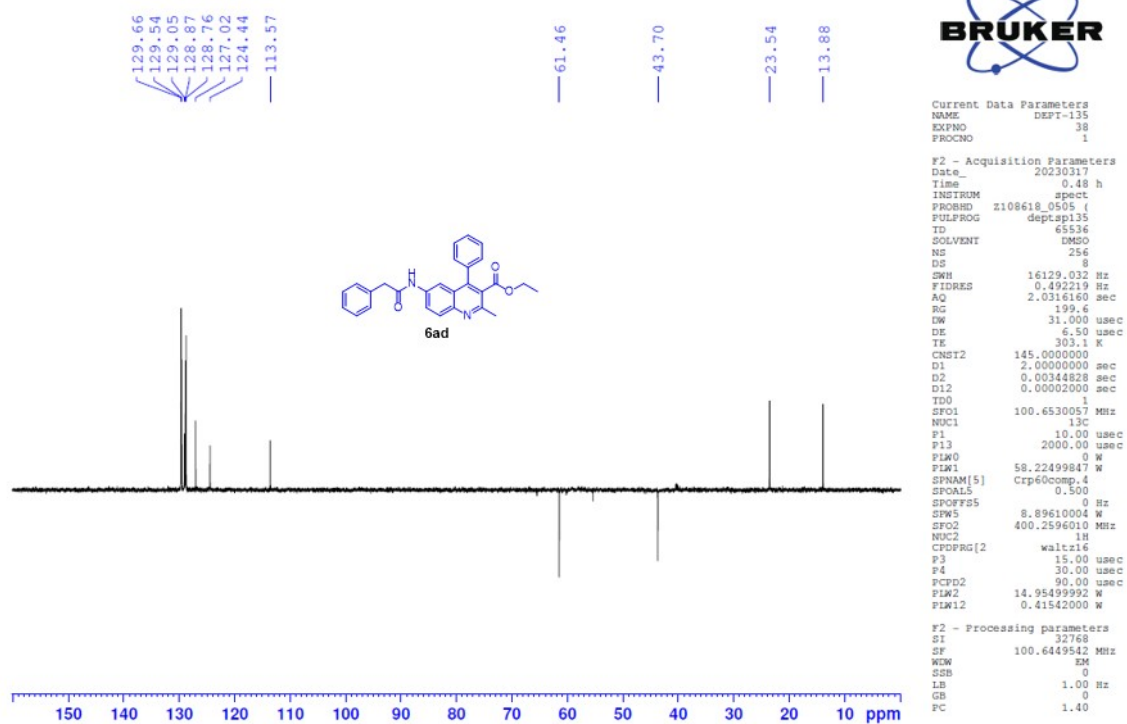


Fig.S178 DEPT-135 of Ethyl 2-methyl-4-phenyl-6-(2-phenylacetamido) quinoline-3-carboxylate(6ad).

HBR-DN-066 #2-15 RT: 0.02-0.06 AV: 4 SB: 63 0.32-1.20 NL: 7.10E8  
T: FTMS + p ESI Full ms [50.0000-750.0000]

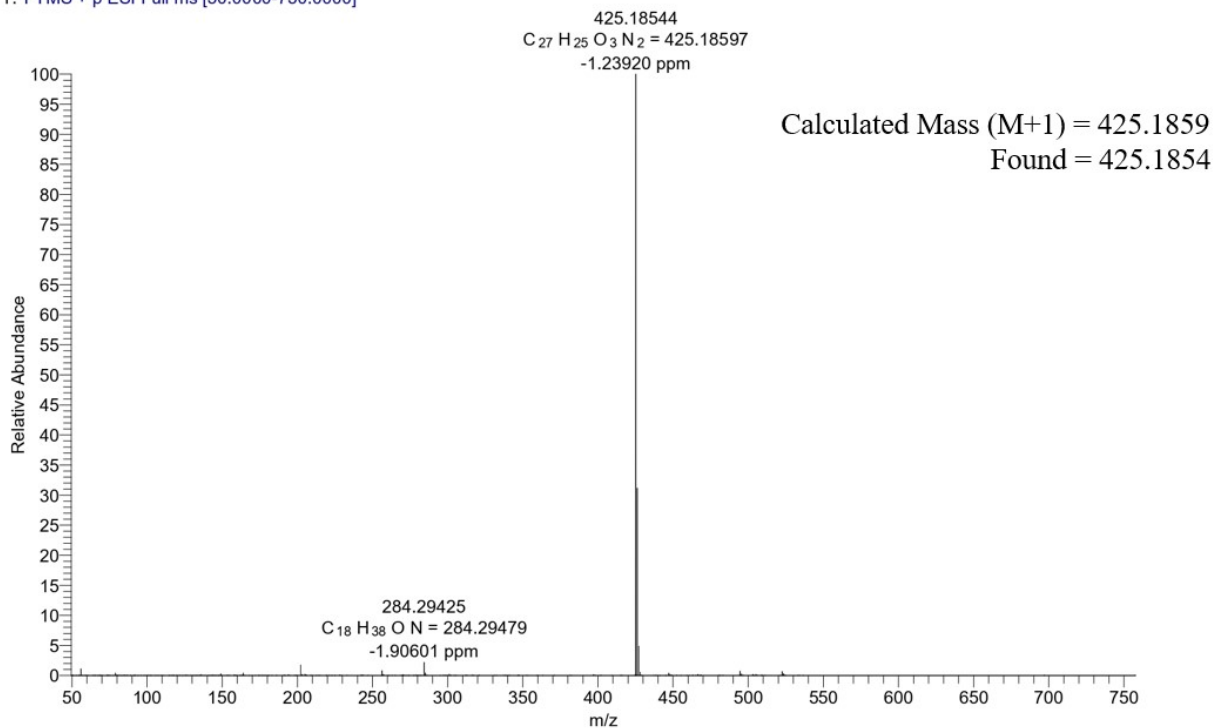
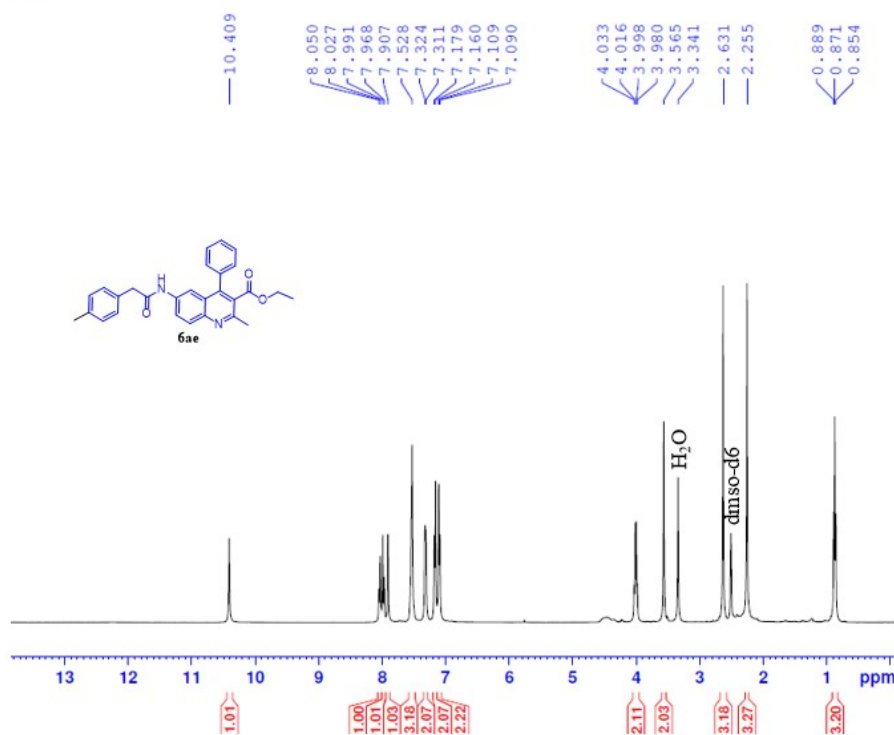


Fig.S179 HRMS of Ethyl 2-methyl-4-phenyl-6-(2-phenylacetamido) quinoline-3-carboxylate(6ad).

Signature SIF VIT VELLORE  
VN-061



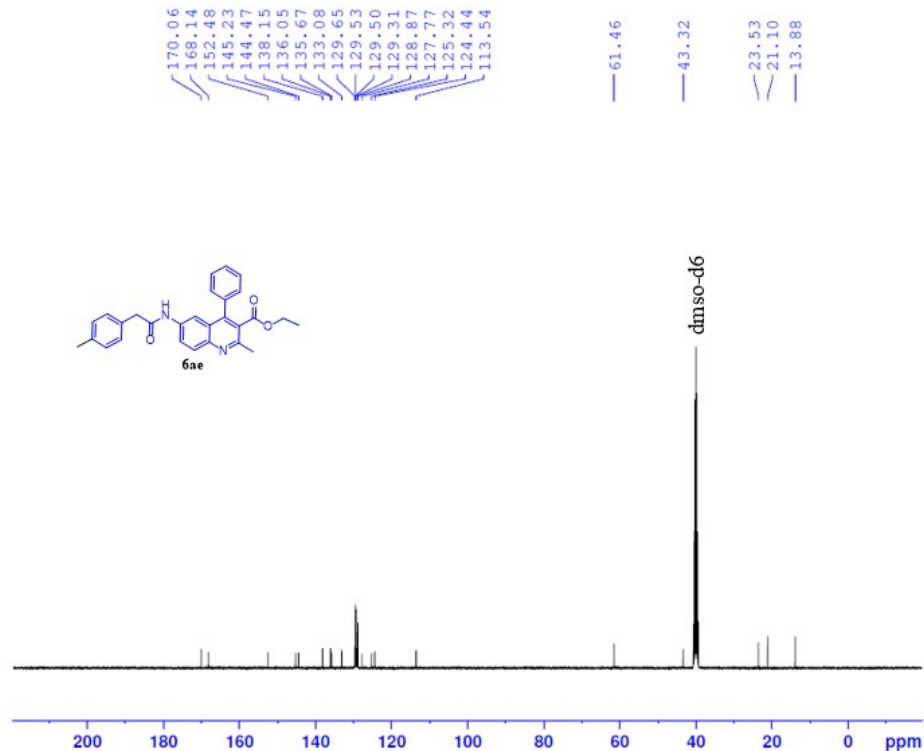
Current Data Parameters  
NAME 1H NMR  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230302  
Time 16.17 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 98.85  
DW 62.400 usec  
DE 6.50 usec  
TE 304.6 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.2604716 MHz  
NUC1 1H  
P1 15.00 usec  
PLW1 14.95499992 W

F2 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Fig.S180 <sup>1</sup>H NMR of Ethyl 2-methyl-4-phenyl-6-(2-(p-tolyl)acetamido)quinoline-3-carboxylate (6ae).

Signature SIF VIT VELLORE  
VN-061



Current Data Parameters  
NAME 13C NMR  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230302  
Time 21.18 h  
INSTRUM spect  
PROBHD Z108618\_0505 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.732596 Hz  
AQ 1.3631488 sec  
RG 156.91  
DW 20.800 usec  
DE 6.50 usec  
TE 302.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6550186 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 58.22499847 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 14.95499992 W  
PLW12 0.41542000 W  
PLW13 0.20895000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S181 <sup>13</sup>C NMR of Ethyl 2-methyl-4-phenyl-6-(2-(p-tolyl)acetamido)quinoline-3-carboxylate (6ae).

Signature SIF VIT VELLORE  
VN-061

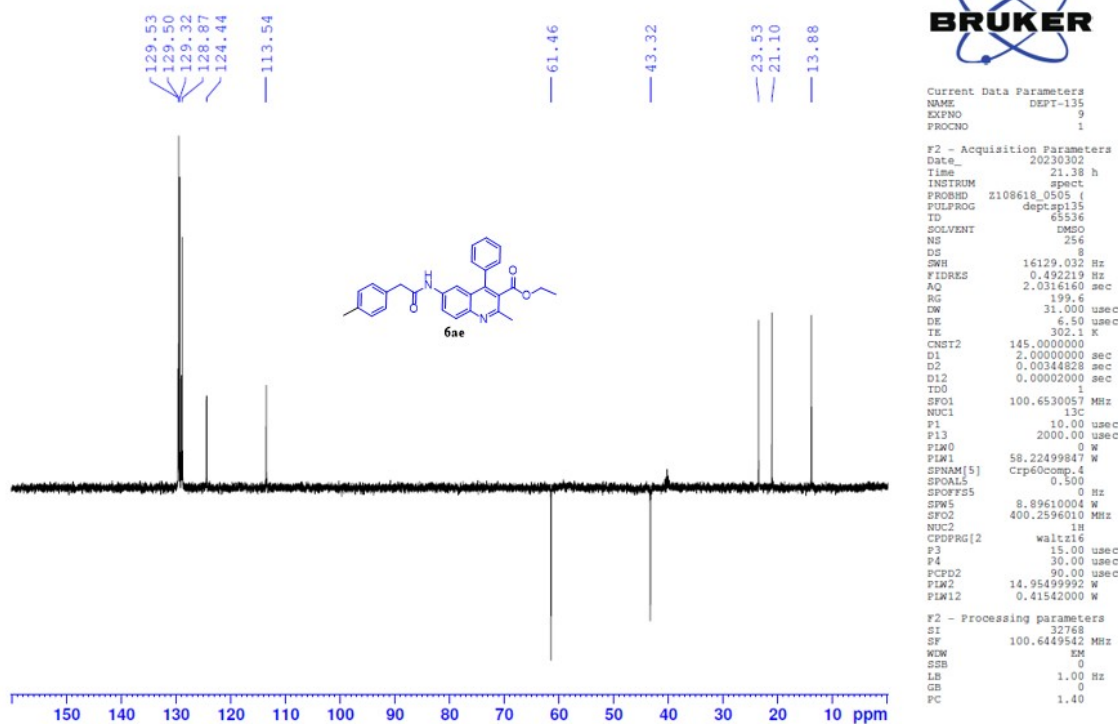


Fig.S182 DEPT-135 of Ethyl 2-methyl-4-phenyl-6-(2-(p-tolyl)acetamido)quinoline-3-carboxylate (6ae).

HBR-DN-61 #1-29 RT: 0.00-0.13 AV: 10 SB: 64 0.32-1.20 NL: 2.71E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

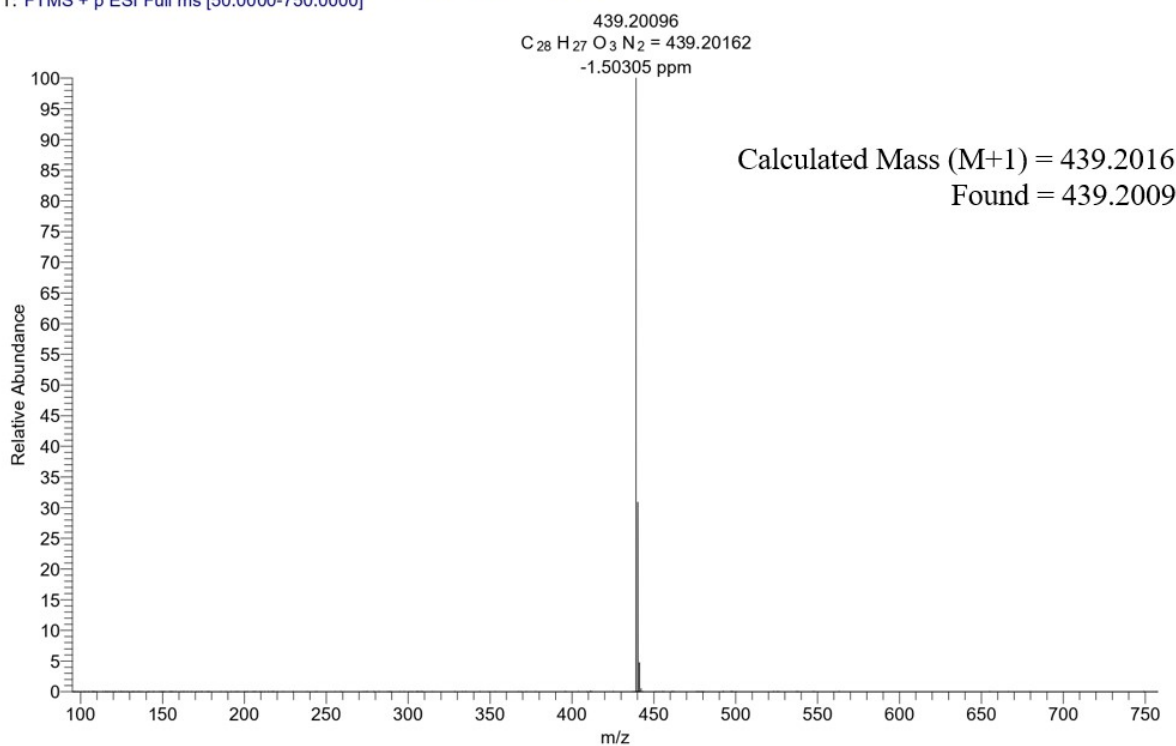


Fig.S183 HRMS of Ethyl 2-methyl-4-phenyl-6-(2-(p-tolyl)acetamido)quinoline-3-carboxylate (6ae).

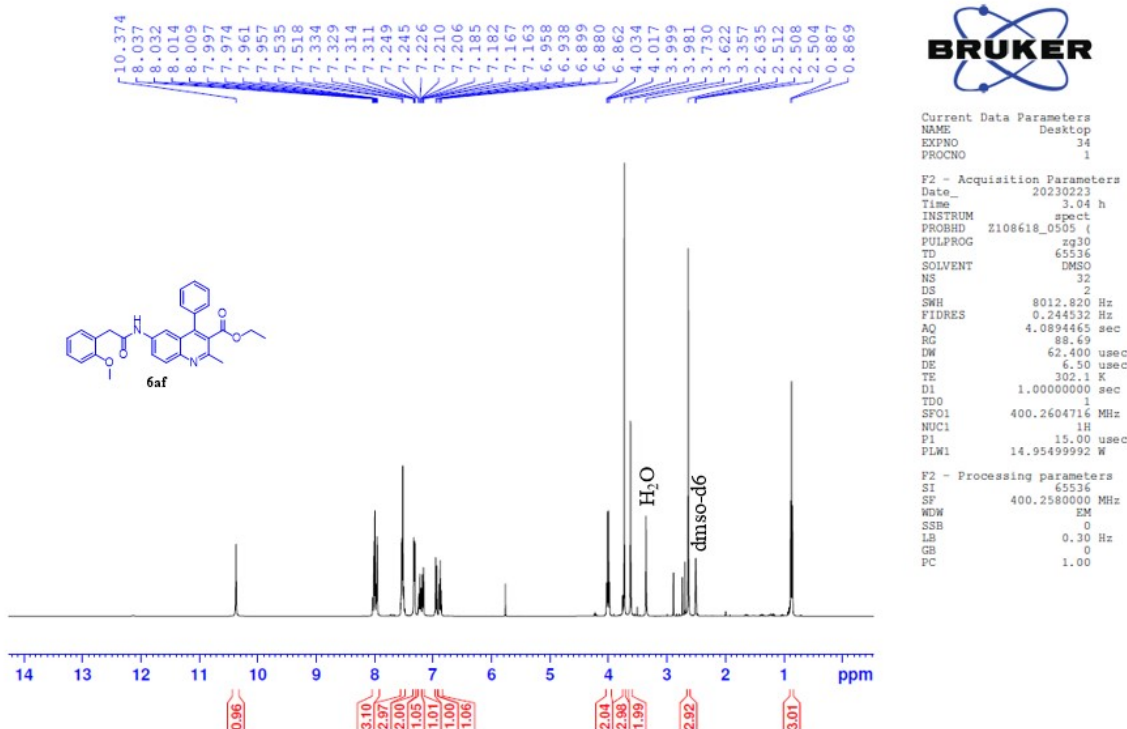


Fig.S184 <sup>1</sup>H NMR of Ethyl 6-(2-(2-methoxyphenyl)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6af).

Signature SIF VIT VELLORE  
 VN-059

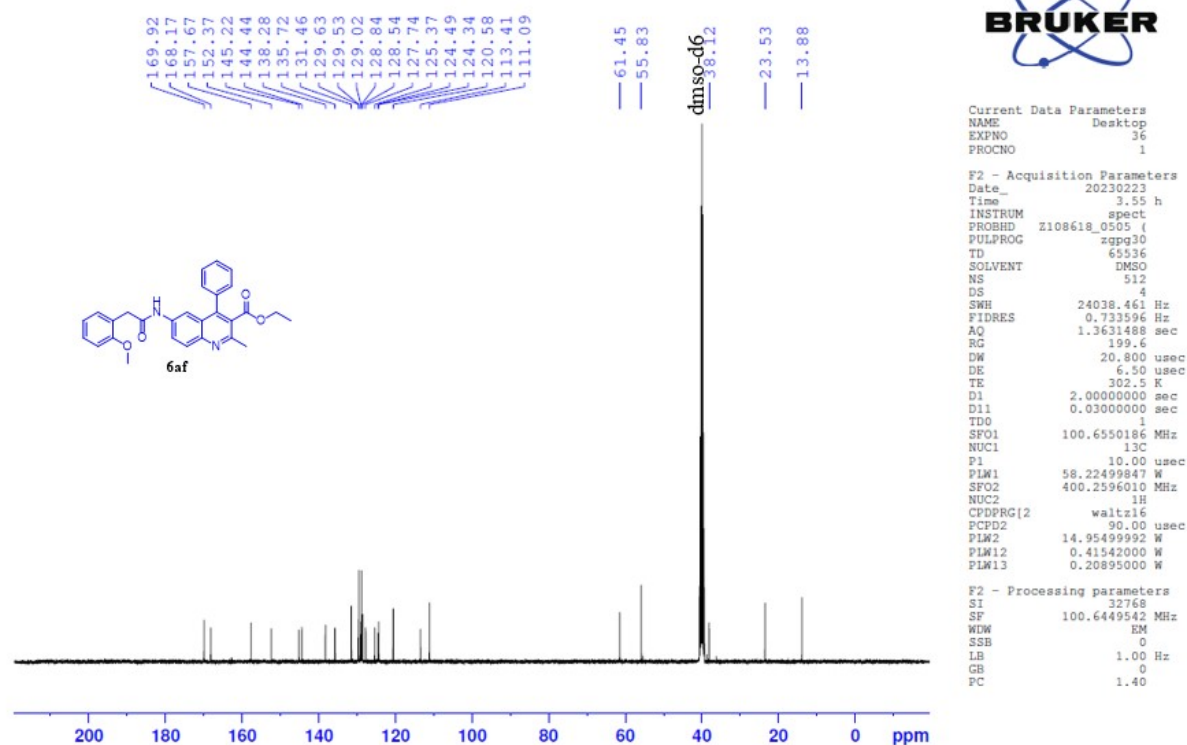


Fig.S185 <sup>13</sup>C NMR of Ethyl 6-(2-(2-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6af).

Signature SIF VIT VELLORE  
VN-059

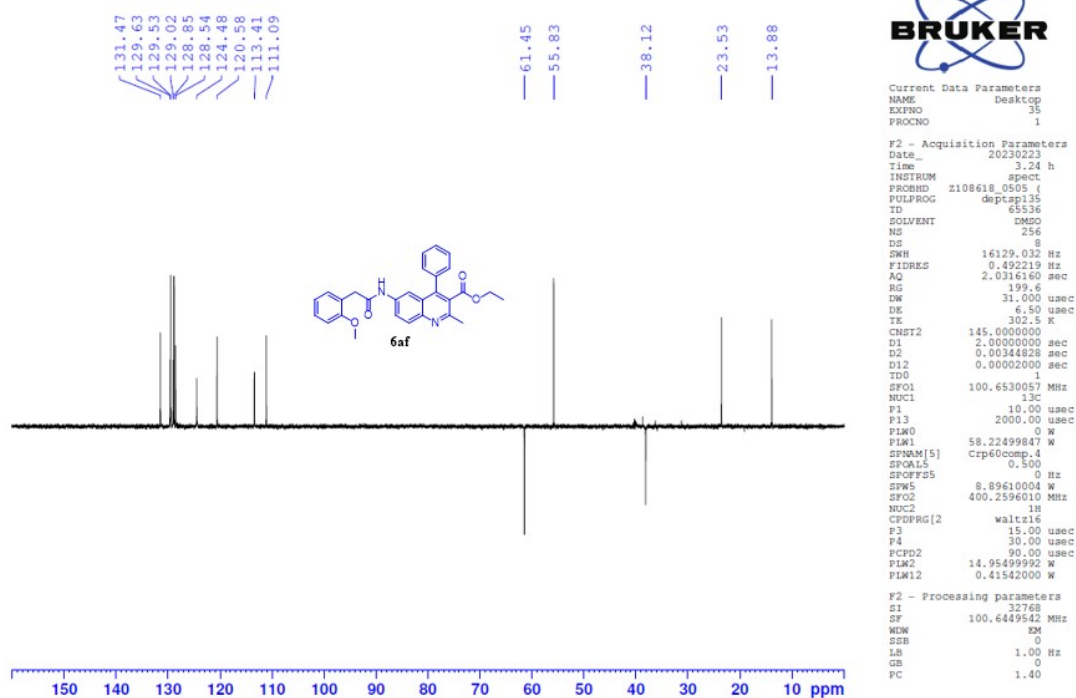


Fig.S186 DEPT-135 of Ethyl 6-(2-(2-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6af).

HBR-DN-059 #2-13 RT: 0.02-0.06 AV: 4 SB: 63 0.32-1.20 NL: 2.33E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

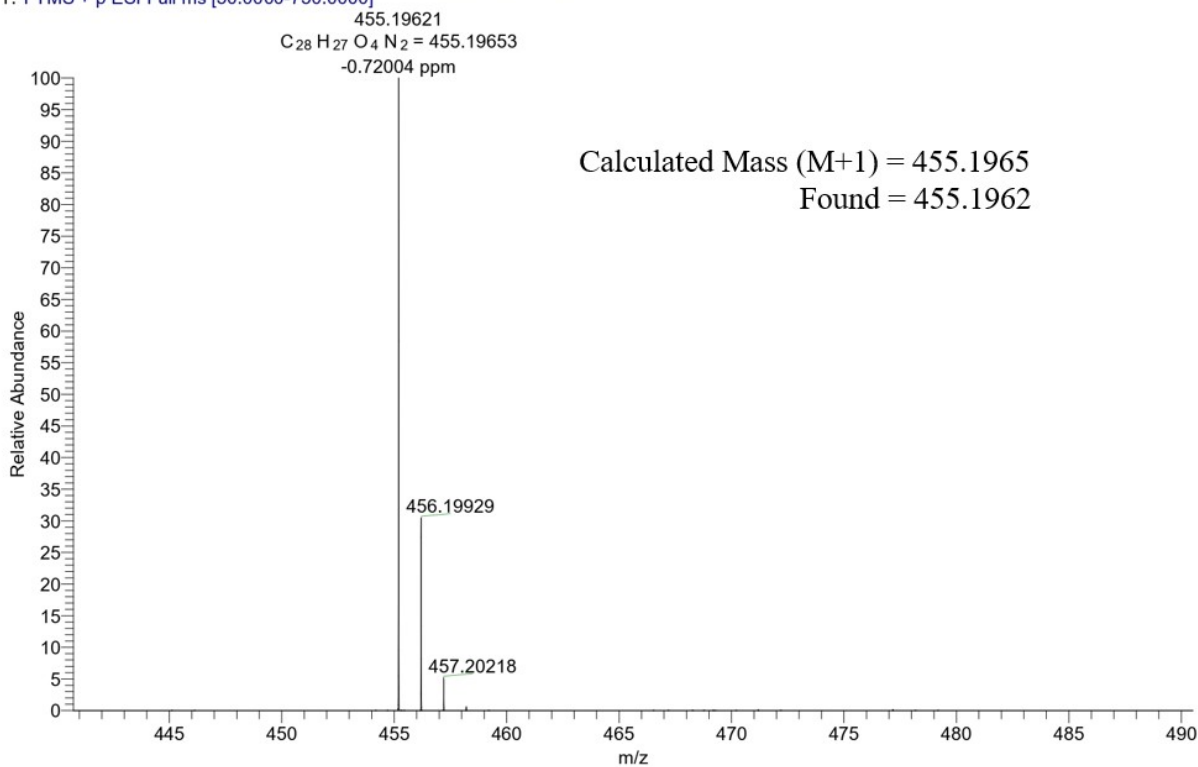


Fig.S187 HRMS of Ethyl 6-(2-(2-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6af).

