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Synthesis, quantum chemical computation, molecular docking analysis and biological activity of chlorophenyl thiazolyl naphthyl methanone as dendrodoine analogs

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A series of chlorophenyl thiazolyl naphthyl methanone derivatives have been synthesized and found to possess a wide spectrum of biological activities. Chlorophenyl thiazolyl naphthyl methanone has been synthesized and characterized by elemental analysis IR, ^{1}H and ^{13}C NMR and mass spectral data. Quantum chemical computation and vibrational spectral analysis of chlorophenyl thiazolyl naphthyl methanone have been carried out using DFT level B3LYP with 6-31G basis set. Electric dipole moment (μ) values have been computed by utilizing *ab initio* and DFT quantum mechanical calculations. The energy gap is an indicator of chemical reactivity, kinetic stability and polarizability. The novel compounds show very good antioxidant and anticancer activity. Docking studies have been performed for target molecules using the molecular docking software. The antioxidant activity of chlorophenylthiazolylnaphthylmethanone has been analyzed using the DPPH radical scavenging assay. Among the studied compounds, (4-chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl)methanone **2b** is highly active on the SKMEL cell line.

Keywords: IR, ^{1}H NMR, ^{13}C NMR, Mass spectra, Quantum chemical computation, Antioxidant, Anticancer

Heterocyclic chemistry is a branch of organic chemistry responsible for the synthesis, structure and application of heterocycles. Heterocyclic compounds are cyclic compounds with a ring containing carbon and other elements, including oxygen, nitrogen and sulfur[1]. Drugs containing thiazole are approved for clinical use, such as sulphathiazole, ravuconazole, ritonavir and meloxicam. It is important to note that thiazole can be used as a promising supplement for the development of anticancer agents[2]. The naphthalene ring is highly present in active natural products[3], contributing to the fight against inflammation[4], antibacterial[5], antioxidant[6] and antifungal properties[7] in molecules containing the naphthalene moiety. Naphthalene derivatives have attracted significant attention in the field of medical chemicals due to their widespread use in drug discovery[8]. It is an important component of many anticancer agents. Bioactive substances are gaining interest in phytomedicine, which includes their clinical use, suspension, quality control, mechanism of action and potential drug interactions. These have emerged as the most exciting advances in modern medicine[9].

An antioxidant is a molecule that inhibits the oxidation of other molecules. Since 1990s, antioxidant research has grown significantly due to its potential benefits in disease prevention and health promotion[10]. Cancer is the most frequent disease that affects humans worldwide. New medications are desperately needed to treat and prevent this life-threatening condition. The interest in science and research is drawing attention to naturally occurring computers as they are considered to have fewer toxic side effects compared to current treatments such as chemotherapy[11]. The aim of this research was to generate unique compounds by connecting the thiazole and naphthalene rings together. To learn more about their structure and type of bonds, spectroscopy is used and combined with standard DFT calculations.

Experimental Section

All start up items and reagents are purchased from commercial suppliers. FT-IR experimental spectra (400-4000 cm^{-1}) of chlorophenylthiazolylnaphthyl-methanone discharge are recorded. Nuclear magnetic resonance spectra (^{1}H and ^{13}C NMR) and Mass spectra were recorded on the Bruker spectrometer (400 MHz) with TMS as an external reference and reported in parts per million. All characteristic studies

have been conducted by the CSIR-Central Drug Research Institute, Lucknow, India.

Synthesis of target compound

The reaction between 4-chlorobenzoyl thiourea (20 mmol) using a different method of closing the ring of methylene-carbonyl condensation and (2-bromoacetyl)naphthalene (20 mmol) is mixed and ignited with ethyl alcohol. After the reaction is complete, the mixture is left to cool. When the mixture reached 20°C it was poured into cold water (50 mL) and added to water and $NaHCO_3$. Targeted compound reconstruction are done using ethyl alcohol[12].

(4-Chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone, 2a: Yellow solid. Yield 78%. Anal. Found: C, 67.23; H, 4.35; Cl, 9.00; N, 7.11. Calcd for $C_{22}H_{17}ClN_2OS$ (392.90): C, 67.25; H, 4.36; Cl, 9.02; N, 7.13%. IR (KBr): 3867, 3453, 2923, 2851, 1689, 1625, 1592, 1568, 1390, 1275, 1182, 1122, 1088, 1012, 942, 893, 854, 810, 748, 680, 530, 474 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 4.21(6H, s, $N(CH_3)_3$), 7.60-7.79 (4H, m, ArH), 7.99-8.06 (4H, m, naphth H), 8.07-8.21(2H, m, naphth H), 8.71(1H, s, naphth H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 14.15(N-CH_3), 20.34, 39.05, 49.75, 76.81, 77.23, 77.43, 77.65, 110.43, 116.59, 118.62, 119.87, 121.16, 123.58, 124.78, 128.51, 129.78, 131.53, 139.09, 140.32, 144.31, 153.15; ESI-MS: *m/z* 393 (MH^+).

(4-Chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl)methanone, 2b: Yellow solid. Yield 69%. Anal. Found: C, 68.47; H, 5.02; Cl, 8.41; N, 6.63. Calcd for $C_{24}H_{21}ClN_2OS$ (420.96): C, 68.48; H, 5.03; Cl, 8.42; N, 6.65%. IR (KBr): 3725, 3417, 2925, 2851, 2383, 2331, 1688, 1624, 1594, 1548, 1454, 1396, 1332, 1286, 1176, 1123, 1080, 1011, 945, 892, 854, 810, 730, 683, 568, 513, 473 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 1.17-1.32(6H, m, $(CH_3)_3$), 3.52-3.59(4H, q, $N(CH_2)_2$), 6.98 (1H, d, ArH), 7.00(1H, d, ArH), 7.29-7.31(1H, d, ArH), 7.31-7.32(1H, d, ArH), 7.60-7.94 (4H, m, naphth H), 7.95-8.04(2H, m, naphth H), 8.71 (1H, s, naphth H).

