Article

A Review on Procedure of QSAR Assessment in Organic Compounds as a Measure of Antioxidant Potentiality

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Abstract:

Chemical and biological properties of substances may be inferred from their more fundamental physical, chemical, and biological characteristics using QSAR models. An insilico model may be built using QSAR to anticipate the activity of novel molecules before they are synthesised, allowing the author to establish a quantifiable link between structure and behaviour. QSAR is a powerful tool. Although QSAR modelling is a computer area, medicinal chemists are the main users and ultimate assessors, especially when it comes to developing compounds with the necessary biological activity. Several studies were conducted in which medicinal chemists and cheminformaticians collaborated to discover new compounds with specific biological activity. This was done through the development of QSAR models and their use in virtual screening, followed by experimental verification. Despite the fact that QSAR methods have their own set of limitations, their use in molecular prediction and assessment has been effective due to a division of labour in which mathematical professionals ensured the greatest quality of models. The predictions also helped experimental chemists design and test compounds that were expected to be successful. This review is being developed and implemented to look into the development of the QSAR tool in the assessment of antioxidant potentiality for diverse organic chemicals found in our environment.

Keywords:

QSAR Assessment, Organic Compounds, Anti-Oxidant Potentiality

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1. Introduction

Computational models that seek to predict complex physico-chemical/biological aspects of the materials are known as quantitative structure-activity relationships (QSARs). QSAR allows researchers to develop a reliable logical knowledge of the structure and behavior, which can then be utilised to create an in silico model to predict the activity of novel compounds before they are synthesised[18].

Quantitative Structure-Activity Relationship (QSAR) is a statistical tool that permits the numerical correlation of biological activity with changes in molecular structure. This means that each molecule's biological activities and functions may be described by a specific chemical descriptor, and the biological effect can be determined using specialised regression algorithms[17].

Computer techniques that begin with a precise molecular structure description and end with findings on the role molecules play in environmental, physicochemical, and biological systems under inquiry are responsible for this conclusion. The end result of a QSAR study is a set of mathematical equations that connect the chemical structure of a molecule with its biological activity. 4–6 Multiple representations of a molecule are examined in order to find the best accurate chemical descriptors for a certain feature[18].

QSAR arose and evolved in response to the necessity and aim of medicinal chemists to anticipate biological reaction. It ultimately made its way into agrochemistry, medicinal chemistry, and most other branches of chemistry. Drug resistance, toxicity forecasting, and physico-chemical features prediction may all be accurately predicted using QSAR models, according to references in the fields of environmental chemistry and drug development.

As a result, the core principles mentioned here are the most widely studied materials. This literature analysis on Procedure of QSAR Assessment in Organic Compounds As a Measure of Antioxidant Potentiality elaborates on and seeks to go beyond existing theories and practises in order to highlight the long term prospects of QSAR Assessment Models relevant in this study area.

1.1 Emergence and Purpose of QSAR Assessment in Biomedical Observations

A variety of statistical and machine learning techniques have been used to analyse very large datasets containing thousands of different molecular structures, expanding the QSAR representation from small datasets containing thousands of different molecular formats to more complex datasets containing millions of different molecular formats. Few tools used for QSAR calculation is SYBYL-X 2.1, VLifeMDS 4.6, Hypercam 8.0.

Hansch et al. published a paper in 1962 that laid the groundwork for present QSAR practise.

This paper was the sum total of a fifteen-year attempt to learn the justification of plant development supervisory structure-activity relationships (SARs), with the majority of that effort invested attempting to select a decent Hammett relationship, which was the dominant methodology for explaining substituent effects on chemical reactivity at the time. In the absence of a strong association, Hansch pursued Veldstra's views and looked into the effect of lipophilicity on biological potency[16].

Biochemical prescribers, on the other hand, were interested in the impact of molecular partition coefficients on drug uptake at the time. This method was first used by Overton and Meyer fifty years ago, and then by Collander in the 1930s. Notably, in the mid-1900s, Fieser, a famous organic chemist, demonstrated visually the link connecting naphthoquinones' antimalarial efficacy and their ether-water distribution coefficients.[14] For diverse class of compounds, he also discovered a constant optimum lipophilicity[16].

