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Design and Synthesis of Organic Molecules for Anticancer Drug Development

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Abstract- ***Cancer is still one of the largest global health burdens due to the complex biology behind the process, uncontrolled proliferation of cells and mutations, as well as continuous and insistent needs to develop novel effective anticancer agents although established anticancer drugs made some notable success in cancer treatment. Many established chemotherapy drugs suffer from serious disadvantages like resistance development, lack of specificity toward tumor cell and normal cell, toxicity related with dosage, undesirable adverse effects and relatively low therapeutic index, therefore creating an imperative need for novel drugs and chemical entities with better physicochemical and pharmacokinetic properties. Organic molecules form a quintessential backbone for the development of medicinal chemistry today with its potential for structural variation, ability to participate in chemical transformations and to interact with particular cellular targets which in turn enable them as valuable molecular species to design selective anticancer agents, affecting the cellular pathways which were reported to be crucial in cancer promotion, survival and pathogenesis. This conceptual research article aims to present the systematic process of design and synthesis of novel organic molecules which has the potential to be used as novel anticancer agent using rational molecular design approaches, functionalization/modification of privileged structure and advanced organic synthesis approaches towards the identification of molecular features corresponding to an enhanced activity, selectivity and druglike properties. The presented strategy to design and synthesis novel cancer static entities comprises structural optimization via derivatization, heterocyclic moiety inclusion and molecular architecture modification as strategy to explore relation between molecular structure and anti-cancer activity and to identify beneficial groups for anti-cancer activity; The developed molecules were hypothetically suggested to have their structural elucidation using various Spectroscopic characterizations such as fourier transform infrared spectrum, Nuclear Magnetic Resonance spectrum and Mass spectroscopy while potential interaction with tumor related proteins was predicted with computational approach using docking; Moreover the molecular models were designed by applying a knowledge of relation between molecular structure and anti-cancer activity, which includes molecular modeling and QSAR prediction as well as ADMET analysis to have an idea of interactions between target molecules and predicted drug molecules and drug-like characters which is useful to identify promising lead compounds before the biological assay.***

Keywords: ***Anticancer Drug Development, Organic Molecules, Medicinal Chemistry, Rational Molecular Design, Organic Synthesis, Structure–Activity Relationship (SAR)***

I. INTRODUCTION AND BACKGROUND RELATED TO THE STUDY

One of the most complicated and challenging world public health disorders is Cancer, the result of abnormal unchecked cell division and accumulated genetic alterations and abnormality of normal mechanism of control and abnormality activation or silencing of signaling pathways that have role in cell proliferation, differentiation, survival and programmed cell death. Normal cells differentiate into the malignant type by multistage process of mutations in oncogenes, tumor suppressors genes, genes related with DNA damage and control genes that control homeostasis of cells which in result is uncontrolled tumor growth (Hanahan & Weinberg, 2011) Cancer burden in terms of new case and deaths caused by different kinds of tumor have resulted in a high, growing requirement of advanced treatments and drugs for increasing outcome and limiting their side effects. As in contrast to important growth achievement of drugs such as surgery, Radiotherapy, immunotherapy and chemotherapy many cases have treatment failure with drugs due to the resistance development of resistant types of tumor, tumor heterogeneity and narrow specificity, chemotherapy is the most applied therapeutic system due to using the effective cytotoxin or cytostatic compound that damage normal or malignant cells by interfering with growth factors in cells such as DNA replication, RNA