(4-Chlorophenyl-2-pyrrolidin-1-ylthiazol-5-yl-2-naphthyl)methanone, 2c: Yellow solid. Yield 72%. Anal. Found: C, 68.80; H, 4.55; Cl, 8.46; N, 6.68. Calcd for $C_{24}H_{19}ClN_2OS$ (418.94): C, 68.81; H, 4.57; Cl, 8.46; N, 6.69%. IR (KBr): 3420, 3056, 2920, 2850, 2317, 1927, 1667, 1626, 1595, 1549, 1489, 1466, 1393, 1353, 1295, 1248, 1176, 1122, 1090, 1014, 942, 895, 851, 818, 747, 590, 474 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 3.43-3.69(8H, m, Pyrrolidine), 7.59-7.79(4H, m, ArH), 7.82-7.84(4H, m, naphth H), 7.91-8.15(2H, m, naphth H), 8.70(1H, s, naphth H).

(4-Chlorophenyl-2-piperidin-1-ylthiazol-5-yl-2-naphthyl)methanone, 2d: Yellow solid. Yield 65%. Anal. Found: C, 69.34; H, 4.87; Cl, 8.19; N, 6.46. Calcd for $C_{25}H_{21}ClN_2OS$ (432.97): C, 69.35; H, 4.89; Cl, 8.19; N, 6.47%. IR (KBr): 3056, 2360, 1694, 1627, 1596, 1550, 1463, 1444, 1398, 1353, 1294, 1185, 1123, 1087, 1013, 950, 889, 861, 823, 750, 683, 585, 475 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 1.47-1.62(6H, s, $(CH_2)_3$), 3.59-3.65(4H, q, $N(CH_2)_2$), 6.99(1H, d, ArH), 7.01(1H, d, ArH), 7.29-7.30(1H, d, ArH), 7.31-7.32(1H, d, ArH), 7.60-8.06(4H, m, naphth H), 8.08-8.14(2H, m, naphth H), 8.70(1H, s, naphth H).

(4-Chlorophenyl-2-morpholin-1-ylthiazol-5-yl-2-naphthyl)methanone, 2e: Yellow solid. Yield 76%. Anal. Found: C, 66.26; H, 4.39; Cl, 8.15; N, 6.43. Calcd for $C_{24}H_{19}ClN_2O_2S$ (434.94): C, 66.28; H, 4.40; Cl, 8.15; N, 6.44%. IR (KBr): 3436, 2987, 2885, 2360, 1693, 1624, 1592, 1468, 1435, 1386, 1360, 1268, 1175, 1126, 1028, 960, 896, 854, 811, 741, 677, 568, 475 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 3.58(8H, s, Morpholine), 7.63-7.67(4H, m, ArH), 7.95-8.01(4H, m, naphth H), 8.03-8.10(2H, m, naphth H), 8.76 (1H, s, naphth H).

Computational details

A quantum mechanical modelling method for investigating the electronic structure of molecules is Density Functional Theory (DFT) and the determination of the properties of a many-electron system using this method is based on electron density. The force constant matrix of Cartesian co-ordinates is transformed to force field internal co-ordinates in the B3LYP/6-31G level of calculations[13]. Based on experimental comparisons and very high levels of electronic structure theory, it has been demonstrated that B3LYP (Becke-3Lee-Yang-Parr) performance is extremely strong in predicting geometry in this region for organic electrocyclic processes.

For *ab initio* computations of the structure of atoms, molecules, crystals, surfaces and their interactions, DFT is one of the most used techniques. It may be employed for atoms, molecules, solids as well as nuclei. Gaussian 09 takes the input as .gif

produced by Gauss view and runs the analyzer to produce a typical solution to the problem. Output is produced as a text file (.out) and a checkpoint file (.chk). The checkpoint file may be processed by a computer to produce further detailed information.

An additional feature of Gaussian works, which is utilized to represent the motion of atoms individually, is one that is not optimal[14]. The Linear Combination of Atomic Orbital method (LCAO) is the main basis of these quantum chemical calculations and is routinely used as variables in linear regression procedures. The HOMO-LUMO energy gap and other relevant functional characteristics (chemical strength, electronegativity, electrophilicity, hardness, and softness) were also obtained using DFT at the same time as a low molecular set[15].

Results and Discussion

Molecular Geometry

The geometrical parameters that assist to determine the position of the atom are distance between the nuclei, angles of three connected atoms and angle of three consecutive bonds. The Gaussian 09 package is used to obtain the molecular structure using an atom numbering scheme. Minimum energy obtained by DFT structure optimization using 6-31G basis sets for the synthesized compounds are as -1881.8 amu, -1960.0 amu, -1958.8 amu, -1997.9 and -2043.9 amu, respectively. The optimized compound's structural properties (bond length, bond angle, and dihedral angle) were also determined and summarized. The C-S bond length is greater than C-N, C=O and C-H because when the size of the atom increases, bond length also increases. For computational chemistry, we need to be more precise by using Cartesian coordinates, bond lengths, and bond angles to find the optimal molecular geometry (Fig. 1 and Table 1).

