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# MOLECULAR DOCKING SIMULATION ON ISATIN- A MAGICAL MOLECULE

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**Keywords:**

Isatin, Covid-19, Molecular docking, Isatin derivatives, Anticancer

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**ABSTRACT:** Isatin is magical molecule widely used in drug discovery of many areas like anticancer, anti-inflammatory, antiviral, anti-convulsant, anti-tubercular, antimicrobial, antidiabetic most important it was found effective in COVID-19 as well as on Lumpy Skin Diseases. Isatin can be synthesized by different methods like Sandmeyer method, Gassman synthesis. Isatin was modified by researchers at C2, C3, C5, position and contribute its magic into the medicinal field. In this research article, main focus has been done on design and docking of various derivatives possessing promising biological activity, novel drug design strategies and their respective drug target. It will provides different approaches to design new drug entity along with docking studies to the young researcher to dig new aspect of molecule.

**INTRODUCTION:** Isatin (1H-indole-2,3-dione), an indole derivative of plant origin, add a value in a place of chemistry of nitrogen heterocyclic compounds [1]. This versatile scaffold has appreciable therapeutic value like antiallergic, antimalarial, antiviral and antimicrobial [2, 3] antitumor, antifungal, antiparasitic, antioxidant, anti-inflammatory [3], anticonvulsant, anthelmintic, anti-HIV, CNS depressant, analgesic [4]. Due to their wide range of therapeutic activity, Isatin and its derivative continuously studied by researchers for the development of the new useful drugs. Structure of Isatin had fused six-member benzene ring had aromatic character and five-member ring had anti-aromatic character, containing nitrogen [5]. Isatin was first isolated as an oxidative product of indigo by using nitric acid and chromic acid further re-crystallized from water, alcohol, acetic acid in orange colour monoclinic prism crystal having melting point 200 ºC. Isatin is metabolite of adrenaline hormone in human being, and it also found in plant as methoxy phenylpentyl Isatins, 5-(3'-methylbut-2'-yl) isatin, 6-(3'-methylbuten-2'-yl) isatin *etc* [6].

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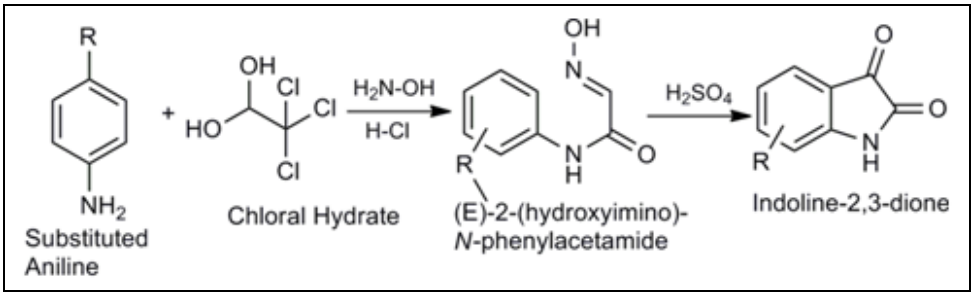
**General Methods for the Synthesis of Isatin:** Isatin is synthesized by different ways most used method is Sandmeyer Isatin synthesis and second is Stolle Isatin synthesis. Sandmeyer Isatin synthesis is condensation reaction between arylamine and chloral hydrate in the presence of hydroxylamine and aqueous sodium sulfate. Stolle Isatin synthesis is the cyclization reaction between aniline with oxalyl chloride to get chlorooxalylanilide in presence of acid [5, 7].