synthesis and cell division processes, most antitumor agents in chemotherapy target fast dividing cells and apply to their activities such as inhibiting their cell cycle, forming lesions in DNA, interfering mitotic apparatus, disrupting the signaling pathways controlling abnormal division etc. (DeVita & Rosenberg, 2012) cell apoptosis also plays an important role in malignant cell destruction by an antitumor agent, induction of cell apoptosis a process controlled strictly by cell itself is also mechanism of the antitumor drugs to target and annihilate the tumor, intrinsic mitochondrial related pathways, extrinsic receptor mediated pathways, cascades of caspases, and cellular stress related pathways, are signaling pathway the that activated the programmed death by antitumor drugs, In order of effectiveness on tumor certain cytotoxic chemo agent have limitation their activity by system toxicity, tumor no selectivity, cross resistance and damage to normal cells and require further new agent to be developed. Since ancient, organic compounds are considered important role in designing anticancer drugs due to its high diversities, synthetic accessibility, and the opportunity of its modification for a highly targeted and specific compound capable to affect a cancer related signaling molecules, today modern methods of chemistry with new designs using scaffolds of different organic structures equipped with functional group and hetero-cyclic structures have make it possible to target any signal molecules that controlling many cellular pathway related with cancer cell, for instance the signaling pathway controlling the cell cycle or angiogenesis or apoptosis or DNA interaction, hence it could be consider that rational designing and synthesis using some methods of computational analysis along with advance experimental measurement represents another future development on anticancer target finding and therapy.
Importance of Organic Molecules in Anticancer Research

Organic molecules are crucial therapeutic platforms in cancer drug discovery. They offer significant advantages such as immense structural diversity, chemical tractability and selectively target biomolecules, which aid in the design and development of improved cancer therapeutic agents. In order to produce more active, selective, soluble, bio-compatible and potent drug candidates, medicinal chemists systematically vary and modify their structural scaffolds using extensive structure–activity relationship studies, an achievement which is possible through the synthetic versatility of organic molecules, Patrick, 2017. Nitrogen-containing organic entities gained considerable attention in anti-cancer studies as they can form H-bonds, ionic bonds or coordinated bond with the biological target thereby affecting molecular recognition and activity. Quinolone derivatives are extensively explored for potential anti-cancer activity and are known to modulate DNA–binding, enzyme inhibitions and cell signaling pathway for proliferation. Pyrimidine and imidazole-based derivatives are known to modulate the various kinases. They serve as key role of anti-metabolic and cell-signaling pathways regulator. Pyrimidine, for example, serve as DNA and RNA bases and many analogs have been synthesized with anti-cancer and anti-microbial activity (Mishra et al., 2017). Oxygen-containing organic entities like flavonoids and coumarins have also been gained considerable interest as some could affect the cancer cell viability via oxidative stress modulation, inducing apoptosis and inhibiting tumor growth with its electron-donating potential or interaction to cell signaling pathway (Ren et al., 2018). Moreover, heterocyclic organic molecules play significant role of important molecular scaffolds due to biological relevance of these structures. Compounds containing indole and thiazoles derivatives display anti-cancer property by binding the corresponding targets and have been applied in the development of medicinal drugs targeting enzymes (e.g. CDK/cyclin dependent kinase inhibitors), receptors (e.g. Tumor associated antigen-targeted drugs) and proteins (e.g. Cancer related protein) with these values added. In fact, various indole and thiazole derivatives show high potent inhibition or regulation in their respective biological pathway through interaction with cancer target proteins as they share similar feature as biomolecules. Combined with their capability in molecular modification so as to change their electronic properties or incorporate the optimal functional group. Therefore, organic framework is considered as the useful therapeutic molecules by modifying their functional groups to affect desired chemical-modification of the molecules with consideration of structural difference as well as the pharmacophores and active sites to form well characterized drugs, in view of target selectivity, structural and synthetical

varied properties that can promote them as potent medicinal compounds for future application in cancer therapy.

