SUPPLEMENTARY INFORMATION

EXPERIMENTAL SECTION

Experimental protocols

General

Melting points (m.p.) were determined on Mettler FP 51apparatus (Mettler Instruments, Switzerland) and are uncorrected. They are expressed in degree centigrade (°C). A Nicolet Avatar Model FT-IR spectrophotometer was used to record the IR spectra (4000–400 cm^{-1}). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AV 500 (500 MHz (^{1}H) and 125 MHz (^{13}C)) spectrometer using tetramethylsilane (TMS) as an internal reference. The chemical shifts are expressed in parts per million (ppm). Mass spectra (MS), were recorded on Auto Spec EI+ shimadzu QP 2010 PLUS GC-MS mass spectrometer. Microanalyses were performed on a Vario EL III model CHNS analyzer (Vario, Germany) at the Department of Chemistry, Bharathiar University, Coimbatore, India.

General procedure for the preparation of 2-(2'-chloro-benzo[*f*]quinolin-2-ylmethylene)-2,3,4,9-tetrahydro-carbazol-1-one 3:

An equimolar mixture of the appropriate 2,3,4,9-tetrahydro-1*H*-carbazol-l-one, **1**(**a-c**) (0.005 mol) and 2-chloro-benzo[*h*]quinoline-3-carbaldehyde **2** (0.005 mol) was treated with 5 % ethanolic potassium hydroxide (25 mL) solution and stirred for 24 h at room temperature. The product precipitating as a yellow crystalline mass was filtered off and washed with 50 % ethanol. A further crop was obtained on neutralization with acetic acid and dilution with water. The product was recrystallised from ethanol to yield **3**(**a-c**).

2-(2'-Chloro-benzo[f]quinolin-2-ylmethylene)-6-methyl-2,3,4,9-tetrahydro-carbazol-1-one, 3a:

Yellow solid, m.p. 240-243 °C, yield : (90%); IR ν_{max} (cm^{-1}) : 3287 (NH), 1643 (C=O); ^{1}H NMR (δ, ppm $CDCl_3$): 9.11 (b s, 1H, N_9-H), 7.49-9.26 (m, 10H, C_5-, C_7-, C_8-, C_4'-, C_5'-, C_6'-, C_7'- , C_8'-, C_9'-, C_{10}'-H), 7.28 (s, 1H, C_2-H), 3.03-3.24 (m, 4H, C_3-2H, C_4-2H), 2.56 (s, 3H, C_6-CH_3); ^{13}C NMR (δ, ppm, $CDCl_3$): 177.0 (C_1), 152.8 (C_2'), 148.2 (C_{3a}'), 143.3 (C_2), 142.3 (C_{8a}), 137.2 (C_{9a}), 135.5 (C_{10}'), 135.2 (C_2 olefinic), 134.6 (C_{4b}), 130.9 (C_6), 130.5 (C_1'), 130.1 (C_5'), 128.2 (C_6' & C_9'), 127.7 (C_4'), 127.4 (C_{5b}') 126.7 (C_{5a}'), 126.1 (C_{4a}), 125.9 (C_7' & C_8'), 125.2 (C_{3b}'), 121.2 (C_5), 120.3 (C_7), 110.9 (C_8), 27.2 (C_3), 22.8 (C_4), 21.3 (C_6-CH_3); MS : m/z(%)

422.91. Anal. Calcd. for $C_{27}H_{19}ClN_2O$: C, 76.68; H, 4.53; N, 6.62. Found: C, 76.65; H, 4.55; N, 6.64 %.

2-(2'-Chloro-benzo[f]quinolin-2-ylmethylene)-6chloro-2,3,4,9-tetrahydro-carbazol-1-one,3b:

Yellow solid, m.p. 250-253 °C, yield : (87%); IR ν_{max} (cm^{-1}) : 3271 (NH), 1645 (C=O); ^{1}H NMR (δ, ppm $CDCl_3$): 8.90 (b s, 1H, N_9-H), 7.45-9.29 (m, 10H, C_5-, C_7-, C_8-, C_4'-, C_5'-, C_6'-, C_7'- , C_8'- , C_9'-, C_{10}'-H), 7.30 (s, 1H, C_2-H), 3.02-3.22 (m, 4H, C_3-2H, C_4-2H); ^{13}C NMR (δ, ppm, $CDCl_3$): 177.4 (C_1), 151.8 (C_2'), 147.5 (C_{3a}'), 141.4 (C_2), 140.1 (C_{8a}), 137.0 (C_{9a}), 135.1 (C_{10}'), 135.0 (C_2 olefinic), 133.7 (C_{4b}), 130.7 (C_6), 129.9 (C_1'), 129.1 (C_5'), 127.7 (C_6' & C_9'), 128.0 (C_4'), 127.7 (C_{5b}') 126.2 (C_{5a}'), 126.0 (C_{4a}), 125.2 (C_7' & C_8'), 125.0 (C_{3b}'), 122.2 (C_5), 121.3 (C_7), 110.3 (C_8), 27.0 (C_3), 22.4 (C_4); MS : m/z (%) 443.32. Anal. Calcd. for $C_{26}H_{16}Cl_2N_2O$: C, 70.44; H, 3.64; N, 6.32. Found: C, 70.46; H, 3.67; N, 6.30 %.

2-(2'-Chloro-benzo[f]quinolin-2-ylmethylene)-2,3,4,9-tetrahydro-carbazol-1-one, 3c:

Yellow solid, m.p. 242-244 °C, Yield : (83%); IR ν_{max} (cm^{-1}) : 3218 (NH), 1652 (C=O); ^{1}H NMR (δ, ppm $CDCl_3$): 8.48 (b s, 1H, N_9-H), 7.32-9.09 (m, 11H, C_5-, C_6-, C_7-, C_8-, C_4'-, C_5'-, C_6'-, C_7'-, C_8'-, C_9'-, C_{10}'-H), 7.27 (s, 1H, C_2-H), 2.85-3.00 (m, 4H, C_3-2H, C_4-2H); ^{13}C NMR (δ, ppm, $CDCl_3$): 177.1(C_1), 151.8 (C_2'), 147.2 (C_{3a}'), 140.4 (C_2), 140.2 (C_{8a}), 137.3 (C_{9a}), 135.7 (C_{10}'), 134.9 (C_2 olefinic), 133.4 (C_{4b}), 130.2 (C_6), 130.1 (C_1'), 129.0 (C_5'), 128.5 (C_6' & C_9'), 128.0 (C_4'), 127.1 (C_{5b}'), 126.5 (C_{5a}'), 126.0 (C_{4a}), 125.0 (C_7' & C_8'), 124.9 (C_{3b}'), 122.1 (C_5), 121.0 (C_7), 110.1 (C_8), 27.2 (C_3), 22.3 (C_4); MS : m/z (%) 408.88. Anal. Calcd. for $C_{26}H_{17}ClN_2O$: C, 76.37; H, 4.19; N, 6.87. Found: C, 76.34; H, 4.22; N, 6.89 %