Martinet Isatin synthesis is reaction between aromatic amine and oxomalonate ester to form oxindole carboxylic acid derivative upon decarboxylation Isatin will form [6]. Gassman Isatin Synthesis method used to synthesize substituted isatin derivatives from substituted aniline by using *t*-butyloxychloride and ethoxycarbonyl sulfide. The latest method for synthesis of Isatin is methylation of anilide is *o*-methylation of N-pivaloyl and N-(*t*-

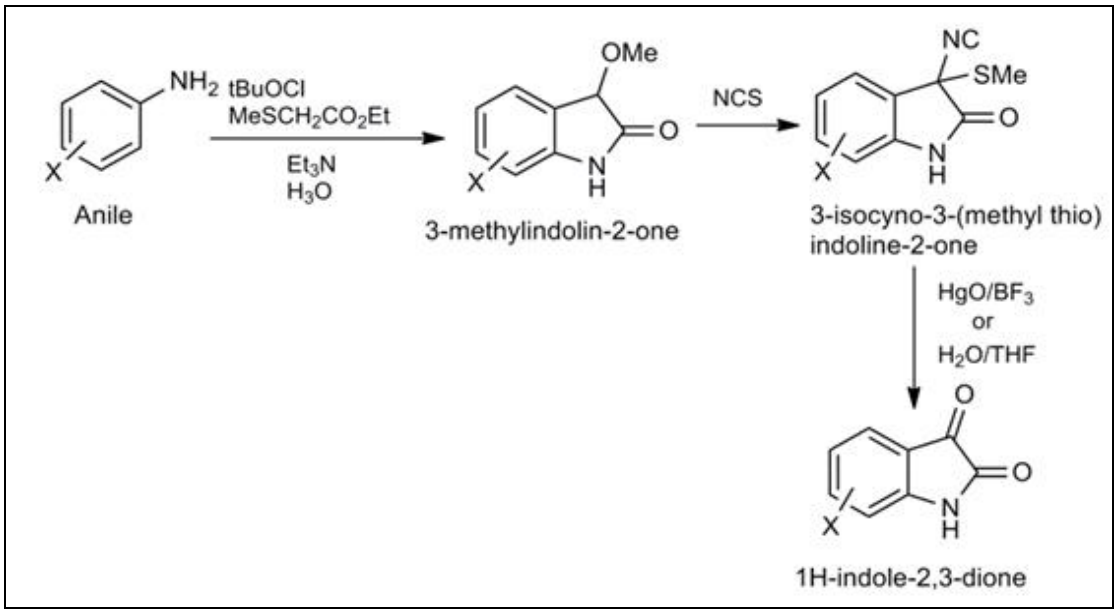
butoxycarbonyl)-anilines following de-protection and cylization of α-ketoesters [1].

**Synthesis of Isatin Derivatives:**

**Sandmeyer Method:** Most famous method to synthesis of Isatin and achieved by refluxing aniline and chloral hydrate in the presence of hydroxyl amine and sodium sulphate to form an intermediate (E) – 2 - (hydroxyimino) – N –phenyl-acetamide, cyclization and indoline-2,3-dione can be achieved by strong acid i.e. sulfuric acid [1, 8, 9].




**Grassman Method:** As discussed in Sandmeyer synthesis aniline was used as starting material, *N*-Chlorosuccinimide was used for cyclization to obtain 3-isocyano-3-(methyl thio) indoline-2-one was obtained. Further treating with mercury (II) oxide/boron trifluride etherate get 1H-indole-2,3-dione [7, 10, 12].




These two methods are more convenient methods for synthesis of novel Isatin and their derivatives. Here we first screened Isatin moiety for their probable uses on the basis of literature available and found that Isatin will act as antiviral on SARS Covid-19 Virus[7]. Following literature we refer to know the Isatin-A versatile Moiety [8, 11].

**Drug Design Study of Isatin:** A. Frediansyah, *et al*. (2021) in his review highlights important information including multiplication of virus, molecular docking and modeling analyses[9,13], in vitro studies, as well as results from clinical uses of these antiviral against COVID-19 pandemic [10]. No specific drug was approved for COVID-19 they reviewed a different fusion inhibitor, protease inhibitor, neuraminidae inhibitors and M2 ion channel protein blockers [11]. P. Pakravan1, *et al.* (2013) reviewed biochemical and pharmacological characterization of isatin and its derivatives from structure to activity [9, 12].