Useful in the early stages of the drug development process, in silico techniques Molecule formulation, biological activity prediction, lead compound optimization and virtual screening, classification of pharmacological action mechanism diagnostics and understanding, environmental toxic effects projection and drug-induced toxic evaluation[19] have all employed QSAR. Screening libraries that closely mimic drugs are being created using phytochemistry methods. QSARs, pharmacophores, and virtual screening can speed up the development of better medications. 48 QSAR models have been developed using traditional medicinal plants' phenolic components and flavonoids (such curcuminoids and tannins) for antibacterial and wound-healing properties.

1.2 QSAR Processes Applied in Biomedical Assessment

Quantitative structure-activity relationship (QSAR) interactions are becoming more significant in the drug development process because they are the most cost-effective choice for mid-throughput testing and low vivo performance testing. Predicting biological activities of unknown substances, drug resistance, hazardousness, and physicochemical properties in drug development and environmental toxicity are all made possible via the use of QSAR models, which are now widely regarded as academically acceptable approaches.[17].

Various researchers have conducted previous research on the subject. Adenosine antagonists were tested using a QSAR study in a series of 8-substituted xanthines. Exploring preferred binding mode for selected chemicals, multilayer neural feed networks and docking courses. With toxicity of polycylic aromatics hydrocarbons (PAHs), QSAR models were developed (PAHs).

The QSAR for N-Amino-N'-hydroxyguanidine Hydrazones as Xanthine Oxidase Electron Acceptors was created. For the first time in the publication, antiviral QSAR models were utilised to estimate the mt-QSAR model of 500

medicines tested on 40 distinct viruses. Using Markov Chain theory, generate a new multi-target entropy comparable to the QSAR model.

1.3 General QSAR Biomedical Assessment Steps

The inclusion of cellular components and the creation of 3-D representations are essential first steps in QSPR/QSAR research. Geometric calculations need the use of three-dimensional molecule models. The creation of molecular structure definitions is the second critical phase in QSPR / QSAR research. Feature selection methods can be used to choose the most important definitions in the third step. Fourth in QSPR/QSAR research is the development of QSPR/QSAR models using descriptive sets.

Topological, geometrical, electronic, and hybrid adjectives are the four categories of adjectives. Topological adjectives are graph variants produced utilising graph theory concepts in chemistry. Examples of topological adjectives include atomic figures, ring counts, molecular weight, weighted lines, molecular connections, subcutaneous computations, molecular distance descriptors, kappa indices, electro-topological status indicators, and other rules.

Calculation of electrical adjectives includes the features required for electrons. Part-time atomic costs, HOMO or LUMO power, and dipole moment are examples of electronic adjectives. Inertia times, melting point, height and width measurements, shadow regions, and gravitational index are some of the 3-D elements of a coded molecule structure using geometric adjectives[17].

The charged component adjectives are a composite formula that incorporates the proclivity of a polar cohesive compound. Charge descriptions of the Charge partial surface area (CPSA) are built on the atomic charge of each component and the surface area.

In the fifth and final phase, an external prediction set is used to test the model's ability to anticipate the activity of objects. In order to quickly discover the model's suitability, the outcomes of prediction should be compared with those of a training set and a sample confirmation of the opposite.

1.4 Limitations and Challenges in QSAR Biomedical Assessment

Although commonly utilised in drug design and molecular predictions, QSAR techniques have a number of flaws that cause them to be inaccurate in some situations. In most circumstances, when two or more samples are used in a single interpretation to construct a QSAR model in vitro, the model's coherence is jeopardised.

In addition, as long as two descriptors are strongly collinear, they supply the same information twice in a QSAR response, resulting in a complicated statistical connection and making it much more difficult to comprehend the QSAR.

Thousands of molecular descriptors are currently available for QSAR, and many of them are challenging to understand in a physical-chemical sense.

Descriptors in published QSAR models aren't usually well-defined or recognised, and mechanistic explanations aren't always supplied[16].

2. Objective

The Literature Review on application of QSAR assessment in identifying antioxidant potentiality present in organic compounds for medical purpose attempts to locate the correctness and scope of the tool so that it can be enhanced in its features and applicability ensuring more satisfying result with least possible difficulties or complexities that the current researches are facing.