Historical Development of Anticancer Organic Molecules

The evolution of anticancer organic drugs throughout the history can be considered as a pathway from a simple cytotoxic to a targeted therapeutic. The history can be traced to the discovery and applications of certain chemotherapeutic compounds, the oldest examples of which are nitrogen mustards derived from warfare researches, among the first recognized organic compounds that cause anti-tumor activity through inducing cancer cell division arrest and modulating the activity of DNA to impair cell proliferation as well as to initiate DNA alkylation and replication cycle disruption (DeVita & Rosenberg, 2012). Although these drugs are proved to initiate major progress on cancer treatment, limitation in selectively targeting the cancer cells or low potency under systemic circumstances require a better strategy. Subsequent research is focused on the anti-metabolite therapy where a structurally similar organic compound was utilized to compete with a normal one for enzyme synthesis, producing effective treatment options such as methatrexate and fluoropyrimidines, which interfere with nucleic acid biosynthesis pathway specifically damaging cancer cell growth and proliferation through blocking the synthesis of DNA or RNA. Discovery of organic molecules from natural sources further expanding the area where compounds such as taxanes, camptothecin derivatives and vinca alkaloids exhibit remarkable anticancer activity by different mechanisms such as microtubule stabilization, inhibition of topoisomerase I, as well as mitotic blockage (Newman & Cragg, 2016). Derivatives of taxanes and particularly paclitaxel has become an important sample to illustrate the successful drug discovery through nature source as well as how it works to impair cancer growth through microtubule destabilization. Camptothecin derivatives have gained their place in drug history by targeting the topoisomerase I enzyme playing vital role on DNA replication, in a very similar way, Vinca alkaloid acts through prevention of microtubule assembly to cause cell cycle arrest. Latest development is around rational design and synthetic design targeted molecular abnormalities involved in tumorigenesis, exemplified by kinase inhibitors for signaling pathway disruption and hormone therapies inhibiting hormone-dependent cancer. Both inhibition on protein tyrosine kinases and modulation on estrogen or androgen receptor can represent specific biological target mediated targeted cancer drug (Sawyers, 2004). Therefore, from a simple cytotoxic compound to a high specificity molecular targeted drug, history of anticancer organic molecules seems successfully illustrate the transition by means of rationally targeted drug discovery strategies

II. RESEARCH PROBLEM

Despite remarkable progress in cancer treatment through chemotherapy, targeted therapy, and combination treatment strategies, the development of effective anticancer medicines remains a major scientific challenge due to the limitations associated with currently available therapeutic agents, including the emergence of drug resistance, dose-dependent toxicity, poor selectivity toward malignant cells, and a narrow therapeutic window between effective and harmful concentrations; cancer cells possess remarkable genetic and biological adaptability that allows them to acquire resistance mechanisms through alterations in drug targets, enhanced DNA repair capacity, increased drug efflux activity, and changes in cellular survival pathways, resulting in reduced treatment effectiveness and disease progression (Gottesman, 2002); furthermore, many conventional anticancer drugs exhibit limited selectivity because they frequently affect rapidly dividing normal tissues along with tumor cells, leading to severe adverse effects such as bone marrow suppression, gastrointestinal toxicity, and damage to healthy cellular systems, which restrict their clinical application and patient tolerance (DeVita & Rosenberg, 2012); the complexity and heterogeneity of cancer biology further contribute to therapeutic limitations because tumors contain diverse populations of cells with different molecular characteristics, making it difficult for single therapeutic agents to achieve complete and long-lasting responses; therefore, there is an urgent need for the discovery and development of novel organic molecules capable of overcoming these challenges through improved molecular targeting, enhanced biological selectivity, optimized pharmacological properties, and reduced toxicity profiles; rational

design of organic compounds based on biologically relevant scaffolds, structural modification strategies, computational prediction methods, and advanced synthetic approaches provides promising opportunities for generating new anticancer lead molecules with improved therapeutic potential; consequently, the development of innovative organic molecules with precise interactions toward cancer-associated targets represents an essential research direction for modern medicinal chemistry and drug discovery programs aimed at producing safer, more effective, and clinically valuable anticancer agents.