Fundamentals of electrophillic aromatic substitution of Isatin with respect to biological activity and structure activity relationship towards the antimicrobial, antibiotic, antifungal, antimalarial, anticancer activity [13, 14, 15]. H. Jebiti, *et al.* (2021) the mono and bi-nuclear copper (II)

complexes containing *N*-substituted isatin thiosemicarbazone(s) were synthesized and characterized by analytical and spectroscopic validated by computational studies [14]. Molecular docking studies showed hydrogen bonding and hydrophobic interactions of both complexes with tyrosinase kinase receptors having considerable cytotoxic activity against Juurkat and HeLa S3 cell line [15, 16]. Following two complexes were synthesized and compared with Cisplatin for activity [16]. P. Shukla *et al.* (2018) in his review focus on recent perspectives on chemistry and biological activity of Isatin derivatives [1]. R. Jarapula *et al.* (2016) in his research article introduced new Isatin derivatives, synthesis of 2-hydroxy -N'-(2 - oxoindolin - 3 - ylidene) benzo-hydrazide from condensation of 2-hydroxybenzohydrazide with suitable Isatin and docked with COX-1 and COX-2 X-ray crystal structure by using PDB ID: 3N8Y, 3LN1 [17]. After completion of the docking process, the minimum interaction energy between each ligand and COX proteins for the best ligand pose inside the receptor cavity was obtained as the PLP score when compared with standard drug celecoxib [18, 19].

G. Singh *et al.* (2018) proposed that Acetylinic Isatin hydrazones and acetylinic spiroisatins was the most potent antibacterial scaffold with $IC_{50}$ 1.95 µM against *E. coli* while bis-isatin assembly was the lead compound against *C. albicans* with IC50 15.67 µM [18, 19]. Molecule has been screened by SAR to check substituent effect on the observed bioactivities of the compounds. Further, docking studies of the selected scaffolds on admissible bacterial and fungal proteins elicited Isatin derivative to exhibit highest ligand efficiency [20]. Molecular interactions disclosed that 3-N substituted Isatin derivatives may be considered as efficient candidates to curb bacterial and fungal diseases [17, 21]. R. Nath *et al.* (2020) analyzed structure activity relationship of Isatin containing heterocycles for the different biological activity [22, 5].

**Target for Isatin:** Frediansyah, *et al.* (2021) has reviewed anti-SARS-CoV-2 potencies of available antiviral drug groups such as fusion inhibitors [6], protease inhibitors [23], neuraminidase inhibitors [24], and M2 ion-channel protein blockers as a target like Baricitinib and Remdesivir [11]. Varun *et al.* (2019) summarized some recently reported biological activities exhibited by Isatin derivatives, like anti-cancer, anti-bacterial, anti-diabetic and others [19, 25]. They said in their article that N-substitituted isatin, C2, C3, C5, Bromo derivatives are more effective against cancer, viral and bacterial infection [6]. Vandana *et al.* (2017) in her reviews give focus in Isatin and its derivatives possess numerous biological properties like anticancer, antimicrobial, anti-inflammatory, analgesic, anticonvulsant, antiviral, anticonvulsant, anti-helmintic, anti-HIV, antioxidant, CNS depressant activities. The present review provides a brief overview on the recent advances and future perspectives on pharmacological aspects of Isatin and its derivatives reported in the last decade [4]. H. Jebiti, *et al.* (2021) finds that N-substitution in isatin thiosemicarbazones decides nuclearity of Cu (II) complexes has potent binding ability toward tyrosine kinase receptor [16, 20]. S. Kumar *et al.* (2021) in his article explain the Isatin medicinal chemistry of carbonic anhydrase inhibitor [26]. K. Swathi *et al.* (2010) evaluate some new 5-[2(3)-dialkylamino alkoxy] Indole 2, 3-diones compounds for antihistaminic activity by histamine chamber method [21, 24]. P. Shukla *et al.* (2018) in his review focus on recent advances in biological application of Isatin derivatives [1]. R. Jarapula *et al.* (2016) in his research article introduced new Isatin derivatives specially designed to target COX enzymes which are responsible to cause inflammation [18, 22]. R. Nath *et al.* (2020) explained docking interaction within the receptor for the Isatin hybrid with cancer cell line [5].