General procedure for preparation of 4,5-dihydro-3-(2'-chloro-benzo[*f*]quinolin-2-ylmethylene) isoxazolo[3,4-*a*]carbazole 4:

The respective 2-(2'-chloro-benzo[*f*]quinolin-2-yl)-2,3,4,9-tetrahydro-carbazol-1-one **3(a-c)** (0.001 mol) was treated with hydroxylamine hydrochloride (1 g, 0.014 mol) in dry pyridine (5 mL) at 130 °C for 8 h. The reaction was monitored by TLC. After completion of the reaction, the crude mixture was poured into ice-cold water and neutralized with 5N HCl, the resulting semi-solid that separated was extracted with ethyl acetate. The combined organic layers were dried over anhydrous sodium sulphate. It was then purified by column chromatography over silica gel using petroleum ether: ethyl acetate (98 : 2) to yield the corresponding, 4,5-dihydro-3-(2'-chloro-benzo[*f*]quinolin-2-ylmethylene) isoxazolo[3,4-*a*]carbazole, **4(a-c)**. The product obtained was recrystallised from ethanol.

4,5-Dihydro-7-methyl-3-(2'--chloro-benzo[f]quinolin-2-ylmethylene)isoxazolo[3,4-a]carbazole, 4a:

Brown solid m.p. 252-244 °C, yield : (72%); IR ν_{max} (cm^{-1}) : 3310 (NH), 1598 (C=N); ^{1}H NMR (δ, ppm $CDCl_3$): 8.43 (b s, 1H, N_9-H), 7.02-9.55 (m, 10H, C_6-, C_8-, C_9-, C_4'-, C_5'-, C_6'-, C_7'- , C_8'-, C_9'-, C_{10}'-H), 3.03-3.24 (m, 4H, C_4-2H, C_5-2H), 2.53 (s, 3H, C_7-CH_3); ^{13}C NMR (δ, ppm, $CDCl_3$): 158.3 (C_3), 155.4 (C_2'), 150.0 (C_1), 147.3 (C_{3a}'), 135.7 (C_{10}'), 134.2 (C_{9a}), 132.0 (C_{5b}), 131.5 (C_1), 131.0 (C_7), 130.6 (C_5'), 129.2 (C_6' & C_9'), 127.1 (C_4'), 127.4 (C_{5b}'), 126.3 (C_{10b}), 126.1 (C_{4a}), 126.0 (C_{5a}'), 125.2 (C_7' & C_8'), 123.4 (C_{10a}), 121.7 (C_6), 120.3 (C_8), 111.9 (C_9), 100.5 (C_{3a}), 27.6 (C_5), 22.6 (C_4), 22.3 (C_6-CH_3); MS : m/z (%) 435.90. Anal. Calcd. for $C_{27}H_{18}ClN_3O$: C, 74.39; H, 4.16; N, 9.64. Found: C, 74.41; H, 4.18; N, 9.63 %.

4,5-Dihydro-7-chloro-3-(2'-chloro-benzo[f]quinolin-2-ylmethylene)isoxazolo[3,4-a]carbazole, 4b:

Brown solid. m.p. 257-259 °C, yield : (74%); IR ν_{max} (cm^{-1}) : 3456 (NH), 1586 (C=N); ^{1}H NMR (δ, ppm $CDCl_3$): 8.50 (b s, 1H, N_9-H), 7.15-9.33 (m, 10H, C_6-, C_8-, C_9-, C_4'-, C_5'-, C_6'-, C_7'-, C_8'-, C_9'-, C_{10}'-H), 3.03-3.24 (m, 4H, C_4-2H, C_5-2H); ^{13}C NMR (δ, ppm, $CDCl_3$): 158.1 (C_3), 155.7 (C_2'), 150.2 (C_1), 147.1 (C_{3a}'), 135.2 (C_{10}'), 134.0 (C_{9a}), 132.9 (C_{5b}), 131.1 (C_1), 131.4 (C_7), 130.1(C_5'), 129.2 (C_6' & C_9'), 127.1 (C_4'), 127.4 (C_{5b}'), 126.2 (C_{10b}), 126.0 (C_{4a}), 125.9 (C_{5a}'), 125.6 (C_7' & C_8'), 123.1 (C_{10a}), 121.4 (C_6), 120.0 (C_8), 111.2 (C_9), 100.1 (C_{3a}), 27.2 (C_5), 22.1 (C_4); MS : m/z (%) 456.32. Anal. Calcd. for $C_{26}H_{15}Cl_2N_3O$: C, 68.43; H, 3.31; N, 9.21. Found: C, 68.40; H, 3.29; N, 9.24%.

4,5-Dihydro-3-(2'-chloro-benzo[f]quinolin-2-ylmethylene) isoxazolo[3,4-a]carbazole, 4c:

Brown solid. m.p. 250-252 °C, Yield : (72 %); IR ν_{max} (cm^{-1}) : 3444 (NH), 1587 (C=N), ^{1}H NMR (δ, ppm, $CDCl_3$): 8.43 (b s, 1H, N_9-H), 7.11-9.21 (m, 11H, C_6-, C_7-, C_8-, C_9-, C_4'-, C_5'-, C_6'-, C_7'-, C_8'-, C_9'-, C_{10}'-H), 3.00-3.29 (m, 4H, C_4-2H, C_5-2H); ^{13}C NMR (δ, ppm, $CDCl_3$): 158.6 (C_3), 155.6 (C_2'), 150.1 (C_1), 147.0 (C_{3a}'), 135.4 (C_{10}'), 134.2 (C_{9a}), 132.3 (C_{5b}), 131.4 (C_1), 131.2 (C_7), 130.2 (C_5'), 129.0 (C_6' & C_9'), 127.2 (C_4'), 127.6 (C_{5b}'), 126.6 (C_{10b}), 126.3 (C_{4a}), 126.0 (C_{5a}'), 125.2 (C_7' & C_8'), 123.4 (C_{10a}), 121.7 (C_6), 120.3 (C_8), 111.9 (C_9), 100.5 (C_{3a}), 27.6 (C_5), 22.6 (C_4); MS : m/z (%) 421.88. Anal. Calcd. for $C_{26}H_{16}ClN_3O$: C, 74.08; H, 3.82; N, 9.96. Found: C, 74.06; H, 3.84; N, 9.94 %.

General procedure for preparation of 4-(2'-chloro-benzo[f]quinolin-2-ylmethylene)-2-ethoxy-5,6-dihydro-pyrido[2,3-a]carbazole-3-carbonitriles, 5:

The respective 2-(2'-chloro-benzo[*f*]quinolin-2-ylmethylene)-2,3,4,9-tetrahydro-carbazol-1-one **3**(**a-c**) (0.001 mol) in dry ethanol (20 mL) was added to an ice-cooled solution of 1.00 g of sodium hydride (degreased with petroleum ether) in dry benzene (10 mL). To this malononitrile (0.005 mol) was added and the mixture was refluxed on an oil bath for 5 h. The reaction was monitored by TLC indicated the formation of the product. The excess solvent was removed by distillation and the mixture was poured into ice-water. The brown solid that separated was neutralized with 5N HCl, filtered and dried. It was purified by column chromatography over silica gel using petroleum ether : ethyl acetate (98 : 2) as eluent to yield the corresponding pyrido carbazoles 4-(2'-chloro-benzo[*f*]quinolin-2-ylmethylene)-2-ethoxy-5,6-dihydro-pyrido[2,3-*a*]carbazole-3-carbonitriles, **5**(**a-c**). The products obtained were recrystallised from ethanol.