Signature SIF VIT VELLORE  
VN-060

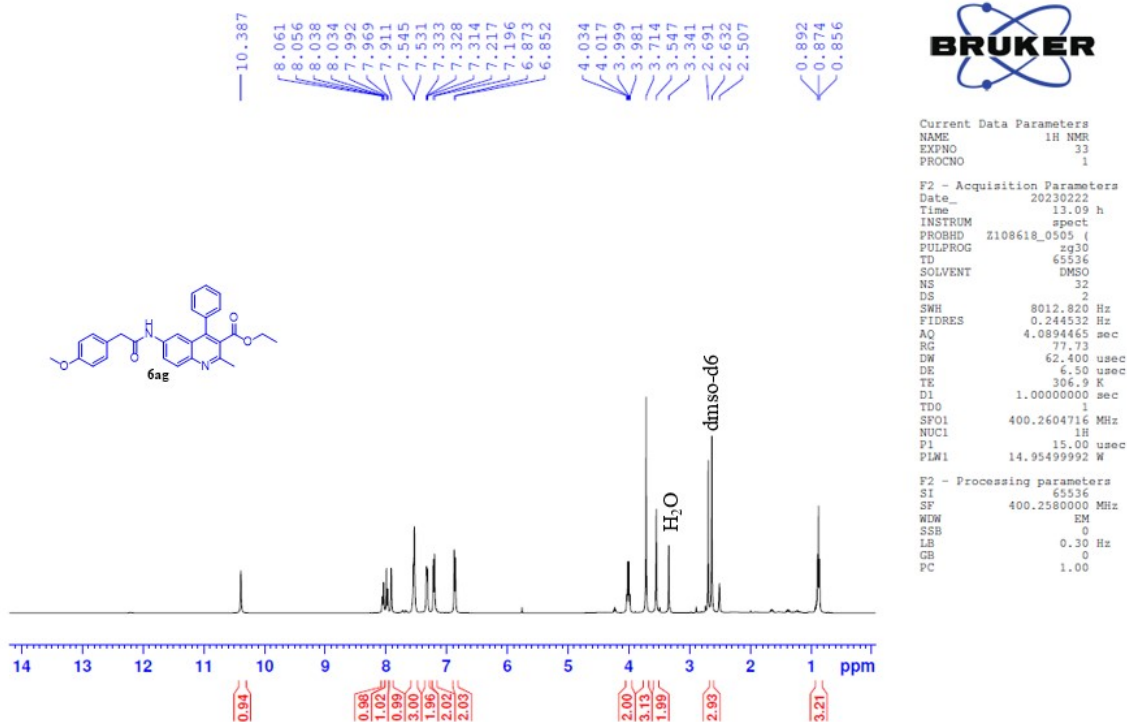


Fig.S188 <sup>1</sup>H NMR of Ethyl 6-(2-(4-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ag).

Signature SIF VIT VELLORE  
VN-06

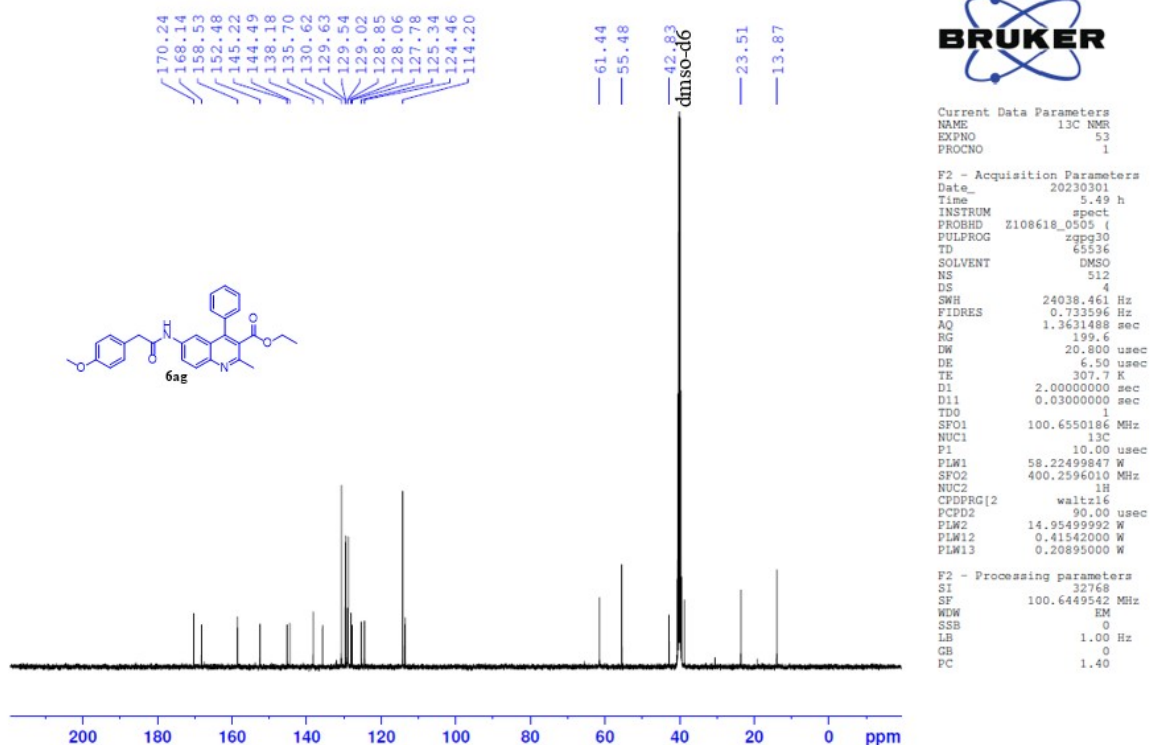


Fig.S189 <sup>13</sup>C NMR of Ethyl 6-(2-(4-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ag).



Signature SIF VIT VELLORE  
VN-06

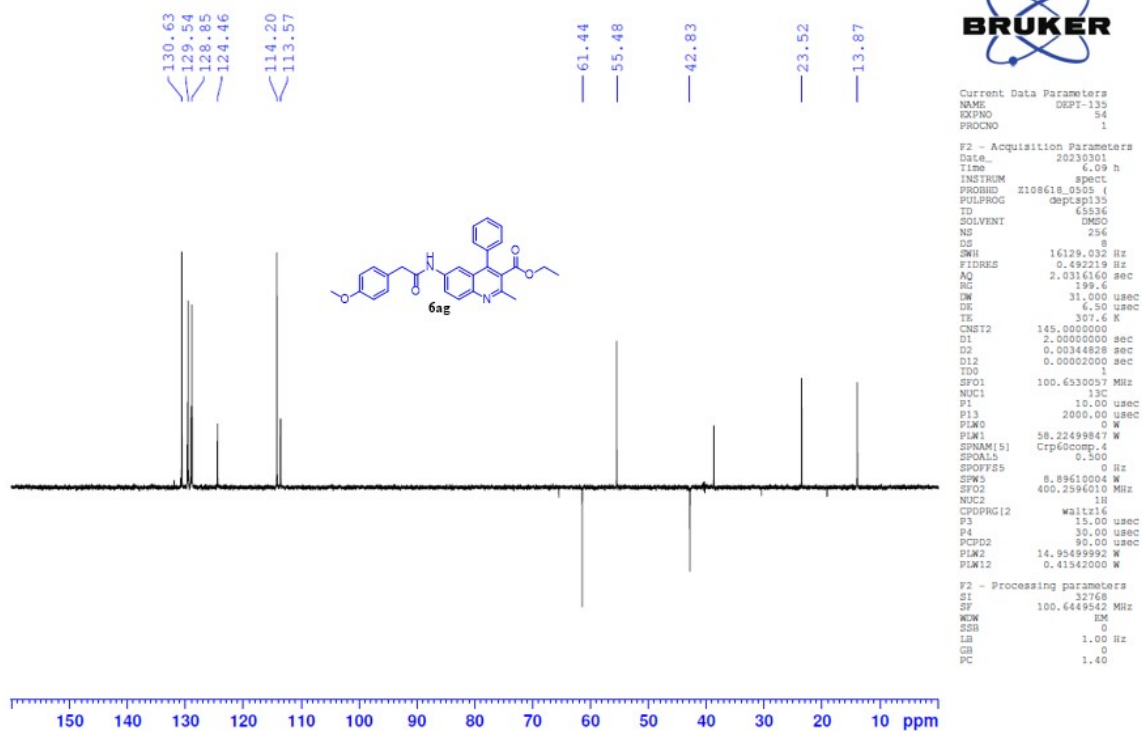


Fig.S190 DEPT-135 of Ethyl 6-(2-(4-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ag).

HBR-DN-060 #4-24 RT: 0.02-0.10 AV: 7 SB: 63 0.32-1.20 NL: 3.33E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

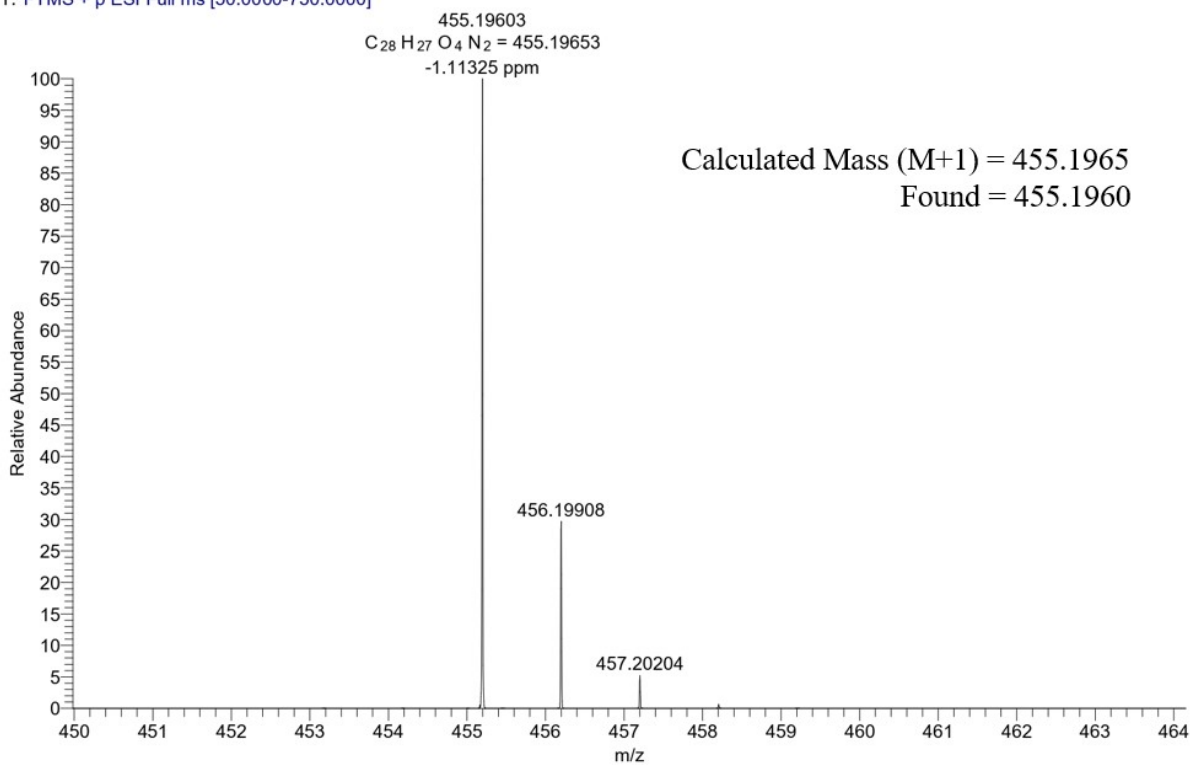


Fig.S191 HRMS of Ethyl 6-(2-(4-methoxyphenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ag)

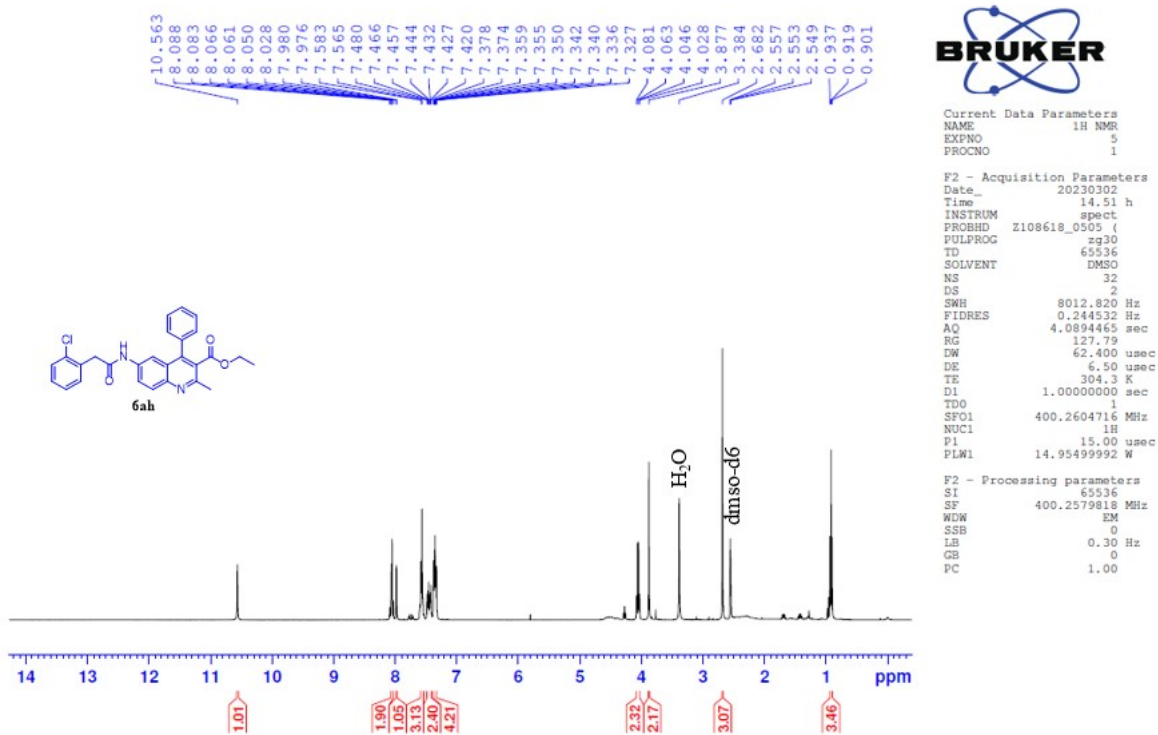


Fig.S192 <sup>1</sup>H NMR of Ethyl 6-(2-(2-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ah).

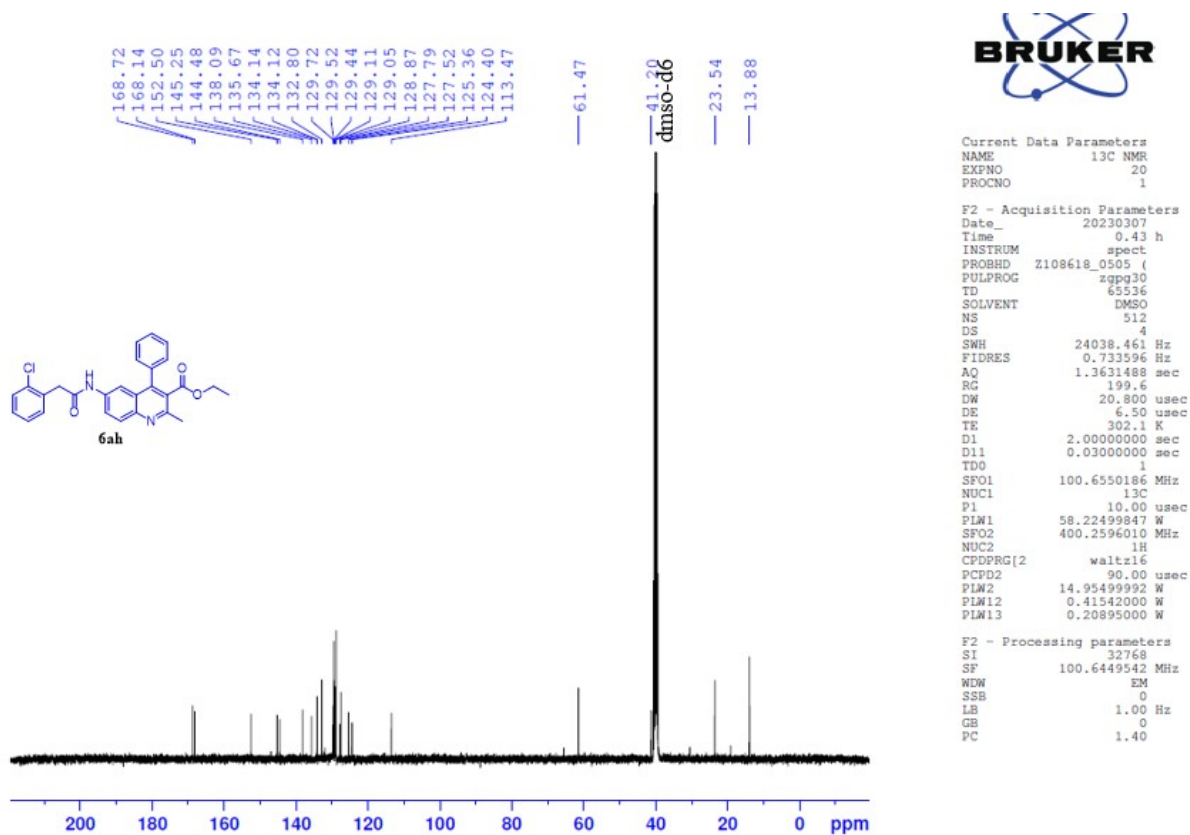


Fig.S193 <sup>13</sup>C NMR of Ethyl 6-(2-(2-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ah).

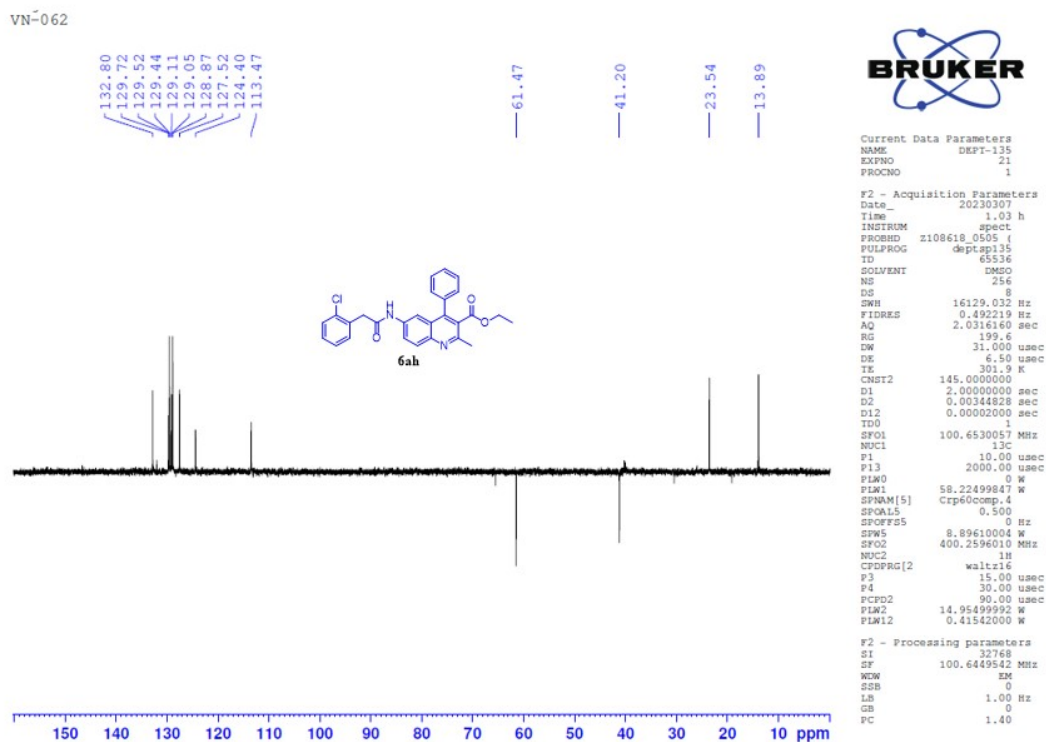


Fig.S194 DEPT-135 of Ethyl 6-(2-(2-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ah).

HBR-DN-062 #4-24 RT: 0.02-0.10 AV: 7 SB: 63 0.32-1.20 NL: 5.21E8  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

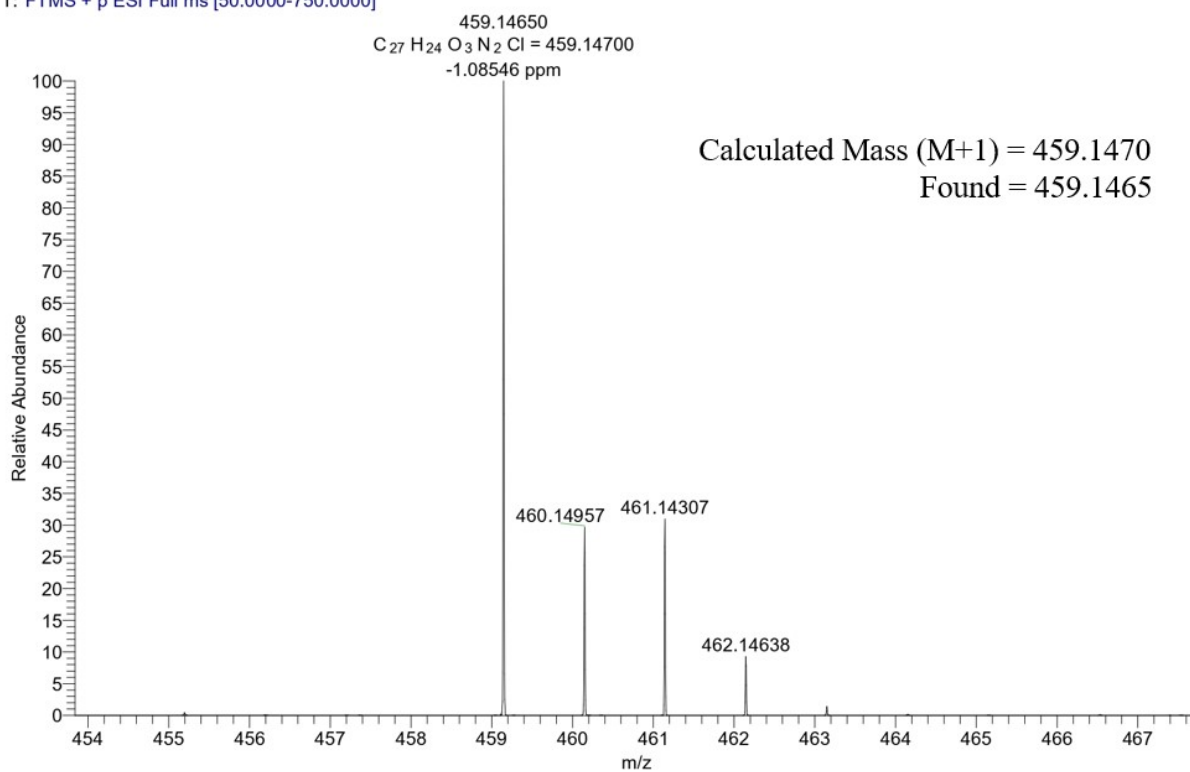


Fig.S195 HRMS of Ethyl 6-(2-(2-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ah).

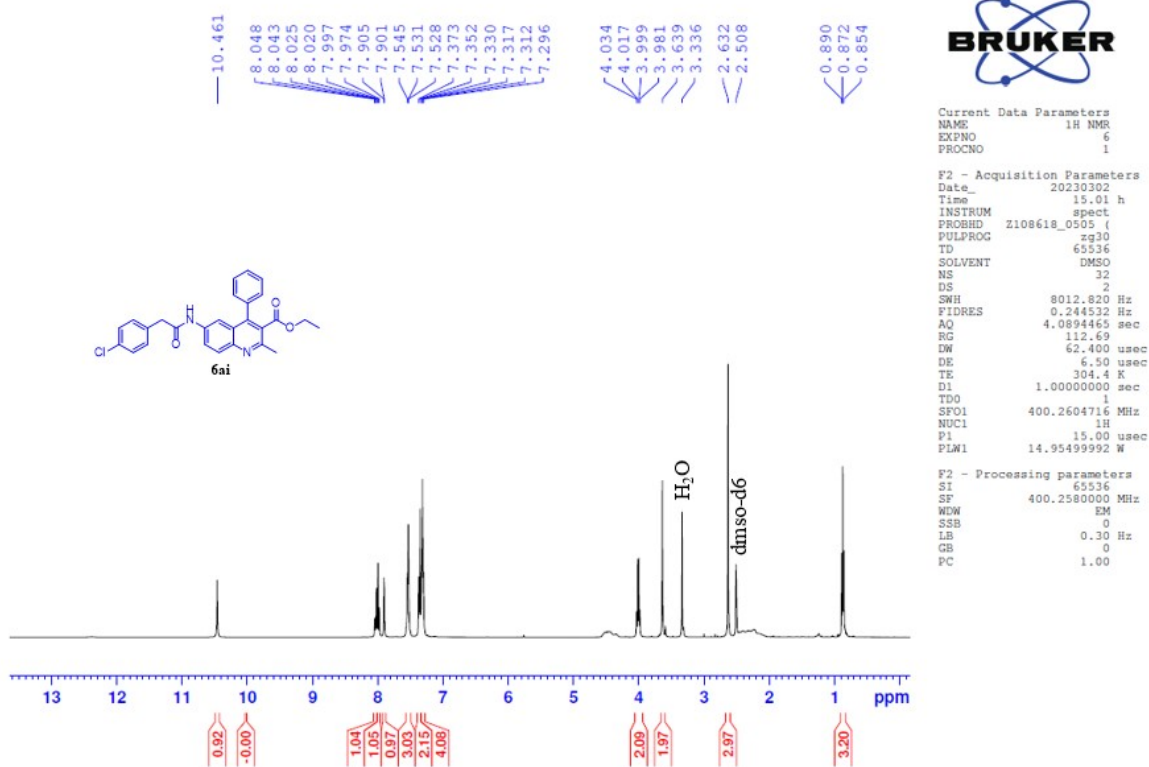


Fig.S196 <sup>1</sup>H NMR of Ethyl 6-(2-(4-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ai).