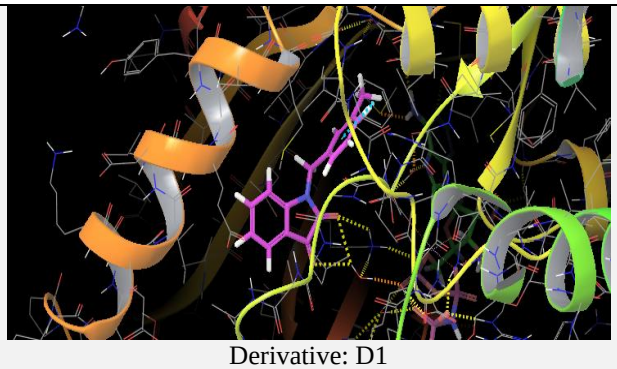
**Eligible Target and Molecular Docking:** Effect of sulfonamide-derived isatins, which molecular hybrid on hepatocellular carcinoma (HCC) HepG2 and Huh7 cell line and found that four compounds were highly toxic using MTT assay. These molecular hybrids comparatively decrease the concentration of angiogenic marker epithelial growth factor receptor (EGFR) level that further confirmed by molecular docking with PDB: 1M17 and results were compared with Erlotinib [36] Isatin and derivative was found to be active against ACE-2, M Pro, SARS-3CL Protease, Spike protein, PL Pro, Helicase, DNA depending on RNA polymerase, HIV Protease Inhibitor, TMPRSS2 inhibitor. These all are the Covid-19 target [23, 37]. The present study aims that Design Synthesis and

Biological Evaluation of Isatin Derivatives. We studied synthetic scheme of various derivatives also molecular hybrid of isatin and found effective in COVID-19 main protease [24, 38]. We designed synthetic derivative library to check the interaction of the molecule with respective target protein for this we choose SARS CoV-2 main protease is a potential target for that crystal structure. PDB-ID: 6VXX, 7V7Q, 7DF4, 7V8B was selected and used for the docking study [5] and it was found that is have some activity towards these targets as mentioned in previous report [25, 9, 35]. This report includes study of designed derivatives against lung cancer. In this study we used PDB-ID: 6DUK. Allosteric kinase inhibitors offer a potentially complementary therapeutic strategy to ATP-competitive kinase inhibitors due to their distinct sites of target binding [10]. In this study, we identify and study a mutant-selective EGFR allosteric inhibitor, JBJ, which as a single agent can inhibit cell proliferation and EGFR signaling *in-vitro* and *in-vivo* [15]. However, increased EGFR dimer formation limits treatment efficacy and leads to drug resistance. Remarkably, Isatin an ATP-competitive covalent EGFR inhibitor, uniquely and significantly enhances the binding of different derivatives to EGFR [20, 26, 34]. The derivatives results in an increase in apoptosis, a more effective inhibition of cellular growth, and an increased efficacy *in-vitro* and *in-vivo* compared with either single agent alone [21, 27, 33]. Collectively, our findings suggest that isatin based EGFR inhibitor may be an effective therapeutic approach for patients with EGFR-mutant lung cancer. For more precise findings needed as in EGFR-mutant lung cancer is limited by acquired drug resistance, thus highlighting the need for alternative strategies to inhibit EGFR [22]. Here, we identify a EGFR inhibitor [21, 28, 32].

