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A Literature Review On The Structure-Activity Relationship (SAR) Approach In The Optimization And Development Of Anticancer Compounds As Drug Candidates

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Abstract

Cancer is one of the leading causes of death worldwide, with increasing incidence and mortality rates, highlighting the urgent need for more effective and selective therapeutic strategies. One widely used approach in medicinal chemistry is the Structure–Activity Relationship (SAR), which aims to understand the relationship between the chemical structure of compounds and their biological activity. This study aims to analyze the role of the SAR approach in the optimization and development of anticancer compounds as drug candidates through a literature review of 15 scientific journals. The method used is a descriptive-comparative approach by evaluating parameters such as compound structure, types of substituents, biological activity, and mechanisms of action. The results indicate that structural modifications, including the addition of hydroxyl, methoxy, and halogen groups, as well as molecular hybridization strategies, significantly enhance anticancer activity, as reflected by IC_{50} values in the micromolar to nanomolar range. Furthermore, modified compounds tend to exhibit higher selectivity and more specific mechanisms of action toward biological targets. Therefore, the SAR approach is proven to be effective as a foundation for the rational design of more optimal anticancer compounds. The implications of this study suggest that integrating SAR with biological evaluation and formulation development may lead to more effective and safer anticancer drug candidates.

Keywords: ***SAR, Anticancer, Structural Optimization, Biological Activity, Drug Candidates.***

INTRODUCTION

Cancer is a complex disease characterized by uncontrolled proliferation of abnormal cells and the ability to invade and metastasize to other tissues.(Constantinescu & Lungu, 2021). To date, cancer remains one of the leading causes of death worldwide. According to reports*World Health Organization*, (2026)Cancer caused nearly 10 million deaths in 2020, making it the second leading cause of death globally. Furthermore, global epidemiological data reported by the International Agency for Research on Cancer through GLOBOCAN 2022 shows that there were 19,976,499 new cases of cancer, with 9,743,832 deaths, and 53,504,187 cases of prevalence (5 years) worldwide.((IARC), 2022).

Figure 1. Global Cancer Overview (Incidence, Deaths, Prevalence) (Source((IARC), 2022)

These figures not only reflect the high incidence and mortality of cancer but also illustrate the significant long-term burden this disease places on the global health system. The high prevalence of cancer indicates that cancer is chronic and requires ongoing treatment, significantly impacting patients' quality of life and healthcare needs. Although various therapeutic modalities such as chemotherapy, radiotherapy, and targeted therapy have experienced rapid development, their effectiveness remains suboptimal due to the frequent presence of significant side effects and the emergence of drug resistance in cancer cells.(Hashmi et al., 2025b)Therefore, the development of more selective, effective, and safe therapeutic strategies is an urgent need in the fields of pharmacy and medicinal chemistry.

In line with the increasing need for more effective therapies, the development of anticancer compounds based on natural and synthetic materials is a growing approach. Bioactive compounds are

known to inhibit cancer cell growth through various mechanisms, such as apoptosis induction, proliferation inhibition, and modulation of molecular signaling pathways involved in carcinogenesis.(Burc et al., 2026)However, the utilization of these compounds still faces various obstacles, including low bioavailability, poor chemical stability, and suboptimal selectivity against cancer cells.(Amin, Fariidah, et al., 2025)This shows that the effectiveness of a compound is not only determined by the type of compound itself, but also by the characteristics of its chemical structure. Therefore, a rational approach is needed in optimizing molecular structures. One approach that is widely used is the Structure–Activity Relationship (SAR), which allows the analysis of the relationship between changes in chemical structure and the biological activity of a compound, so that it can be used as a basis for designing more effective and selective drugs.(Cybulski et al., 2024).

The Structure–Activity Relationship (SAR) approach is an important method in medicinal chemistry for understanding the relationship between a compound's chemical structure and its biological activity. Through this approach, structural modifications such as the addition of functional groups, changes to the ring framework, and adjustments to physicochemical properties can be analyzed for their effect on anticancer activity.(Bina et al., 2025)In general, hydroxyl (–OH), methoxy ($–OCH_3$), carbonyl, and heteroatoms such as nitrogen and oxygen play a role in enhancing interactions with biological targets through hydrogen bonds and hydrophobic interactions. Furthermore, the balance between lipophilicity and polarity also determines a compound's ability to penetrate cell membranes.(Cybulski et al., 2024)Therefore, the SAR approach is the basis for optimizing and developing anticancer compounds as more effective and selective drug candidates.