Molecular orbital (HOMO and LUMO) of chlorophenyl thiazolyl naphthyl methanone

The electronic properties of isolated molecules are associated with their geometry and the electronic

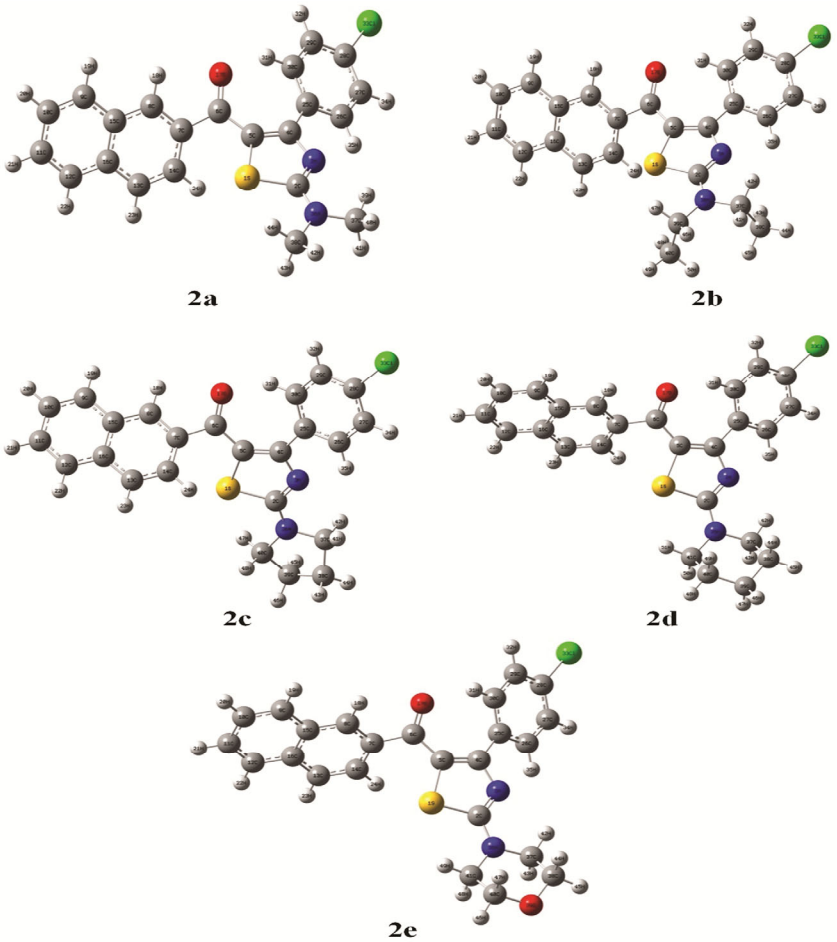

Fig. 1 — Optimized structure of chlorophenylthiazolylnaphthylmethanone

Table 1 — Bond length (in Å) of chlorophenylthiazolylnaphthylmethanone

Position	Parameter	2a	2b	2c	2d	2e
Thiazole	C-S	1.835	1.837	1.832	1.838	1.828
Thiazole	C=N	1.310	1.311	1.312	1.311	1.315
Thiazole	C-N	1.389	1.390	1.389	1.388	1.392
Naphthalene	C-C	1.423	1.415	1.415	1.415	1.418
Naphthalene	C-H	1.084	1.083	1.083	1.083	1.085
Phenyl	C-C	1.410	1.411	1.411	1.410	1.413
Phenyl	C-H	1.081	1.081	1.081	1.081	1.083
Phenyl	C-Cl	1.834	1.834	1.834	1.834	1.828
Chain	C=O	1.083	1.254	1.254	1.254	1.261
Chain	N-C	1.477	1.488	1.490	1.485	1.479
Chain	C-H	1.093	1.095	1.092	1.096	1.099
Chain	C-C	-	1.540	1.546	1.541	1.528
Chain	C-O	-	-	-	-	1.457

Table 2 — Calculated electronic parameters

Parameters	2a	2b	2c	2d	2e
Total Energy (a.u)	-1881.85	-1960.06	-1958.86	-1997.96	-2043.96
Dipole Moment (Debye)	8.0066	8.0293	8.6854	8.2922	6.4855
HOMO	-0.2418	-0.2417	-0.2405	-0.2408	-0.2397
LUMO	-0.0353	-0.0346	-0.0318	-0.0338	-0.0371
HOMO-LUMO (ΔE)	0.2065	0.2071	0.2087	0.2070	0.2026
Ionisation potential (I)	0.2418	0.2417	0.2405	0.2408	0.2397
Electron affinity (A)	0.0353	0.0346	0.0318	0.0338	0.0371
Electronegativity (χ)	0.1385	0.1381	0.1361	0.1373	0.1384
Hardness (Ƞ)	0.1032	0.1035	0.1043	0.1035	0.1013
Softness (S)	4.8449	4.8309	4.7938	4.8309	4.9358

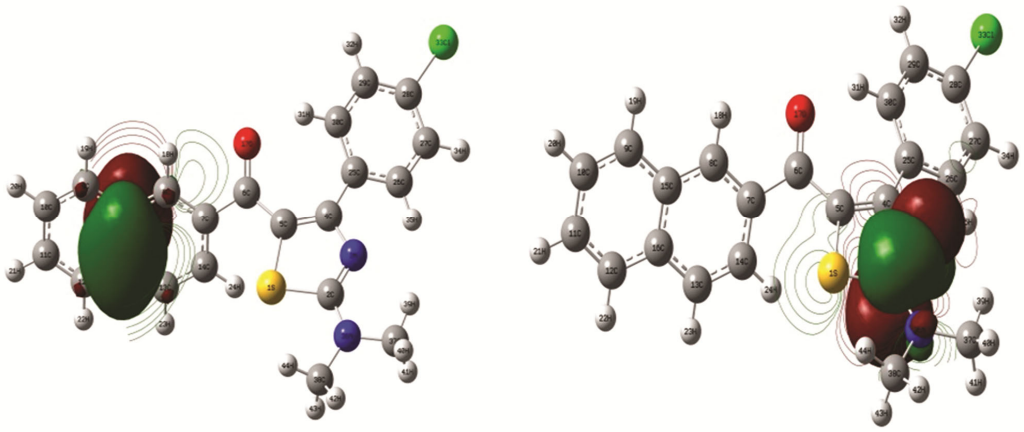

Fig. 2 — HOMO and LUMO of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone **2a**