Signature SIF VIT VELLORE  
 VN-063

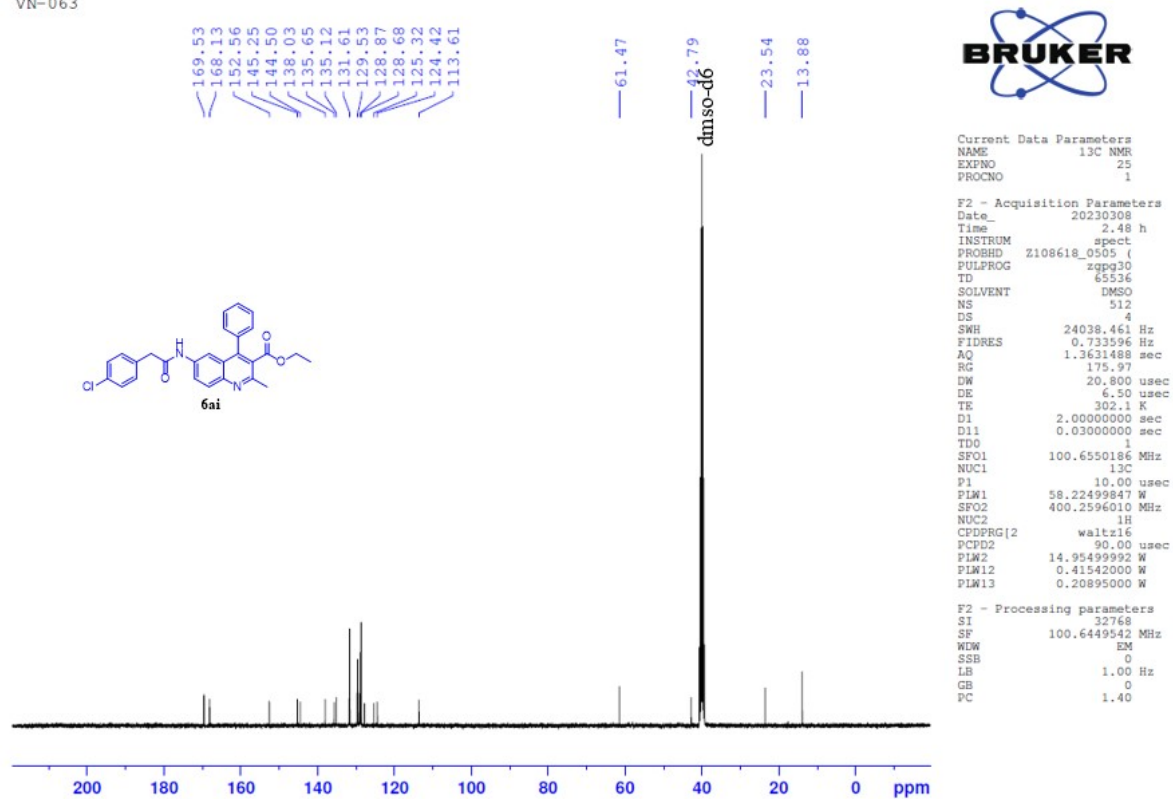


Fig.S197 <sup>13</sup>C NMR of Ethyl 6-(2-(4-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ai).

Signature SIF VIT VELLORE  
VN-063

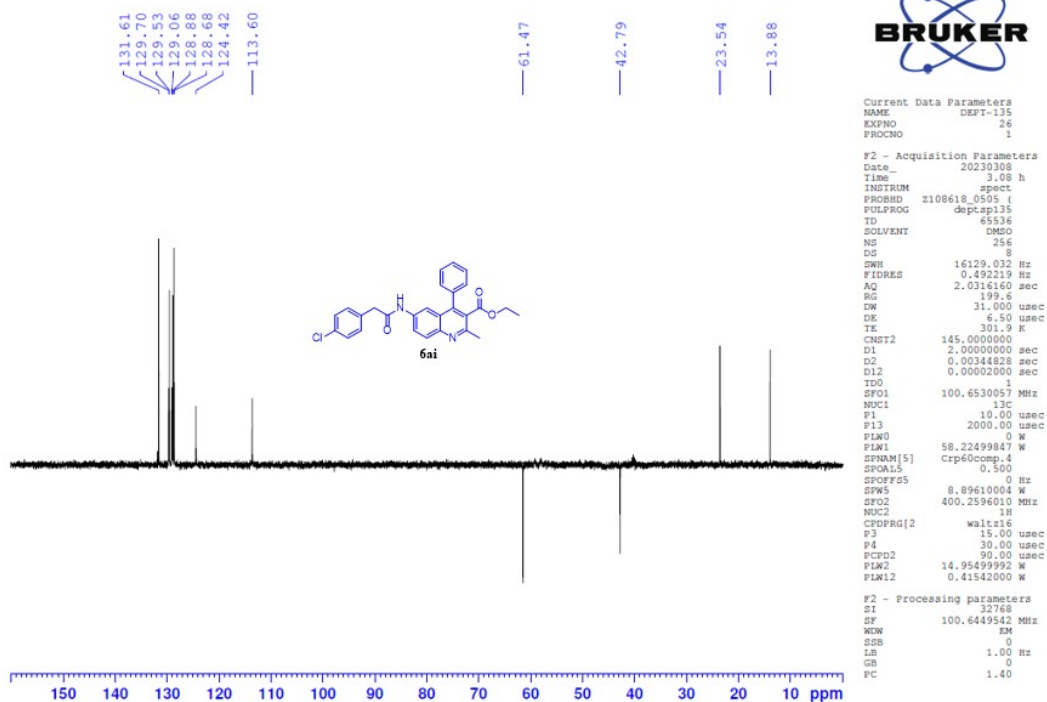


Fig.S198 DEPT-135 of Ethyl 6-(2-(4-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ai).

HBR-DN-063 #4-24 RT: 0.02-0.10 AV: 7 SB: 63 0.32-1.20 NL: 8.88E8  
T: FTMS + p ESI Full ms [50.0000-750.0000]

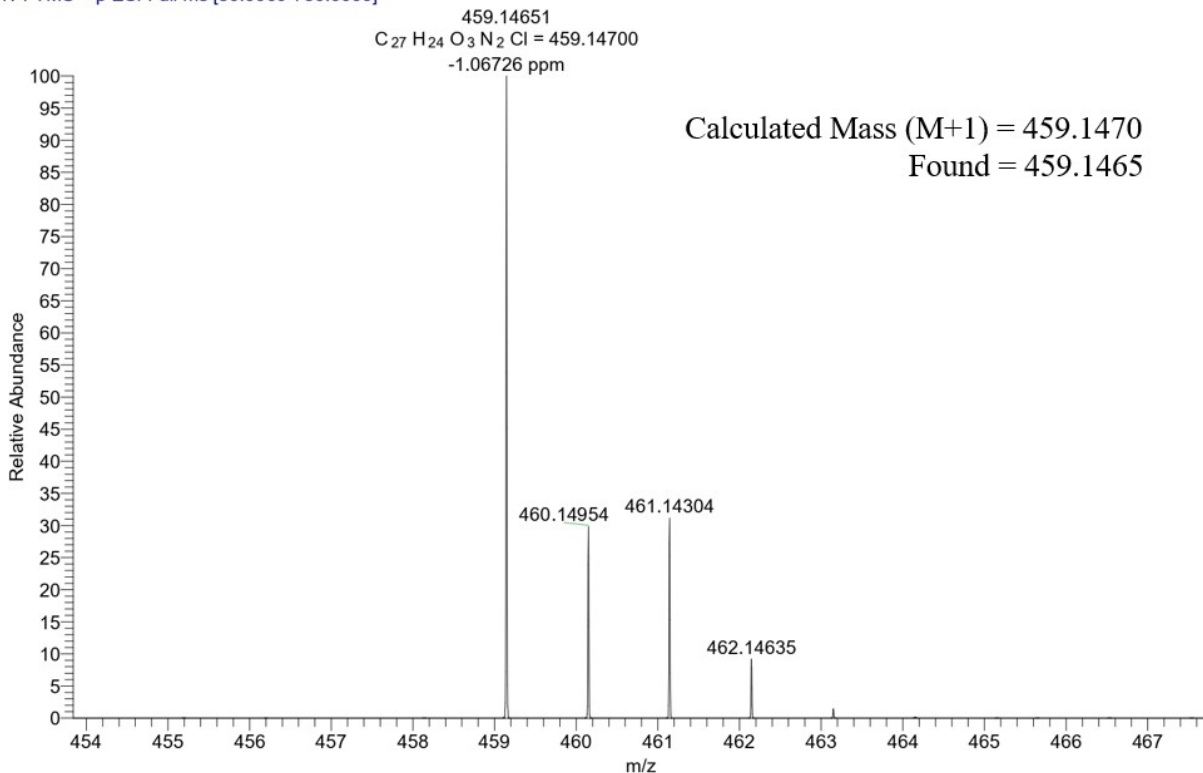


Fig.S199 HRMS of Ethyl 6-(2-(4-chlorophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ai).

VN-064

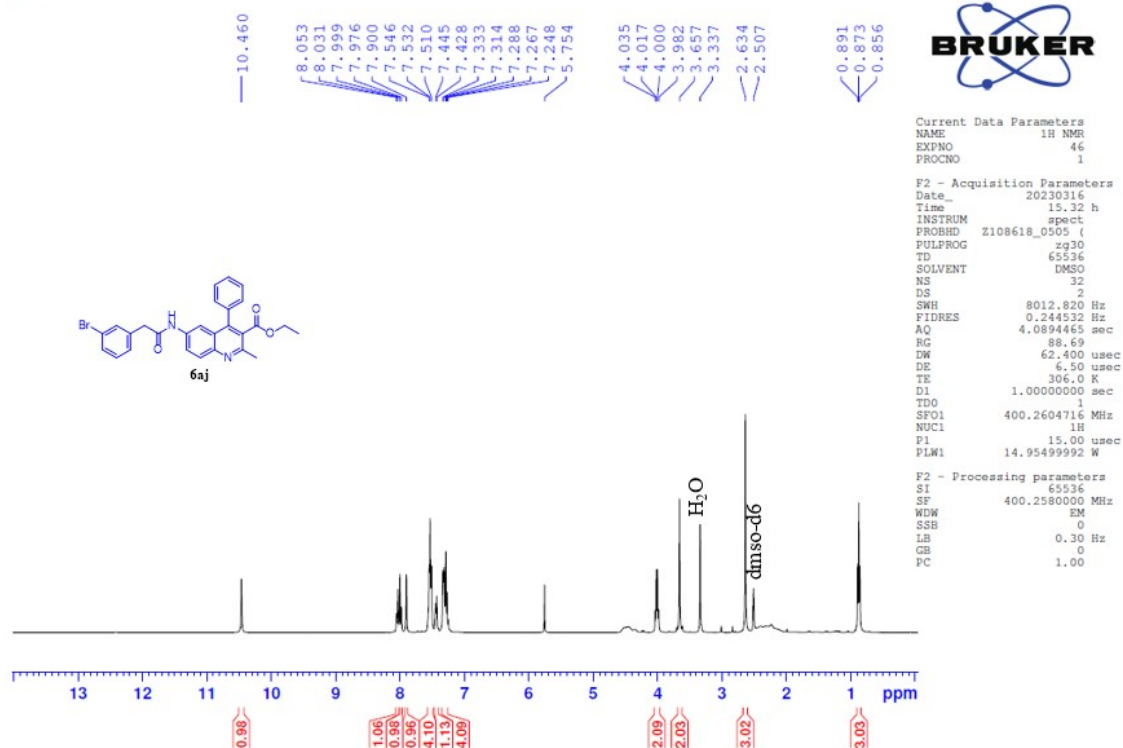


Fig.S200 <sup>1</sup>H NMR of Ethyl 6-(2-(3-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aj).

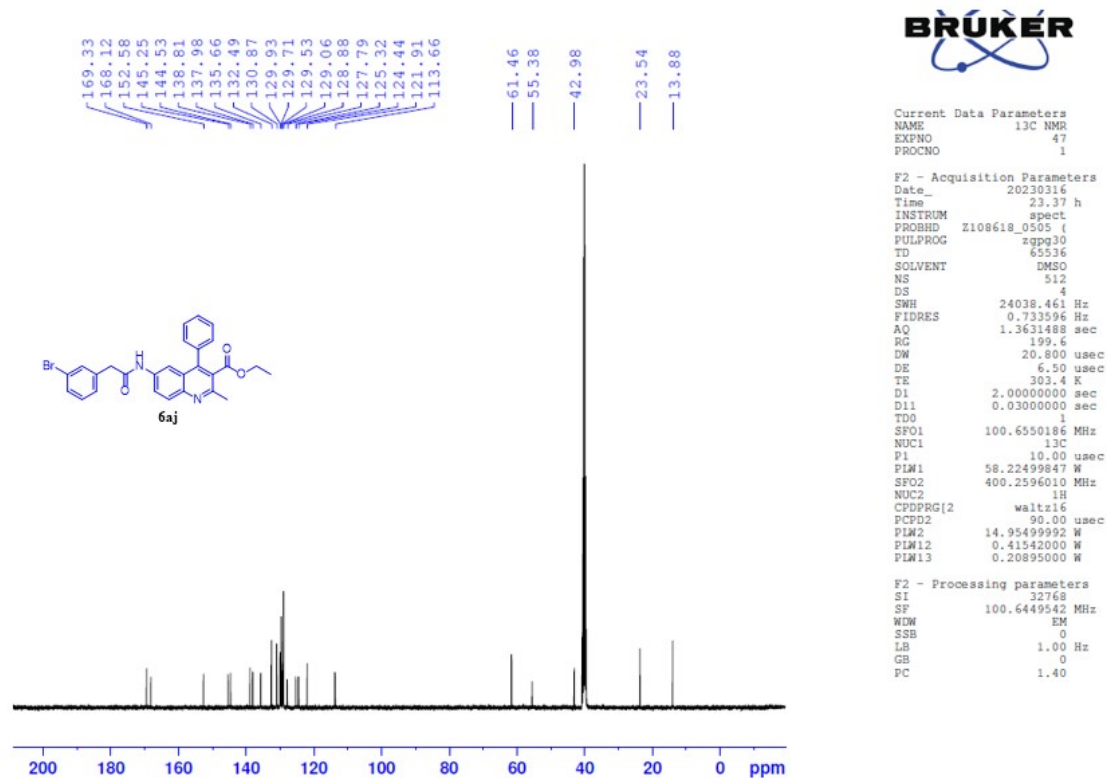


Fig.S201 <sup>13</sup>C NMR of Ethyl 6-(2-(3-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aj).

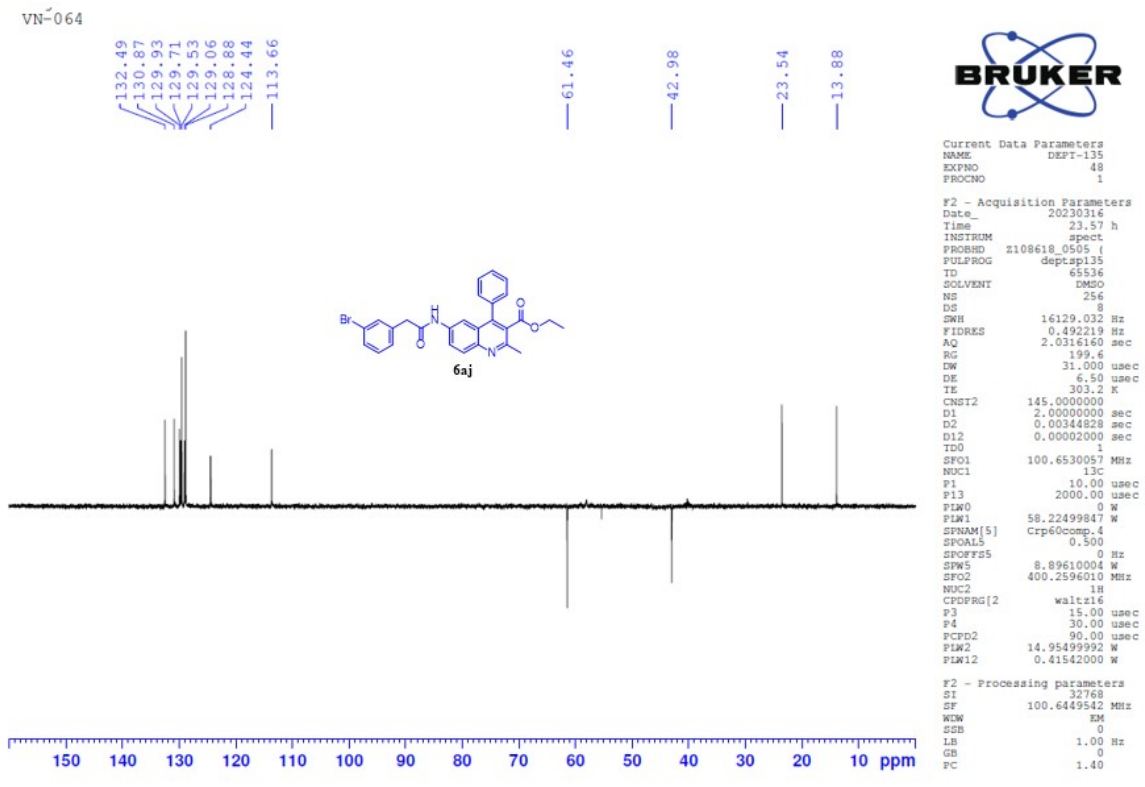


Fig.S202 DEPT-135 of Ethyl 6-(2-(3-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aj).

HBR-DN-064 #4-21 RT: 0.02-0.08 AV: 6 SB: 63 0.32-1.20 NL: 2.73E8  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

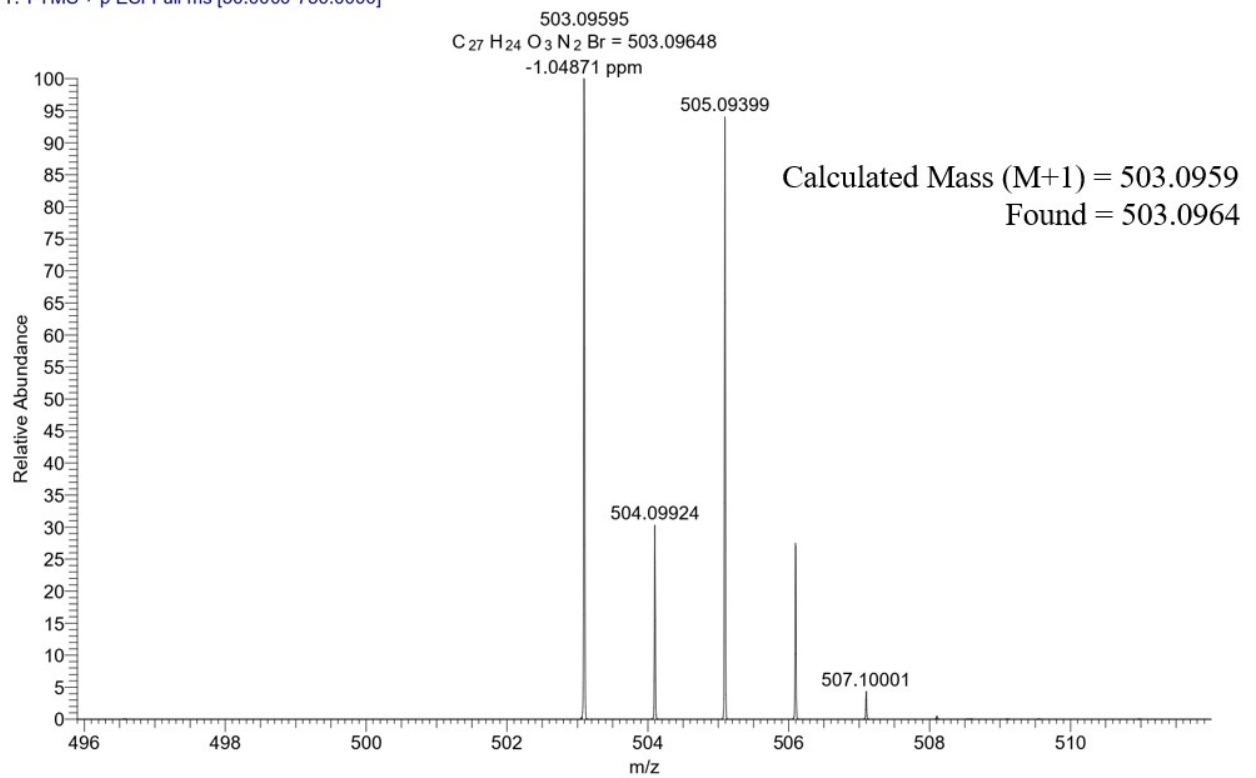


Fig.S203 HRMS of Ethyl 6-(2-(3-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aj).

VN-065

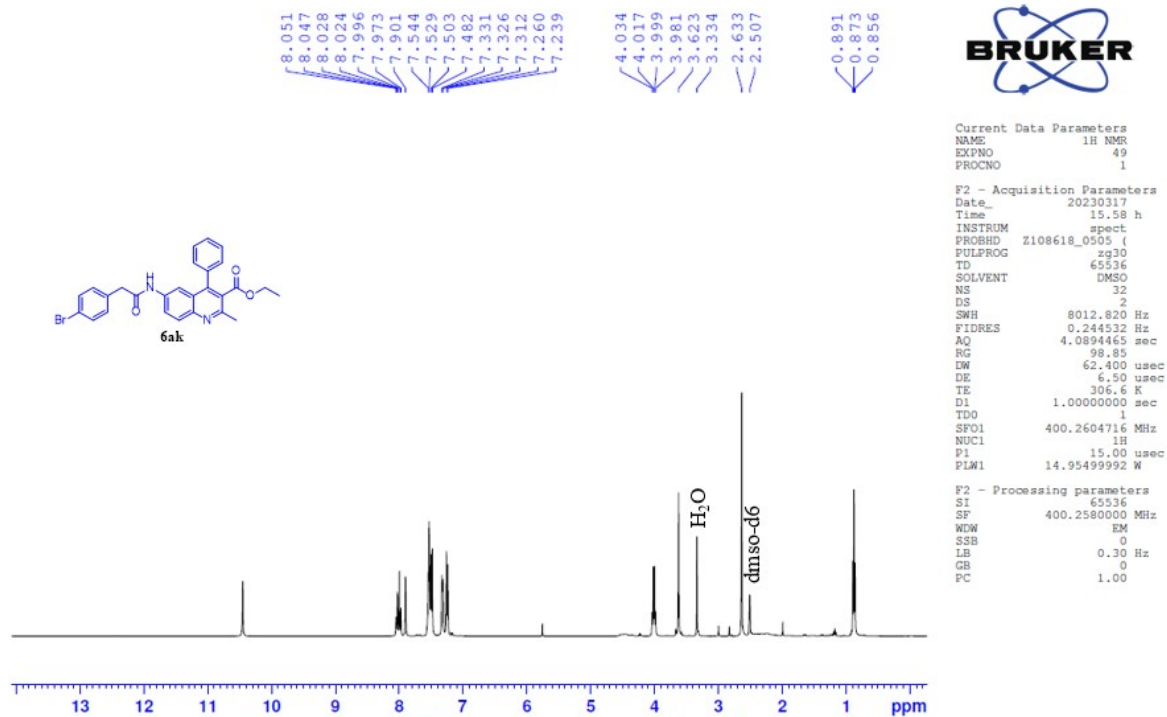


Fig.S204 <sup>1</sup>H NMR of Ethyl 6-(2-(4-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ak).

VN-065

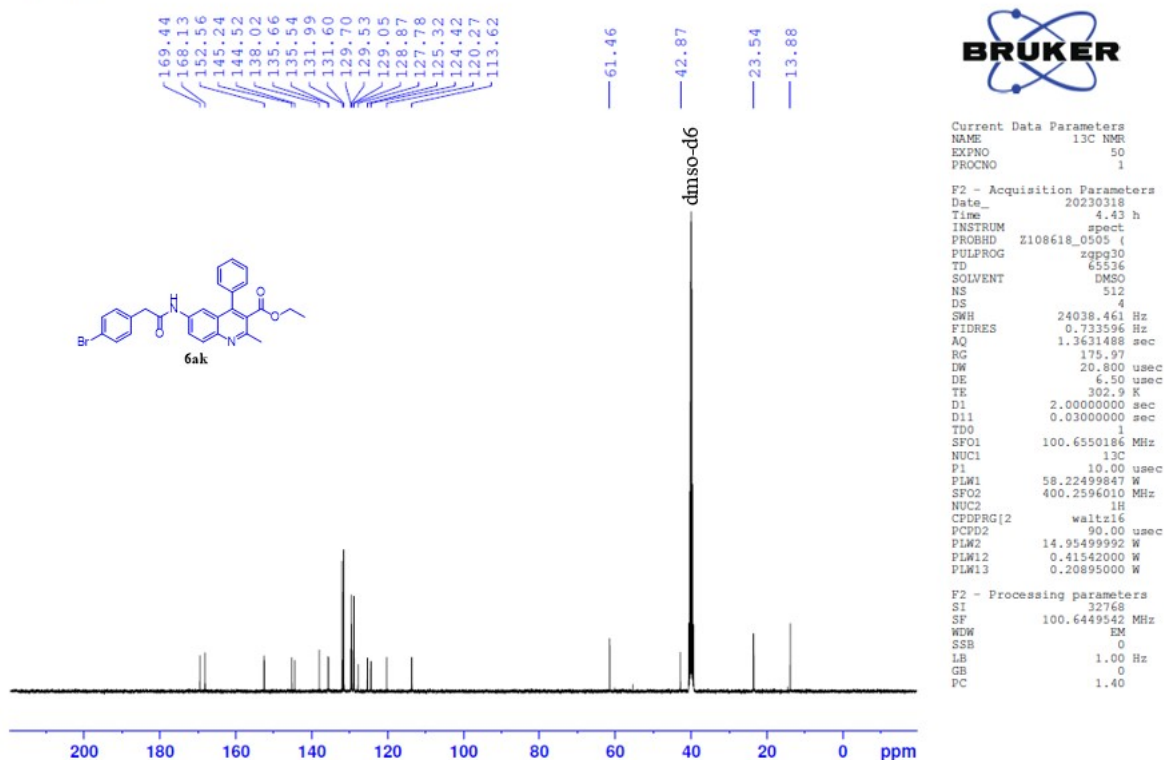


Fig.S205 <sup>13</sup>C NMR of Ethyl 6-(2-(4-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ak).



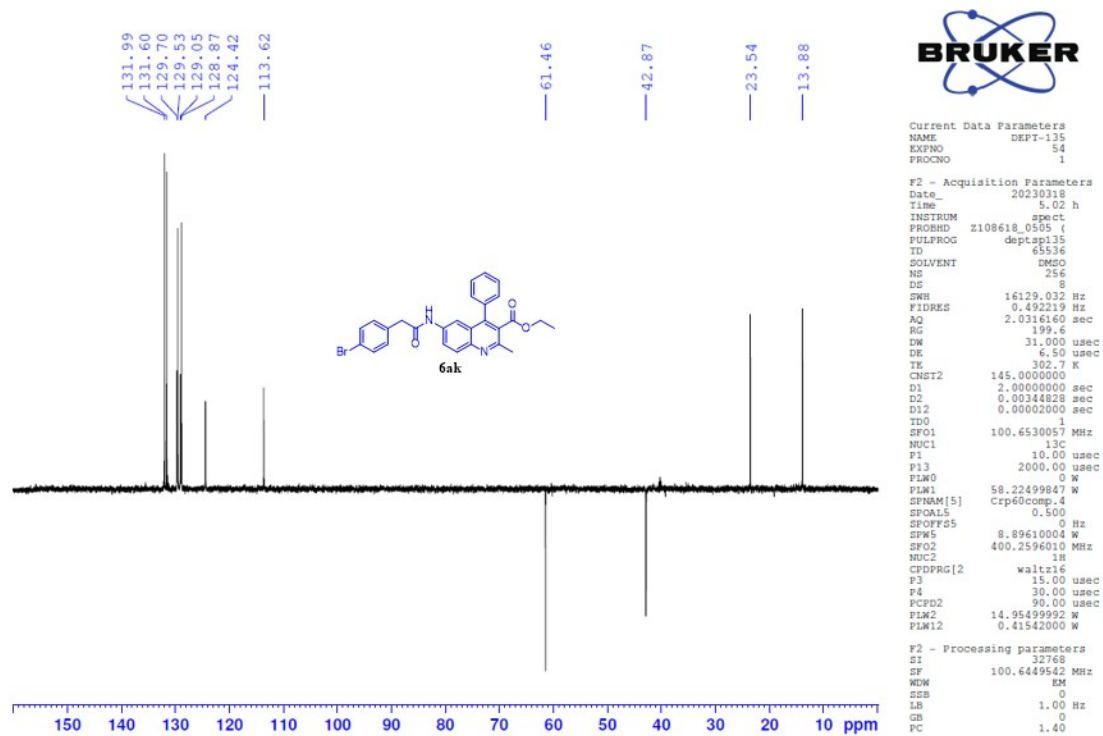


Fig.S206 DEPT-135 of Ethyl 6-(2-(4-bromophenyl) acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ak).