4-(2'-Chloro-benzo[f]quinolin-2-ylmethylene)-2-ethoxy-5,6-dihydro-8-methylpyrido[2,3-a]carbazole-3-carbonitriles, 5a :

Yellow solid, m.p. 240-244 ^{o}C, yield: (70%); IR ν_{max} (cm^{-1}): 3327 (NH), 2216 (C≡N), 1641 (C=N); ^{1}H NMR (δ, ppm $CDCl_3$): 8.66 (b s, 1H, N_{11}-H), 7.22-9.30 (m, 10H, C_7-, C_9-, C_{10}-, C_4'-, C_5'-, C_6'-, C_7'-,C_8'-, C_9'-, C_{10}'-H), 4.71 (q, 2H, C_2-OCH_2- J = 7.00 Hz), 3.00-3.06 (m, 4H, C_5-2H, C_6-2H), 2.62 (s, 3H, C_8-CH_3), 1.58 (t, 3H, C_2-$OCH_2C\mathbf{H_3}$, J = 7.00 Hz); ^{13}C NMR(δ, ppm $CDCl_3$): 166.7 (C_2), 159.4 (C_{11b}), 155.3 (C_2'), 150.2 (C_4), 147.1 (C_{3a}'), 135.7 (C_{10}'), 134.3 (C_{10a}), 132.1 (C_{6b}), 131.5 (C_1'), 131.0 (C_8), 130.1 (C_5'), 128.5 (C_4'), 127.4 (C_{5b}') 127.9 (C_6' & C_9'), 126.5 (C_{5a}'), 126.3 (C_{3b}'), 125.5 (C_7' & C_8'), 123.9 (C_{4a}), 123.2 (C_{11a}), 121.1 (C_7), 120.2 (C_9), 118.3 (C_3-CN), 112.0 (C_{6a}), 111.3 (C_{10}) 97.3 (C_3), 28.7 (C_5), 27.6 (C_6), 21.1 (C_8-CH_3), 64.3 (C_2-CH_2), 14.4 (C_2-CH_3); MS: m/z (%) 515.00; Anal. Calcd. for: $C_{32}H_{23}ClN_3O$: C, 74.63; H, 4.50; N, 10.88. Found: C, 74.60; H, 4.52; N, 10.85 %.

4-(2'-Chloro-benzo[f]quinolin-2-ylmethylene)-2-ethoxy-5,6-dihydro-8-chloropyrido[2,3-a]carbazole-3-carbonitriles, 5b :

Yellow solid, m.p. 261-264 ^{o}C, yield: (71%); IR ν_{max} (cm^{-1}): 3325 (NH), 2219 (C≡N), 1640 (C=N); ^{1}H NMR (δ, ppm, $CDCl_3$): 8.51 (b s, 1H, N_{11}-H), 7.21-9.23 (m, 10H, C_7-, C_9-, C_{10}-, C_4'-, C_5'-, C_6'-, C_7'-,C_8'-, C_9'-, C_{10}'-H), 4.45 (q, 2H, C_2-OCH_2- J = 6.00 Hz), 3.04-3.12 (m, 4H, C_5-

2H, C_6-2H), 1.45 (t, 3H, C_2-$OCH_2C\mathbf{H_3}$, J = 6.00 Hz); ^{13}C NMR(δ, ppm, $CDCl_3$): 166.5 (C_2), 159.1 (C_{11b}), 155.0 (C_2'), 149.7 (C_4), 146.5 (C_{3a}'), 135.1 (C_{10}'), 134.0 (C_{10a}), 131.7 (C_{6b}), 131.2 (C_1'), 131.1 (C_8), 129.5 (C_5'), 128.0 (C_4'), 127.9 (C_{5b}'), 127.5 (C_6' & C_9'), 126.0 (C_{5a}'), 125.9 (C_{3b}'), 125.2 (C_7' & C_8'), 123.3 (C_{4a}), 123.0 (C_{11a}), 120.6 (C_7), 120.1 (C_9), 118.5 (C_3-CN), 111.9 (C_{6a}), 111.0 (C_{10}), 97.0 (C_3), 28.3 (C_5), 27.1 (C_6), 64.0 (C_2-CH_2), 14.0 (C_2-CH_3); MS: m/z (%) 534.42; Anal. Calcd. for: $C_{31}H_{20}Cl_2N_4O$: C, 69.54; H, 3.77; N, 10.46. Found: C, 69.51; H, 3.75; N, 10.44 %.

4-(2'-Chloro-benzo[f]quinolin-2-ylmethylene)-2-ethoxy-5,6-dihydro-pyrido[2,3-a]carbazole-3-carbonitriles, 5c :

Yellow solid, m.p. 244-246 ^oC, yield: (72%); IR ν_{max} (cm^{-1}): 3327 (NH), 2215 (C≡N), 1641 (C=N); ^{1}H NMR (δ, ppm, $CDCl_3$): 8.51 (b s, 1H, N_{11}-H), 7.32-9.02 (m, 11H, , C_7-, C_8-, C_9-, C_{10}-, C_4'-, C_5'-, C_6'-, C_7'-,C_8'-, C_9'-, C_{10}'-H), 4.43 (q, 2H, C_2-OCH_2- J = 9.00 Hz), 2.94-3.00 (m, 4H, C_5-2H, C_6-2H), 1.40 (t, 3H, C_2-$OCH_2C\mathbf{H_3}$, J = 9.00 Hz); ^{13}C NMR(δ, ppm, $CDCl_3$): 166.1 (C_2), 159.0 (C_{11b}), 154.3 (C_2'), 149.2 (C_4), 146.9 (C_{3a}'), 135.1 (C_{10}'), 134.0 (C_{10a}), 132.3 (C_{6b}), 131.2 (C_1'), 131.4 (C_8), 130.2 (C_5'), 128.1 (C_4'), 127.2 (C_{5b}') 127.0 (C_6' & C_9'), 126.2 (C_{5a}'), 126.1 (C_{3b}'), 125.2 (C_7' & C_8'), 123.4 (C_{4a}), 123.0 (C_{11a}), 121.5 (C_7), 120.0 (C_9), 118.5 (C_3-CN), 112.4 (C_{6a}), 111.5 (C_{10}), 97.7 (C_3), 28.4 (C_5), 27.6 (C_6), 64.1 (C_2-CH_2), 14.7 (C_2-CH_3); MS: m/z (%) 500.98; Anal. Calcd. for: $C_{31}H_{21}ClN_4O$: C, 74.32; H, 4.23; N, 11.18. Found: C, 74.30; H, 4.20; N, 11.16 %.