3. Methodology

The present review article on QSAR Assessment Application to examine Antioxidant Potentiality of

Organic Compounds is entirely composed based on the existing authentic biochemical and medical analyses and articles that as published in acknowledged online portals, such as, Pub Med, Google Scholar, Science Direct, etc.. Genuine facts and informations are gathered from trusted web libraries and institute portals are thoroughly studied, sorted and selected based on their relevance to be

4. Literature Review

Sapra et al. (2014)[1] Antibacterial activity was investigated for a number of p-hydroxy benzoic acid derivatives (1–29). Generally, antimicrobial tests have indicated that schiff bases are more active than esters, with compound 14 being the most potent agent (pMICam=1.50 M/ml). The antibacterial activity of the synthesised compounds was examined using a QSAR method, Valence first-order molecular connectivity index, first-order shape index, and first-order valence index were employed to measure antibacterial activity in this experiment.

P. Erzincan et al. (2015)[2] identified 37 novel antioxidant coumarin derivatives as well as structural remodeling options for improving antioxidant activity. They were tested for antioxidant capabilities using QSAR models based on ferric-reducing antioxidant power (FRAP). Coriolic derivatives were optimised using a semi-empirical PM6 approach and the SPARTAN 10 computer programme.

The DRAGON 6.0 programme was used to generate the descriptors. An MLR model was created using the QSARINS 2.2.1 tool and evaluated using a variety of training/test set pairs. A mix of internal and external validations assessed the models' robustness, dependability, and predictive capacity. Antioxidant action was described in the model as being complex, H-bond donor, and lipophilic. Additionally, we synthesised 31 novel antioxidant coumarin derivatives, whose

antioxidant activity was predicted using the best two-descriptor approach. Antioxidant properties are seen in the majority of these compounds.

QSAR analysis was used by Vashist et al. (2015)[3] to link antibacterial activity of substituted benzimidazole derivatives to their physico-chemical characteristics. Leave one out was utilised to cross-validate QSAR models created before. In order to do cross-validation, a number of statistical measures were used, including Friedman's lack of fit, the standard error of prediction, and the quality value. Antibacterial activity of substituted benzimidazole compounds was described by WAP, Mlog P, and UI in QSAR tests.

Baldim et al. (2017)[4] investigated the structure and activity of 40 flavonoids with the goal of correlating leishmanicidal, trypanocidal, antioxidant, and prooxidant characteristics using integrated networks and QSAR models. To understand the influence of antioxidant and prooxidant activities on antiparasitic properties, the classical groups for flavonoids' antioxidant properties were merged. These studies will aid in the development of effective leishmaniasis and trypanosomiasis treatments. The experimental findings indicate that flavonoids with both anti- and prooxidant properties had dual action, implying that finding a balance between these two properties could be crucial in developing effective therapeutic solutions.

In a mini-review, Neves et al.[5] described and critically examined recent advances in QSAR-based virtual screening (VS) in drug discovery, demonstrating successful applications in identifying potential compounds with desired features. In addition, the study included some recommendations for best practises for QSAR-based VS, as well as the approach's future prospects.

Ogadimma Alisi et al. (2019)[6] The free radical scavenging characteristics of 1,3,4-oxadiazoles were studied using a quantitative structure activity relationship (QSAR). Using Becke's three-parameter Lee-Yang-Parr (B3LYP) hybrid functional and the 6-311G basis set, the whole oxadiazole derivative data set was reduced and then optimised in DFT. To separate the data into training and testing sets, we employed the Kennard Stone approach.

The training set was used to generate QSAR models using the genetic function technique, while the test set was utilised to assess the developed models (GFA). To get to the usefulness space of the constructed model, the leverage strategy was applied. The variance inflation factor, degree of contribution, and mean effect of each descriptor were calculated. Quantum chemical and molecular descriptors were constructed for each molecule in the data set. Five prediction models were developed that satisfied all of the acceptance requirements and performed well in validation. The QSAR analysis revealed that the sum of e-state descriptors of power for prospective hydrogen bonds of path length 9 (SHBint9) and topological radius (topoRadius) are the most important descriptors that impact the free radical scavenging activities of 1,3,4-oxadiazole derivatives.