Various studies have reported the potential of various classes of compounds as anticancer agents with diverse and often multi-target mechanisms of action. For example, flavonoids are known to have cytotoxic activity influenced by the presence and position of methoxy and hydroxyl groups, which play a role in interactions with cancer protein targets.(Yun et al., 2021)Isoquinoline alkaloids have also been reported to induce apoptosis and autophagy through interactions with nucleic acids and proteins of cancer cells.(Aidiel et al., 2025). In addition, chalcone compounds and their derivatives exhibit anticancer activity through inhibition of important enzymes such as topoisomerases that play a role in DNA replication.(Al-ghorbani & Alharbi, 2023)Heterocyclic compounds such as quinazoline and purine also show significant activity as protein kinase inhibitors that play a role in regulating cancer cell growth.(Hashmi et al., 2025a)Although these research results show promising potential, most studies still focus on biological activity testing without comprehensively examining the systematic relationship between structural modifications and activity enhancement. Consequently, a comprehensive understanding of the most effective structural optimization patterns for enhancing anticancer activity remains incompletely integrated.

Based on this description, a comprehensive study is needed that not only collects data on the activity of anticancer compounds but also systematically integrates the relationship between chemical structure and biological activity. Therefore, this review aims to analyze the Structure-Activity Relationship (SAR) of various anticancer compounds based on 15 relevant scientific journals. The analysis focuses on identifying structural modification patterns that contribute to increased cytotoxic activity, selectivity against cancer cells, and interactions with specific molecular targets. The novelty of this study lies in the integrative approach that combines various SAR research results from various classes of compounds, both natural and synthetic, thus producing a more comprehensive understanding of structure optimization strategies in anticancer drug development. Thus, the results of this study are expected to provide a scientific basis for the rational design of new drug candidates that are more effective, selective, and have minimal side effects.

RESEARCH METHODS

This research is a literature study with a descriptive approach conducted by searching various electronic scientific journal sources. Data were obtained from several reputable databases, such as Google Scholar, PubMed, ScienceDirect, and ResearchGate, with a total of 15 scientific journals

relevant to the topic of Structure-Activity Relationship (SAR) of anticancer compounds. The literature search process was carried out using a combination of keywords, including: "anticancer", "structure-activity relationship", "SAR", "natural compounds", "synthetic compounds", and "molecular modification". The selected journals are the most recent publications in the period around 2020–2026 and have direct relevance to the study of the relationship between structure and activity of anticancer compounds.

The research procedure was carried out through several stages, namely identification, selection, and literature analysis. The initial stage was carried out by collecting articles based on predetermined keywords, then filtered using inclusion criteria, namely journals that discuss anticancer activity, have clear compound structure data, and contain information related to biological activity such as IC_{50} values or mechanisms of action. Meanwhile, exclusion criteria included articles that did not have measurable activity data, were not relevant to the SAR topic, or were non-scientific publications. The selection process was carried out in stages until 15 journals were obtained that met the criteria. The obtained data were then analyzed using a descriptive-comparative method, by comparing parameters such as the chemical structure of the compound, type of substituent, biological activity, IC_{50} values, and interactions with molecular targets to identify patterns of structure and activity relationships in the development of anticancer compounds.

RESULTS AND DISCUSSION

Based on the results of a review of 15 relevant journals using the Structure–Activity Relationship (SAR) approach, a general overview was obtained that the anticancer compounds studied come from various groups, both natural and synthetic. These groups include flavonoids, chalcones, isoquinoline alkaloids, purine derivatives, quinazolines, and other heterocyclic compounds. In general, all journals indicate that chemical structure plays a significant role in determining anticancer activity. Small changes such as the addition of functional groups, substitutions on rings, or the combination of two compounds (hybridization) can increase or decrease biological activity. Furthermore, in vitro and in silico approaches are widely used to assess the potential activity of compounds against cancer targets such as EGFR, HER2, VEGFR, and other proteins.(Amin, Fariidah, et al., 2025). To facilitate comparative analysis between studies, a summary of the study results is presented in Table 1.