III. LITERATURE REVIEW

Cancer at a molecular level relies on complex networks of genetically, molecularly and cellularly dysregulated processes, whereby normal cells are transformed into malignant growths driven by unrestrained division, resistance to programmed death, altered metabolism, and increased survival pathways. While numerous molecular events trigger carcinogenesis, DNA mutations stand out as initial triggering agents, since a modification of genetic information can deregulate control of cellular growth, DNA repair and programmed death. These alterations result in sequential accumulation of further abnormalities, driving tumor progression (Hanahan & Weinberg, 2011). Oncogenes, overstimulated by a change of genetics through mutations, copy number amplification, or abnormal regulation of its expression. Activate the cascade of signals required for the unlimited proliferation and survival of cells. A loss or inhibition of function of tumor suppressor genes subsequently removes protective mechanisms that normally inhibit excessive cell division, and maintain genomic stability, while facilitating apoptosis (programmed cell death). Key molecular signaling pathways involved in carcinogenesis are PI3K/Akt pathway that plays a critical role in regulation of cell proliferation, survival, growth and metabolism, MAPK pathway that involves cellular response to extracellular growth signals, and p53 pathway that plays an irreplaceable role as a tumor suppressor. The signaling transduction mediated by these pathways directly impacts both tumor initiation, growth, and even metastasis, and also resistance to current therapies (Vogelstein et al., 2013). Understanding the signaling mechanisms involved provides a prerequisite for developing and synthesizing various organic molecules which precisely target cancer associated targets and effectively regulates tumor signaling transduction pathways and improve tumor therapy strategies.

Organic Scaffolds in Anticancer Drug Development

Heterocyclic organic compounds are among the most useful frameworks for developing anticancer drugs, because diversity in chemical structure and inherent compatibility to form complex with biological molecule and target, allow a wide design choices of selective anti-cancer agents. Quinazoline derivatives attract great interest to discover new anticancer compounds due to their potential as anti-cancer agents, particularly inhibiting the Epidermal growth factor receptor (EGFR) tyrosine kinase activity and the pathway involved in tumor cell proliferation, signaling pathway and survival (Zhang et al., 2009). In addition, indole derivatives are widely studied as a component of new chemical entities since indole nucleus is part of many naturally occurring and synthesized drugs. Mechanistic aspects include cell-cycle regulation, induction of apoptosis, regulation cancer-related pathways (Kaushik et al., 2013). Pyrimidne-based compounds comprise of another major class of the most effective nitrogen-containing heterocyclic rings, which can also serve as excellent scaffolds because of structural similarity to nucleic acid component and therefore inhibit both DNA and RNA biosynthesis leading to suppression of proliferation cancer cell in order to disruption the replication machinery (Jampilek, 2019). Further, the presence of both sulfur and nitrogen atoms in thiazole derivatives indicates their considerable biological value for antimicrobial and anticancer drugs, and suggested mechanism of action including inhibition of enzyme, mediation of oxidates stresses and disruption in cell signaling (Al-Sohaimani, et al., 2014; Sharma and Garg, 2017). Their structures can be modified in many ways making them suitable for targeting specificity and pharmacological performance, hence, further rational drug design and chemical synthesis of heterocyclic organic frameworks have proved very fruitful approaches in search for new anti-cancer molecules with desirable properties.