Sharma et al. (2019)[7] examined physicochemical properties using QSAR and the modelling software Win CAChe 6.1. HOMO and LUMO energies, as well as conformational minimum energies (CME), log P, the ionisation potential (IP), the molar refractivity (MR), and the Shape Index were estimated (SAS). A total of 18 compounds were selected at random for the training set, and 10 were selected at

random for the test set. Using stepwise multiple linear regression analysis, the best models were identified. The correctness of the equation was established. Streptococcus mutans was shown to be ineffective against C5. In contrast, 2,3-dihydroflavan-3-ol derivatives were found to have MICs between 1000 and 500 g/ml for all 3-hydroxyflavone molecules. This is the MIC for the chalcone derivatives.

Duchowicz et al. (2019)[8] Researchers conducted their analysis using experimental data from antioxidant tests of seventeen anthocyanins and six distinct anthocyanidins. The quantitative structure–activity relationship (QSAR) assessment was found. In vitro and ex vivo studies were conducted to determine the inhibitor's ability to protect against lipid peroxidation in emulsified and bulk oil (methyl linoleate) at doses of 50, 250, and 50 M, respectively. The 1,1-diphenyl-2-picrylhydrazyl radical (DPPH) was used in the experiment to anticipate the action of radical scavengers. Quantitative structural analysis of the anthocyanin/anthocyanidin compounds was possible thanks to the QSAR models developed for each test and concentration. It was possible to make predictions about the antioxidant activity of twenty-one substances whose experimental values had not yet been determined.

Gul et al. (2019)[9] As part of their research into the binding mechanisms that might affect anticancer effectiveness, they used a computer-aided computational MOE software programme and a variety of poly (azomethine) esters that they synthesised in the lab. A Schiff base phenol was polycondensed with terephthaloyl chloride in the solution phase to produce PAME (TC). Terpolymers were made by combining various moieties with TC and SB in the main chain. The structure was deduced by the use of spectroscopy and elemental analysis.

Using a docking technique, it was determined that the anticancer protein complex docked in the same active site pocket as the material (PDB code: 1T69). Glitch bonding was shown to be the most common method of contact between the material and double-stranded DNA after molecular docking and quantitative structure activity relationship (QSAR) studies (PDB ID-1BNA). The material's physicochemical qualities were shown to have a direct impact on the binding strength. The formation constant values calculated demonstrated that the polymer-DNA complex had good binding strength. As a result, the synthesised substance was expected to have anticancer properties and might potentially be used as an anticancer medicine.

Drapak et al. (2019)[10] 1-[2-(R-phenylimino) 4-methyl-3-[morpholine-4-yl] propanoic acid]-2,3-dihydro-1,3-thiazol-5-yl] is the name of the 14 derivatives of this compound. they calculated the total number of chemical descriptors for ethane-1-one (electronic, steric, geometric, and energy). Training and test samples were created for QSAR analysis. A multivariate linear QSAR-model was used to show the relationships between antioxidant activity and the above-mentioned chemical descriptors.

When it comes to antioxidant activity, polarisation, dipole moment, lipophilicity, energy parameters, and molecule size and branching all played a role in the QSAR research. The antioxidant activity of the compounds was improved by hydrophilic and reductive features; the antioxidant activity of molecules with

small volume and surface area was stronger. The QSAR models were used to develop new possible antioxidants within the above-mentioned row of chemicals, and predictions of antioxidant activity were presented as a theoretical foundation.

Yan et al. (2020)[11] used 3D-QSAR models to create two new antioxidative tripeptides, GWY and QWY. An enhanced TEAC assay validated their activity. The findings of the experiments revealed that GWY and QWY had good antioxidant activity, with 3.32 mM TE and 2.97 mM TE, respectively. According to the findings, 3D-QSAR models provide a high predictive capacity for drug design. To identify the probable molecular mechanism of antioxidant peptides, molecular docking and molecular dynamics modelling were used.

Spiegel et al. (2020)[12] The antioxidant potential of a collection of 22 phenolic acids was evaluated experimentally and theoretically using several models of aromatic ring hydroxylation and methoxylation. This characteristic was tested using a ferric reducing antioxidant power test. It was shown that 2,3-dihydroxybenzoic acid was the most potent antioxidant, whereas monohydroxylated and methoxylated molecules had the lowest levels of activity.