General procedure for preparation of 2-amino-4-(2'-chloro-benzo[f]quinolin-2-ylmethylene)pyrimido[4,5-a]-carbazoles, 6 :

To 1.00 g of sodium hydride (degreased with petroleum ether) in dry benzene (10 mL), the respective 2-(2'-chloro-benzo[*f*]quinolin-2-ylmethylene)-2,3,4,9-tetrahydro-carbazol-1-one, **3(a-c)** (1mmol) and guanidine nitrate (10 mmol) were added and the mixture was refluxed for 18 h. The reaction was monitored by TLC. After completion of the reaction, the excess solvent was boiled off and the residue was poured into crushed ice. The mixture was then neutralized and extracted with ethyl acetate. The organic layer was washed with water and dried over anhydrous sodium sulphate, upon removal of the solvent a brown mass was obtained. It was purified by column chromatography over silica gel using petroleum ether: ethyl acetate (80: 20) mixture as eluent to afford a yellow solid which was recrystallised from ethanol to the yield 2-amino-4-(2'-chloro-benzo*[f]*quinolin-2-ylmethylene)pyrimido[4,5-*a*]-carbazoles, **6(a-c)**.

2-Amino-4-(2'-chloro-benzo[f]quinolin-2-ylmethylene)-8methyl-pyrimido[4,5-a]-carbazole, 6a:

Yellow prisms, m.p.155-157 °C, yield: (70%); IR ν_{max} (cm^{-1}): 3322 (sym NH_2), 3296 (asym NH_2), 1583 (C=N); ^{1}H NMR (δ, ppm $CDCl_3$): 8.41 (b s, 1H, N_{11}-H), 7.32-9.02 (m, 12H, C_5-, C_6-, C_7-, C_9-, C_{10}-, C_4'-, C_5'-, C_6'-, C_7', C_8', C_9', C_{10}' H), 5.21 (b s, 2H, NH_2), 2.47 (s, 3H, C_8-CH_3); ^{13}CNMR (δ, ppm $CDCl_3$): 177.2 (C_2), 155.3 (C_2'), 154.2 (C_4), 150.1 (C_{11b}), 147.1 (C_{3a}'), 135.6 (C_{10}'), 133.2 (C_{6a}), 132.4 (C_1'), 130.9 (C_8), 130.2 (C_5'), 128.2 (C_4'), 128.0 (C_6' & C_9'), 127.3 (C_{5b}'), 126.7 (C_{5a}'), 126.0 (C_5), 126.1 (C_{3b}'), 125.6 (C_7' & C_8'), 125.2 (C_{11b}), 124.3 (C_{10a}), 123.4 (C_6), 121.1 (C_7), 120.1 (C_9), 118.1 (C_{4a}), 110.3 (C_{10}), 103.3 (C_{6b}), 21.3 (C_8- CH_3); MS: m/z (%) 459.13; Anal. Calcd. for: $C_{28}H_{18}ClN_5$: C, 73.12; H, 3.94; N, 15.23; Found: C, 73.10; H, 3.96; N, 15.25 %.

2-Amino-4-(2'-chloro-benzo[f]quinolin-2-ylmethylene)-8chloropyrimido[4,5-a]-carbazole, 6b:

Yellow prisms, m.p.165-158 °C, yield: (71%); IR ν_{max} (cm^{-1}): 3341 (sym NH_2), 3305 (asym NH_2), 1601 (C=N); ^{1}H NMR (δ, ppm, $CDCl_3$): 8.47 (b s, 1H, N_{11}-H), 7.42-9.10 (m, 12H, C_5-, C_6-, C_7-, C_9-, C_{10}-, C_4'-, C_5'-, C_6'-, C_7', C_8', C_9', C_{10}' H), 5.32 (b s, 2H, NH_2); ^{13}C NMR ($CDCl_3$): 177.0 (C_2), 155.1 (C_2'), 154.0 (C_4), 150.0 (C_{11b}), 147.5 (C_{3a}'), 135.1 (C_{10}'), 133.0 (C_{6a}), 132.2 (C_1'), 130.5 (C_8), 130.0 (C_5'), 128.1 (C_4'), 127.8 (C_6' & C_9'), 127.1 (C_{5b}'), 126.5 (C_{5a}'), 126.2 (C_5) 126.1 (C_{3b}'), 125.4 (C_7' & C_8'), 125.1 (C_{11b}), 124.5 (C_{10a}), 123.8 (C_6), 121.5 (C_7), 120.5 (C_9), 118.0 (C_{4a}), 110.1 (C_{10}), 103.0 (C_{6b}); MS: m/z (%) 480.35; Anal. Calcd. for: $C_{27}H_{15}Cl_2N_5$: C, 67.51; H, 3.15; N, 14.58; Found: C, 67.49; H, 3.17; N, 14.56 %.

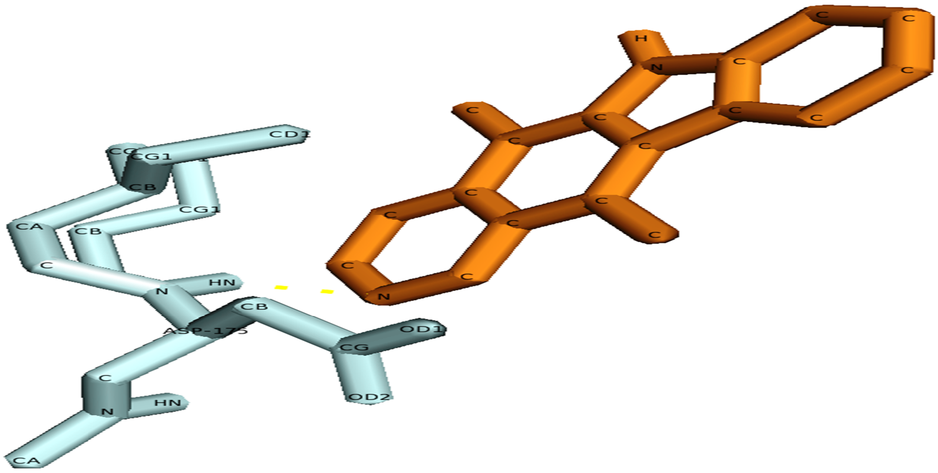
2-Amino-4-(2'-chloro-benzo[f]quinolin-2-ylmethylene)pyrimido[4,5-a]-carbazoles, 6c:

Yellow prisms, m.p.143-146 °C, yield: (70%); IR ν_{max} (cm^{-1}): 3407 (sym NH_2), 3244 (asym NH_2), 1597 (C=N);^{1}H NMR (δ, ppm, $CDCl_3$): 8.36 (b s, 1H, N_{11}-H), 7.31-9.05 (m, 13H, C_5-, C_6-, C_7-, C_8-, C_9-, C_{10}-, C_4'-, C_5'-, C_6'-, C_7', C_8', C_9', C_{10}' H), 5.22 (b s, 2H, NH_2); ^{13}C NMR (δ, ppm, $CDCl_3$): 177.3 (C_2), 155.3 (C_2'), 154.4 (C_4), 150.2 (C_{11b}), 147.2 (C_{3a}'), 135.4 (C_{10}'), 133.5 (C_{6a}), 132.6 (C_1'), 130.7 (C_8), 130.0 (C_5'), 128.4 (C_4'), 127.5 (C_6' & C_9'), 127.3 (C_{5b}'), 126.4 (C_{5a}'), 126.6 (C_5), 126.4 (C_{3b}'), 125.7 (C_7' & C_8'), 125.3 (C_{11b}), 124.4 (C_{10a}), 123.5 (C_6), 121.4 (C_7), 120.3 (C_9), 118.1 (C_{4a}), 110.3 (C_{10}), 103.4 (C_{6b}); MS: m/z (%) 445.90; Anal. Calcd. for: $C_{27}H_{16}ClN_5$: C, 72.73; H, 3.62; N, 15.71; Found: C, 72.70; H, 3.65; N, 15.73.

***in vitro* cytotoxicity evaluation by MTT assay**

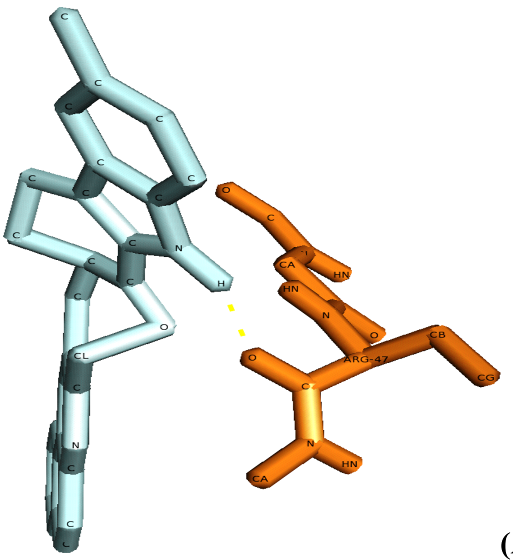
Cytotoxicity studies of the compounds along with ADR were carried out on human cervical cancer cells (HeLa), and breast cancer cells (MCF 7) which were obtained from National Centre for Cell Science, Pune, India. Cell viability was carried out using the MTT assay method. The HeLa and AGS cells were grown in Eagles minimum essential medium containing 10% fetal bovine serum (FBS). For the screening experiment, the cells were seeded into 96-well plates in 100 μL of the respective medium containing 10% FBS, at a plating density of 10000 cells/well, and incubated at 37 °C, under conditions of 5% CO_2, 95% air, and 100% relative humidity for 24h prior to the addition of compounds. The compounds were dissolved in DMSO and diluted in the respective medium containing 1% FBS. After 24 h, the medium was replaced with the respective medium with 1% FBS containing the compounds at various concentrations and incubated at 37°C under conditions of 5% CO_2, 95% air, and 100% relative humidity for 48 h. Triplication was maintained, and the medium not containing the compounds served as the control. After 48 h, 10μL of MTT (5 mg/mL) in phosphate buffered saline (PBS) was added to each well and incubated at 37 °C for 4 h. The medium with MTT was then flicked off, and the formed formazan crystals were dissolved in 100 μL of DMSO. The absorbance was then measured at 570 nm using a microplate reader. The percentage of cell inhibition was determined using the following formula, and a graph was plotted with the percentage of cell inhibition versus concentration. From this, the IC_{50} value was calculated: % inhibition = [mean OD of untreated cells (control)/mean OD of treated cells (control)] × 100. The results were expressed as the concentration at which there was 50% inhibition (IC_{50}).

FIGURES



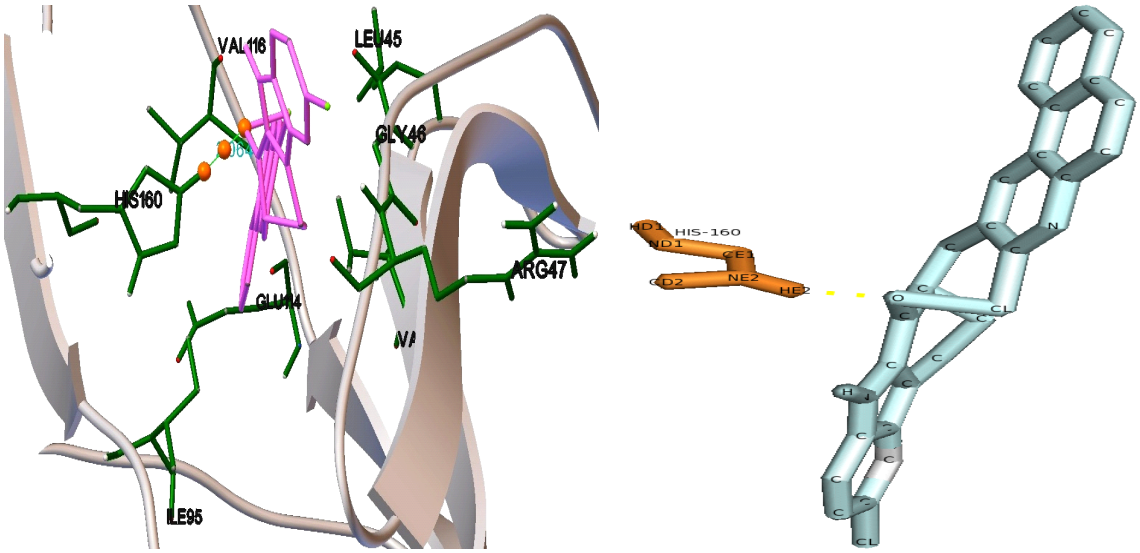
A

Figure S1. Human Protein Kinase CK2 docked with **ellipticine**. (A) The atomic interaction between HN atom of the ASP 175 (Orange color) and Nitrogen atom of Ellipticine (Palecyan color) ligand.