parameters are summarized in Table 2. It also gives knowledge about the macroscopic characteristics of a molecular system in its condensed phase. The HOMO is nucleophilic or electron donating and the LUMO is electrophilic or electron accepting. The energy gap between HOMO and LUMO of a neutral system, *i.e.*, the difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), is related to polarizability, chemical reactivity and kinetic stability.

In chlorophenyl thiazolyl naphthyl methanone, HOMO orbitals are located mainly on the naphthalene ring, while LUMO orbitals are placed on the thiazole ring. The diagrammatic representations of HOMO-LUMO of (4-chlorophenyl-2- dimethylaminothiazol-5-yl-2-naphthyl)methanone are shown in Fig. 2 and the relative energy of the molecular orbitals has been calculated.

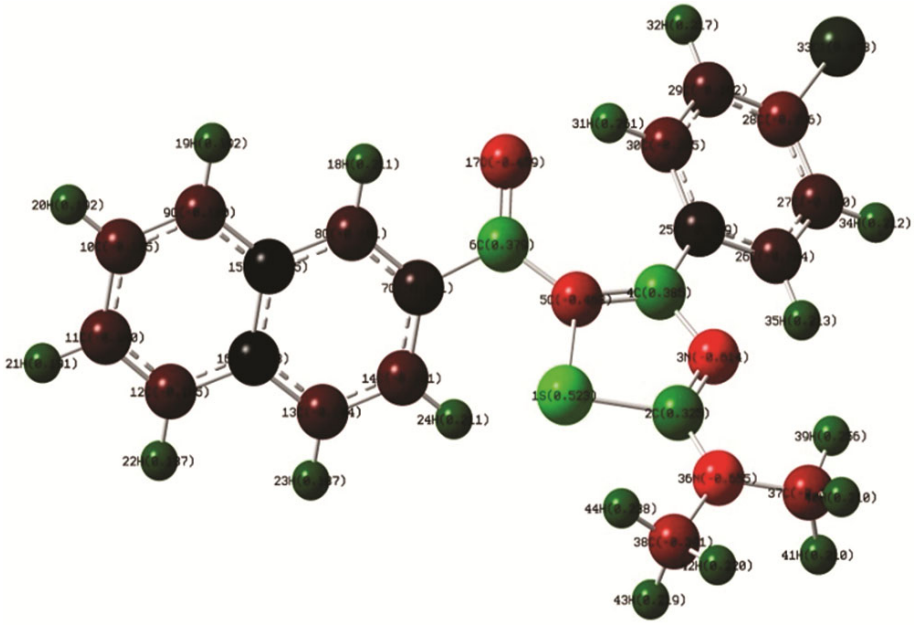

Fig. 3 — Mulliken atomic charge of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone **2a**

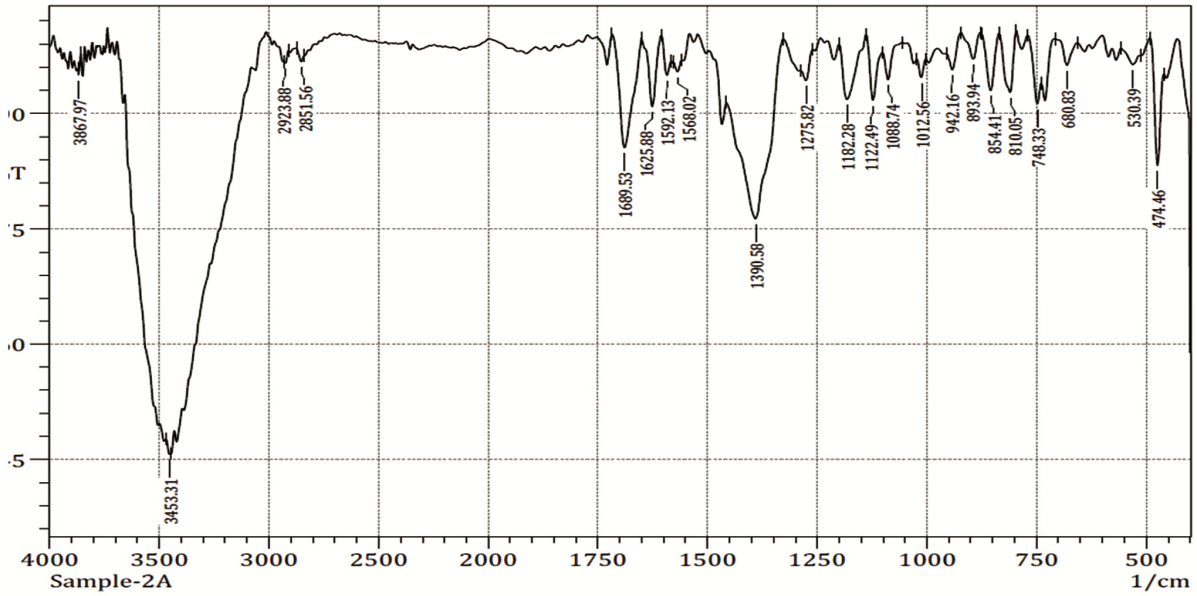

Fig. 4 — FT-IR spectra of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone **2a**

Mulliken Atomic Charges

Mulliken atomic charge values possess an important role in the implementation of quantum chemical calculation since atomic charges affect the dipole moment, electronic structure, molecular polarizability and many other properties of molecular systems. The Mulliken atomic charges of all hydrogens are positive; oxygen and nitrogen atoms contain negative charge and sulphur atom possess a positive charge. The charge distribution structures of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone (2a) are shown in Fig. 3.