Table 1. Summary of the Structure-Activity Relationship (SAR)anticancer compounds based on 15 journals

Journal	**Compound**	**Structural Modification*Structure-Activity Relationship* (SAR)**	**Biological Activity & Implications**
(Hashmi et al., 2025a)	*Purine derivatives (aryl-piperazine, triazole, bis-purine)*	Substitution at the N-9 position with triazole and piperazine groups and the addition of halogen (Cl, Br) and nitro (NO_2) groups	Shows cytotoxic activity with IC_{50} <10 µM on various cancer cells; activity is increased compared to the base compound.
(Toublet, 2025)	*Chalcone (xanthohumol, licochalcone, panduretin)*	Addition of hydroxy and methoxy groups and substitution of aromatic and heterocyclic rings	Anticancer activity with IC_{50} 0.01–2.54 µM; active against various cancer cells such as MCF-7 and A549

(Constantinescu & Lungu, 2021)	*Chalcone–heterocycle*	Hybridization with triazole, pyrazole rings and methoxy and chloro substitutions	Shows increased activity down to low IC_{50} (up to 0.02 µM) and antiproliferative effects
(Hashmi et al., 2025b)	*Purine–chalcone/xanthine hybrid*	Arylpiperazine substitution, halogen, and alkyl chain modification	Cytotoxic activity with IC_{50} around 1.4 µM; shows inhibitory effect on cancer cell growth
(Burc et al., 2026)	*8-quinolinol–diazene*	Diazo coupling with variations of ester, carboxylic, and methyl groups	Compounds active against Hep-G2 cells with IC_{50} around 2.7–2.9 µM; some compounds are more active than control
(Cybulski et al., 2024)	*Indoloquinoline–hydroxycinnamic acid*	Conjugation via amide group with hydroxycinnamic acid	Shows high activity with IC_{50} of around 336 nM against pancreatic cancer cells
Journal	**Compound**	**Structural Modification*Structure-Activity Relationship* (SAR)**	**Biological Activity & Implications**
(Yun et al., 2021)	*Isoquinoline alkaloids (berberine, sanguinarine)*	Natural structure without synthetic modification	Shows activity through induction of apoptosis, autophagy, and inhibition of cell proliferation.
(Aidiel et al., 2025)	*Methoxyflavone*	Variations in the position of methoxy and hydroxy groups	Anticancer activity with IC_{50} around 2.6 µM in several cancer cell lines
(Al-ghorbani & Alharbi, 2023)	*Quinoline–isoindoline hybrid*	Heterocyclic ring integration (tetrazol, triazole, pyrazole)	The main activity is reported as antioxidant, relevant as structural design but limited to anticancer.
(Kinase et al., 2024)	*Quinazoline derivative*	Hydrophobic substitution and addition of active groups such as N-acetohydrazide	Shows high activity with IC_{50} of around 0.29 µM against targets such as VEGFR-2

(Setiawan & Amin, 2025)	*Neoechinulin, Galangin, Belisnostat*	Natural compounds flavonoids and alkaloids	Binding energy -7.2 to -8.9 kcal/mol to HPV protein, indicating potential as an inhibitor
(Amin, 2026)	*Quercetin, Oleandrin, α-terpineol*	Flavonoid, glycoside, and terpenoid compounds	Activity with IC_{50} of approximately 48 µg/mL and interaction with HER2 and STAT3 targets
(Amin & Pratama, 2025)	*EF24, GO-Y030, Curcumin-Nanoform*	Modification of curcumin through substitution and nano-formulation	Shows increased activity compared to native curcumin as well as increased stability
Journal	**Compound**	**Structural Modification*Structure-Activity Relationship* (SAR)**	**Biological Activity & Implications**
(Amin, Sheryl, et al., 2025)	*Genistein, Luteolin, Apigenin*	Flavonoids from Moringa leaves	High binding energy (up to -96 kcal/mol) to the estrogen receptor
(Amin, Fariidah, et al., 2025)	*Squalene, Kaempferol, β-bourbonene*	Natural compounds resulting from molecular docking	Shows high affinity for targets such as EGFR, HER2, and CDK2