IV. MECHANISMS OF ANTICANCER ACTION

Some molecular designs have been explored, and are targeting key interactions and pathways within cancer cells and tumor development process, thus achieving the desired effect. The binding with nucleic acid is a fundamental way whereby various organic anti-tumor drugs cause damage to cancer cells and exhibit cytotoxic effects by inducing DNA intercalation, disruption, interference of replication process, and initiation DNA damages responses that ultimately inhibits cell growth (Hurley, 2002). It does not only directly target nucleic acid, but enzyme inhibition by some organic molecule. These agents work by interacting selectively with key regulatory proteins related to the pathogenesis of cancer, such as inhibiting receptor tyrosine kinases responsible for the proliferation of cells driven by abnormal signals, inhibiting topoisomerase required for DNA replication as well as the chromosome organization, and altering gene expression by interfering with histone deacetylase dependent epigenetic regulation (Roskoski, 2016). In addition to the inhibition to the nucleic acid and enzyme, the organic compounds can induce the apoptotic processes that program for the death of cells. By stimulating caspase cascade, disrupting of mitochondrial membrane, release of cytochrome c to cytoplasm and generating ROS, the cancer cells undergoing apoptosis is activated to kill by programmed cell death pathway (Pfeffer & Singh, 2018). Anti-cancer drug can also be designed by targeting tumor angiogenesis since neovascularization is a crucial process contributing to both tumor growth and development of the metastatic capability. Some molecule capable of antagonize VEGE signals thus can reduce the generation of tumor neo-angiogenesis that nourishes cancer cells and limits distant spread of cancer (Ferrara, 2004). So, it is believed that all these mechanisms provide evidence in design and synthesis of new organic anti-cancer molecules with a high target selectivity, biological activity, and therapeutic prospect.

V. CHARACTERIZATION METHODS

As mentioned above, characterization of newly synthesized organic molecules is also an important part of designing new potential anticancer drugs as proper structurally determined would help one to establish correlation between molecular structure and activity. Among the available spectroscopic methods, FTIR spectrum provides a great source of information on the identification of functional group through specific absorption bands which correspond to the stretching vibrations of some important chemical bonds such as imine (C=N), carbonyl (C=O), and N-H bond stretches. Thus, this spectrum will enable confirming whether a particular carbon skeleton was correctly synthesized or it was transformed appropriately as required (Silverstein et al., 2014). NMR is one of the most versatile techniques for structurally elucidated organic molecules. While H NMR analysis of an organic compound gives detail about proton in a given molecule. Proton NMR has chemical shifts and splits of signal provide the environment of the proton and also a direct conclusion on the number of symmetry available with each proton present. The C NMR give one confirmation on presence of carbon skeleton of the proposed molecule as also on its surroundings. (Claridge, 2016). MS determines molecular weight of the molecule and conclusive evidence for presence of an atom, also its fragmentation pattern will give a clue on the architecture of the molecules. MS analysis will confirm structure after comparing with the calculated value and even helps to have knowledge on elemental composition and structure of new molecules after predicting its structure with the help of MS fragment data. Further, X-ray crystal structure analysis if suitable crystal of synthesized molecule can be obtained, will provide detailed and unambiguous data on the position and connectivity of every atom within the crystal along with information on bond lengths, bond angles, bond torsion and stacking among the molecules, thus confirming 3D structure of a given molecule (Giacovazzo et al., 2011). Combining all the above-mentioned studies together will provide with most acceptable evidence for structurally confirmation of new organic molecules thus enabling one to investigate further toward its application as a potent drug target for cancer.

VI. COMPUTATIONAL DRUG DESIGN APPROACHES

Computational drug design methods-Computational methods provide key prediction information to the