Spectral Analysis

The FT-IR spectra of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone (2a) is shown in Fig. 4. Proton nuclear magnetic resonance (proton NMR, hydrogen -1 NMR or

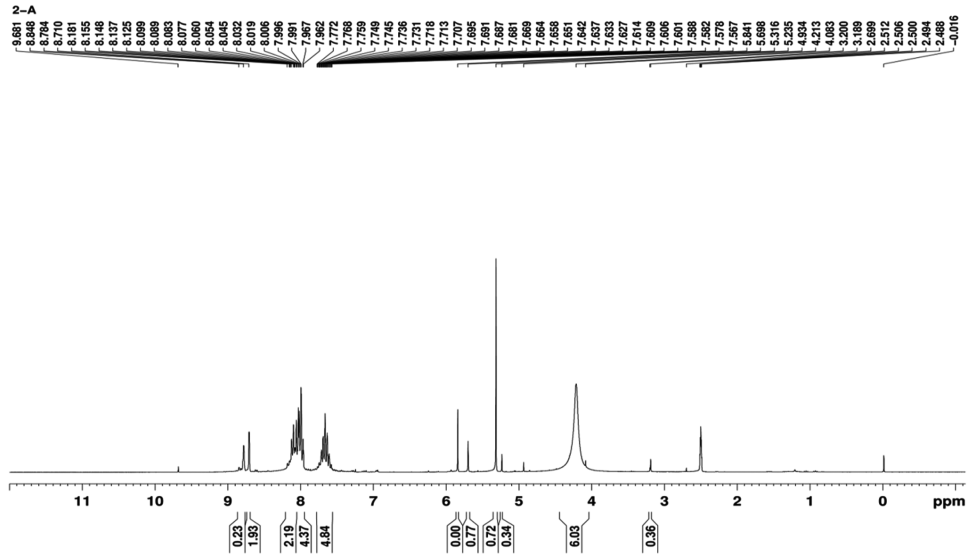

Fig. 5 — ^{1}H NMR spectrum of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone **2a**

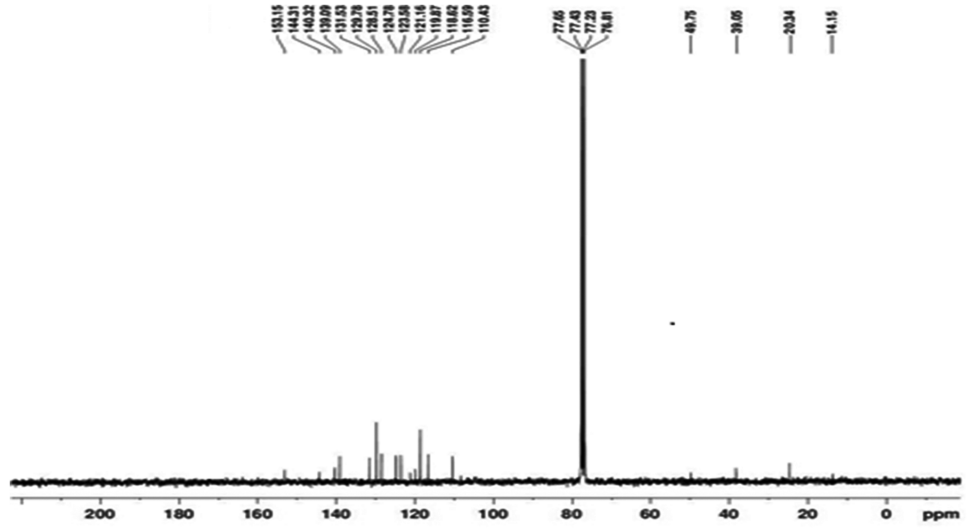

Fig. 6 — ^{13}C NMR spectra of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone **2a**

^{1}H NMR) is the use of nuclear magnetic resonance in NMR spectroscopy in relation to hydrogen-1 nuclei within an object molecule, in order to determine the composition of its molecules[16]. ^{1}H NMR is a method that helps to identify or confirm the formation of organic or proton-containing compounds. Electron-linked electronegative groups reduce the density of electrons around the proton, leading to a reduction in protection for chemical reactions. ^{1}H NMR spectrum of the types of functional group of amine active groups δ 1-5 ppm, alkene 4.5-7.5 ppm, aromatic proton 6-9 ppm, *etc*.

The ^{1}H NMR compound (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone (2a) showed singlet δ 4.21 ppm representing CH proton for dimethyl amine. The 4-chlorophenyl protons appear as a multiplet of four protons at δ 7.60-7.79 ppm. The remaining seven aromatic signals were assigned to the nucleus of naphthalene in the compound δ 7.99-8.71 ppm (Fig. 5).

The ^{13}C NMR spectrum gives twenty two peaks corresponding to the twenty two carbon atoms. From the above evidences, the compound was formulated as (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone (2a) (Fig. 6). The ESI Mass Spectrum exhibits a MH^{+} peak at 392, which confirms the molecular mass of the compound to be 393 which is in accordance with the elemental analysis data (Fig. 7).