Characteristics of Compounds and Structure

Based on a review of 15 journals, the anticancer compounds studied exhibited a wide range of structural diversity, including flavonoids, chalcones, isoquinoline alkaloids, purine derivatives, quinazolines, and various other heterocyclic compounds. In general, these compounds possess an aromatic or heterocyclic framework that acts as the primary pharmacophore in interactions with biological targets. In the chalcone group, the α,β-unsaturated carbonyl structure is a crucial component that enables interactions with enzymes such as topoisomerases through an electrophilic mechanism.(Toublet, 2025)Meanwhile, purine derivatives have structural similarities to DNA and RNA components, thus facilitating interaction with the biological systems of cancer cells and are widely used in the design of heterocyclic-based drugs.(Hashmi et al., 2025b).

This finding is in line with the study by Leite et al., (2023), which reported that chalcone derivatives have important structural features related to their anticancer activity, particularly the presence of the α, β-unsaturated carbonyl system and substituents such as hydroxyl and methoxy groups. These structural characteristics influence the interaction of compounds with biological targets and contribute to their antiproliferative activity against cancer cells. Therefore, the results of this review are consistent with previous SAR-based research, showing that the anticancer potential of a compound is strongly influenced by its core structure, functional groups, and substituent position.

Biological Activity of Compounds

In terms of biological activity, the analyzed compounds showed significant potency variations, ranging from micromolar to nanomolar. Structurally modified compounds generally exhibited higher activity than their unmodified counterparts. For example, indoloquinoline conjugates exhibited very potent activity with an IC_{50} value of approximately 336 nM against pancreatic cancer cells, indicating increased potency due to the molecular conjugation strategy.(Cybulski et al., 2024).

In addition, quinazoline derivatives are known to have high activity as protein kinase inhibitors with low IC_{50} values against targets such as VEGFR and EGFR, which play a role in the proliferation and angiogenesis of cancer cells.(Kinase et al., 2024). In natural compounds, molecular docking approaches show that several compounds such as squalene, kaempferol, and β-bourbonene have high binding affinity to cancer targets such as EGFR, HER2, and ER-α, with stable binding energies.(Amin, Fariidah, et al., 2025)This shows that both experimental (in vitro) and computational (in silico) approaches provide a consistent picture of the potential anticancer activity of a compound.

The results of this review are consistent with the study by Cybulski et al., (2024), which demonstrated that structural modification through molecular conjugation can significantly improve anticancer activity. In that study, indoloquinoline–hydroxycinnamic acid conjugates showed strong cytotoxic activity against pancreatic cancer cells, with IC_{50} values reaching the nanomolar range. This supports the present review, indicating that modified compounds tend to exhibit higher biological activity than their parent structures. Therefore, molecular modification, conjugation strategy, and target interaction are important factors in improving the potency of anticancer drug candidates.

SAR Analysis (Activity Increase and Decrease)

Structure–Activity Relationship (SAR) analysis from 15 journals shows that the increase in anticancer activity is strongly influenced by structural modifications, particularly through the addition of functional groups and molecular hybridization. The addition of hydroxyl groups (–OH) increases the ability to form hydrogen bonds with protein targets, while methoxy groups ($–OCH_3$) increase lipophilicity, which supports cell membrane penetration.(Aidiel et al., 2025). In purine derivatives, substitution with heterocyclic rings such as triazoles and piperazines has been shown to increase cytotoxic activity through enhanced interactions with biological targets.(Hashmi et al., 2025b).

In addition, hybridization strategies such as the incorporation of chalcones with heterocycles or conjugation with other compounds also increase activity because they result in more effective multitarget interactions.(Constantinescu & Lungu, 2021)However, not all modifications have a positive effect. Excessive lipophilicity can decrease the solubility and distribution of compounds, while steric hindrance due to large molecular size can reduce their ability to interact with targets. Therefore, structure optimization through SAR must consider the balance between electronic properties, molecular size, and the ability to interact with biological targets.