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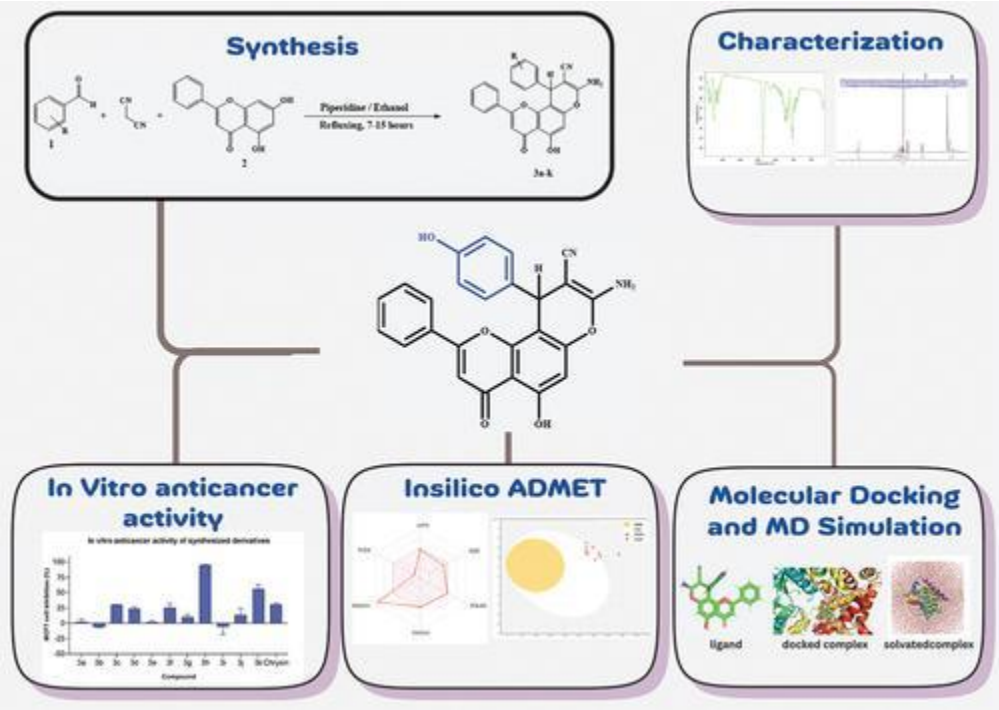
discovery, optimization, and development of potent anti-cancer candidates prior to their extensive empirical investigation, where docking methods are extensively used for investigating the ligand-target interactions with prediction of binding orientation, binding energies, hydrogen bonds, hydrophobic interactions and the active site compatibility between designed organics and its targets; and in discovery of anti-cancer candidates, molecular docking strategy is quite common that target various signaling molecules responsible in cellular growth and proliferation or angiogenesis or DNA replication pathways such as EGF receptor (EGFR),VEGFR and topoisomerase enzymes (Sliwoski et al., 2014); Meanwhile ADMET (absorption, distribution, metabolism, excretion, toxicity) prediction model allows to study the drug likability of designed molecules and also to predict their absorption, distribution, excretion and toxicity properties thus to eliminate potential candidate molecules having unfavorable physicochemical characteristics (Hughes et al., 2011); Also, QSAR (quantitative structure activity relationship) modeling approach relies on correlation study on the relationship between the biological activity and quantitative descriptor of molecule (electron features, hydrophobicity, etc) and allows predict relationship and direction for structural modifications to maximize the potency of derived compounds, thereby, it's important to establish a whole process including molecular docking, ADMET prediction, and QSAR analysis coupled with synthesis and bio-evaluation for rational drug designing toward highly efficient and safe anti-cancer therapeutics.



Above diagram showing Design and Synthesis of Organic Molecules for Anticancer Drug Development

VII. BIOLOGICAL EVALUATION STRATEGY

Biological evaluation is a crucial stage of developing a new drug for the cancer, because the structure of organic molecule in a particular chemical design needs to be screened against cells to measure the ability of molecule against suppressing cancer cell growth, selective toxic on cancer cells and molecular pathway regulation in tumor cells (Abdolrasoul M., et al, 2011). Anti-cancer screening usually starts with the in vitro evaluations including MTT assay that indicates metabolic status of cell by measuring the converting of tetrazolium to colored formazan under the enzymatic activity of mitochondria to provide the quantitative result about viability and potential to inhibit

proliferation of tested compound (Mosmann, 1983). Other evaluation methods including cell viability assay and cytotoxicity assay using cancer cell models are then carry out in order to get know about cell viability against organic molecules based on the concentration to distinguish the favorable ones with favorable selectability profiles; Apoptosis assay can investigate about if candidate molecules induce apoptosis through particular ways, such as activated caspase activation, mitochondrial dysfunction, release of apoptogenic factors, DNA damage pathway, and DNA fragmentation, etc (Elmore, 2007). Cell viability, cell cycle analysis and apoptosis will be typically performed by using a flow cytometry. Cell cycle analysis is a critical step since most anti-cancer drug has the activity based on targeting cell cycle to maintain the controlled proliferation to prevent uncontrollable growing and lead tumor to die; Hence, the integration with cytotoxicity, apoptosis assays and cell cycle analysis can represent sufficient biologically evidence to understand therapeutic prospects, molecular mechanism and the application of new organic anti-cancer molecule.