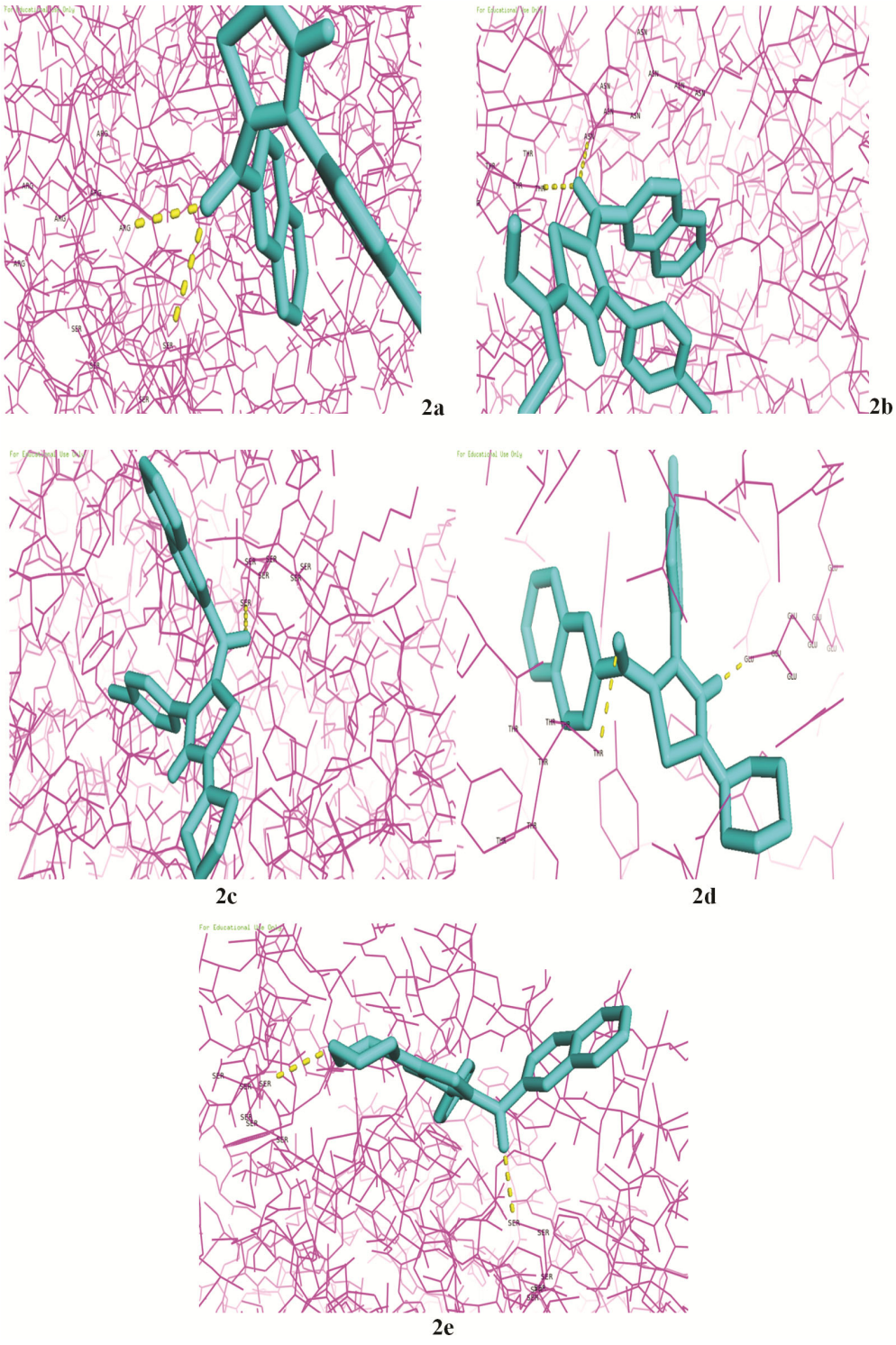

Fig. 7 — Mass spectra of (4-chlorophenyl-2-dimethylaminothiazol-5-yl-2-naphthyl)methanone **2a**

Molecular Docking

The protein ligand docking aims at predicting the predominant binding mode of a ligand with a protein of known three-dimensional structure. We get a ligand-protein complex with optimized conformation, possessing less binding free energy. The predicted binding energy is revealed in terms of hydrogen bonding and hydrophobic interaction between