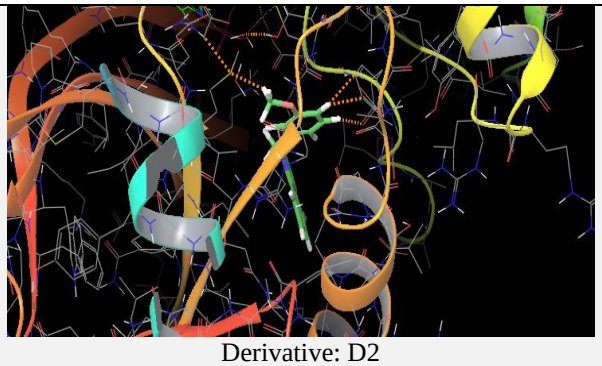
**MATERIAL AND METHODS:** Data Sources and preparation of the target protein: Here we designed a novel derivative of Isatin which are active one having potent biological activity depend on structural activity relationship. We have prepared a list of eighteen potent derivative and one standard molecule used for limiting the interaction.

**Molecular Docking:** Molecular docking was done by Schrodinger docking suits with a standard precision. The receptor which is used is EGFR (PDB ID: 6DUK) was prepared by restrained minimization using force field OPLS3E [23, 31]. The grid site was created using Glide receptor grid generator with site coordinated X=, Y=, Z=, and docking length of 20A$^{o}$. Ligands were prepared using force field OPLS3E and possible states were generated from pH 7. More negative number of docking sore is the better binding; score are reported in kcal/mol [24, 29, 30].

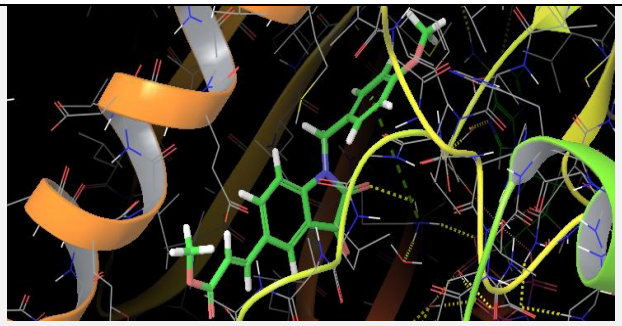
**RESULT AND DISCUSSION:** The potential binding interaction of all ten derivatives of the isatin and standard drug with the EGFR (PDB ID: 6DUK) have done by Schrodinger molecular docking suites molecular docking studies using Glide. Docking score, Glide Emodel and Glide energy has been described. The docking score in the table reflects potential binding site and favorable binding interaction with target of EGFR (PDB ID: 6DUK). Standard molecule in the given study is showing potential binding interaction with the target. Best docked structure has been identified using model energy score i.e. Glide Emodel and shows best pose of ligand docked with the target. Widely used antiviral drugs are the most potent molecule had high score with the target (PDB ID: 6DUK) Docking interactions are provided in below figures.