VIII. DISCUSSION RELATED TO THE STUDY

The conceptual designing of a new organic scaffold intended to identify new candidates of anti-cancer agents is an efficient way for developing enhanced potential therapeutic compounds combining approaches with rational molecular design, organic synthesis, structure examination, and biology evaluation. Successful formation of new frameworks enables researchers to detect compounds possessing novel potentials regarding their efficacy as agents of anti-cancer nature and pharmacological properties. Evaluation as new promising anti-cancer drugs requires knowledge about impact of individual molecular properties like heterocyclic framework, individual substituents, electronic impacts, molecular geometries as well as physical-chemical impacts on Biological effects and binding toward their cancer target associated elements (Patrick, 2017). Investigation regarding Structure-Activity Relationship (SAR) gives the ability to set up the relationships among molecule modifications and any corresponding change of Biological response enabling enhancement regarding Potency, Selectivity, Solubility, Stability, Therapy Profile through a planned arrangement of individual molecule parts modification. Beyond that, studying potentially involved therapeutical mechanisms gives data concerning effects of developed organic molecules on the progression toward cancer along DNA intercalation/adduction, inhibition of enzymes, induction of apoptosis, the regulation of the cell-cycle and blockage of tumor related signaling mechanisms (Hanahan & Weinberg, 2011). By prediction of target affinities and identification of molecular fragments connected with increasing anti-cancer performance, computational techniques such as docking calculation and Quantitative Structure Activity Relationship (QSAR) also contribute to the explanation of molecule actions. Combination of organic synthesis, molecule examination and comparison, computer-driven analysis of predicted and biological activities finally is an outstanding method for potential therapeutic application of organic molecules.

IX. SIGNIFICANCE OF THE STUDY

The research holds considerable scientific, pharmaceutical and industrial significance due to establishing an understanding of improving innovative therapeutic molecule discovery via the combination of medicinal chemistry, organic synthesis, computational methods, and biological analysis; scientifically, it is concerned with moving forward of medicinally organic chemistry as it will expand our knowledge over the designing of molecular scaffolds, chemical modifying strategies, and chemical structure-bioactivity relationships, hence, enhancing effective rational designing ways for acquiring more selectively and biologically active anticancer molecules(Patrick, 2017); studying various organic scaffolds and modified ways to introduce chemical functional groups would lead to an understanding on how chemical properties determine molecules targeting cancer-associated molecules as well as the therapeutic outcome; from a pharmaceutical view, the research aims to provide potential anticancing drug lead molecules through researching on new chemicals effective on critically important cellular functions of tumors regarding growth, proliferation, apoptosis regulation, cellular signal pathway(Hanahan & Weinberg, 2011); Additionally, rational designs and evaluations on organic molecules will assist the progress of addressing negative aspects like drug

resistance and toxicity on many known anticancer treatments(Zhu & Hu, 2011); Industrially, the organic scaffold design contributes to a greater drug discovery pipeline via newly designed candidates of lead compounds on high screening and further studies and it helps in drug development towards efficient and biologically potent drugs.