Compound topology, resonance stabilisation, and intramolecular hydrogen bonding were all shown to have a role in the structure–activity connection. An ortho- or para-positional arrangement of two or more hydroxyl groups was the most significant finding. When all of these characteristics were taken into account, a multiple linear regression model was created that showed a connection between compound structure and antioxidant capacity.

Wijianto et al. (2020)[13] MOE 2018.01.01 software was utilised to do molecular modelling study using the semi-empirical quantum chemistry method AM-1 approach. Build QSAR was used to develop an equation model for the development of novel curcumin mono-ketone analogues. As a result of an aldol condensation process, a new chemical is created. To investigate antioxidant activity, the lipid peroxide concentration was determined using the thiobarbituric acid reactive substance (TBARS) approach. The QSAR analysis found inhibitory action based on potential lipid peroxidation prediction performance.

2,6-bis-(3'-ethoxy,4'-hydroxybenzylidene)-cyclohexanone,2,6-bis-(3'-Bromo,4'- thoxybenzylidene)-cyclohexanone, and 2, 6-bis-(3',4'-dimethoxybenzylidene)-cyclohexanone showed good inhibitory activity against lipid peroxidation in vitro, with IC50 values of 2.95; 0.95; and 2.45 μM respectively. The new mono-ketone analogues of the curcumin molecule demonstrated antioxidant activity in the QSAR study by lowering lipid peroxidation and scavenging free radicals.

Ying Shi (2021)[14] The quantitative structure–activity relationships of 75 phenolic compounds with Trolox-equivalent antioxidant ability were examined using support vector regression (QSAR). Applied to MOPAC's geometric structures, this method had a positive effect. In order to calculate Pearson correlation coefficients, we used n(OH), Cosmo Area (CA), Core-Core Repulsion (CCR), and Final Heat of Formation (FHF) (FHF).

The leave-one-out cross-validation (LOOCV) correlation coefficient was used to assess the prediction capability of the QSAR model after it was developed using the training set of 57 compounds. An artificial neural network (ANN) and multiple linear regression (MLR) were used to analyse the data (MLR). Simply expressed, the RMSE values for LOOCV are 4.44 for SVR, 0.546 for ANN, and 0.54 for (MLR). For the prediction of 18 external compounds, the RMSE for SVR, ANN, and MLR models was 0.41, 0.39, and 0.54, respectively. SVR models were able to properly predict phenolic compounds' TEAC using SVR data, according to the results.

Khairullina et al. (2021)[15] employed 9 QSAR consensus models that were statistically significant. They were able to predict the lgk7 values for the compounds in the training sets with a high degree of accuracy. Also, using atomic and molecular descriptors, could accurately predict lgk7 for test materials.

The RBF-SCR method was used to narrow the list of potential descriptors down to a manageable number. For 8-PPDA, an established antioxidant, our theoretical prediction of the lgk7 is in agreement with the experimental value measure. They were able to use the GUSAR 2013 tool to predict the kinetic parameters of hydrocarbon oxidation processes in this experiment. These 74 compounds were tested for their quantitative structure–antioxidant activity correlation in this study. They ranged from 0.01 to 6.55, and were found to have a lgk7 of 0.01 to 6.55.

5. Findings and Conclusions

The Literatures on QSAR Assessments in ensuring Antioxidant Potentiality from potential organic compounds indicates a varied area of applications for the tool to predict the potentiality of herbal drugs in a number of tough medical disorders, such as, anticancer, diabetes, immunity boosters, etc. However, the process is highly dependent on selection and computation of descriptors where the result may impact the final output and that may vary with change of experimental set up. Since the process is currently being largely connected with computer based machine learning approaches, feature selection and use of datasets need to be considered for result accuracy.

6. Recommendations and Suggestions

Based on the literature review presented for QSAR based Antioxidant Assessment for Organic Compounds, it is observed that QSAR tool needs robust datasets to achieve effective result in the conducted study supported by ideal choice of predictors and cross-validation methods. As the area of application of this tool is expanding with machine learning algorithms to aid for its computation, more

specified sample dataset should be constructed to ease the decision-making and prediction process. Suitable comparison and cross-validation should be planned to obtain least faulty and more effective result.

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