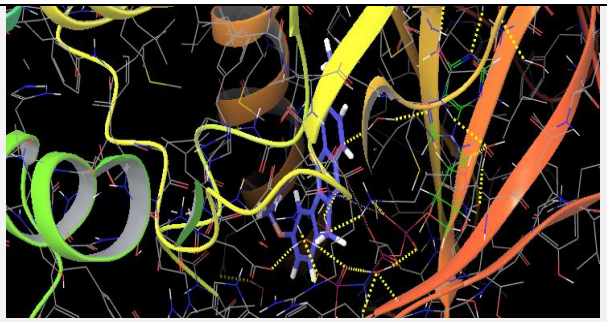
Derivative: D1



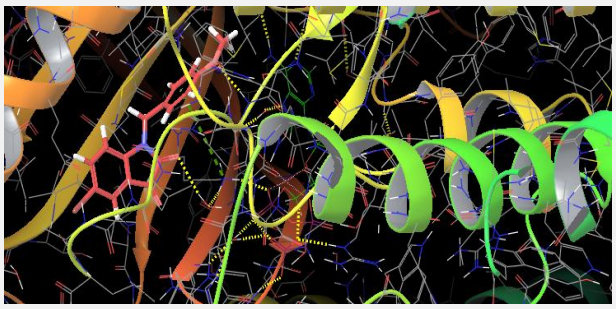
Derivative: D2



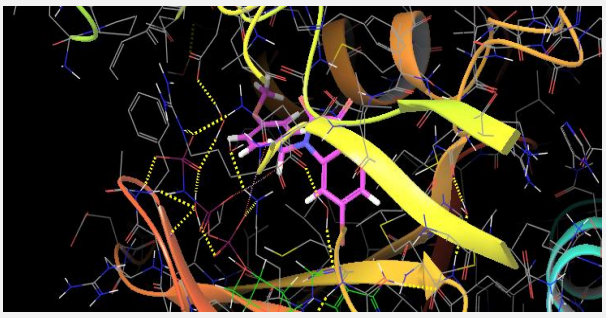
Derivative: D3



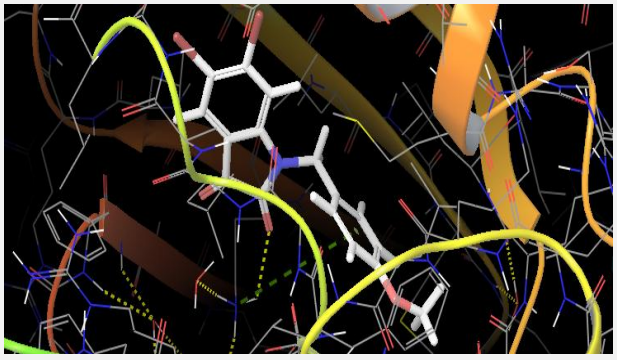
Derivative: D4



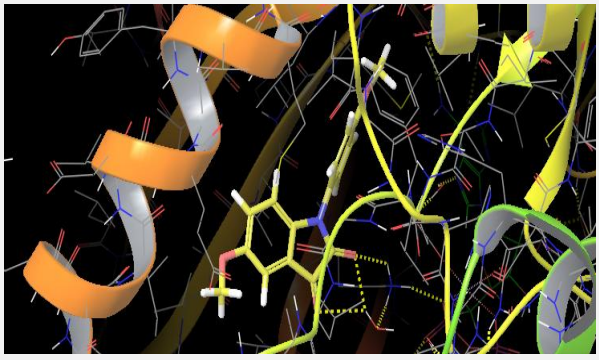
Derivative: D5



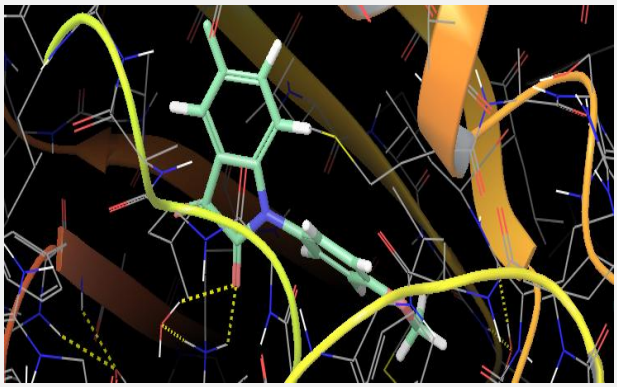
Derivative: D6



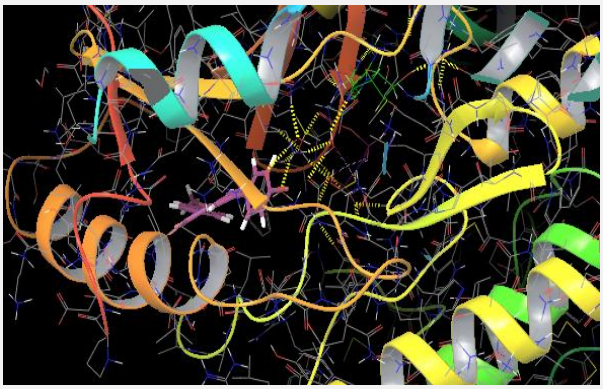
Derivative: D7



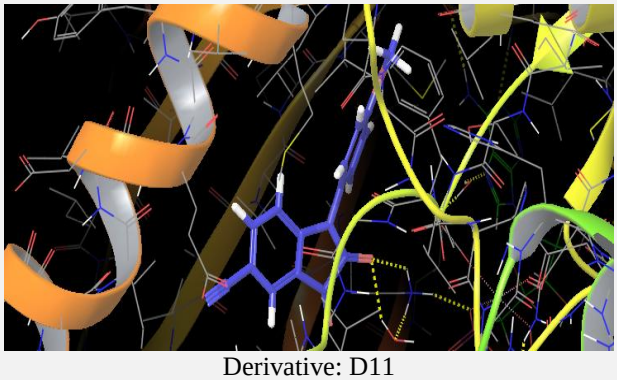
Derivative: D8



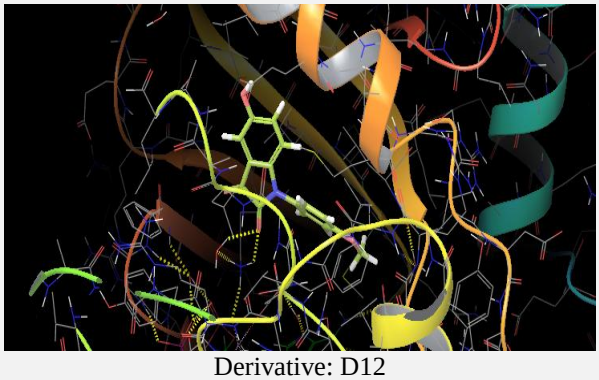
Derivative: D9



Derivative: D10



Derivative: D11



Derivative: D12

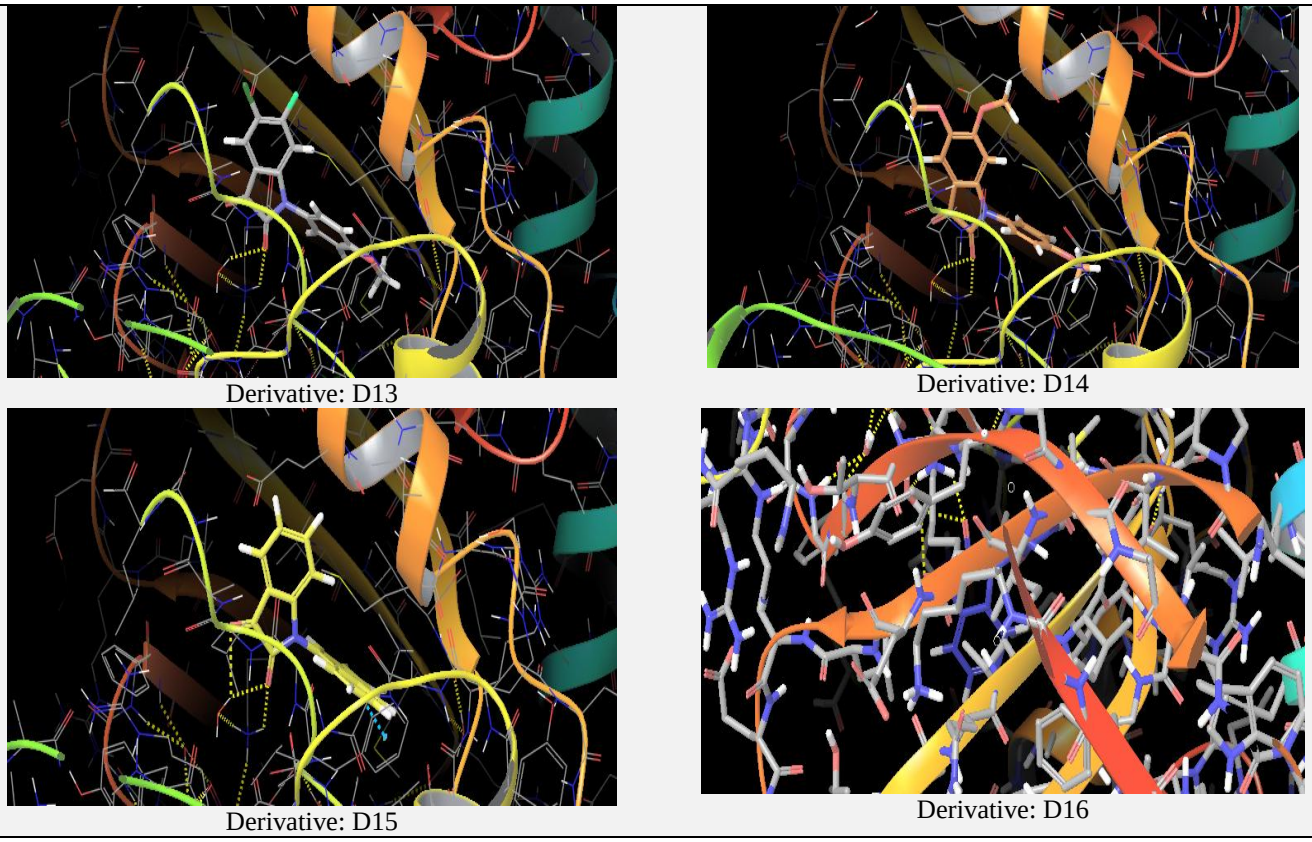



**FIG 1: DOCKING INTERACTION**

Derivatives D1 to D16 has better docking score from -7 to -9.46 as compare with standard drug. is moderately active. Standard drug JBJ molecule show consistent interaction with the amino acid residue and these are the strong interaction site of the target EGFR (PDB ID: 6DUK) as shown in below Figure:

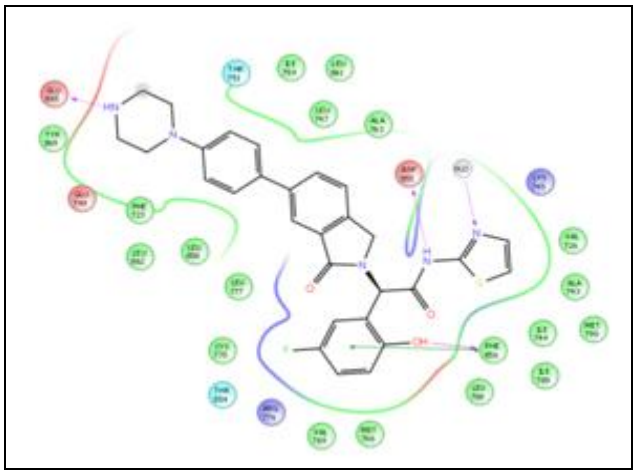


**FIG 2: LIGAND INTERACTION OF MOLECULE JBJ**

GLU 865, ASP 855, PHE 856 Amino acid residues and $H_2O$ molecule which have strong interaction with the ligand JBJ. Molecular docking suggests that GLU 865, ASP 855, PHE 856 and LYS745 are the greatest important amino acid for the H-Bonding interaction. In this study lys745 residue is forming H-Bond interaction with almost all molecules as well as with standard molecule JBJ. This is the most important for polar interaction. Interaction pocket was formed between LEU 747, PHE 723, LEU 858, MET 766, LYS 745, ASP 855, THR 854, ARG 776, MET 790, CYS 775, LEU777, PHE 856, LEU 788, ALA 763, GLU 762, ILE 759.

**CONCLUSION:** Our study concludes that the molecular hybrid of Isatin and derivatives is inhibiting the EGFR with high binding affinity. The strength of binding affinity and the interaction at the site of inhibition reveals that it is a good source of synthetic remedy to inhibit EGFR. Further experimental studies required to check efficacy of these agent to inhibit EGFR and treatment of Lung Cancer. The Superfluity research comprehends in this review which explained great diversity of isatin molecules as anticancer, antiviral, and anti-inflammatory. Study gives clue about the further modification in the main nucleus may provide potent therapeutic application toward the Lumpy Virus. We can

substitute isatin with different aromatic and heterocyclic groups and go for further molecular docking study with respective target.

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**CONFLICTS OF INTEREST:** Authors declare no conflict of interest.

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