Consistent with Toublet, (2025), the anticancer activity of chalcone derivatives is strongly influenced by structural modification, particularly the variation of substituents on the aromatic ring and hybridization with other pharmacophoric groups. Appropriate structural modification can enhance interactions with biological targets such as topoisomerase enzymes, whereas unfavorable changes may reduce activity due to steric effects or an imbalance in physicochemical properties. Thus, the SAR pattern discussed in this study supports previous research, indicating that functional group variation, molecular hybridization, and the balance between electronic and lipophilic properties are important determinants in increasing or decreasing anticancer activity.

Working Mechanism and Development Potential

The mechanisms of action of the anticancer compounds analyzed generally involve several main pathways: apoptosis induction, enzyme inhibition, and interaction with specific receptors. Chalcones work by inhibiting topoisomerases, which play a role in DNA replication, thereby causing DNA damage and cell death.(Toublet, 2025). Meanwhile, isoquinoline alkaloids show mechanisms through the induction of apoptosis, autophagy, and interaction with DNA and target proteins.(Yun et al., 2021). In modified compounds, such as modified curcumin (EF24 and GO-Y030), increased

activity occurs through activation of the apoptosis pathway, inhibition of NF-κB, and decreased VEGF expression.(Amin & Pratama, 2025).

In addition, computational approaches such as molecular docking allow the identification of multitarget compounds capable of interacting with multiple cancer receptors simultaneously, thereby increasing the chances of developing more effective drug candidates.(Amin, Fariidah, et al., 2025)Overall, the modified and hybridized compounds showed the highest potential for development as anticancer drug candidates due to their high activity, specific mechanisms of action, and opportunities for further optimization through the SAR approach.

Consistent with Fouad et al., (2025), structurally modified heterocyclic compounds can exert anticancer effects through multiple mechanisms, including interactions with cancer-related molecular targets and improved cytotoxic potency. Their review reported that benzimidazole-based hybrids and metal complexes showed enhanced anticancer activity with lower IC_{50} values, while SAR analysis helped explain how structural modification contributed to improved biological activity and target interaction. Therefore, the mechanism patterns discussed in this study are in line with previous research, indicating that modified and hybridized compounds have strong development potential as anticancer drug candidates because they can act through specific and multitarget mechanisms.

CONCLUSION

Based on a review of 15 journals, the Structure–Activity Relationship (SAR) approach has been shown to play a crucial role in the optimization and development of anticancer compounds as drug candidates. Structural modifications such as the addition of functional groups, ring substitutions, and molecular hybridization consistently enhance biological activity, as indicated by a decrease in IC_{50} values down to the micromolar and nanomolar scales. Furthermore, the structure–activity relationship also contributes to increased selectivity and mechanism of action of compounds against specific targets such as enzymes and cancer receptors. Thus, SAR can be used as a scientific basis for the rational design of more effective and selective anticancer drugs. However, this study still has limitations, such as method variation between studies and the dominance of in silico studies without further experimental validation. Therefore, further research needs to integrate computational approaches with in vitro and in vivo assays, as well as evaluate pharmacokinetic and toxicity aspects. Furthermore, compound development through SAR-based structure optimization and molecular hybridization approaches needs to be continued to produce more potential and applicable anticancer drug candidates.

Further research is recommended to integrate the Structure–Activity Relationship (SAR) approach with more comprehensive experimental tests, such as in vitro and in vivo tests, to validate the results of in silico studies, which are still dominant in some studies. Furthermore, evaluation of pharmacokinetic, toxicity, and bioavailability aspects is necessary to ensure the safety and effectiveness of compounds as anticancer drug candidates. Furthermore, the development of SAR-based compounds through molecular hybridization strategies and functional group optimization needs to be continuously improved to produce compounds with more specific and selective multitarget activity. Research also needs to be directed at the development of modern formulations, such as nanoformulations, to improve the stability and efficiency of drug delivery, thus optimizing their potential clinical applications.

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