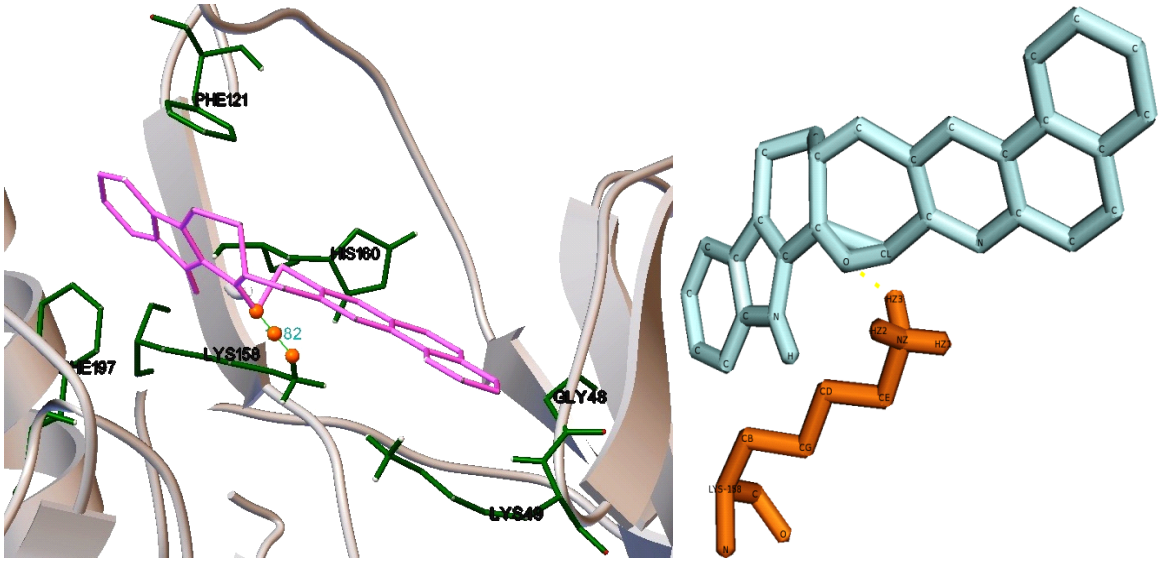
(A)

Figure S2. Human Protein Kinase CK2 docked with **3a**. (A) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Hydrogen atom of 1 (Palecyan color) ligand.



• **(B)**

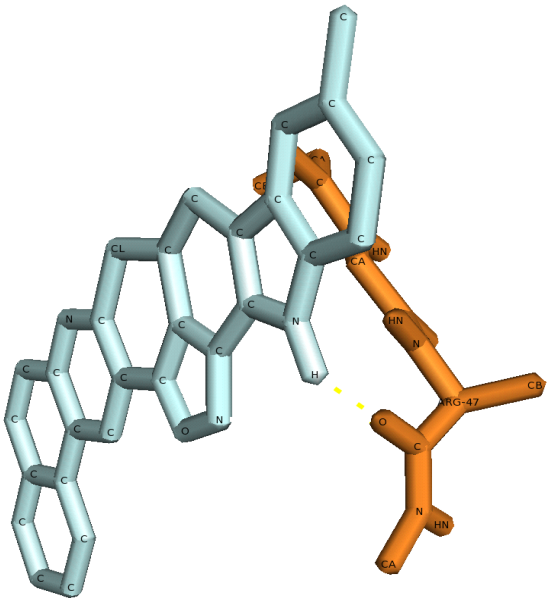
Figure S3. Human Protein Kinase CK2 docked with **3b** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic interaction between HE2 atom of the His 160 (Orange color) and oxygen atom of 5 (Palecyan color) ligand.



• **(B)**

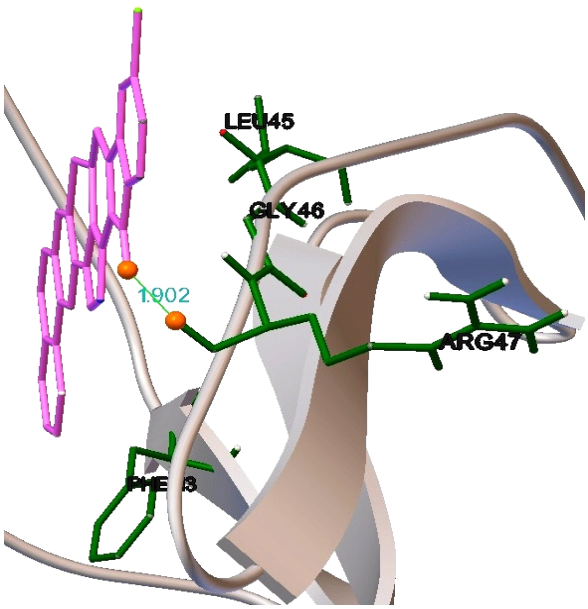
Figure S4. Human Protein Kinase CK2 docked with **3c** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic

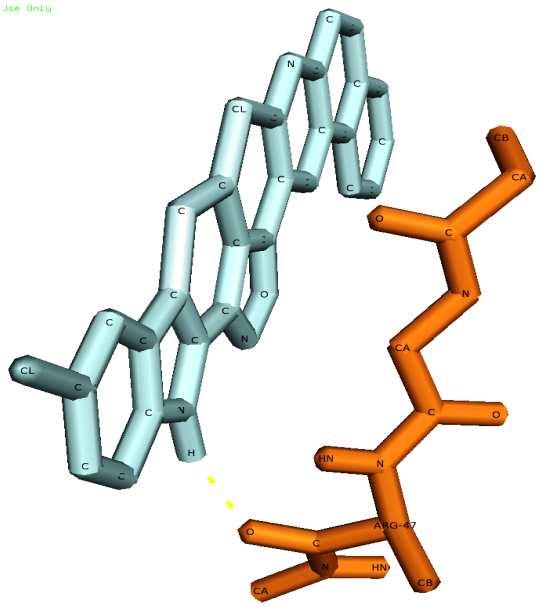
interaction between HZ3 atom of the Lys 158 (Orange color) and Oxygen atom of 9 (Palecyan color) ligand.



(B)

Figure S5 Human Protein Kinase CK2 docked with **4a**. (B) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Hydrogen atom of 4 (Palecyan color) ligand.

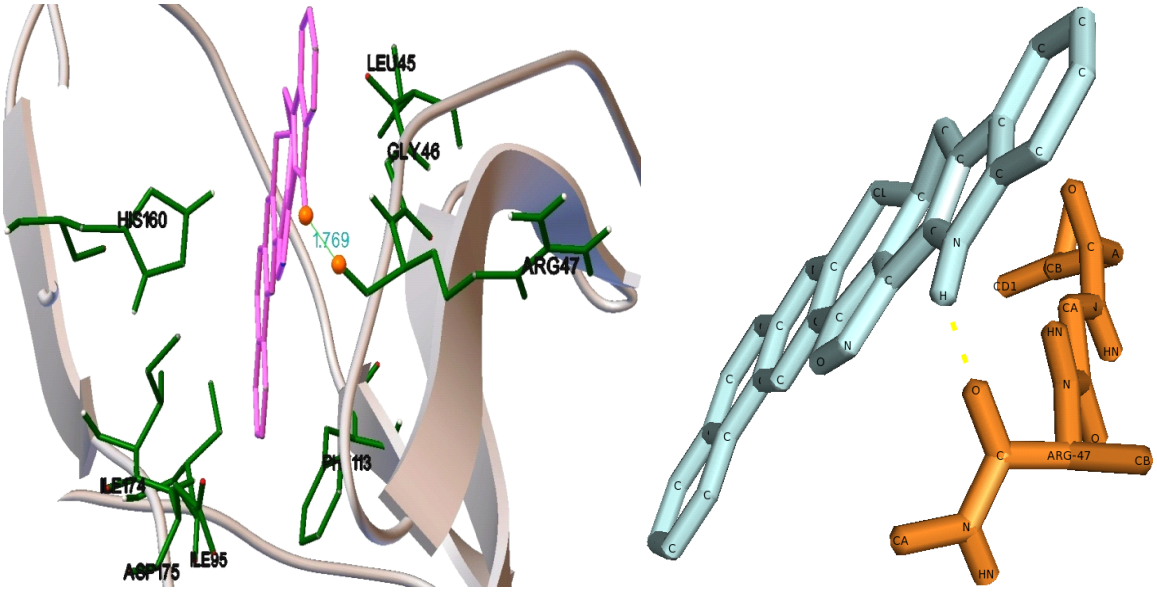




•

(B)