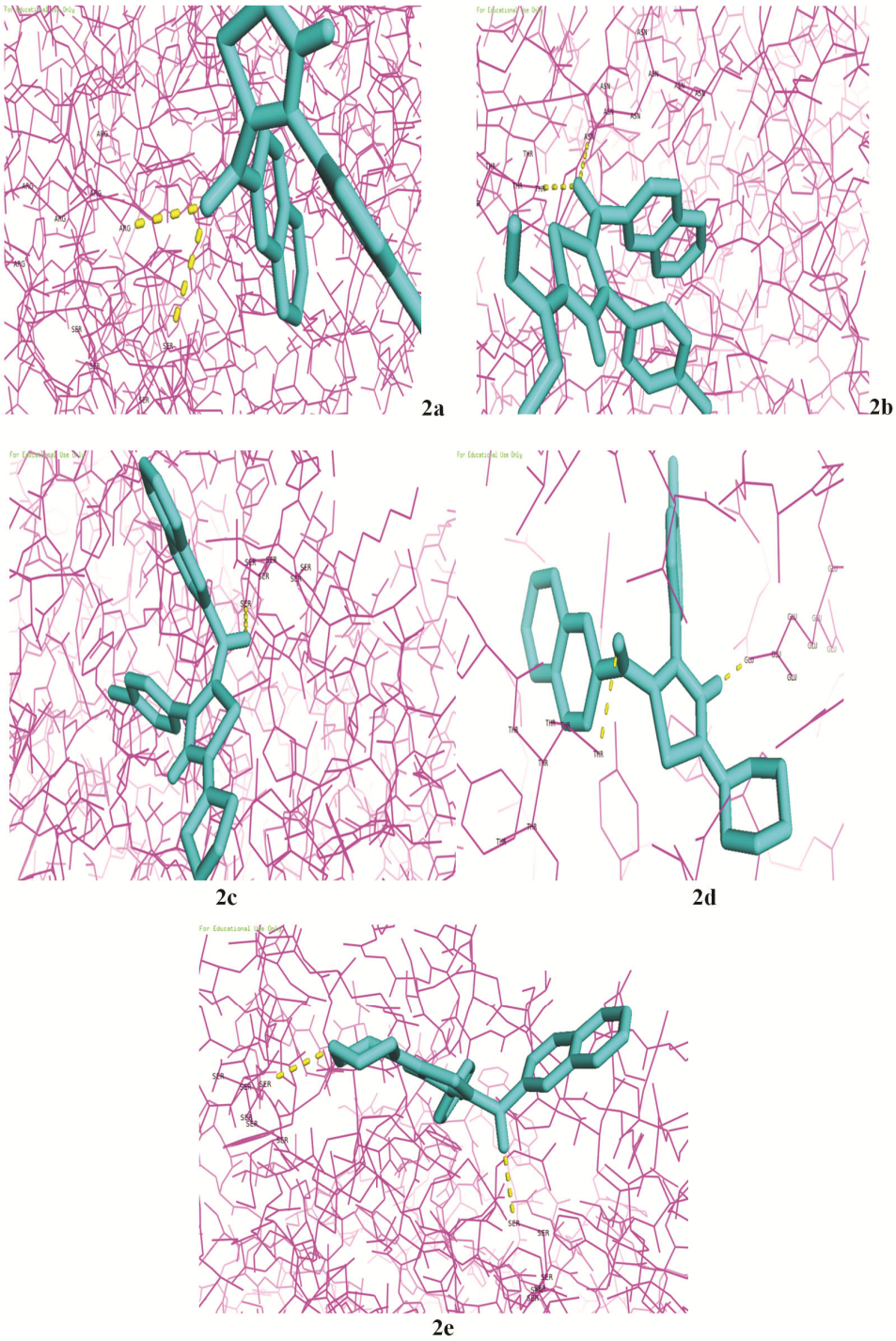

Fig. 8 — Docking image of chlorophenylthiazolylnaphthylmethanone

thiazoles and DNA. The target protein in required format was obtained from Protein Data Bank (PDB). The ligand was made in the PDB format using Openbabel GUI (C) 2006. Proper organization of the ligand in the particular groove of the target DNA is provided by PyRx-Python prescription 0.8.

Molecular docking studies were performed to determine the binding effect of ligand and the active naphthalene-1,2-dioxygenase containing naphthalene and the interactions from docking are shown in Fig. 8. From Protein Data Bank (PDB ID: 107G), 3D crystalline formations of naphthalene-1,2-dioxygenase-

containing naphthalene. The more the negative value of the energy of binding, the better is affinity of the molecule[17]. At physiological *p*H, hydrogen atoms were added to the structure, allowing for proper ionization.

In addition, the protein structure was created by removing repetitive chains, water molecules, and any surfactants, adding hydrogens to the receptor's atom, and calculating partial charges. Other derivatives of chlorophenylthiazolylnaphthylmethanone with the highest dosage value (Table 3) have shown a better molecular binding affinity. 2d is the highest amount of docking against both proteins (-8.1 kcal/mol). Computed dock complex compound 2a is in the active binding mode ARG-577 and SER-575.

Lipinski's rule of five

Drug likeness is a complex balance of structural features and a molecular property which determines whether the molecule has pharmacological activity which is similar to drugs. The Lipinski rule of five explains the molecular characteristics of a drug's pharmacokinetics in the human body, including its absorption, distribution, metabolism, and excretion (ADME). The drug likeliness data and Lipinski's rule of five are given in Table 4. It was found that chlorophenylthiazolylnaphthylmethanone obeyed the Lipinski rule of five and hence these compounds are docked into the active site of naphthalene-1,2-dioxygenase-containing naphthalene (PDB code: 107G).

Antioxidant Studies

The newly synthesized compound was tested for its antioxidant capacity, a DPPH test for ascorbic acid was used as a reference level. A 60 µM solution of DPPH in methanol was prepared and 200µL of this solution was combined with a 50µL test sample. Ascorbic acid (standard) solutions for different concentrations (1.56, 3.12, 6.25, 12.5, 25, 50, 100, 200, 400, 800 µg/mL) were adjusted. Control absorption and test solutions were recorded at 515 nm. By following the same procedure the absorption will be measured with ascorbic acid solutions. From the absorption values, the inhibition percentage was set by different concentrations of different samples and ascorbic acid. The reduction percentage and IC_{50} value are calculated (Table 5). The IC_{50} value indicates that the compound with low IC_{50} has strong antioxidant properties. A typical ascorbic acid shows an IC_{50} value of 90 µM.

$$\text{Percentage of inhibition} = \frac{\text{Aborbance of Control - Absorbance of test}}{\text{Absorbance of Control}} \times 100$$

The Table 5 and Fig. 9 shows that the compound (4-chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl) methanone **2b**, has a value of IC_{50} µM and has excellent antioxidant activity. The order of the highest activity of chlorophenylthiazolylnaphthyl-methanone is 167 > 136 > 130 > 80 > 69.