VN-073

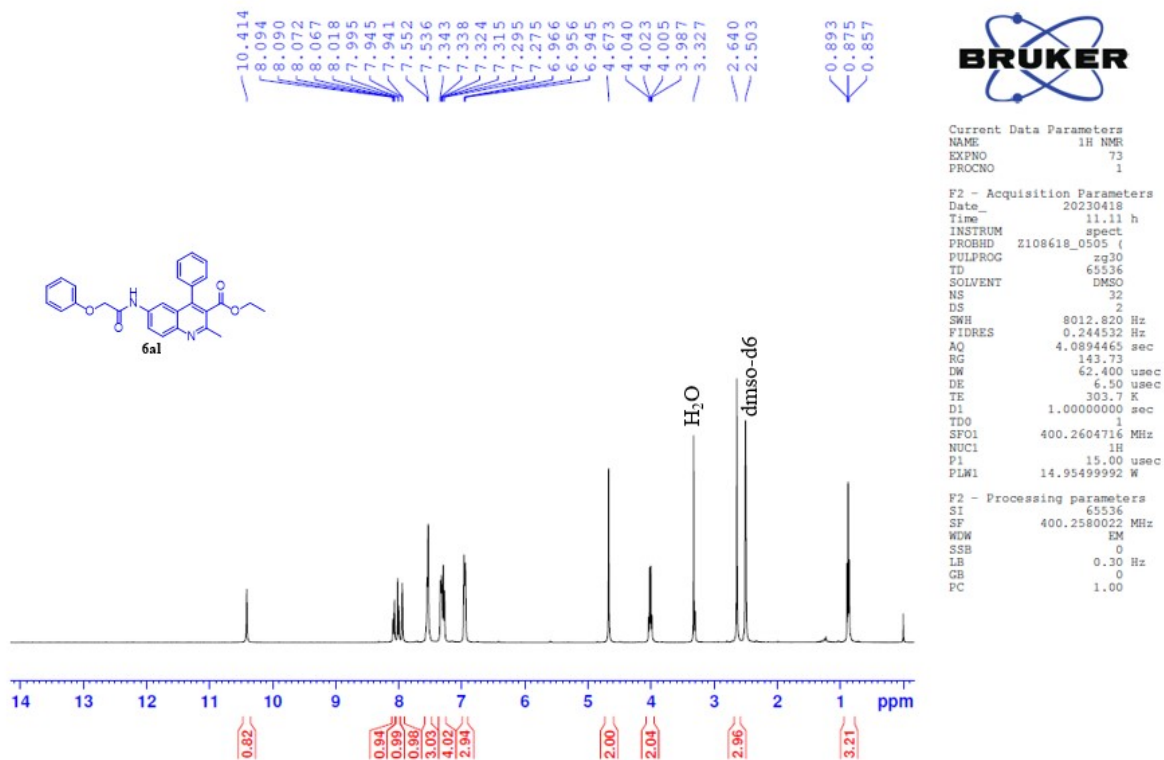
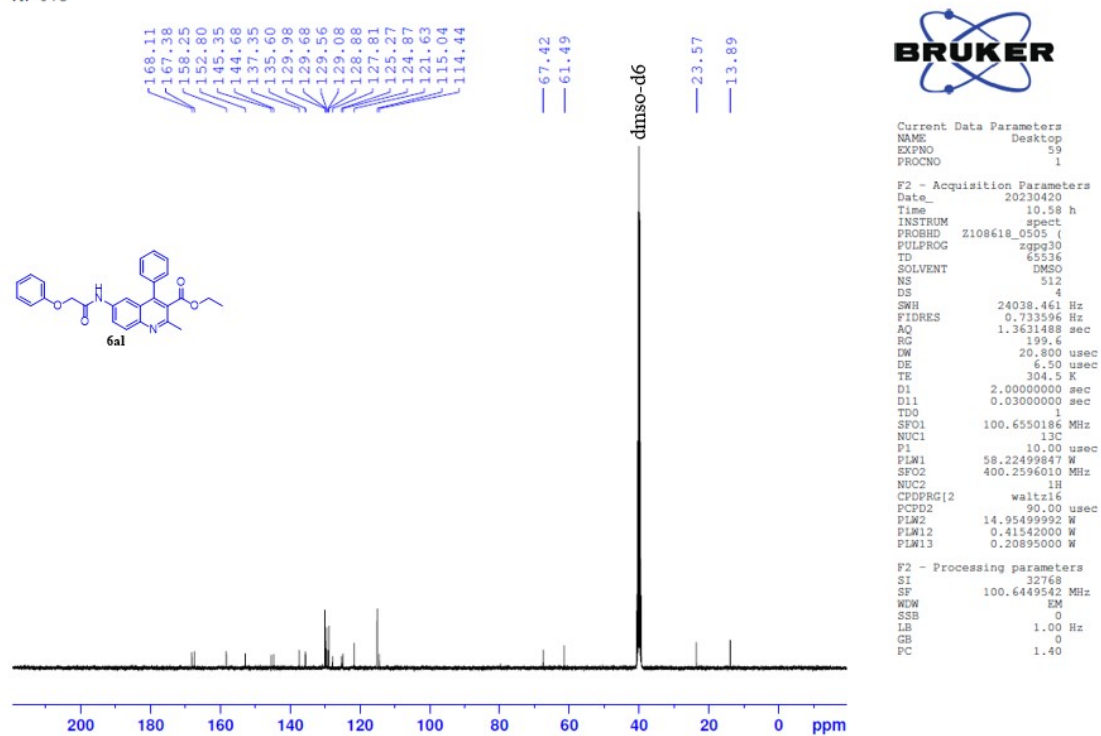


Fig.S207 <sup>1</sup>H NMR of Ethyl 2-methyl-6-(2-phenoxyacetamido)-4-phenylquinoline-3-carboxylate (6al).

VN-073

Fig.S208 <sup>13</sup>C NMR of Ethyl 2-methyl-6-(2-phenoxyacetamido)-4-phenylquinoline-3-carboxylate (6a1).

VN-073

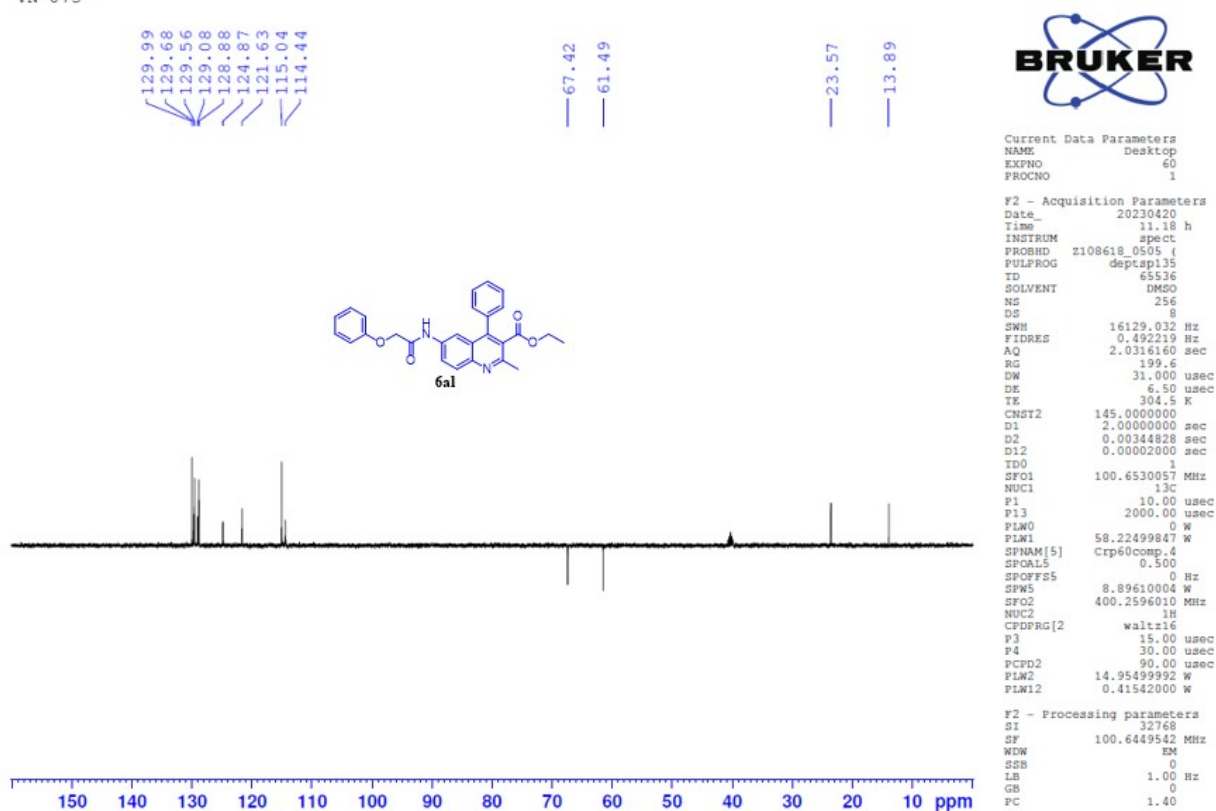


Fig.S209 DEPT-135 of Ethyl 2-methyl-6-(2-phenoxyacetamido)-4-phenylquinoline-3-carboxylate (6a1).

HBR-DN-073 #3-17 RT: 0.02-0.07 AV: 5 SB: 63 0.32-1.20 NL: 9.37E8  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

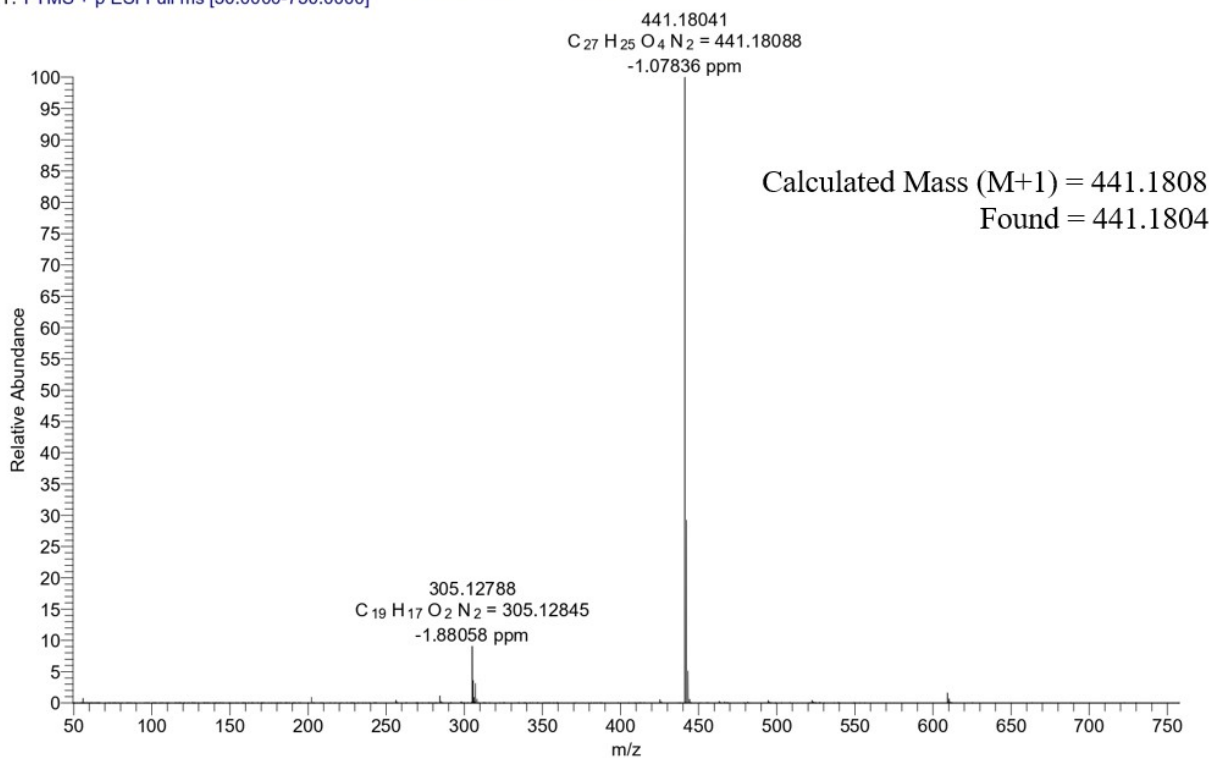


Fig.S210 HRMS of Ethyl 2-methyl-6-(2-phenoxyacetamido)-4-phenylquinoline-3-carboxylate (6al).

VN-074

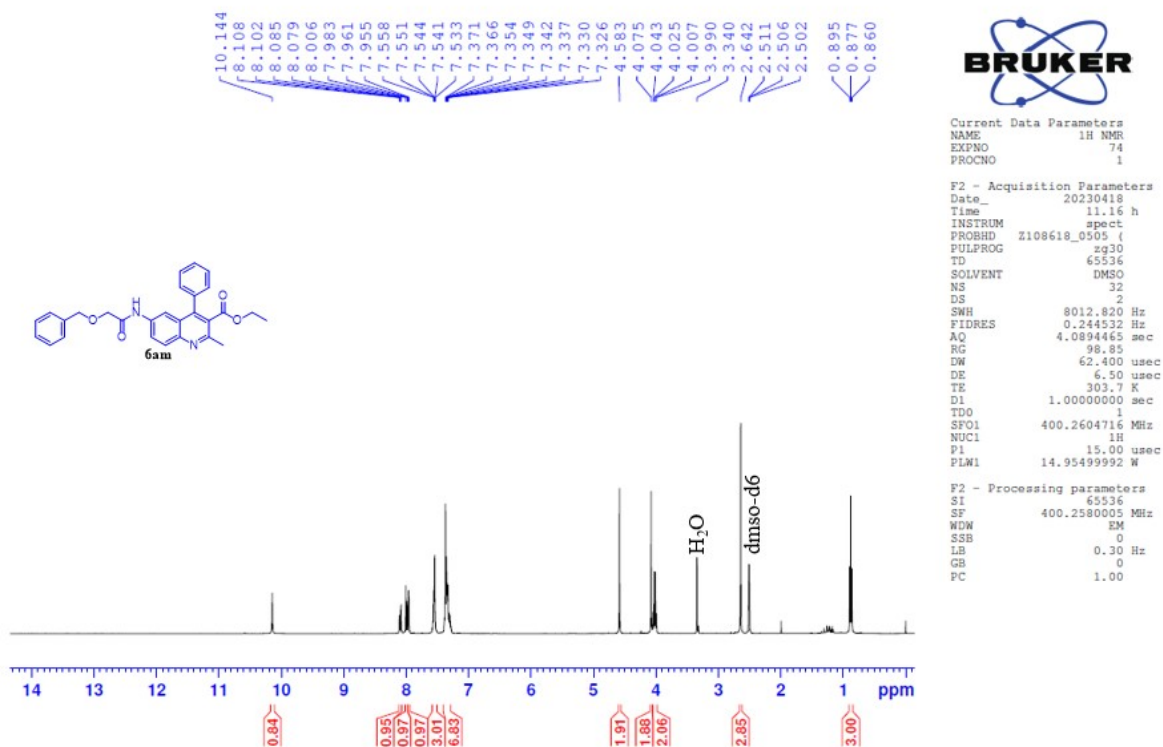


Fig.S211 <sup>1</sup>H NMR of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).

Signature SIF VIT VELLORE  
VN-074

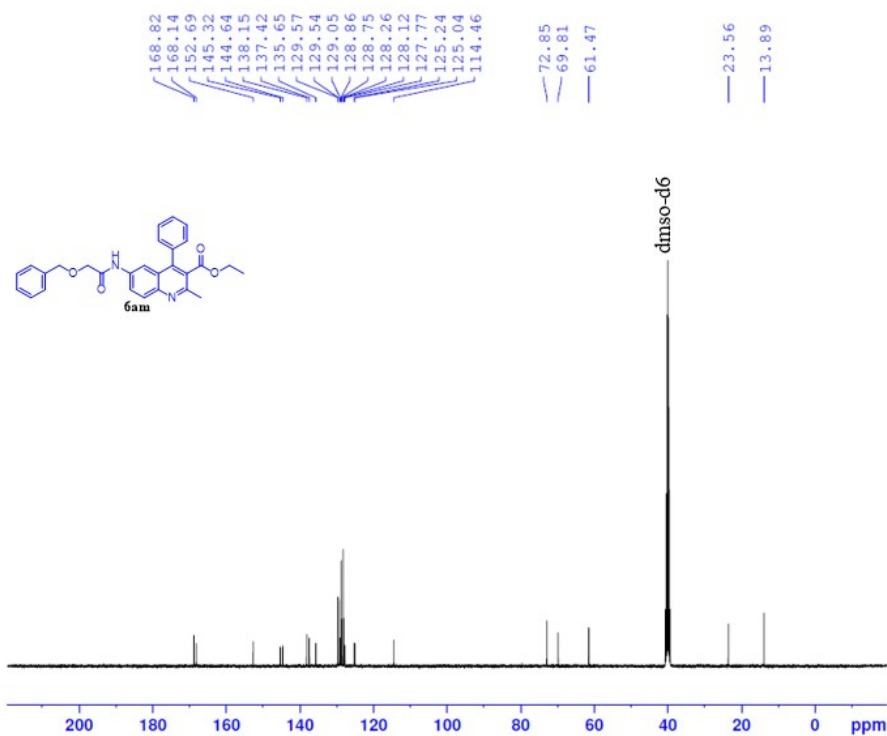


Fig.S212 <sup>13</sup>C NMR of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).

Signature SIF VIT VELLORE  
VN-074

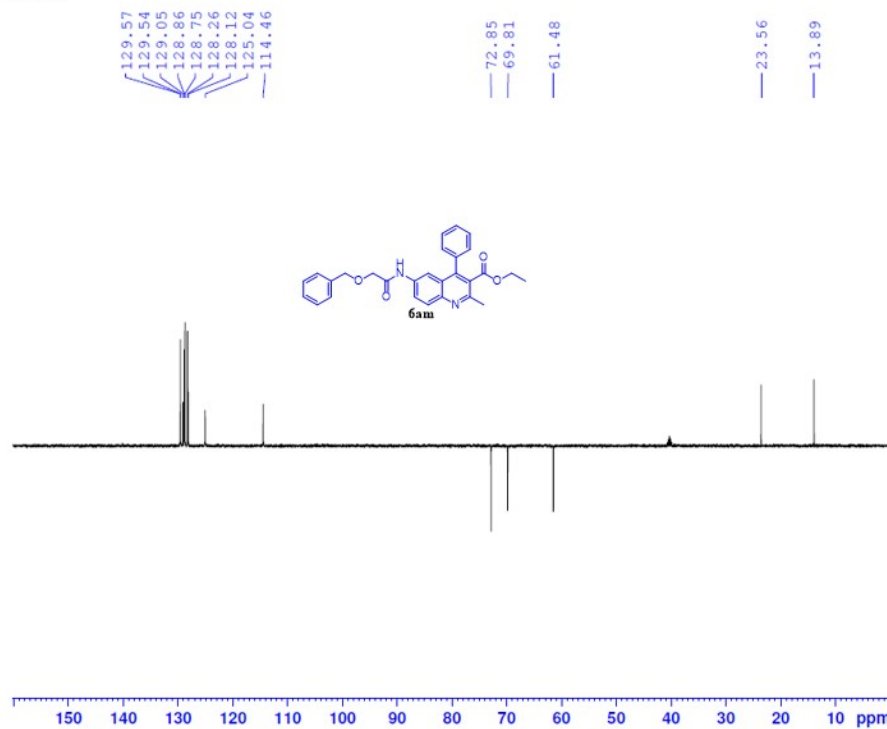


Fig.S213 DEPT-135 of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).

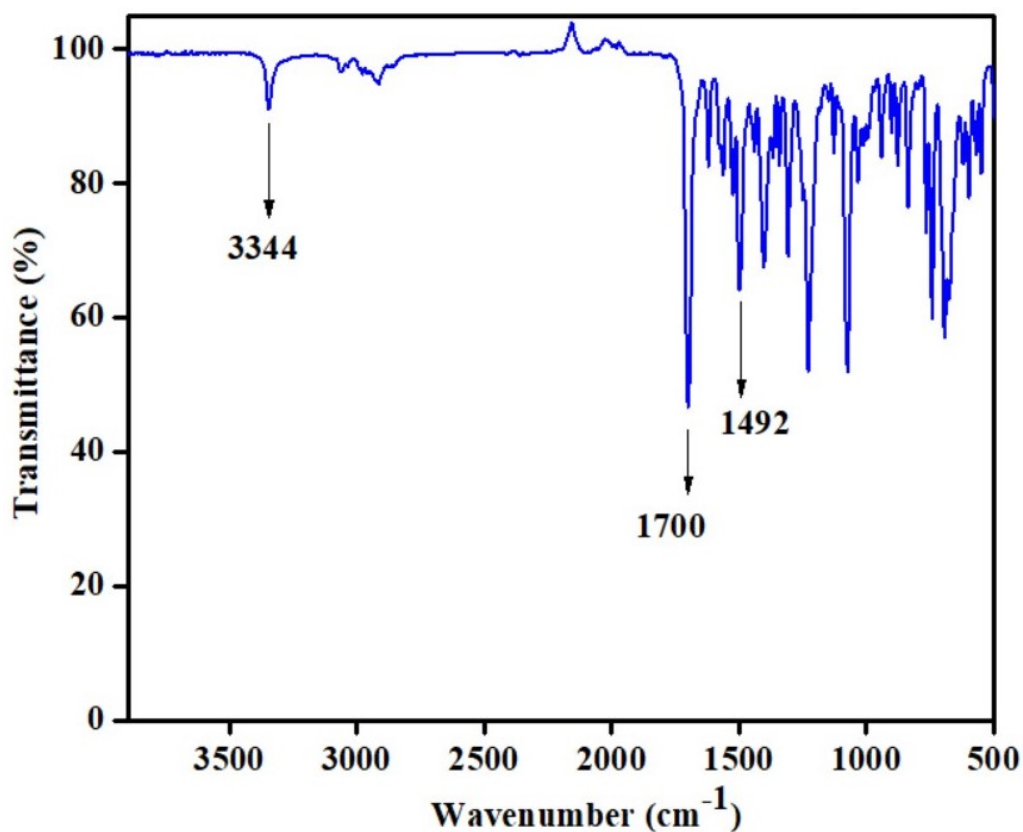


Fig.S214 FT-IR of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).

HBR-DN-074 #8-26 RT: 0.04-0.11 AV: 6 SB: 63 0.32-1.20 NL: 2.07E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

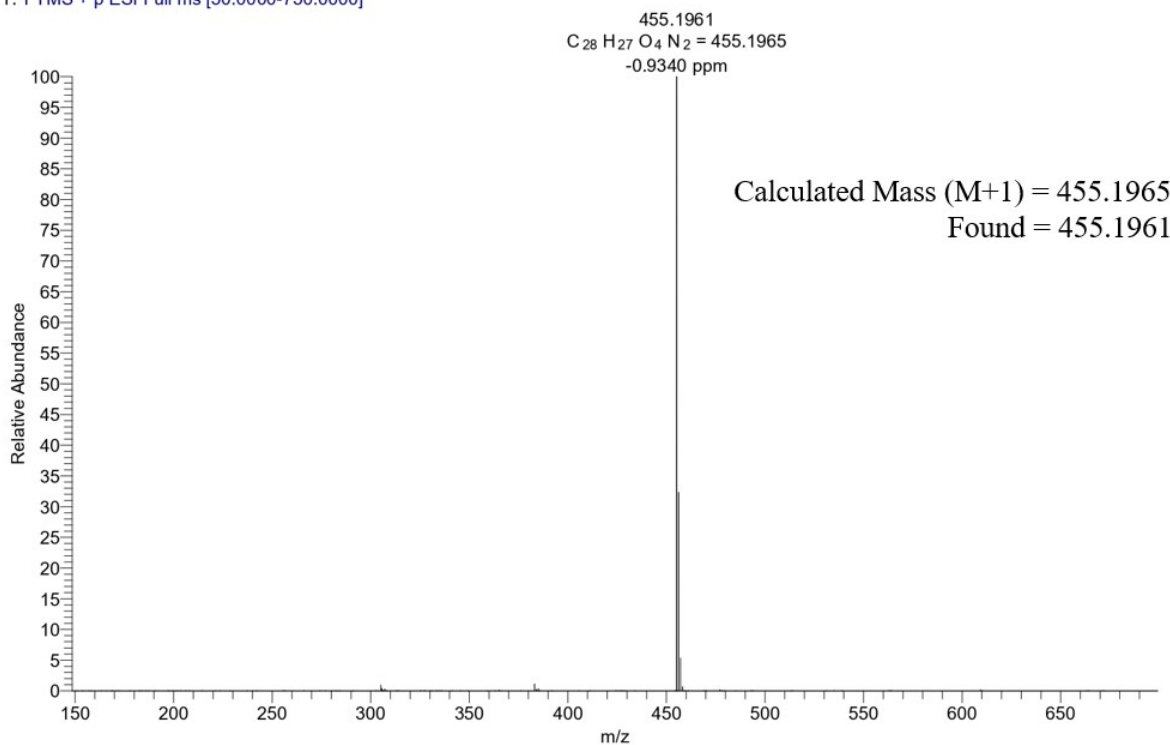


Fig.S215 HRMS of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6am).

Signature SIF VIT VELLORE  
VN-087

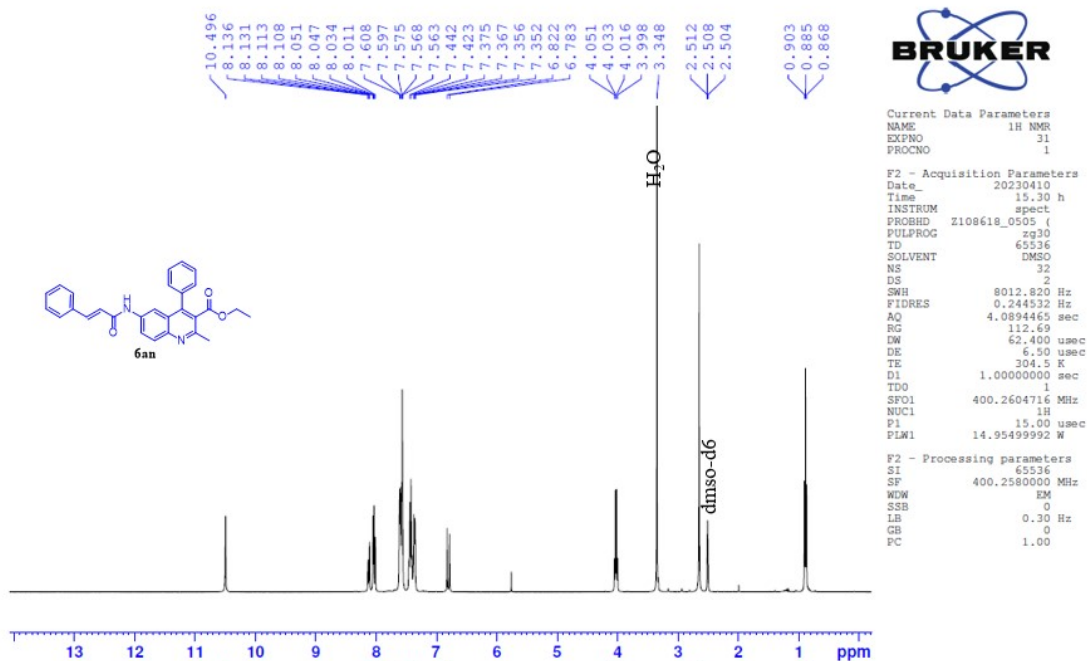


Fig.S216 <sup>1</sup>H NMR of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6an).