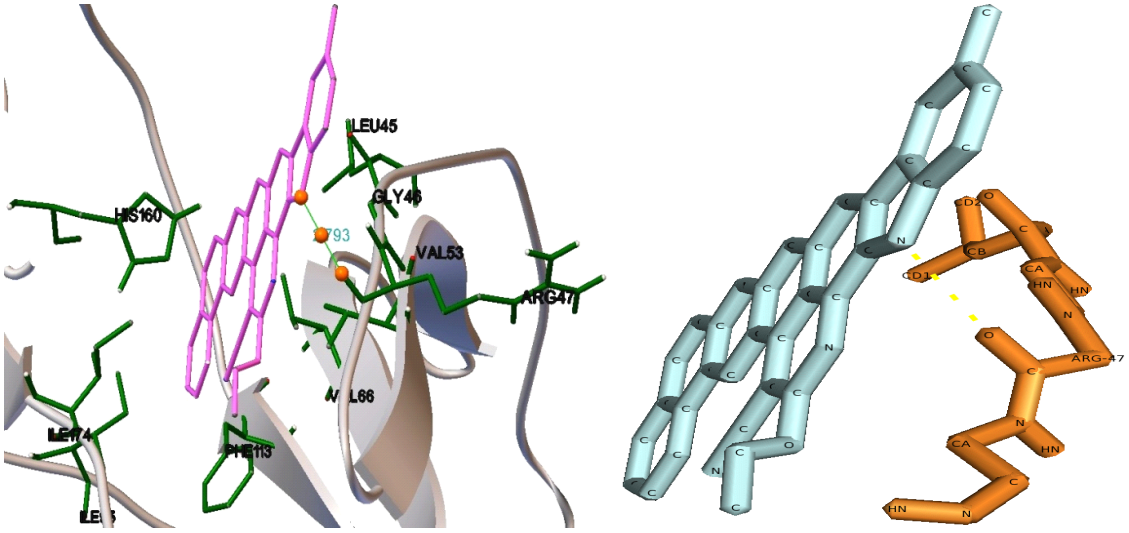
Figure S6. Human Protein Kinase CK2 docked with **4b** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Hydrogen atom of 8 (Palecyan color) ligand.



•

(B)

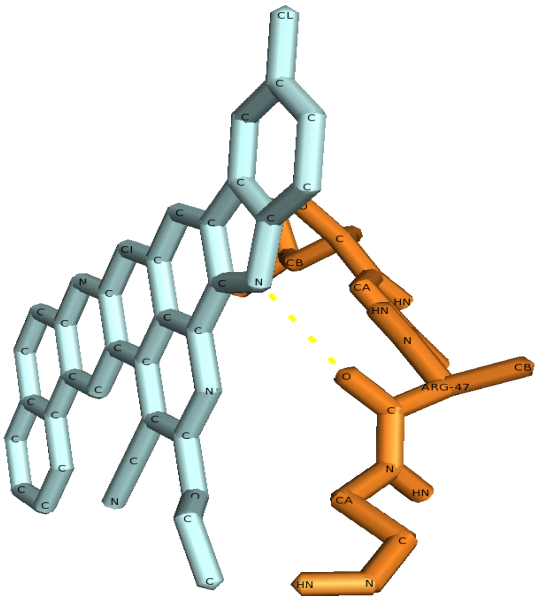
Figure S7. Human Protein Kinase CK2 docked with **4c** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Hydrogen atom of 12 (Palecyan color) ligand.



•

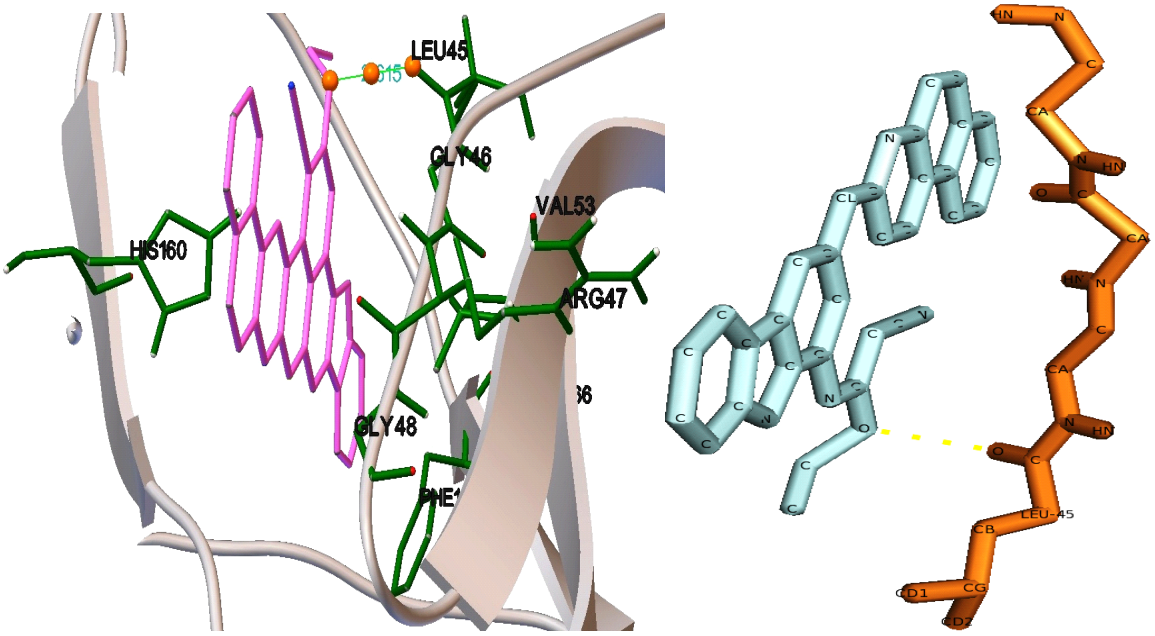
(B)

Figure S8 Human Protein Kinase CK2 docked with **5a** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Nitrogen atom of 2 (Palecyan color) ligand.