Anticancer Studies

SKMEL (2500 cells/well) were seeded on ninety six well plates and allowed to acclimatize to the subculture situations consisting of 37°C and 5% CO_2 surroundings inside the incubator for 24 h. The test samples were prepared in DMEM media (100 mg/mL) and sterilized with the usage of 0.2 µm

Table 3 — Docking Score and hydrogen bonding interactions of chlorophenylthiazolylnaphthylmethanone

Compound	Docking Score (kcal/mol)	Residue involved in Hydrogen bonding
2a	-7.4	ARG-577, SER-575
2b	-7.5	ASN-365, THR-212
2c	-7.8	SER-425
2d	-8.1	GLU-570, THR-43
2e	-7.7	SER-425, SER-437

Table 5 — Antioxidant activities of chlorophenylthiazolylnaphthylmethanone

Compound	IC_{50} (µM)
2a	80
2b	69
2c	136
2d	167
2e	130
Ascorbic acid (Std)	90

Table 4 — Lipinski rule of chlorophenylthiazolylnaphthylmethanone

Compound	Molecular Weight <500 Dalton	HB Donar <5	HB Acceptor <10	Log P <5	Molecular Refractivity 40-130
2a	392	1	3	3.39	113.45
2b	420	1	3	3.71	119.90
2c	418	1	3	3.51	117.79
2d	432	1	3	4.79	122.41
2e	434	1	4	4.72	119.38

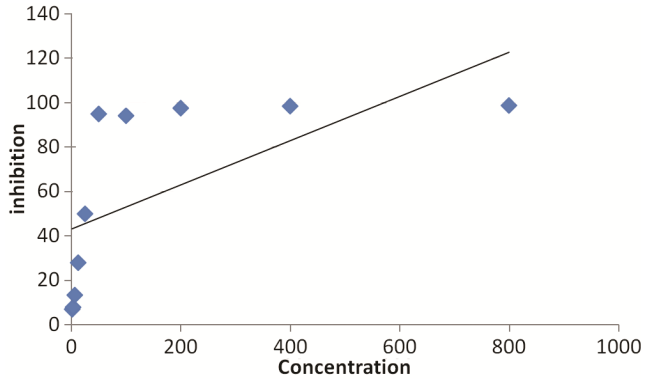

Fig. 9 — Plot of % inhibition *vs* concentration of (4-chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl)methanone **2b**

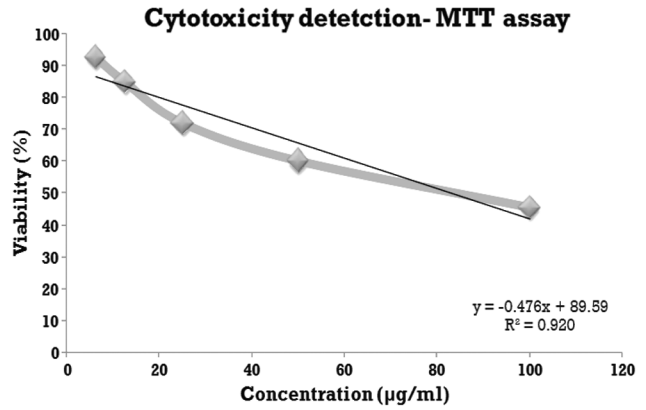

Fig. 10 — Plot of % viability *vs* concentration of (4-chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl)methanone **2b**

millipore syringe filter out. The samples have been in addition, diluted in DMEM media and introduced to the wells containing cultured cells at very low concentrations of 6.25, 12.5, 25, 50, 100 µg/mL respectively. Untreated wells had been kept as control. All the experiments were achieved in triplicate and average values were taken so as to limit mistakes. The plates had been similarly incubated for 24 h. After the incubation period, the media from the sources were desecrated and discarded. 100 µL of 0.5 mg/mL MTT answer in PBS became introduced to the wells. The plates have been similarly incubated for 2 h for the development of formazan crystals. The supernatant was then eliminated and 100 µL DMSO (100%) was introduced. The absorbance at 570 nm was measured with the micro plate reader. Two wells, according to the plate without cells served as blank. All experiments were achieved in triplicates. The mobile viability turned into expressing the use of the following components:

Table 6 — Anticancer activity of (4-chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl)methanone (2b)

Sample Concentration (µg/mL)	Percentage Viability
6.25	92.73
12.5	85.06
25	72.10
50	60.23
100	45.59
IC_{50}	84.17

$$Percentage of cell\ viability = \frac{Average\ absorbance\ of\ treated}{Average\ absorbance\ of control} \times 100$$

The anticancer activities of the studied compound thus obtained are given in Table 6 and illustrated in Fig. 10.

Conclusion

The newly compiled novel compounds were developed on the basis of basic analysis, IR, ^{1}H and ^{13}C NMR, Mass and tested for antioxidant and anticancer activity. With the ultimate goal of testing and planning rapid, accurate density functional theory (DFT) for chlorophenyl thiazolyl naphthyl methanone compound was completed using the Gaussian 09 program with the B3LYP method. The 6-31G basis set is successfully used to determine advanced geometry, binding features, vibration wave numbers, NBO analysis and Mulliken population research on low-level nuclear charges. All the compounds are screened for better docking scores. The molecular docking result indicates that chlorophenyl thiazolyl naphthyl methanone derivative may possess inhibitory activity on 107G. It can be concluded that the new compound (4-chlorophenyl-2-diethylaminothiazol-5-yl-2-naphthyl)methanone (2b) has excellent antioxidant activity and anticancer activity against the SKMEL cell line.

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