VN-087

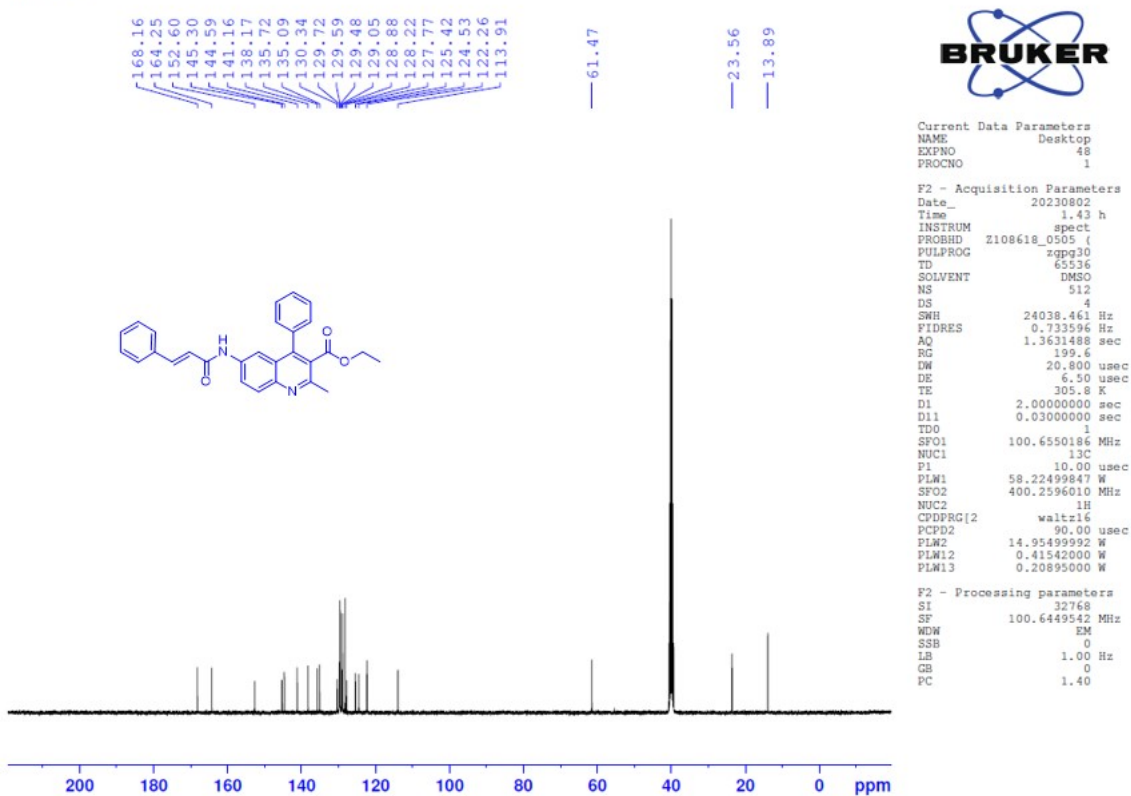


Fig.S217 <sup>13</sup>C NMR of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6an).

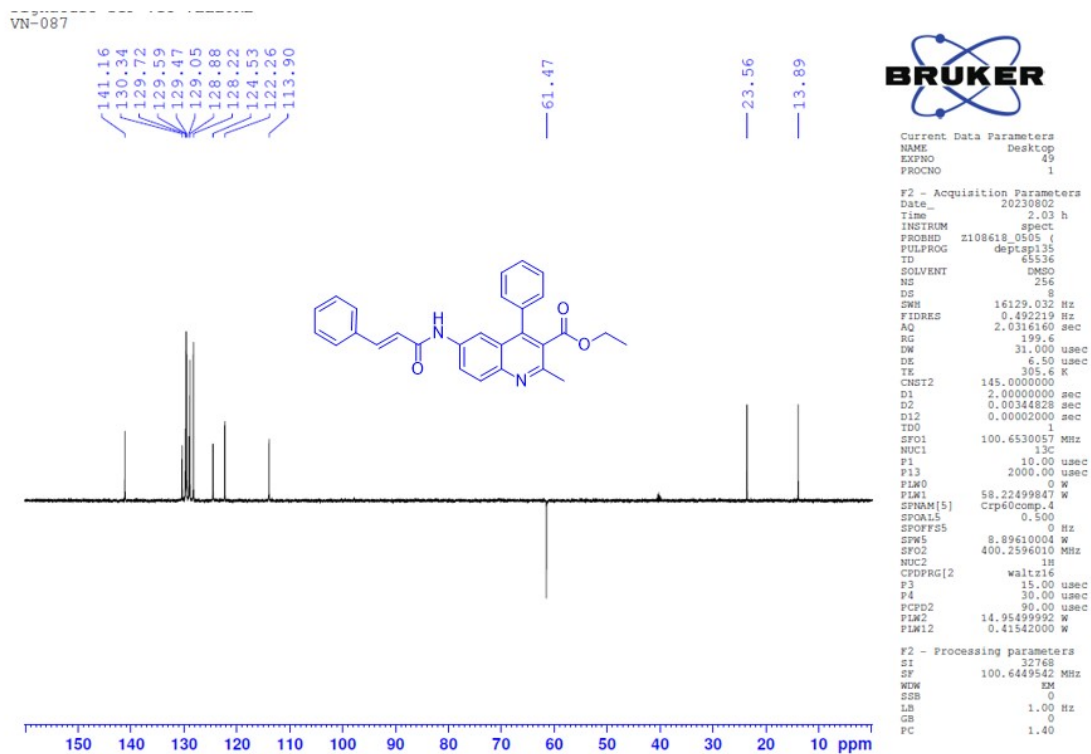


Fig.S218 DEPT-135 of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6an).

HBR-DN-087 #3-28 RT: 0.02-0.13 AV: 9 SB: 63 0.32-1.20 NL: 1.61E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

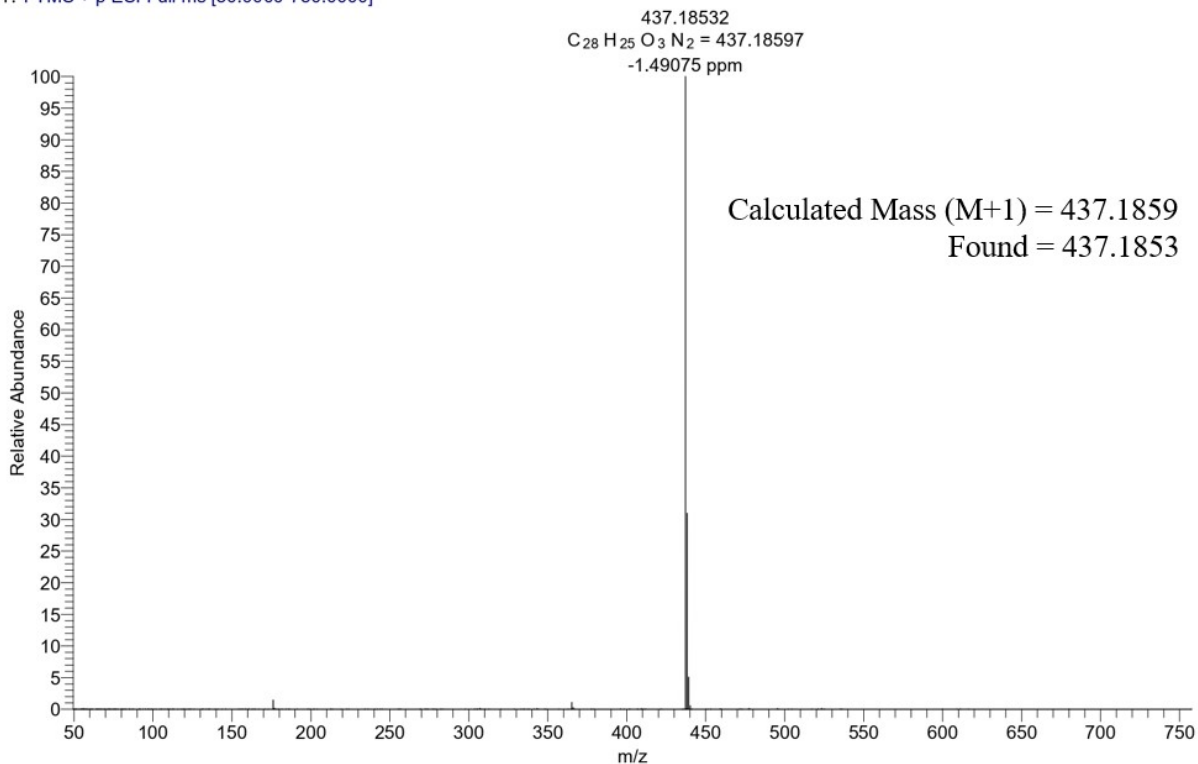
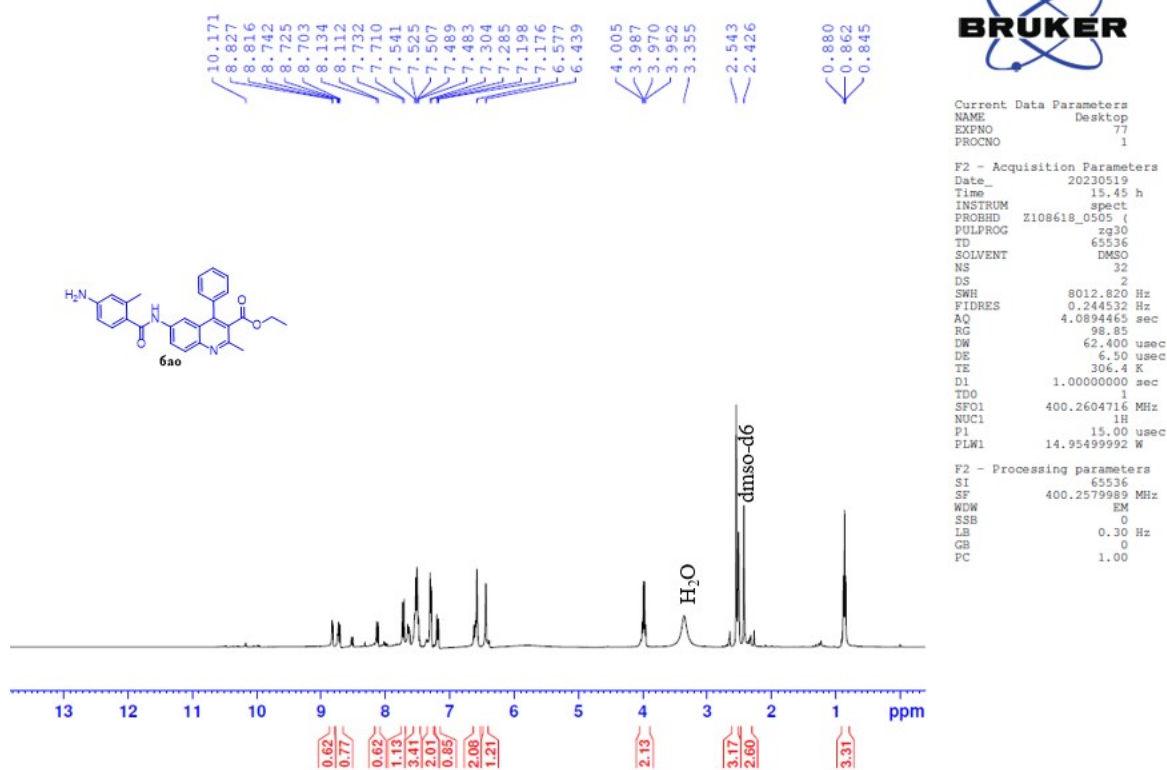
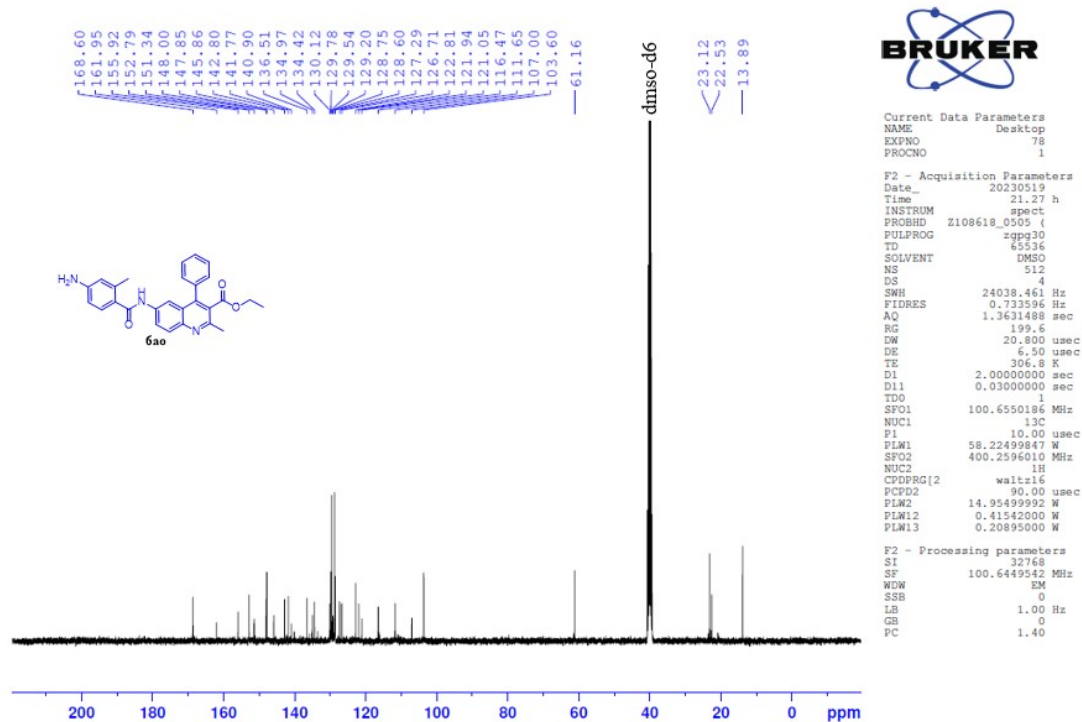


Fig.S219 HRMS of Ethyl 6-(2-(benzyloxy)acetamido)-2-methyl-4-phenylquinoline-3-carboxylate (6an).

VN-080

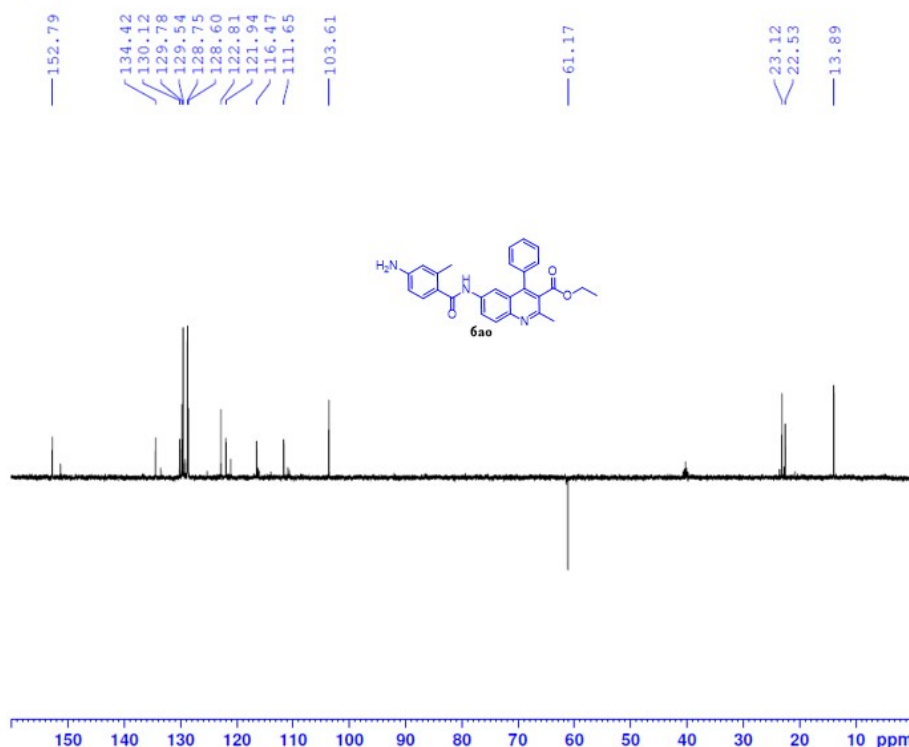
Fig.S220 <sup>1</sup>H NMR of Ethyl 6-(4-amino-2-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ao).

VN-080

Fig.S221 <sup>13</sup>C NMR of Ethyl 6-(4-amino-2-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ao).



Signature SIF VIT VELLORE  
VN-080



Current Data Parameters  
NAME Desktop  
EXPNO 79  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230519  
Time 21.47 h  
INSTRUM spect  
PROBHD Z108618\_0508 f  
PULPROG deptap135  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 8  
SWH 16129.032 Hz  
FIDRES 0.492219 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DE 6.50 usec  
TE 306.6 K  
CNST2 145.000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TDO 1  
SFO1 100.6530057 MHz  
NUC1 13C  
P1 10.00 usec  
PLM0 0 W  
PLM1 58.22499847 W  
SFOFF5 0 Hz  
SFW5 8.89610004 W  
SFO2 400.2596010 MHz  
NUC2 1H  
CDEPRG2 waltra16  
P3 15.00 usec  
P4 30.00 usec  
PCPD2 90.00 usec  
PLM2 14.95499992 W  
PLM12 0.41542000 W

F2 - Processing parameters  
SI 32768  
SF 100.6449542 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Fig.S222 DEPT-135 of Ethyl 6-(4-amino-2-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ao).

HBR-DN-80 #2-23 RT: 0.02-0.10 AV: 7 SB: 63 0.32-1.20 NL: 1.06E8  
T: FTMS + p ESI Full ms [50.0000-750.0000]

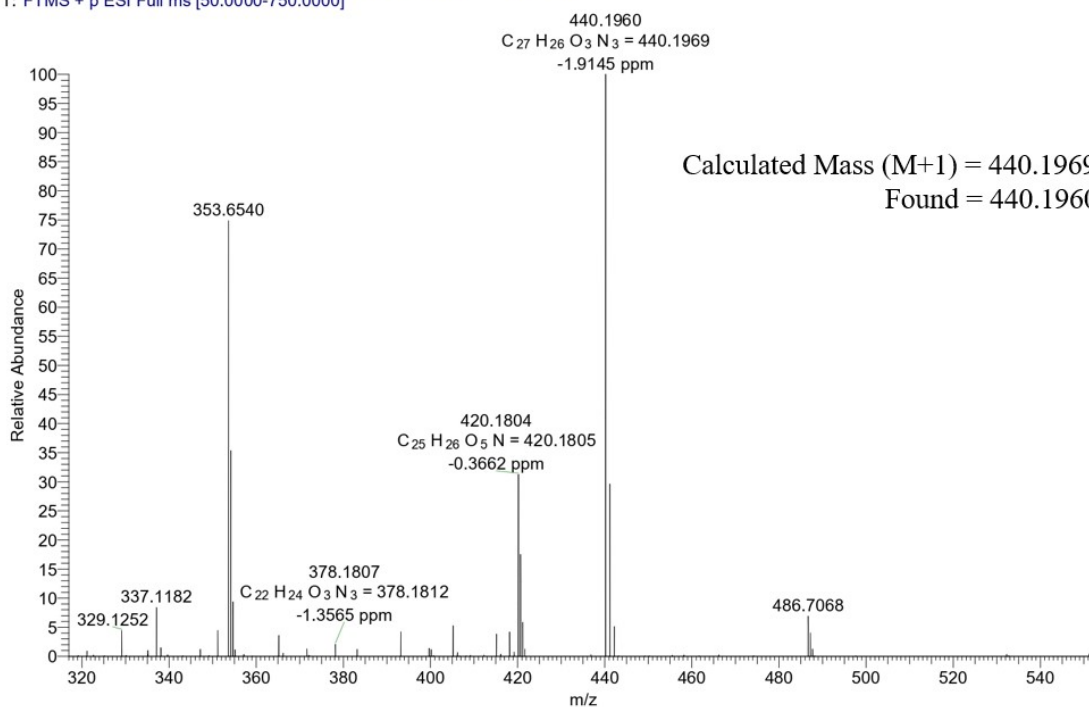
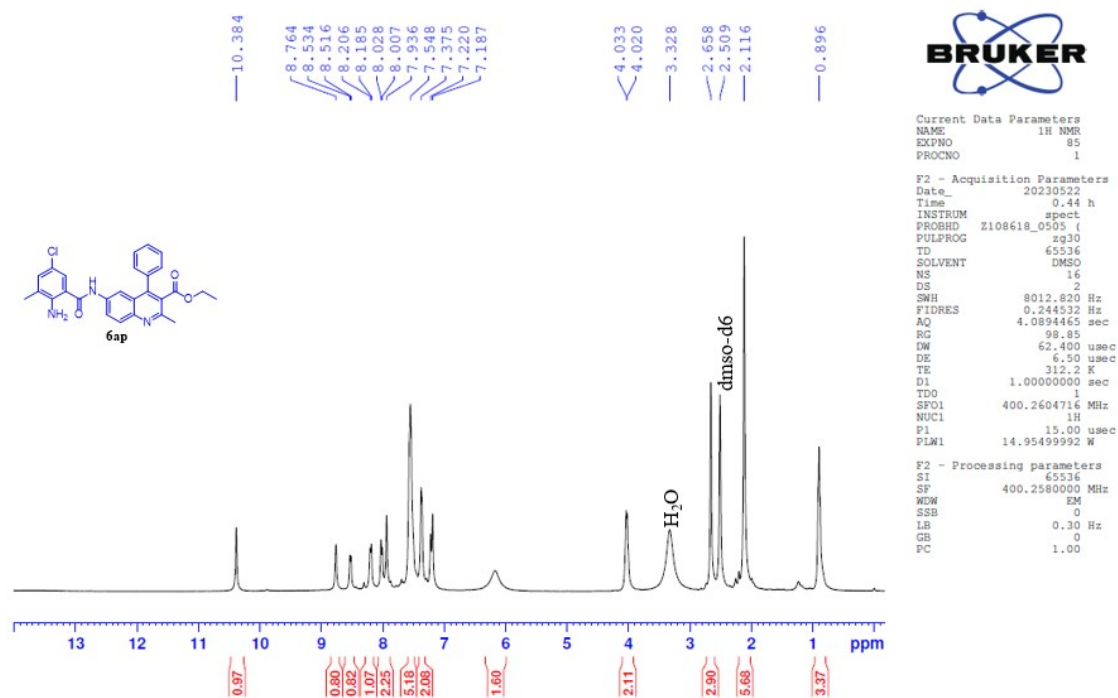
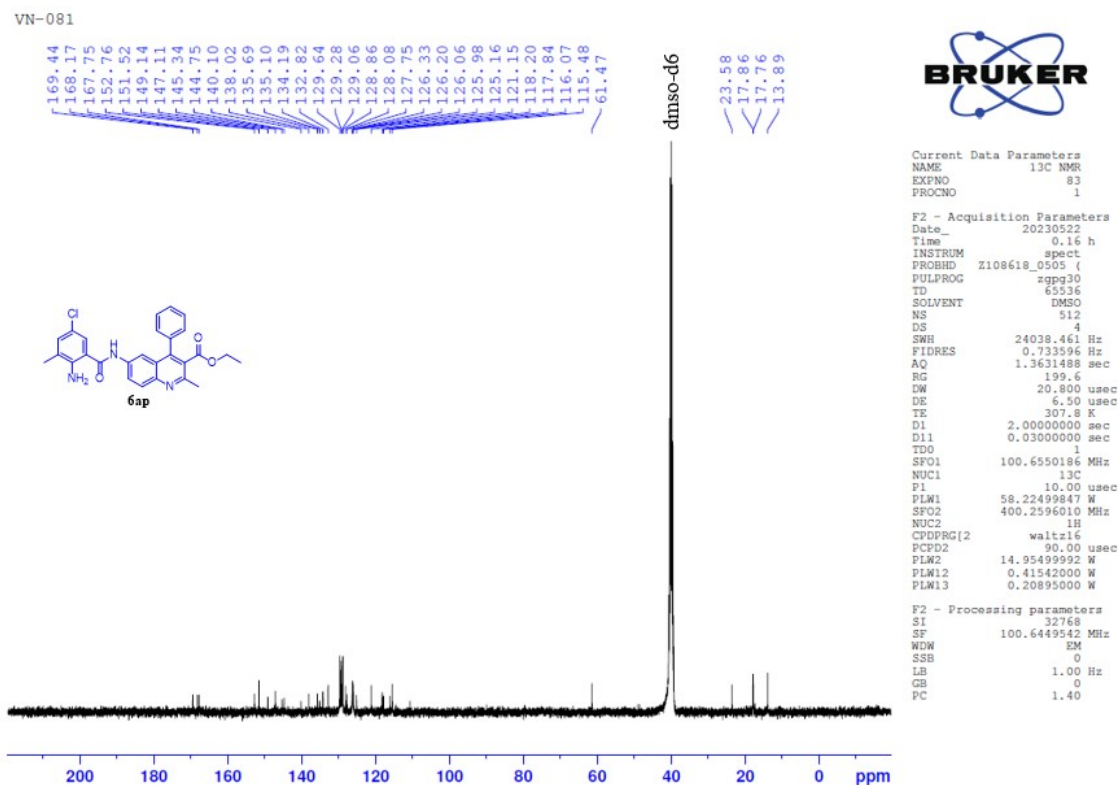


Fig.S223 HRMS of Ethyl 6-(4-amino-2-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ao).

VN-081

Fig.S224 <sup>1</sup>H NMR of Ethyl 6-(2-amino-5-chloro-3-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (**6ap**).Fig.S225 <sup>13</sup>C NMR of Ethyl 6-(2-amino-5-chloro-3-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (**6ap**).

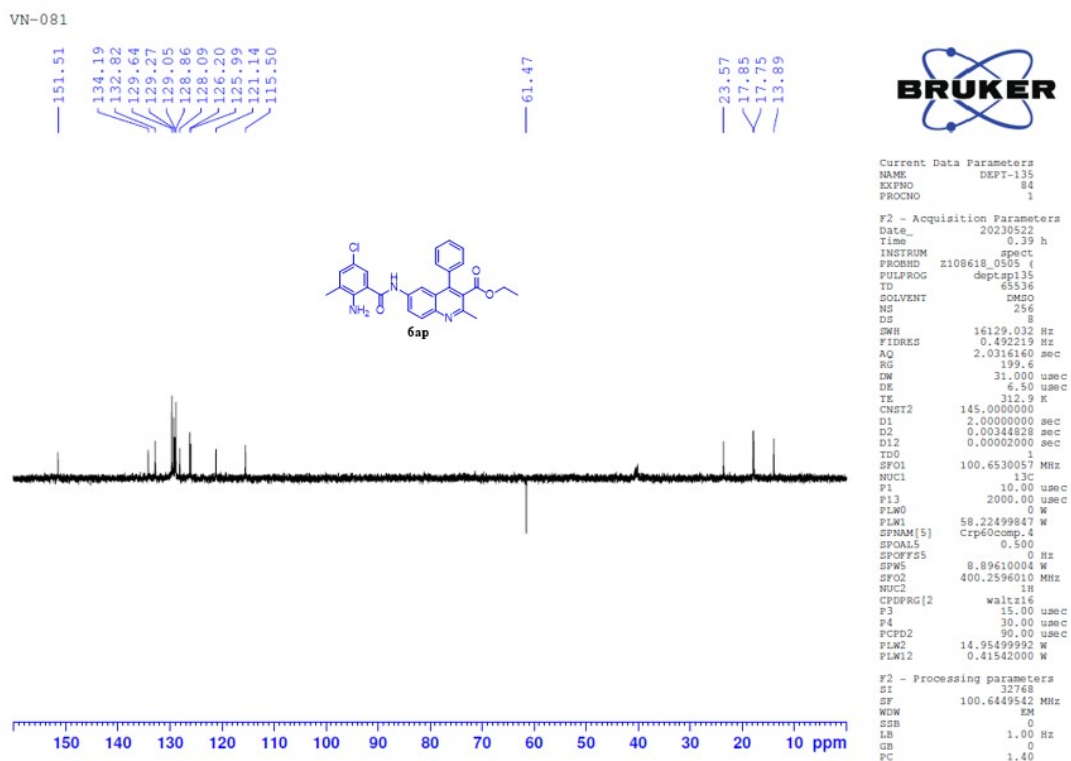


Fig.S226 DEPT-135 of Ethyl 6-(2-amino-5-chloro-3-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ap).