(A)

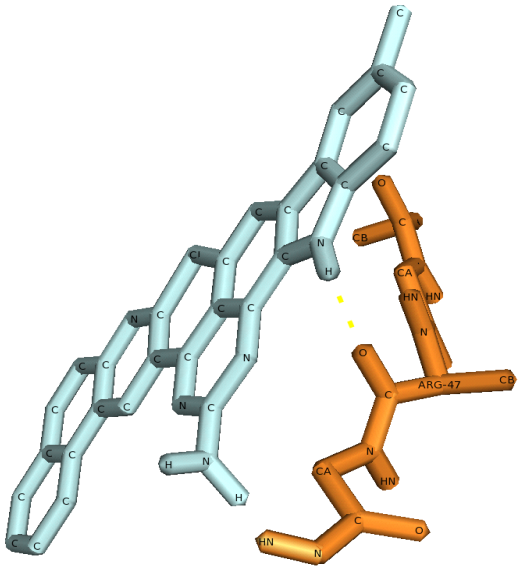
Figure S9. Human Protein Kinase CK2 docked with **5b** (A) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Nitrogen atom of 6 (Palecyan color) ligand.



•

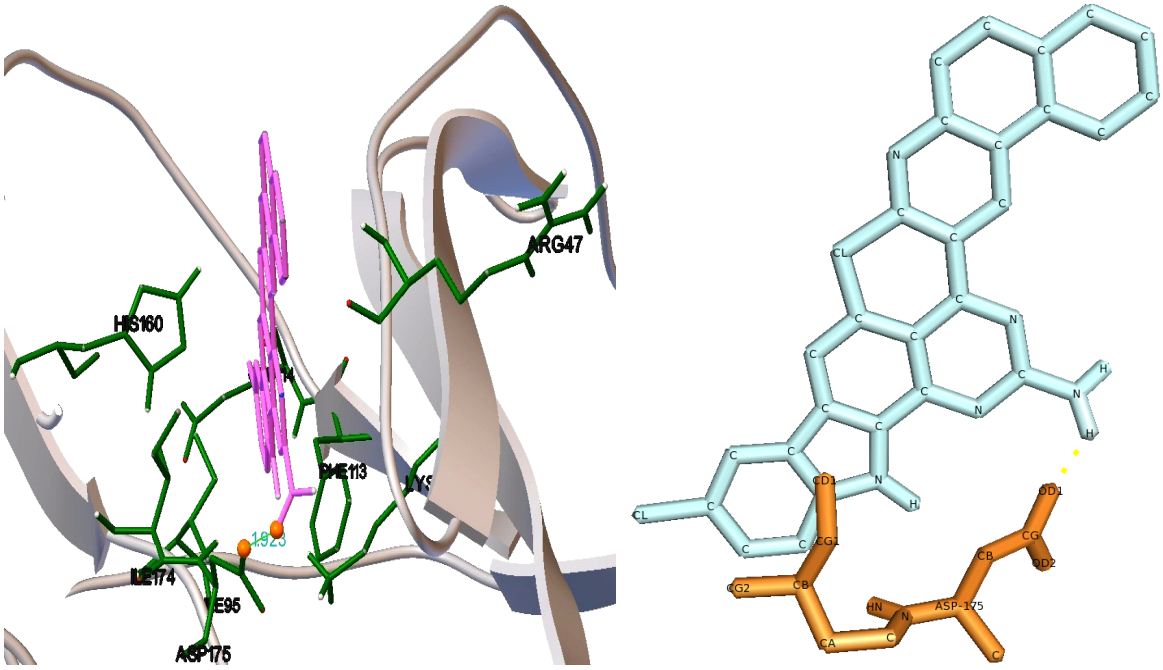
(B)

Figure S10. Human Protein Kinase CK2 docked with **5c** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic interaction between Oxygen atom of the Leu 45 (Orange color) and Oxygen atom of 10 (Palecyan color) ligand.



(A)

Figure S10 Human Protein Kinase CK2 docked with **6a** (A) The atomic interaction between Oxygen atom of the Arg 47 (Orange color) and Hydrogen atom of 3 (Palecyan color) ligand.



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(B)

Figure S11 Human Protein Kinase CK2 docked with **6b** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic

interaction between OD1 atom of the Asp 175 (Orange color) and Hydrogen atom of 7 (Palecyan color) ligand.

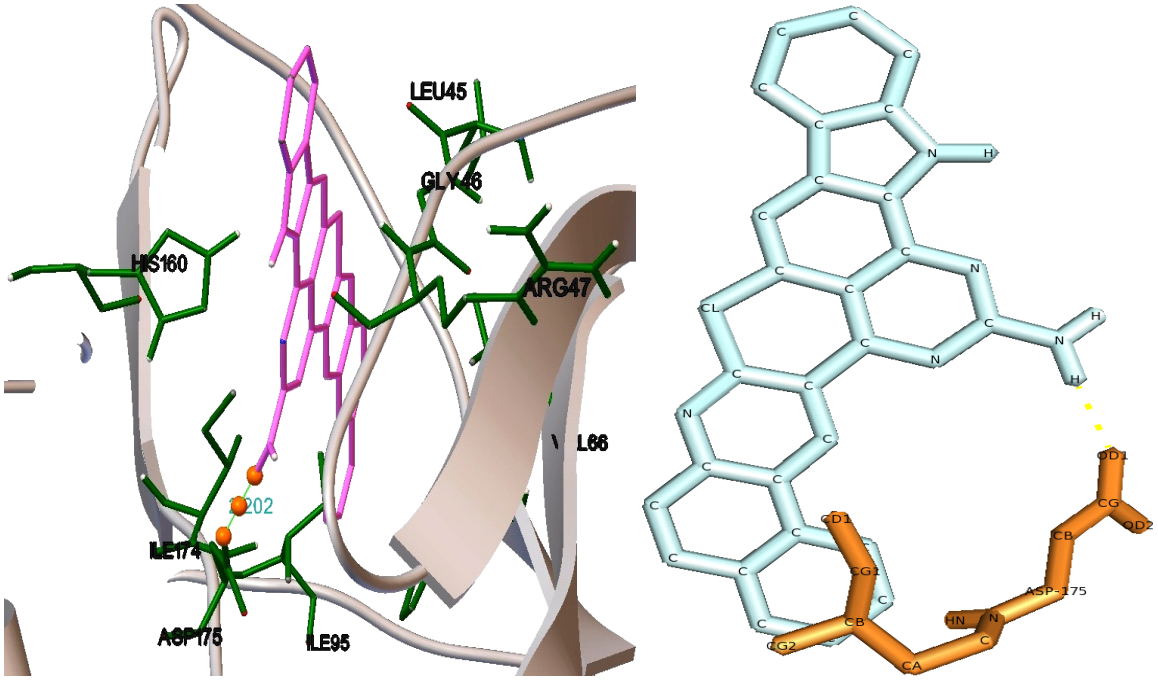

Figure S12 Human Protein Kinase CK2 docked with **6c** (A) The receptor interactions with ligand is represented by Gray, Green, Magenta and Orange colors respectively. (B) The atomic interaction between OD1 atom of the Asp 175 (Orange color) and Hydrogen atom of 11 (Palecyan color) ligand.