X. LIMITATIONS OF THE STUDY

Design and synthesis of novel organic molecules offers good prospect on research for discovery of anticancer drugs however certain challenges need to be explored before its therapeutic utility as computational predictions and theoretical evaluation needs experimental validation to demonstrate biological relevance, safety and therapeutic efficacy in vivo as molecular docking, QSAR modelling and ADMET prediction approaches offer valuable preliminary data to suggest molecular interaction, potential activity and pharmacokinetic parameter; However, none of these cannot fully mimic the intricacies and biological behaviour i.e. Behavior of cellular uptake, metabolism, pharmacology etc within biological system (Sliwoski et al., 2014). Thus, a detailed laboratory-based study needs to establish the anticancer activity by demonstrating efficacy on respective cell lines and examining cytotoxicity, apoptosis studies and study mechanism. Toxicity study is one more of mandatory pre requisites as compound which shows anticancer activity might also affect normal cells and studies related to its safety parameters including selectivity and harmful effects should be carried out (Lombardino & Lowe, 2004). Moving the compound from laboratory bench to clinic involves prolonged pre-clinical and clinical trials that include further pharmacologic study, formulations development, regulatory steps and human safety analysis, though another factor to be focused on is the possibility of producing it on larger scale as the reaction procedures which are successful at laboratory level cannot be readily translated on an industrial scale due to the feasibility of scalability, cost-efficiency, effective purification steps, environmental concerns and reproducibility of manufacturing processes. Hence, by comprehensive and combinatorial use of computational study, empirical results, toxicity evaluations and research in industry; further development for anticancer drugs from the new designs of organic molecules is possible.

XI. FUTURE PERSPECTIVES

Future efforts in anticancer drug development will increasingly utilize a combination of new technologies, greener synthetic procedures, and individualized treatment methodologies in order to circumvent issues encountered in conventional drug discovery as well as treatments. AI is one technology rapidly being incorporated into cancer drug discovery which can be used to predict likely drug candidates, the behavior of their respective chemical compounds, carry out virtual screening experiments and optimize the structure of drug molecules by means of computational models and the large amount of data available about molecular structure and biology (Lavecchia, 2015); the adoption of greener synthetic procedures is currently gaining significance in pharmaceutical chemistry as through approaches such as solvent-free reactions, reactions based on the transformation carried out by a biocatalyst and processes using limited energy, harmful waste produced during synthesis can be eliminated with environmental benefit (Anastas & Warner, 1998). Personalized anticancer treatment is likely to be developed with a focus towards target-specific drugs designed using details about a tumor's molecular makeup and biological state and such drug treatments can be used to tailor therapies more efficiently at specific biological targets to increase efficiency and reduce toxicity to normal cells and tissues (Ashley, 2016); finally, nanotechnology is being utilized to deliver such therapies, with nanoparticles being one example, in order to increase a drugs solubility, maintain a Drugs active form, ensure delivery to a target site and to achieve a controlled release of the Drug once the target has been reached. Overall, such novel methods as AI in conjunction with greener chemistry and personal treatments along with nanotechnology offer unique and powerful strategies toward next-generation anti-cancer drug development.

XII. CONCLUSION

Organic rational design strategy in the discovering modern anti-cancer agents is powerful and effective to design the biological activity, molecular selectivity

and pharmacological parameters systematically according to the knowledge of cancer related target and SAR; the progress in medicinal chemistry indicated that well designed organic scaffold, which are include heterocyclic scaffold and bioactive molecular framework, will offer the useful opportunity in developing molecules capable of interfering with tumor proliferation, survival, and metastasis (Hanahan & Weinberg, 2011). Combining organic synthesis, sophisticated spectroscopic characterization, computer aided analysis and biological investigation, it provides us a robust approach to fast find out promising and to optimize molecule from the relationship of molecular structure and the biological effect and therapeutic response; some computational strategies such as molecular docking, QSAR, ADMET can make it possible and efficient in candidate molecules finding by directing modifications and prioritizing leads prior to extensive testing (Sliwoski et al., 2014). In the following study, the focus of anti-cancer therapeutics is in safe and specific drug molecules that target malignant cells and exhibit minimum toxic on normal cells in order to maximize therapeutic efficiency, overcome problems associated with resistance and transform into viable anti-cancer drugs. Continued cross disciplines cooperate is vital between organic chemists, computer scientists, pharmacologist and biological scientist.

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