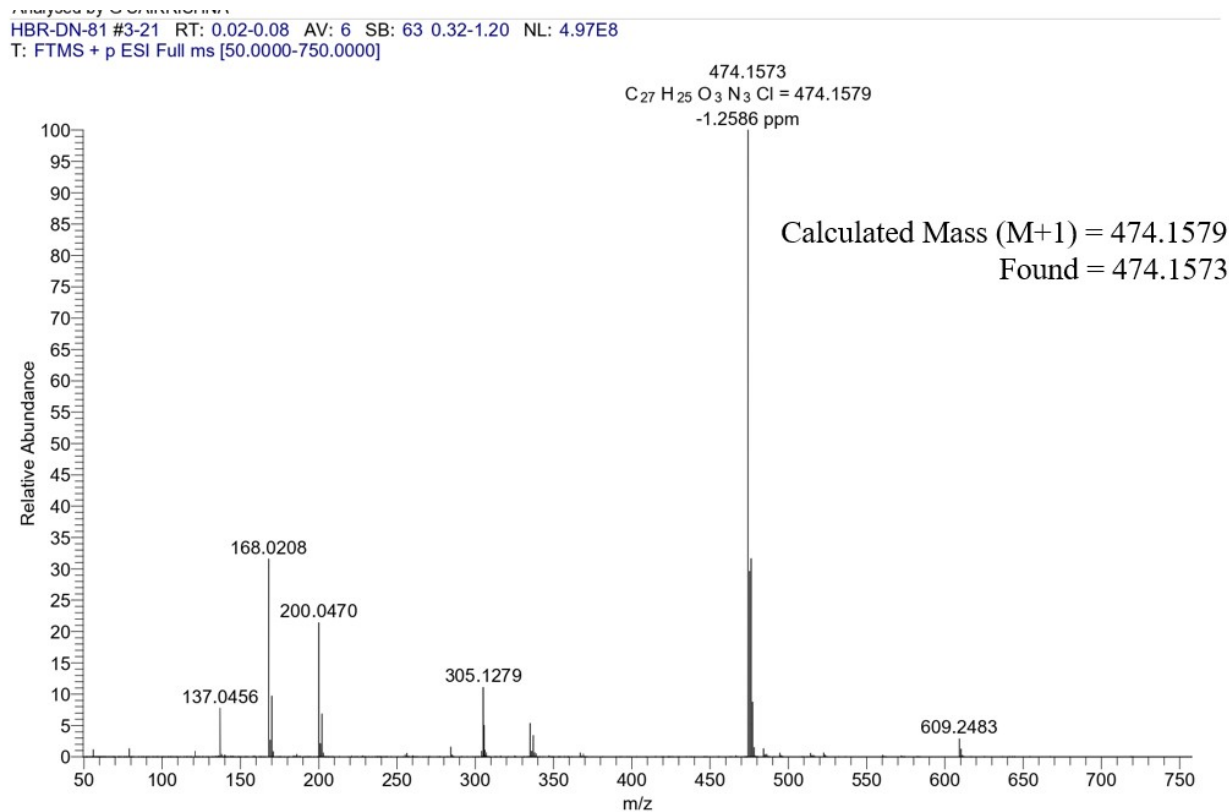
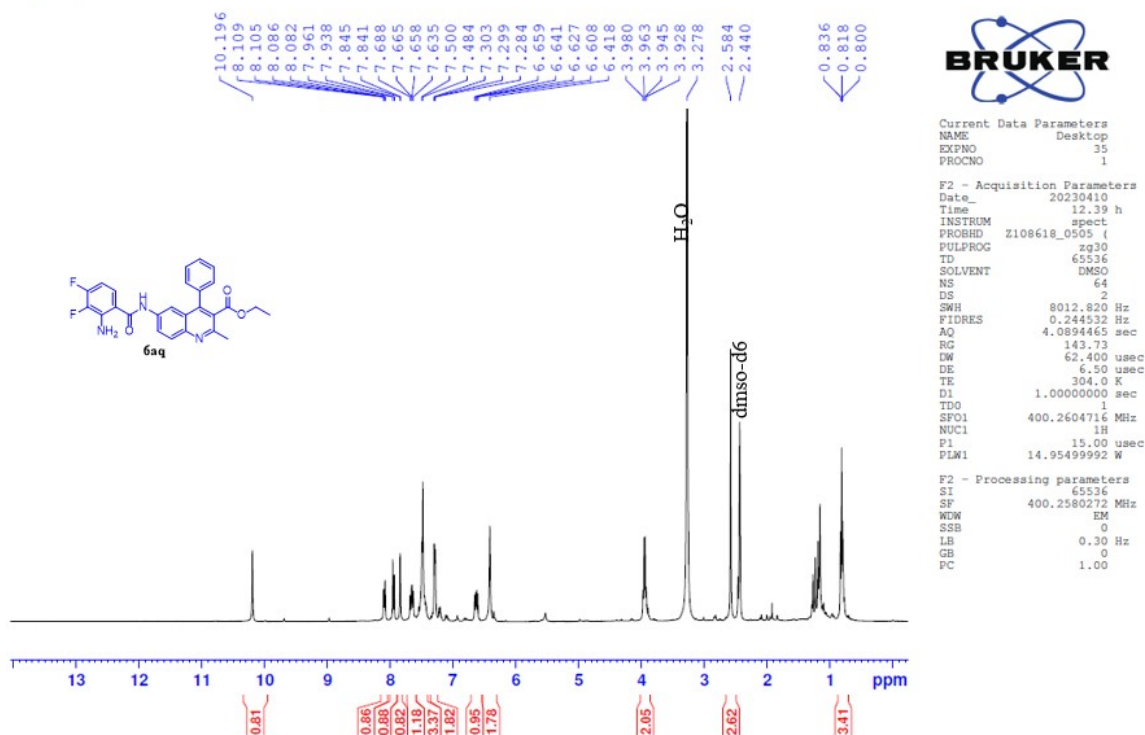
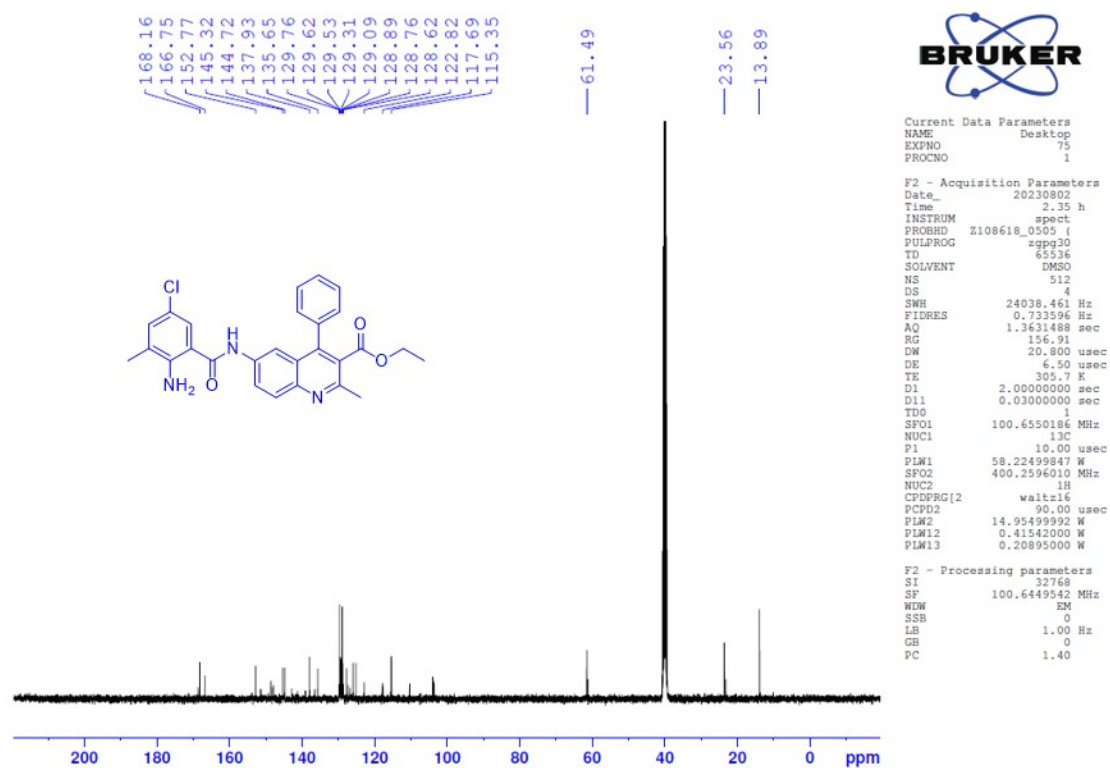


Fig.S227 HRMS of Ethyl 6-(2-amino-5-chloro-3-methylbenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ap).

VN-084

Fig.S228 <sup>1</sup>H NMR of Ethyl 6-(2-amino-3,4-difluorobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aq).

VN-085

Fig.S229 <sup>13</sup>C NMR of Ethyl 6-(2-amino-3,4-difluorobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aq).

Signature SIF VIT VELLORE  
VN-085

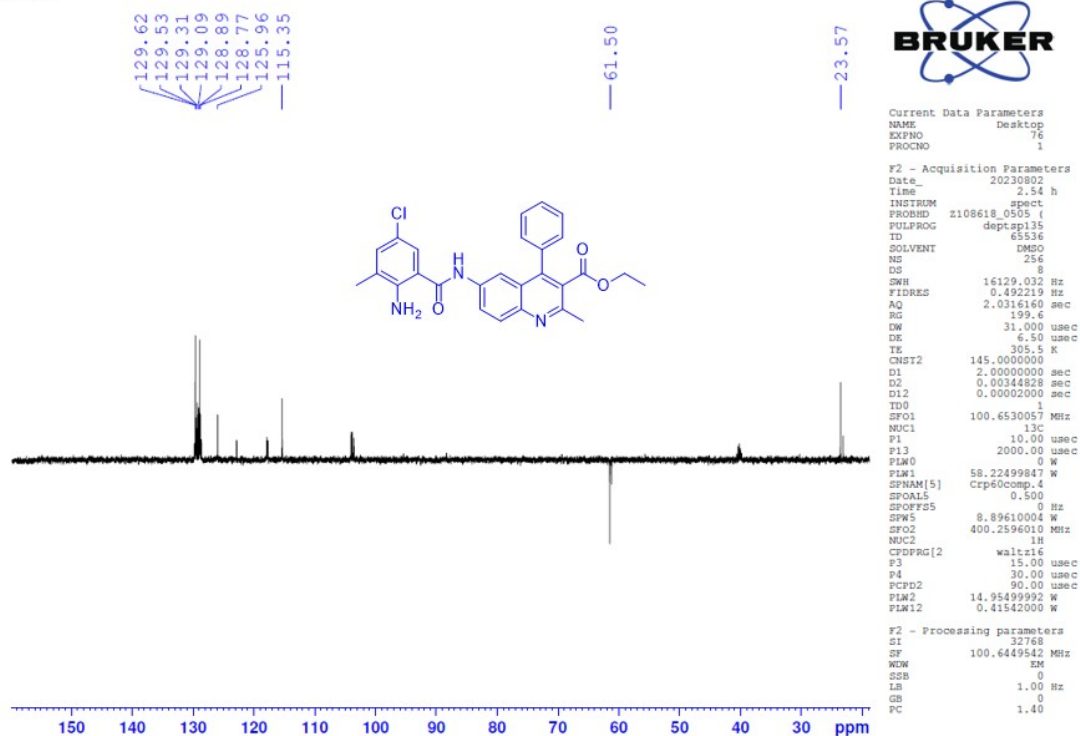


Fig.S230 DEPT-135 of Ethyl 6-(2-amino-3,4-difluorobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aq).

HBR-DN-85 #4-17 RT: 0.02-0.07 AV: 5 SB: 63 0.32-1.20 NL: 1.58E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

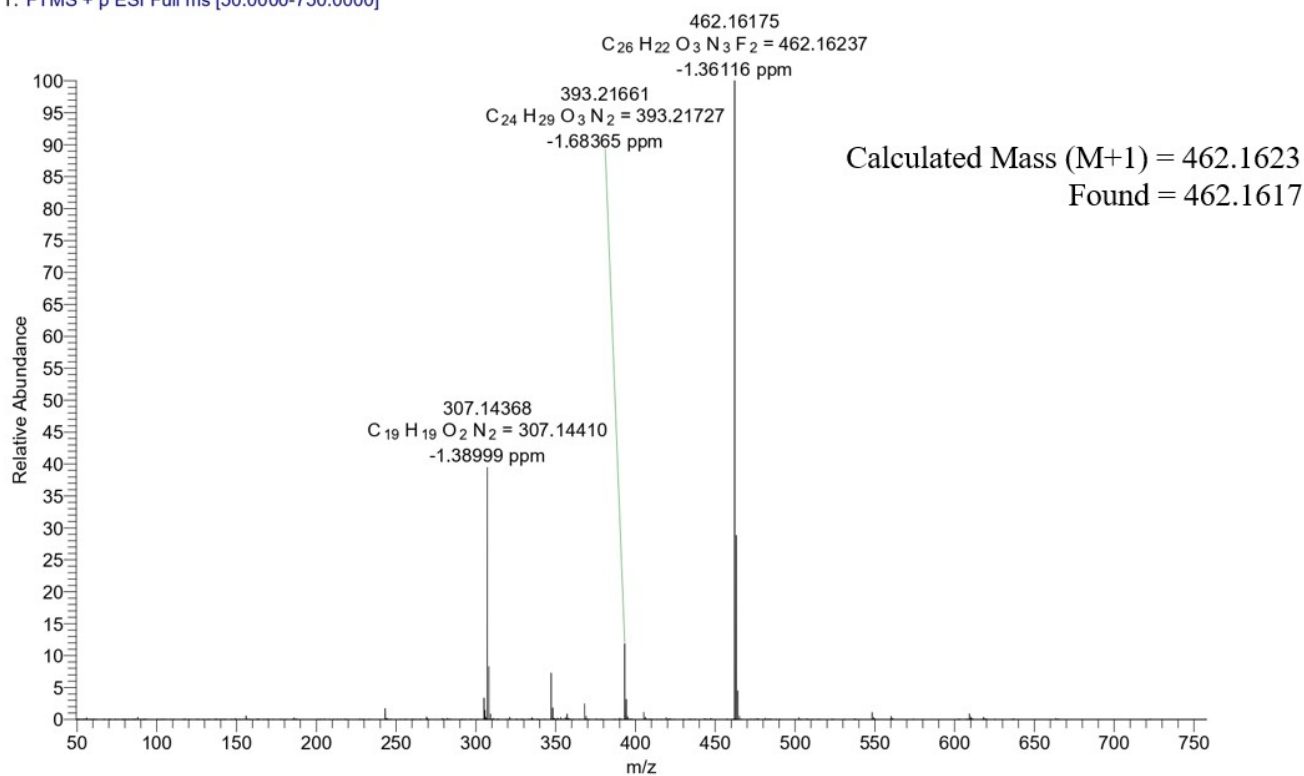


Fig.S231 HRMS of Ethyl 6-(2-amino-3,4-difluorobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6aq).

VN-079

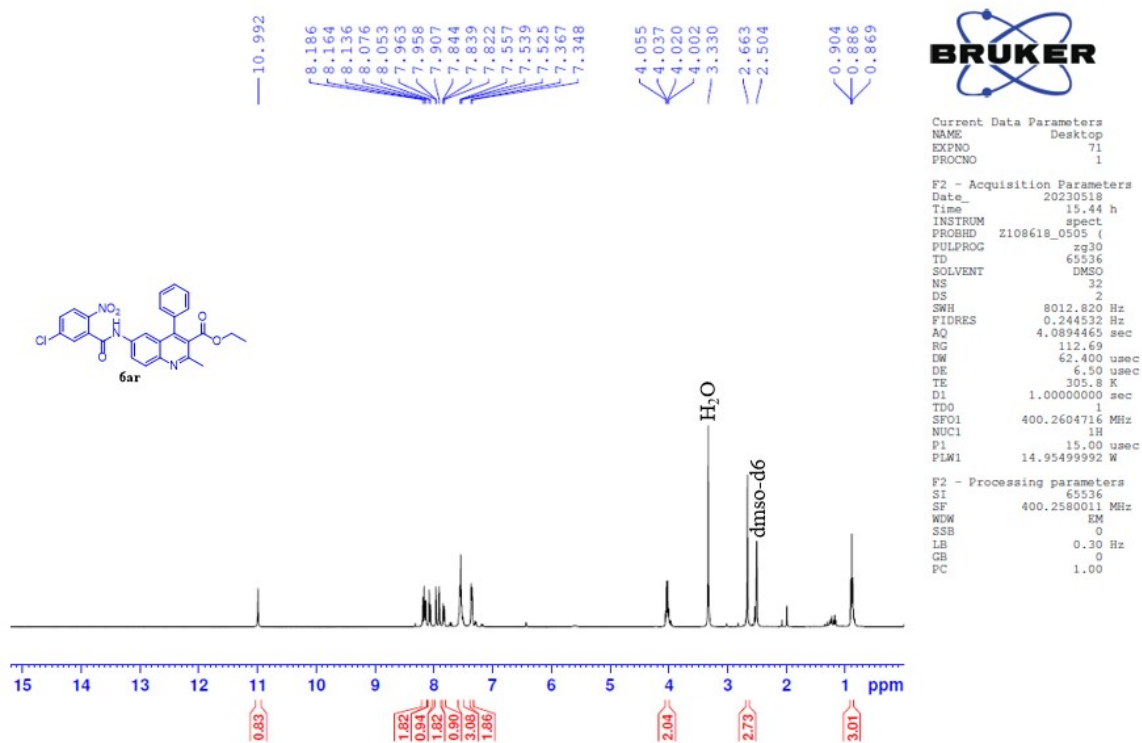


Fig.S232 <sup>1</sup>H NMR of Ethyl 6-(5-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (**6ar**).

VN-079

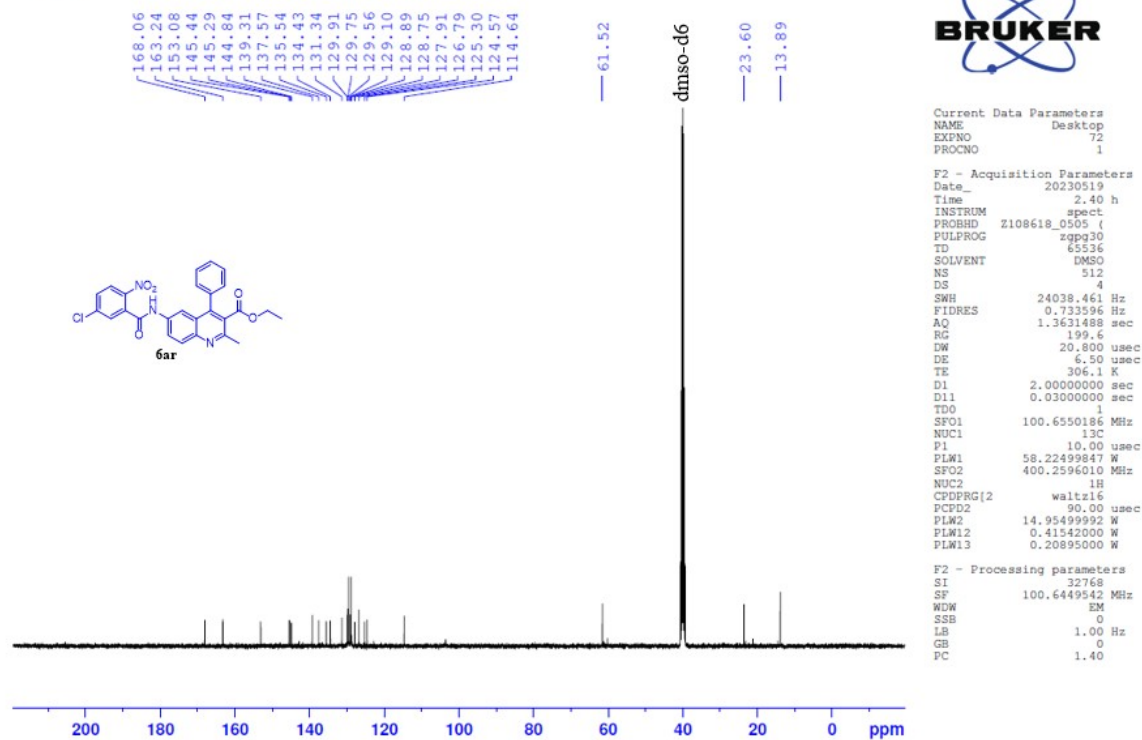


Fig.S233 <sup>13</sup>C NMR of Ethyl 6-(5-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (**6ar**).

VN-079

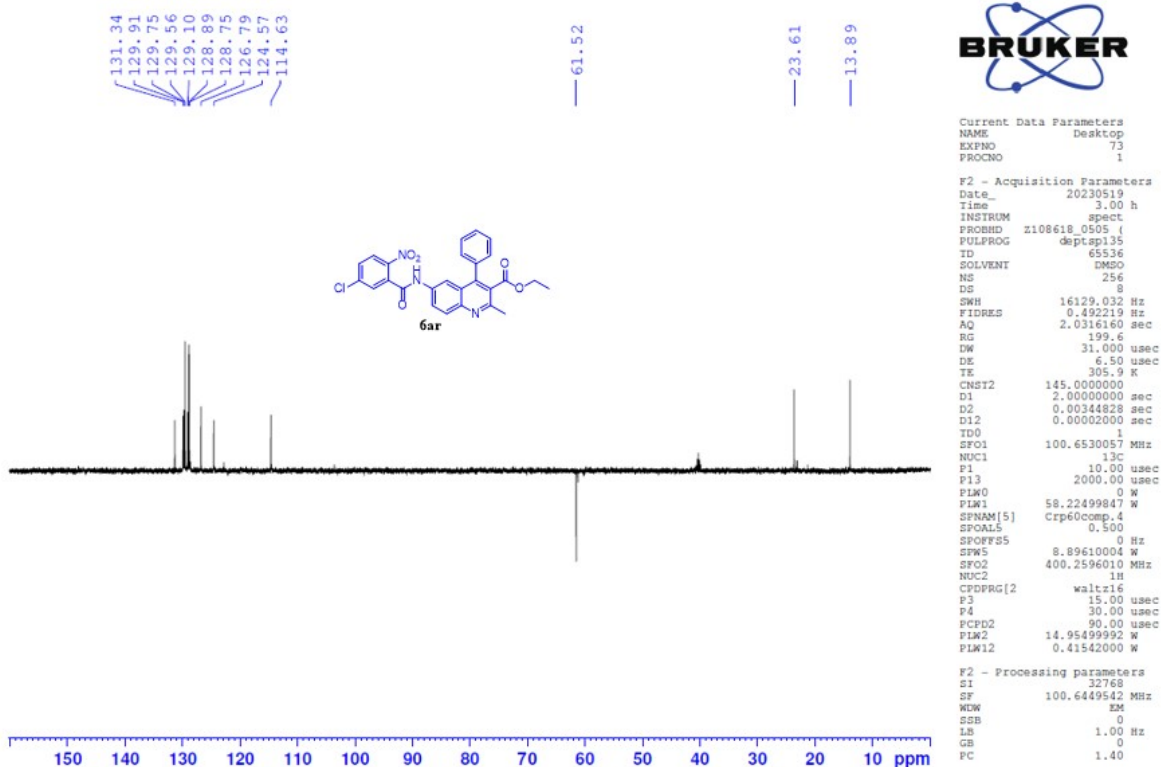


Fig.S234 DEPT-135 of Ethyl 6-(5-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ar).

HBR-DN-079 #4-16 RT: 0.02-0.07 AV: 5 SB: 63 0.32-1.20 NL: 1.75E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

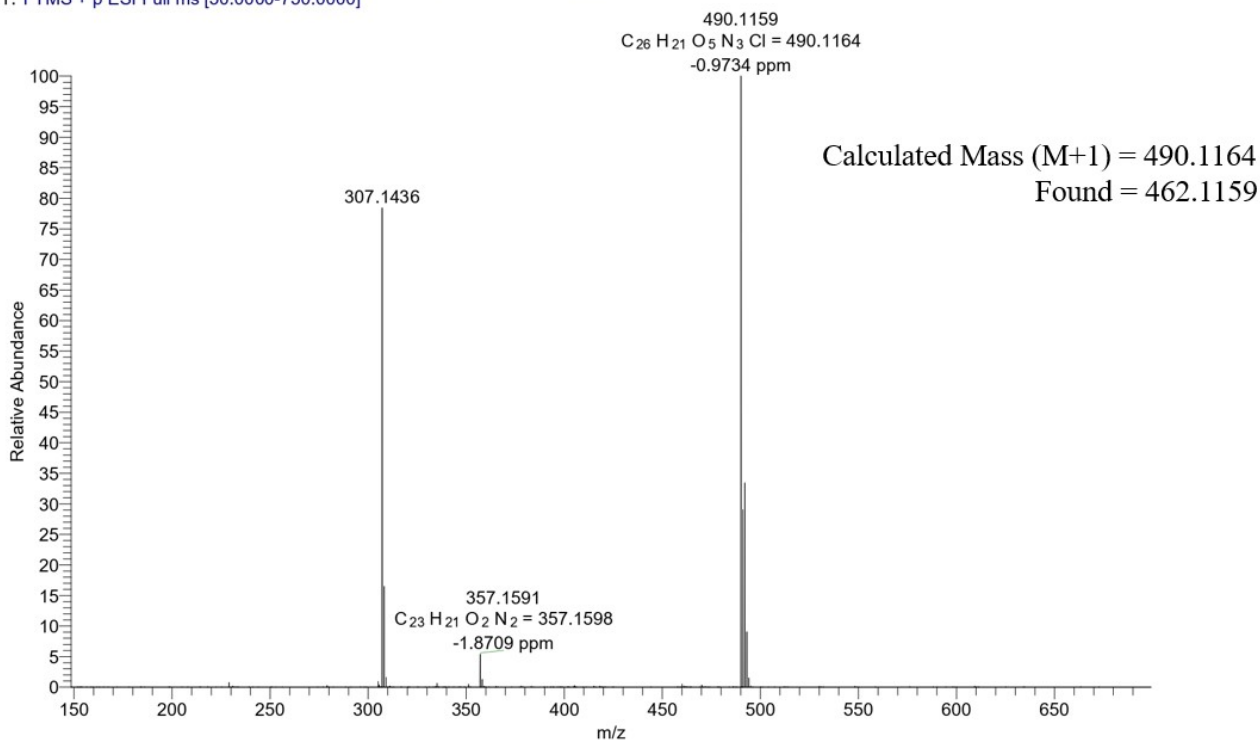


Fig.S235 HRMS of Ethyl 6-(5-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6ar).

VN-082

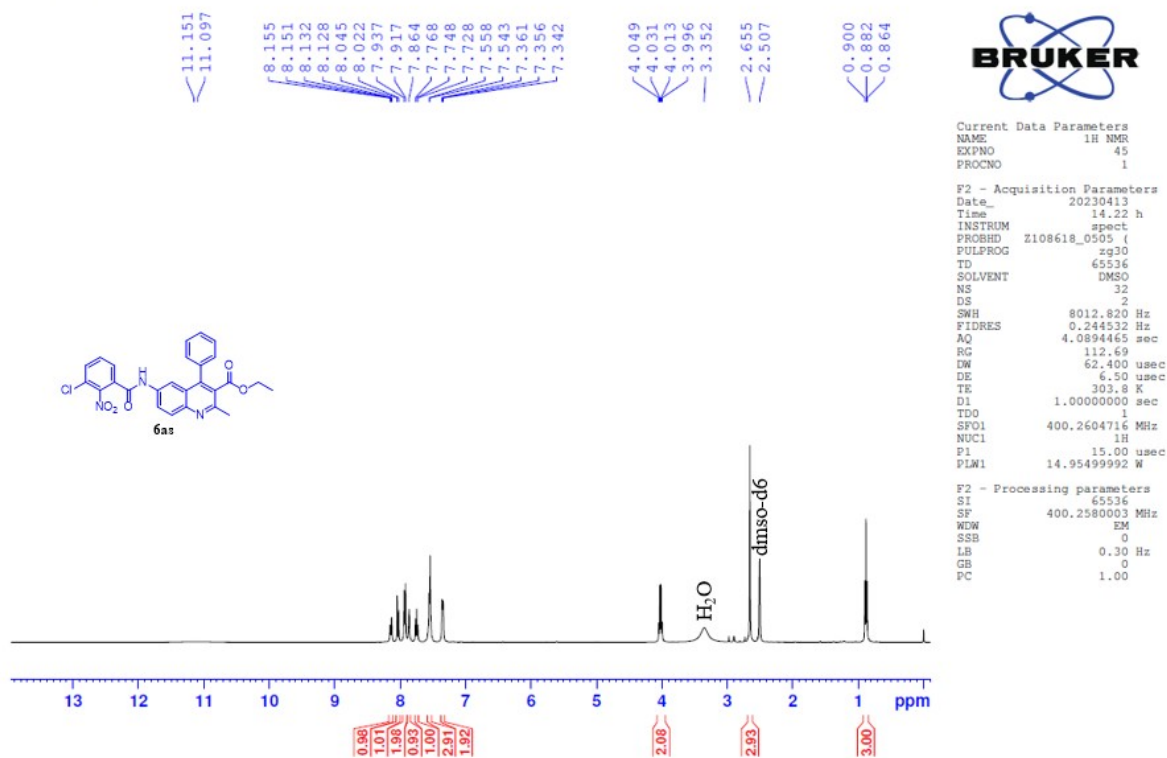


Fig.S236 <sup>1</sup>H NMR of Ethyl 6-(3-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6as).

VN-082

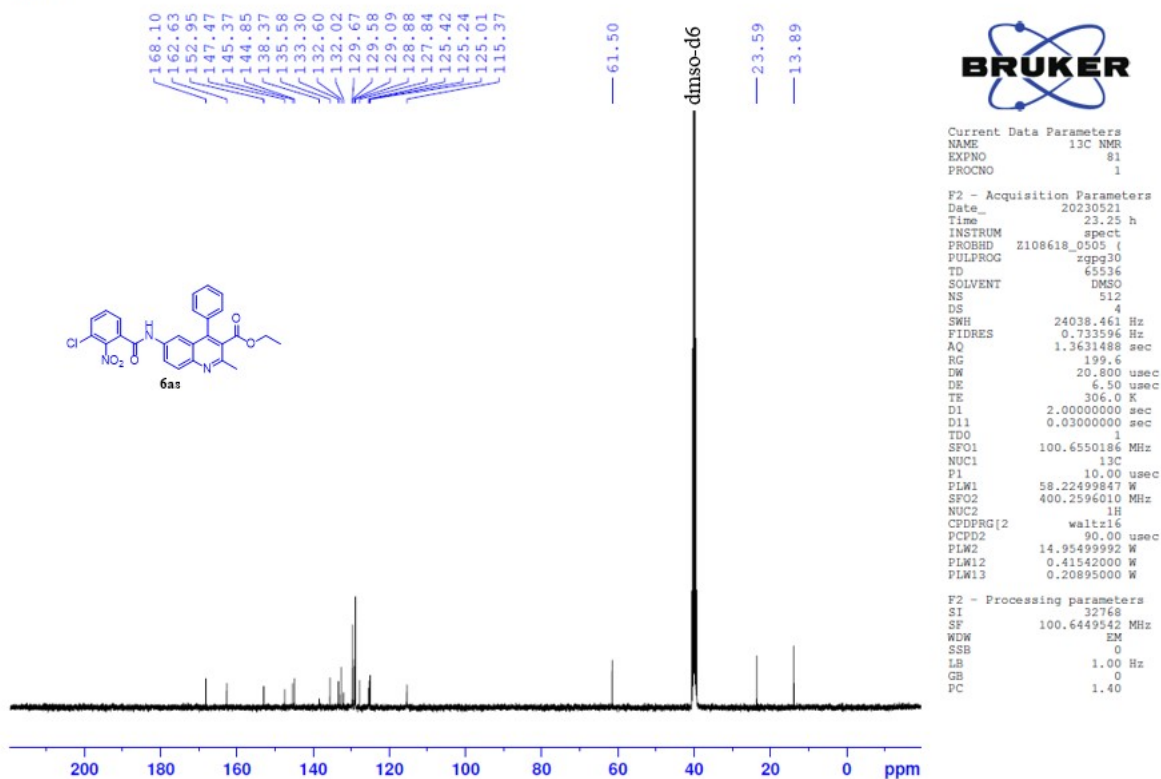


Fig.S237 <sup>13</sup>C NMR of Ethyl 6-(3-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6as).



VN-082

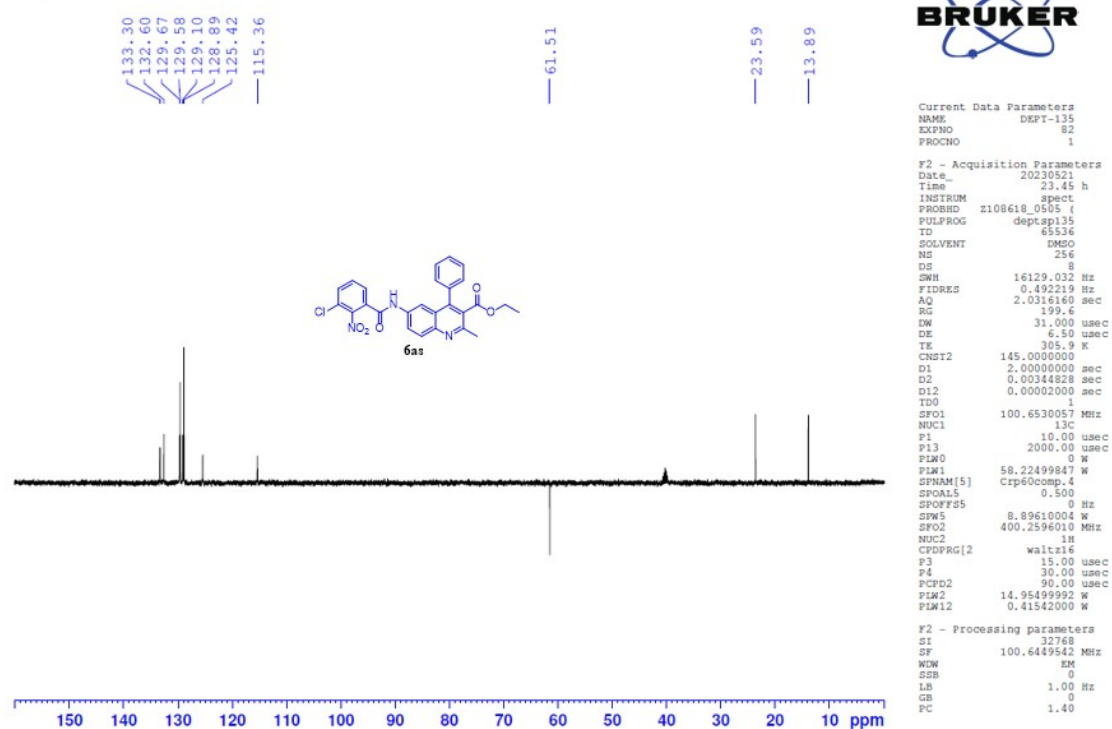


Fig.S238 DEPT-135 of Ethyl 6-(3-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6as).

HBR-DN-82 #4-14 RT: 0.02-0.06 AV: 4 SB: 63 0.32-1.20 NL: 7.95E9  
 T: FTMS + p ESI Full ms [150.0000-2000.0000]

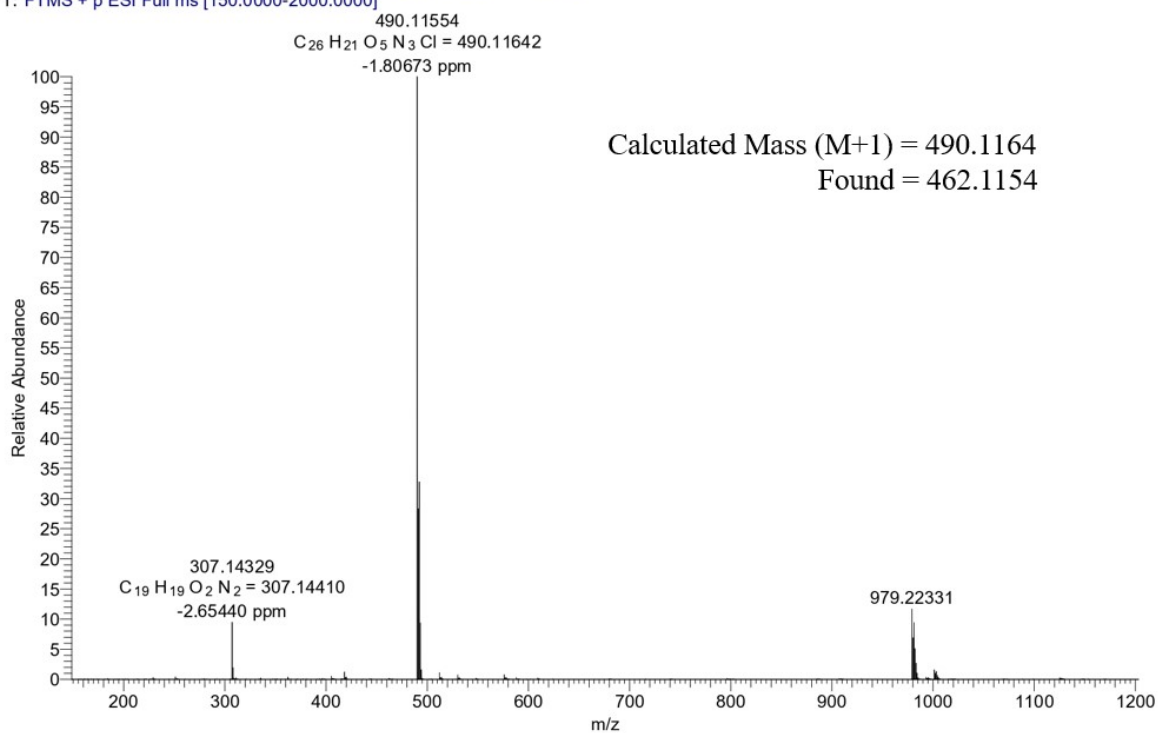
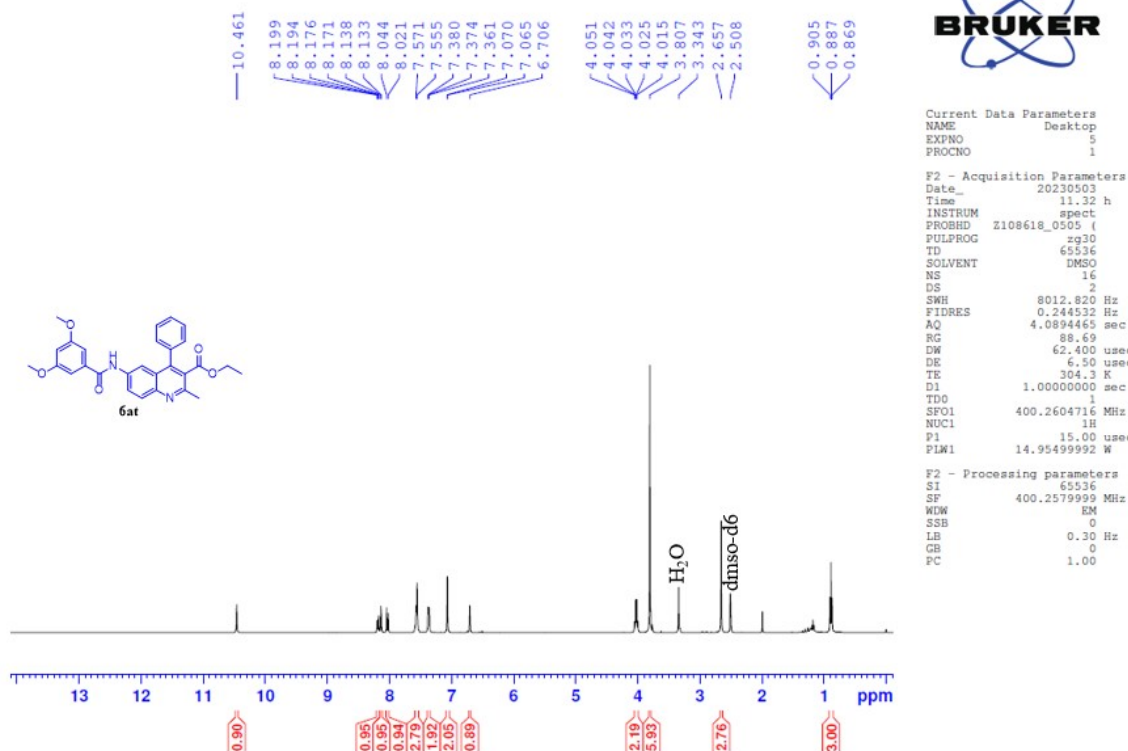
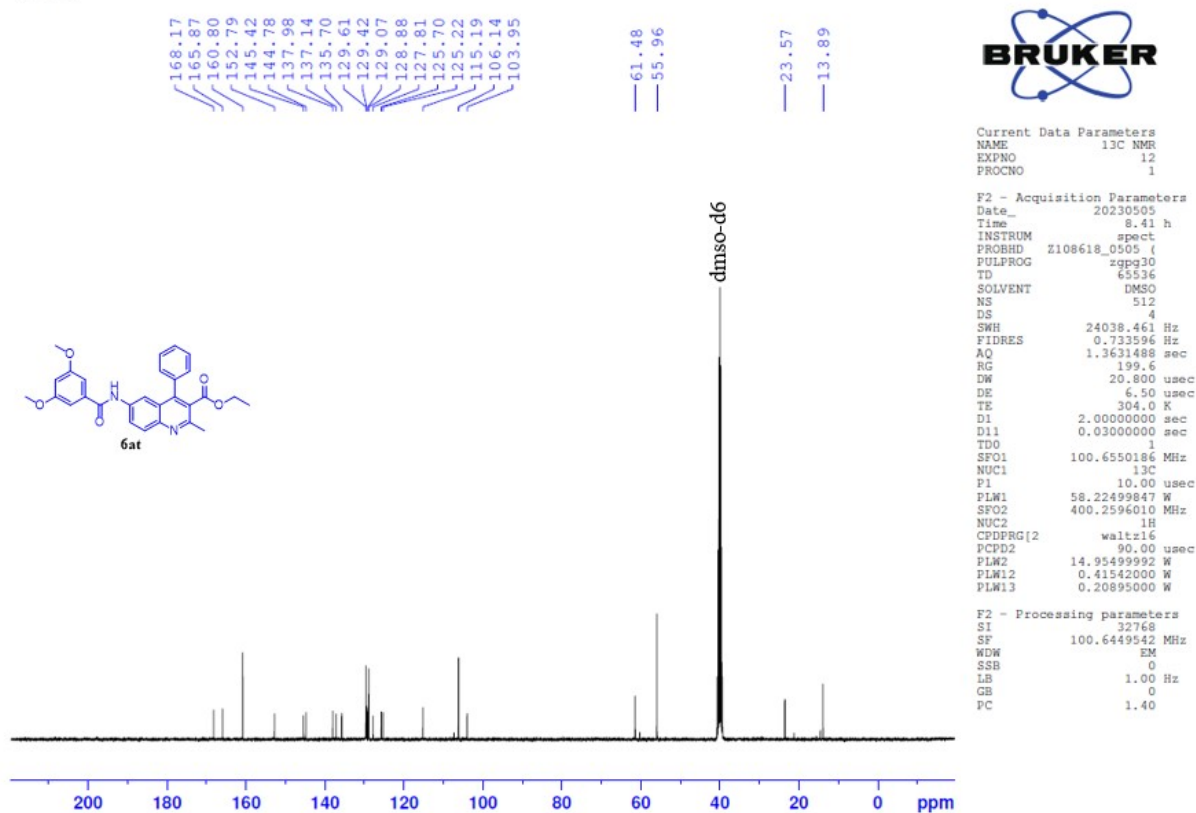


Fig.S239 HRMS of Ethyl 6-(3-chloro-2-nitrobenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6as).

VN-077

Fig.S240 <sup>1</sup>H NMR of Ethyl 6-(3,5-dimethoxybenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (**6at**).

VN-077

Fig.S241 <sup>13</sup>C NMR of Ethyl 6-(3,5-dimethoxybenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (**6at**).

VN-077

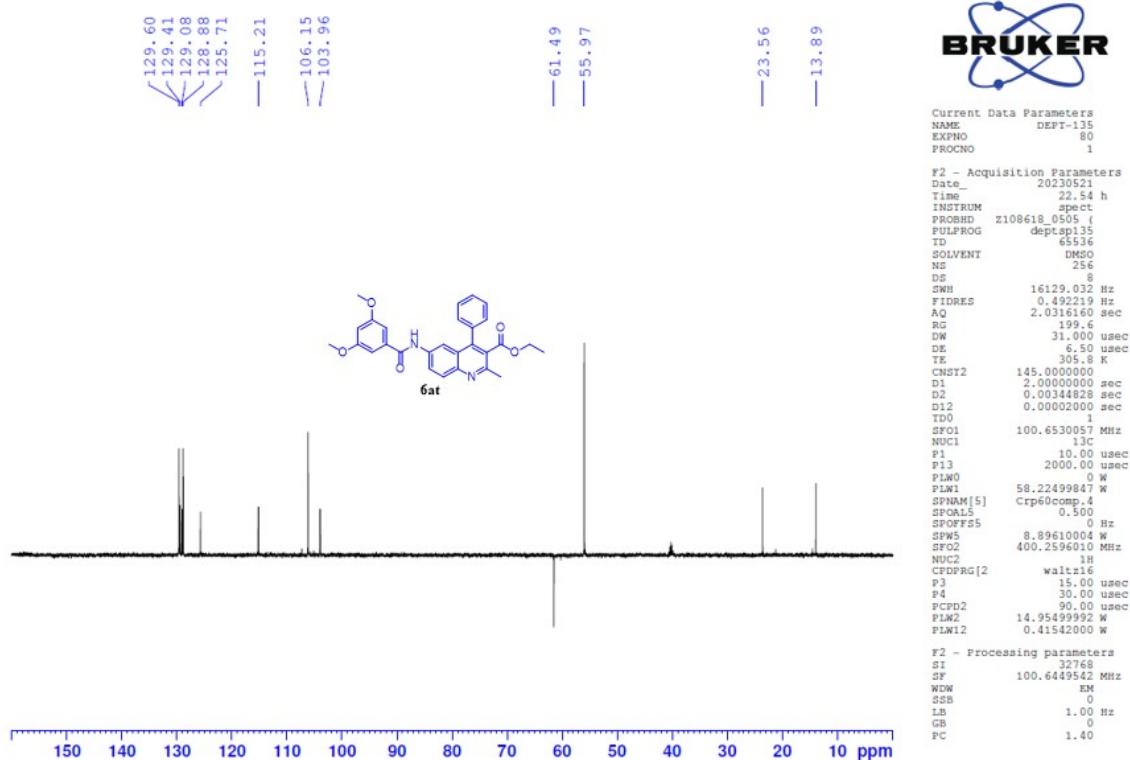


Fig.S242 DEPT-135 of Ethyl 6-(3,5-dimethoxybenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6at).

HBR-DN-077 #3-16 RT: 0.02-0.07 AV: 5 SB: 63 0.32-1.20 NL: 3.14E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

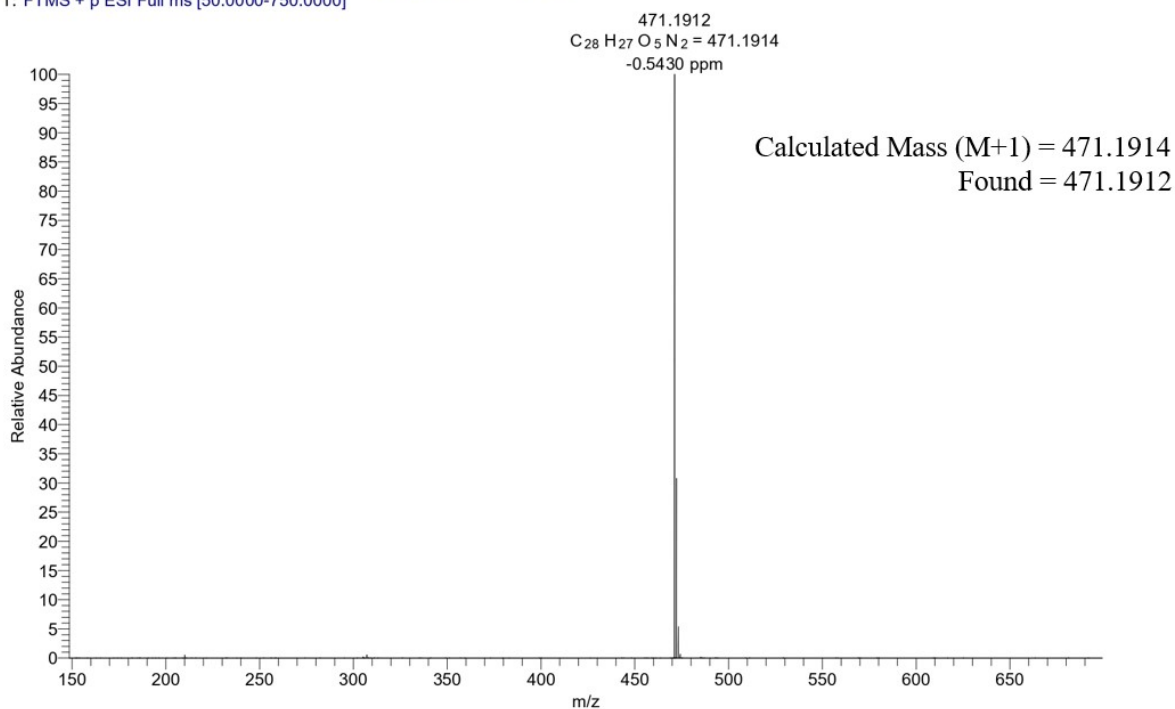
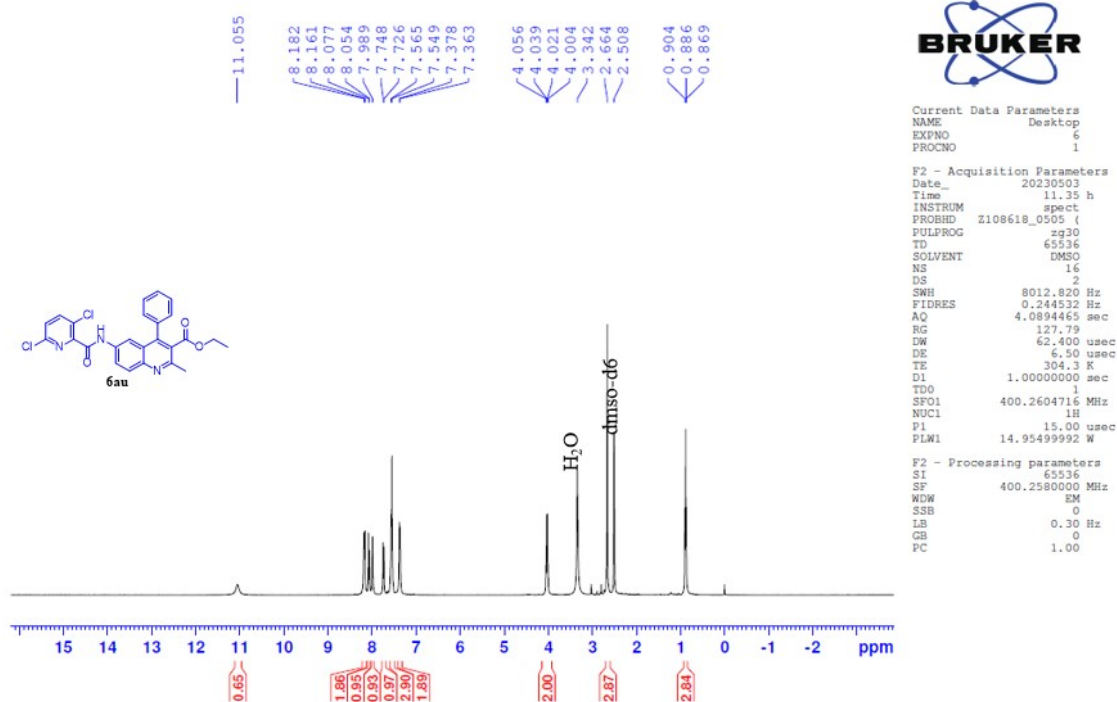
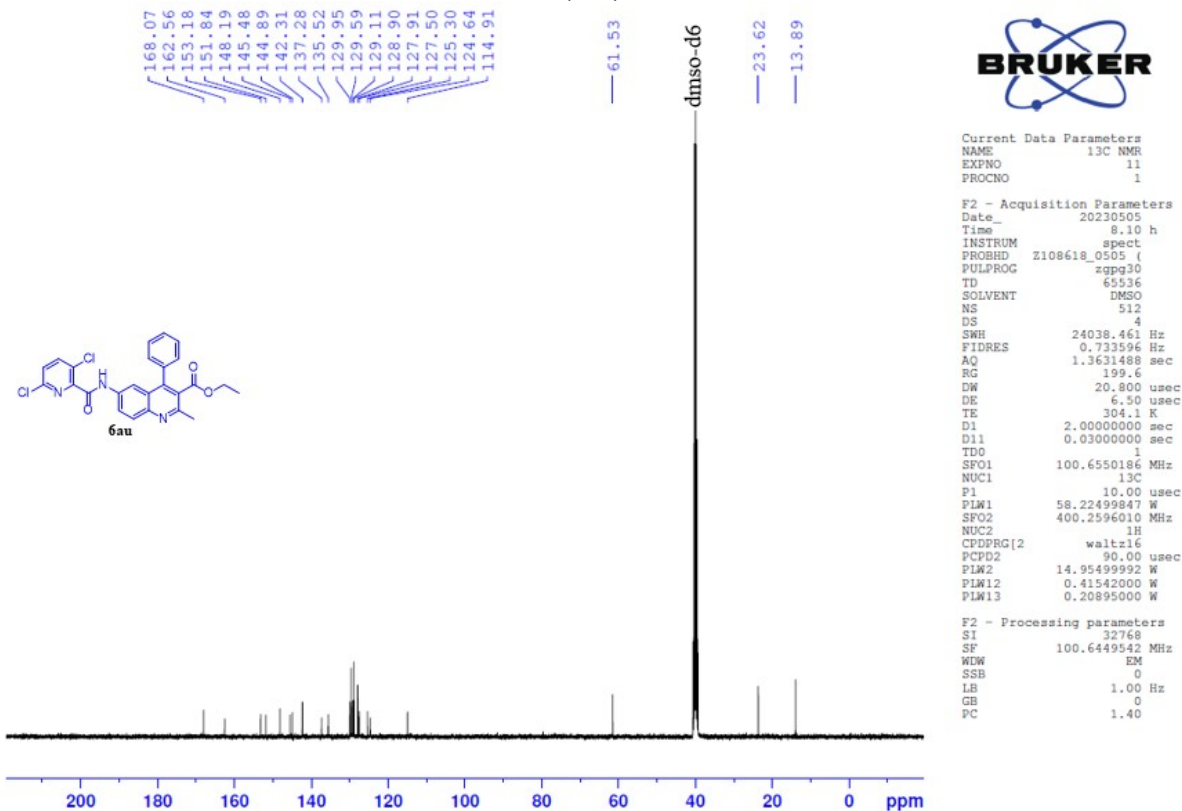


Fig.S243 HRMS of Ethyl 6-(3,5-dimethoxybenzamido)-2-methyl-4-phenylquinoline-3-carboxylate (6at).

VN-078

Fig.S244 <sup>1</sup>H NMR of Ethyl 6-(3,6-dichloropicolinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6au).Fig.S245 <sup>13</sup>C NMR of Ethyl 6-(3,6-dichloropicolinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6au).

VN-078

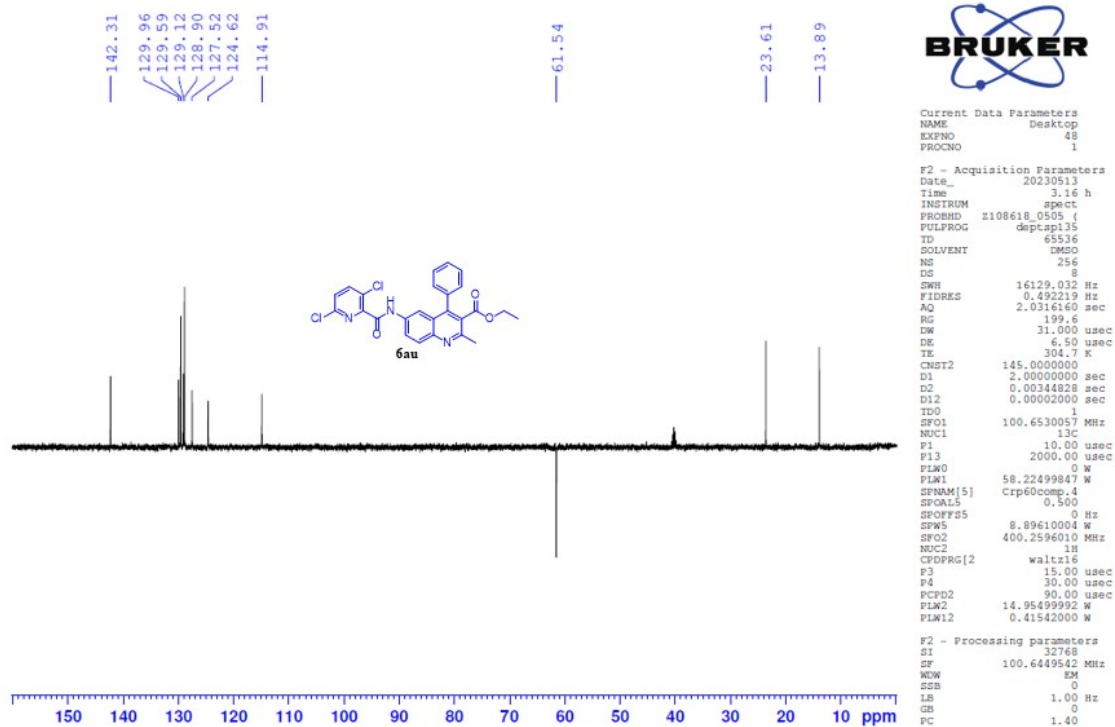


Fig.S246 DEPT-135 of Ethyl 6-(3,6-dichloropicolinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6au).

HBR-DN-078 #5-17 RT: 0.03-0.07 AV: 4 SB: 63 0.32-1.20 NL: 1.71E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

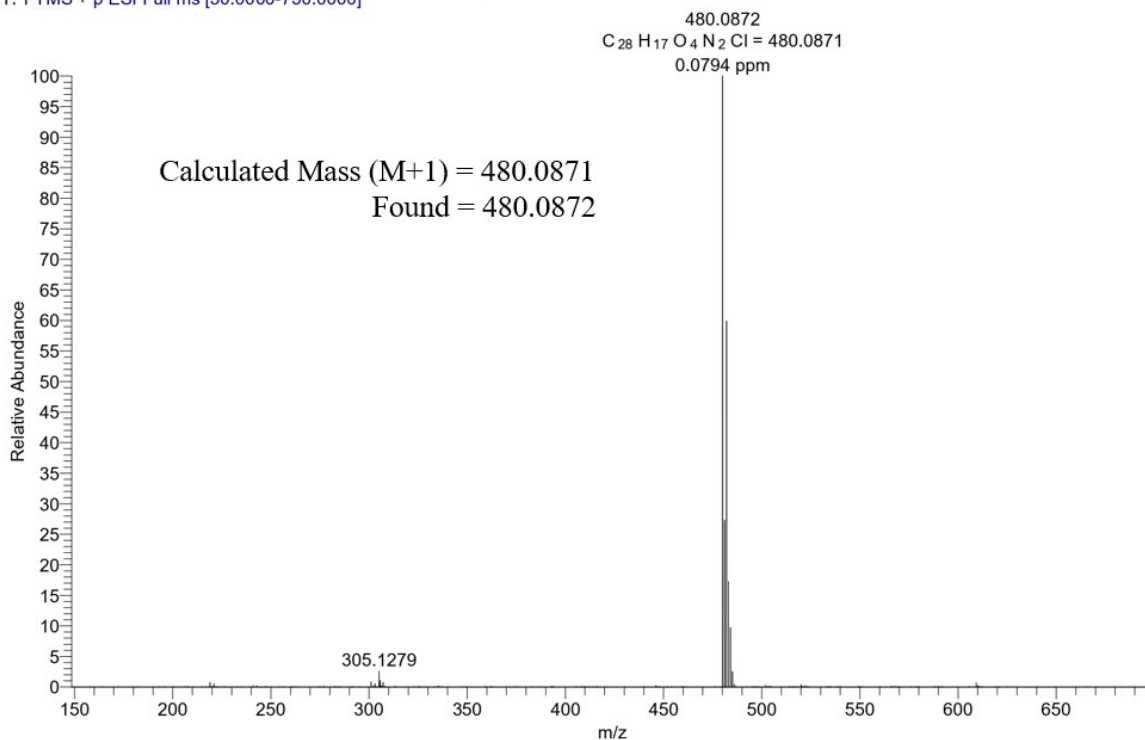


Fig.S247 HRMS of Ethyl 6-(3,6-dichloropicolinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6au).

Signature SIF VIT VELLORE  
VN-083

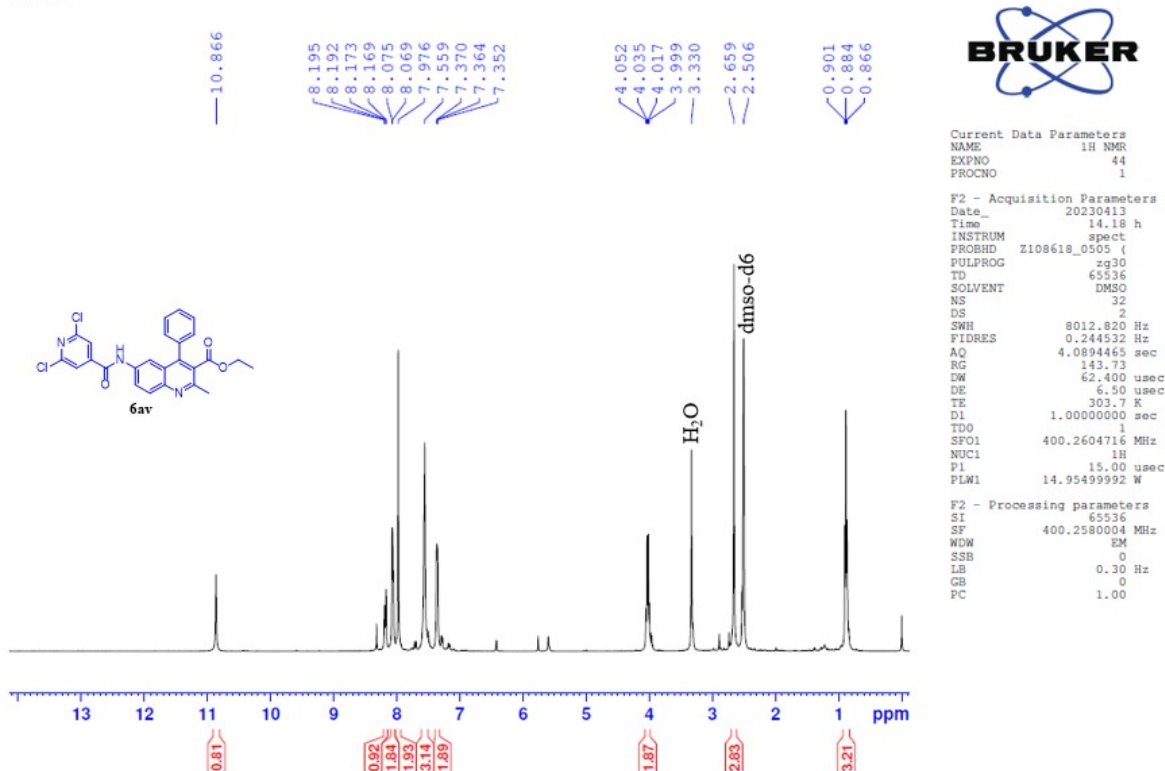


Fig.S248 <sup>1</sup>H NMR of Ethyl 6-(2,6-dichloroisonicotinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6av).

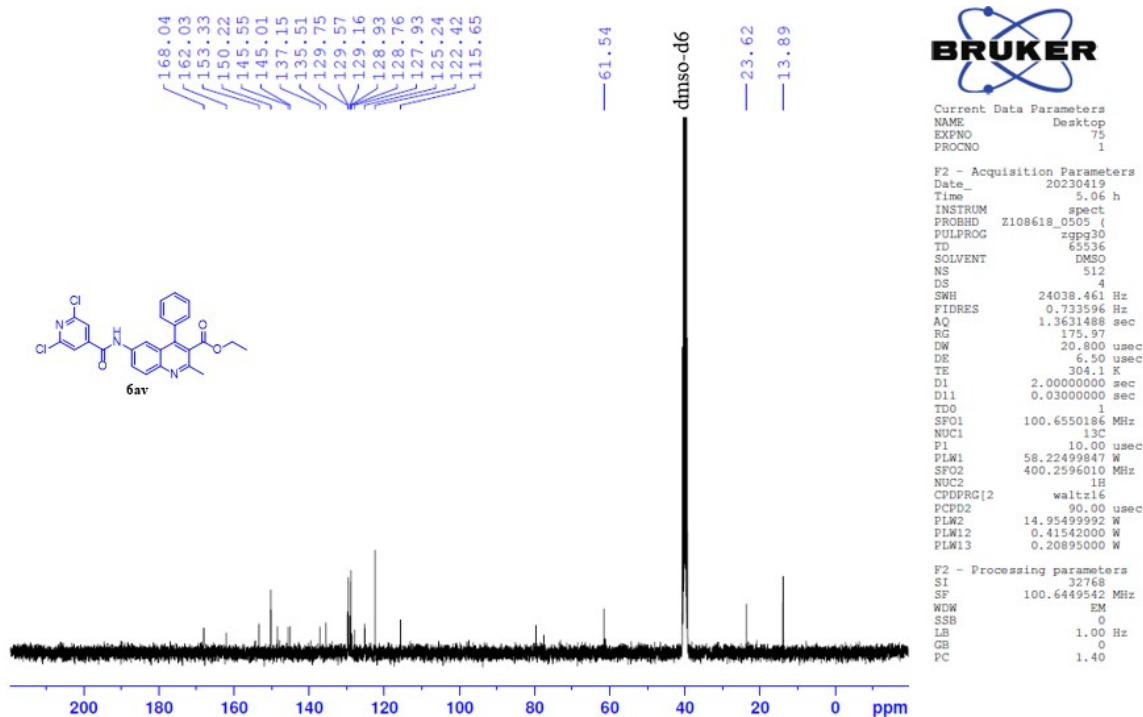


Fig.S249 <sup>13</sup>C NMR of Ethyl 6-(2,6-dichloroisonicotinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6av).

VN-083

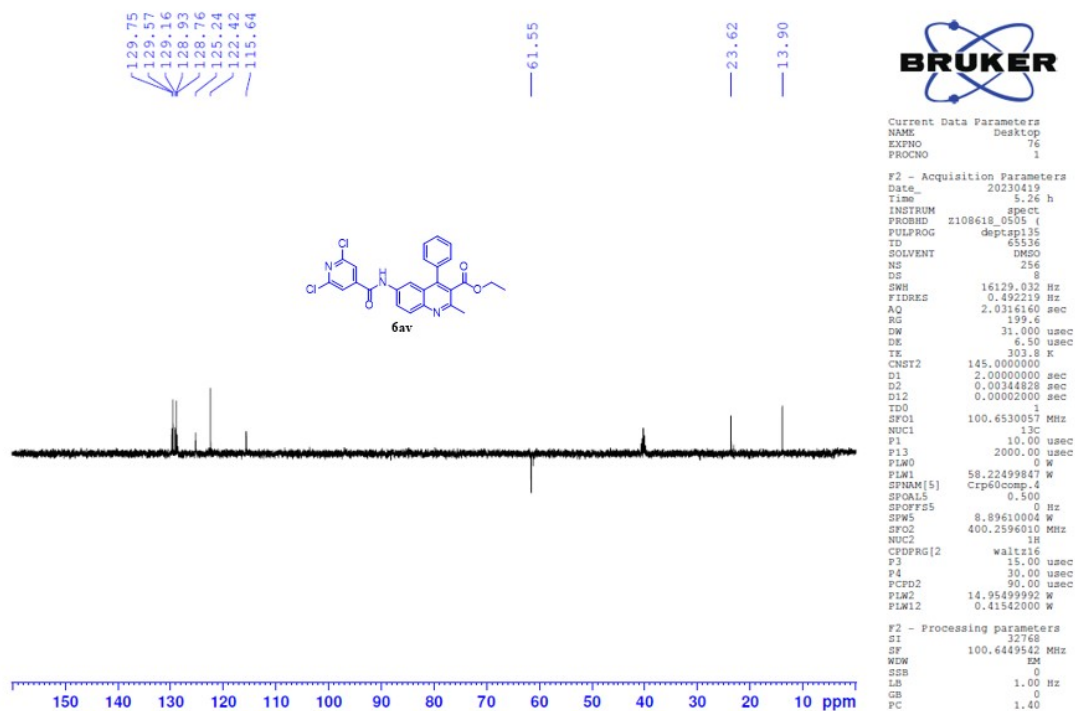


Fig.S250 DEPT-135 of Ethyl 6-(2,6-dichloroisonicotinamido)-2-methyl-4-phenylquinoline-3-carboxylate (6av).

VN-084

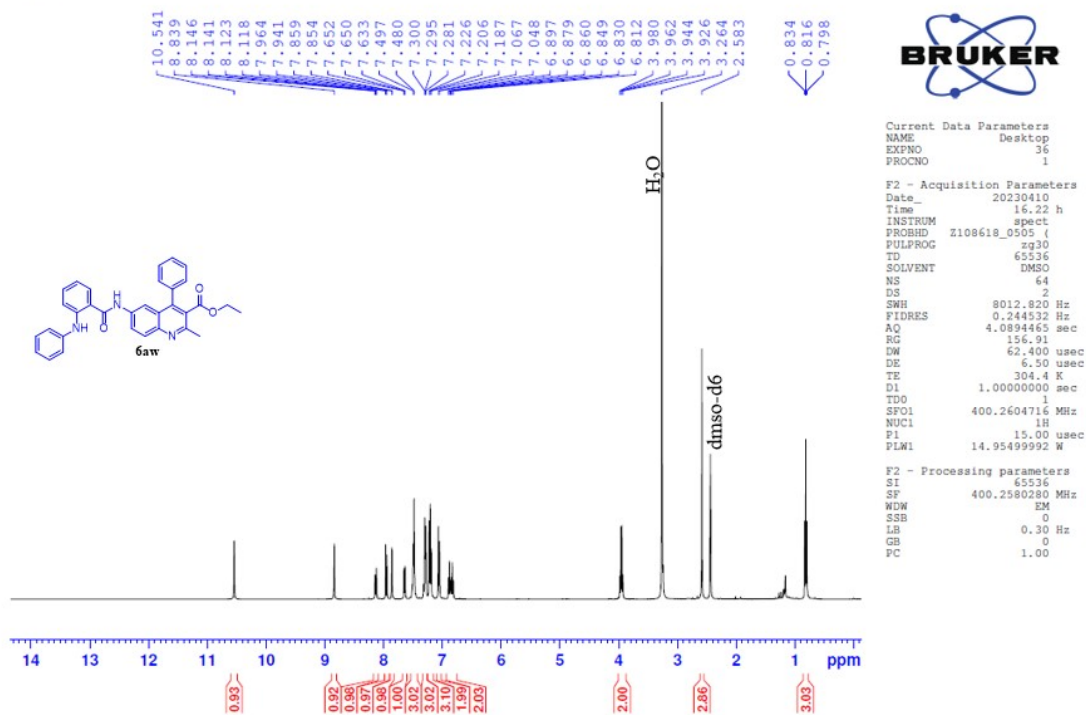


Fig.S251 <sup>1</sup>H NMR of Ethyl 2-methyl-4-phenyl-6-(2-(phenylamino)benzamido)quinoline-3-carboxylate (6aw).

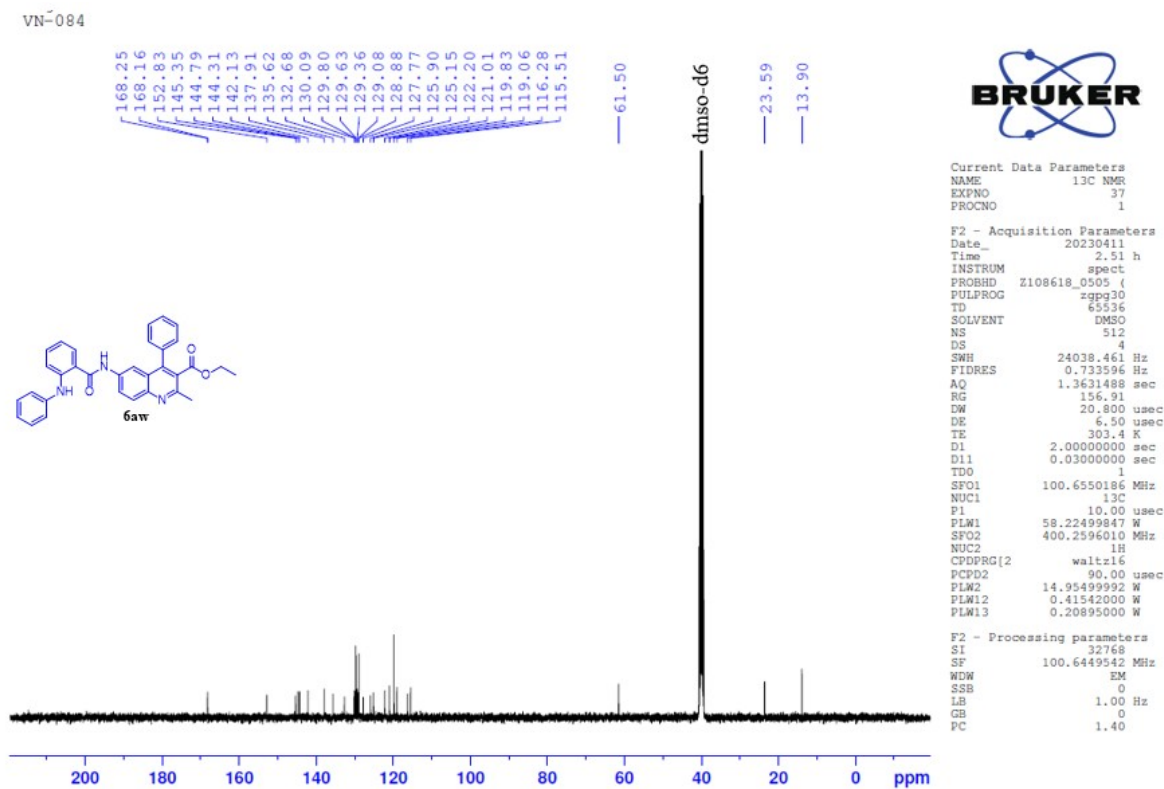


Fig.S252  $^{13}\text{C}$  NMR of Ethyl 2-methyl-4-phenyl-6-(2-(phenylamino)benzamido)quinoline-3-carboxylate (6aw).

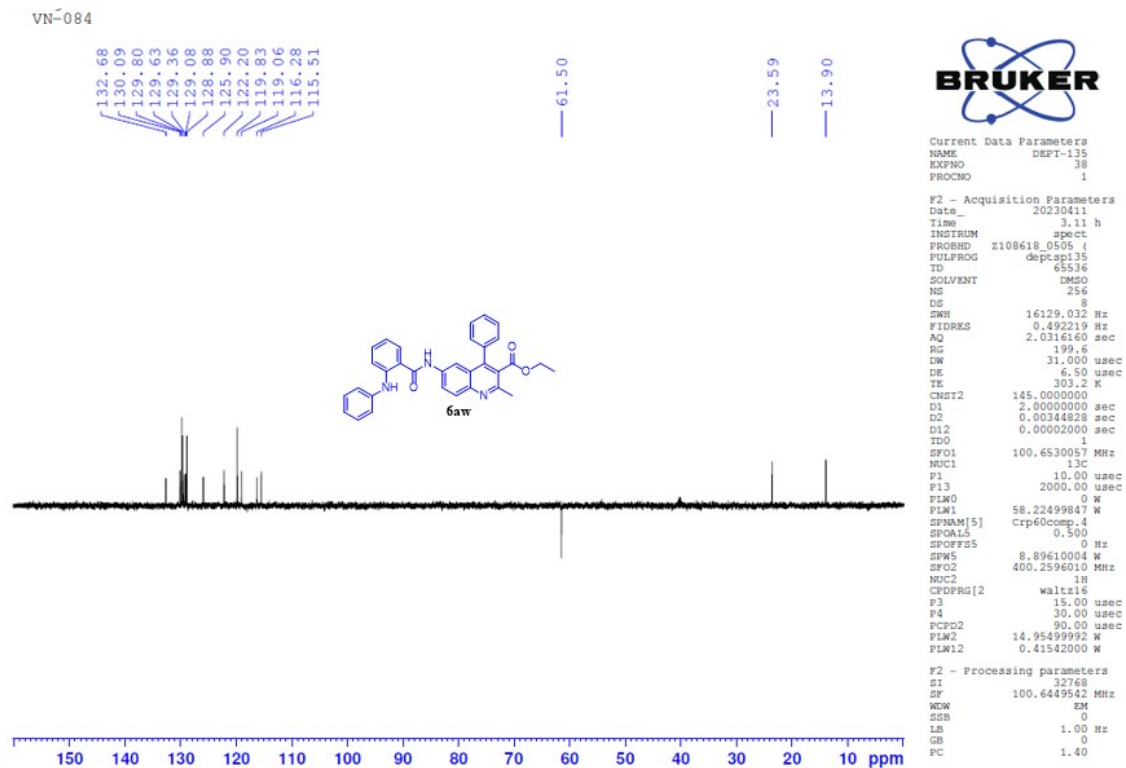


Fig.S253 DEPT-135 of Ethyl 2-methyl-4-phenyl-6-(2-(phenylamino)benzamido)quinoline-3-carboxylate (6aw).



HBR-DN-84 #4-26 RT: 0.02-0.11 AV: 8 SB: 63 0.32-1.20 NL: 1.21E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

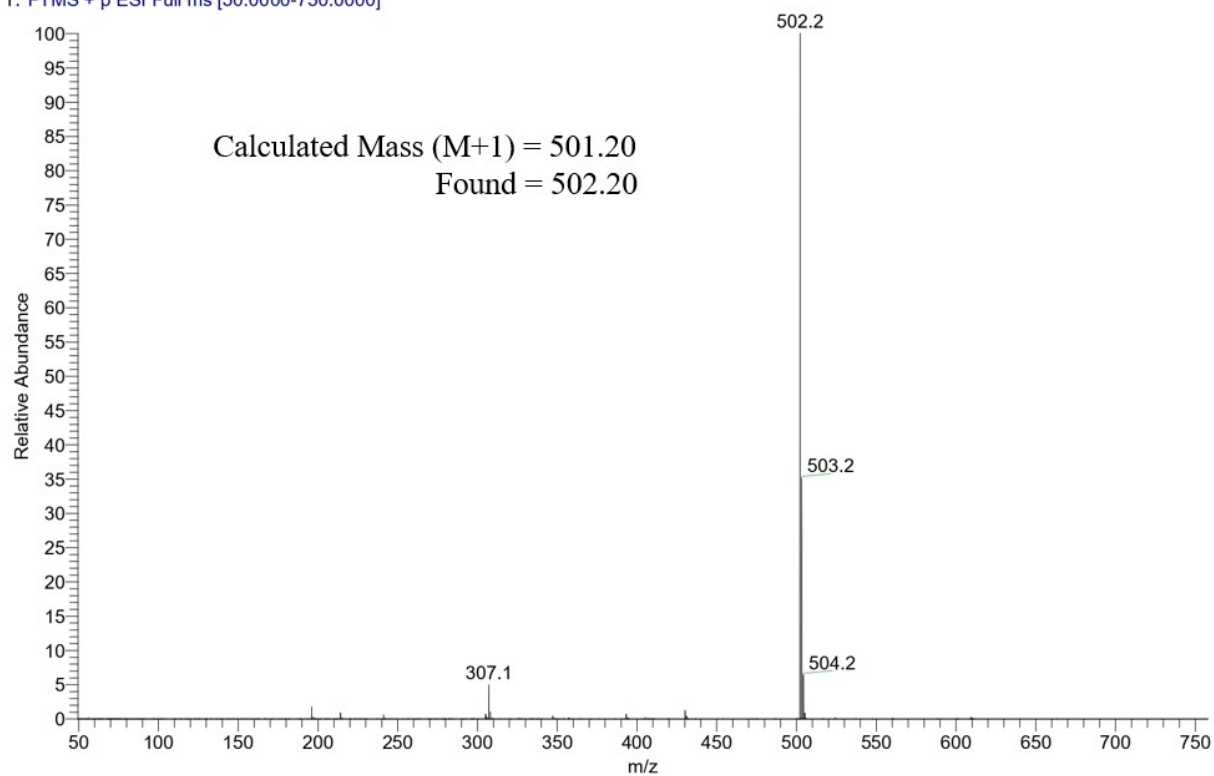


Fig.S254 MS-ESI of Ethyl 2-methyl-4-phenyl-6-(2-(phenylamino)benzamido)quinoline-3-carboxylate (6aw).