

Nano-medicine effectiveness in pediatric patients: An artificial intelligence investigation

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Abstract. Emerge of nanotechnology has affected many aspects of our life and also triggers research studies in many fields. Nano-medicine are proven to be effective in encountering diseases. In the present study, aspects of the applications and effectiveness of nano-medicine in pediatrics patients are studied. In this regard, using experimental data of previous published researches, combination and dose of nano-medicines are optimized using response surface method and neural-fuzzy inference network. The input parameters of the selected multiple nano-medicines are dose and type and the output is the effectiveness of the combinations using IC50 parameter. A detailed parameter study is presented to observe effects of each inputs on the IC50. The results indicate that personalized scaling of nano-medicine is required in therapy of pediatric diseases such as cancers.

Keywords: artificial intelligence; cancer; nano-medicine; nanoparticles; pediatric patients

1. Introduction

Diseases in children are different in many aspects from their equivalent disease in adults and different treatment procedure should be adopted. For an account, there are three main differences in pediatrics and adults cancers (Zou *et al.* 2019, Liu *et al.* 2021c, Hou *et al.* 2022, Xue *et al.* 2022). First, cancer in children is not caused by life style. Second, for the same cancer therapy, a different response is seen in children, and third, type of mutation is different (Dai and Safarpour 2021, Forsat *et al.* 2021, Ghamkhar *et al.* 2021, Khadimallah *et al.* 2021a, Khadimallah *et al.* 2021b, Kumar *et al.* 2021, Madenci 2021, Tlidji *et al.* 2021). Therefore, specific treatments must be sought in the case of pediatric patients.

Using nanomaterials in the medical treatment have found several applications (Fan *et al.* 2022, Luo *et al.* 2022b, Wang *et al.* 2022a, Xia *et al.* 2022). In the ligament injury repair, graphene nanocomposites (Habibi *et al.* 2019a, d, e, Al-Furjan *et al.* 2020d, f, i, j) are utilized in scaffold shape instead of conventional screws (Silva *et al.* 2020). Recent developments in nanotechnology in different fields make drug delivery more efficient and simpler. Using iron oxide nanoparticles (NPs) as carriers of medicine, it is possible to direct the nano-medicine to a specific location in the body. On the other hand, the amount of the chemical medicine is considerably reduced using nano-carriers (Jin and Wang 2019, Gao *et al.* 2020, Li and Wang 2021, Jin *et al.* 2022). Using in vitro experiments, Sunoqrot and Abujamous (2019) demonstrated that effects of drug delivery using NPs was significantly higher than conventional drug administration. They used a polymeric NP of the drug with mean diameter 66.8nm. The results showed that the

parameter IC₅₀ in nano-medicine was extremely lower than conventional drug which indicates its effectiveness. Kim *et al.* (Kim *et al.* 2010) reviewed the application of nano-structure in the drug-delivery applications (Habibi *et al.* 2017, 2019a, c, Safarpour *et al.* 2018, 2019b, 2020, Alipour *et al.* 2020, Ebrahimi *et al.* 2020a, Ghazanfari *et al.* 2020, Chen *et al.* 2022). de Lázaro and Mooney (de Lázaro and Mooney 2021) explored the barriers in the effectiveness of nano-medicines and suggested two possible solutions to improve the efficiency of nano-medicines. Cellot *et al.* (2021) gathered recent studies on the graphene based nano materials used in the brain pathologies. They discussed the wide application of the graphene in the drug delivery system and concluded that successful applications of graphene in multi-purpose nano-devices make them a proper choice of controlling active molecules in different diseases. Nieto González *et al.* (2021) explored applications of polymeric and lipid nanoparticles in development of nano-medicine with emphasis on pediatrics diseases. The various usages of both categories were discussed in detail and it was concluded that these NPs could be utilized not only in cancer treatment but also in chronic diseases. However, there few studies on the actual therapeutic effectiveness of them. Thus, in vivo experiments are necessary to assess effects of these NPs prior to further investigations on the topic. In the case of brain cancer, standard treatment of using chemotherapy usually has the risk of brain damage in children (Guido *et al.* 2022). Thus, the novel treatment development is a must in the case of pediatric brain cancer. Using nano-medicine showed a promising method which could overcome brain and blood obstacles in brain (Ebrahimi *et al.* 2019b, c, 2020b, Hashemi *et al.* 2019, Moayedi *et al.* 2019, 2020a, b, Mohammadgholiha *et al.* 2019, Mohammadi *et al.* 2019, Habibi *et al.* 2020, Oyarhossein *et al.* 2020, Shariati *et al.* 2020a, b, Shokrgozar *et al.* 2020).

First phase in evaluation of nanoparticles as drug

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delivery vehicles is molecular dynamics (MD) method in which a detailed chemical and physical calculations are performed on the interaction of nanoparticles with its circumstances inside the body (Habibi *et al.* 2016, 2018a, b, 2019b, d, e, Ebrahimi *et al.* 2019a, Esmailpoor Hajilak *et al.* 2019, Pourjabari *et al.* 2019, Safarpour *et al.* 2019a, Zhu *et al.* 2022). Lee (2021) gathered published MD simulations on the interaction of NPs' surface with different protein in blood during its journey inside body. The simulations accurately revealed the interactions of proteins and NPs and covering NPs by proteins. These simulations had capability to show reactions which were hardly followed by experiments. Different simulation method in modeling drug delivery system were reviewed by Moradi Kashkooli *et al.* (2021). They mentioned several discrete and continuous mathematical models used in simulations and concluded that using simulation and in vitro experiments drug delivery behavior could be predicted.

Computational costs of the MD and finite elements method (FEM) (Hashemi *et al.* 2019, Al-Furjan *et al.* 2020c, e, g, f, Bai *et al.* 2020, Cheshmeh *et al.* 2020, Li *et al.* 2020a, Lori *et al.* 2020, Najaafi *et al.* 2020, Shariati *et al.* 2020c, Xiong *et al.* 2020, Guo *et al.* 2021b, Liu *et al.* 2021a) triggered employment of novel approaches in predictions of nano-medicines behavior and body responses (Amelirad and Assempour 2019, Amelirad and Assempour 2021). Ho *et al.* (2019) discussed the role of the artificial intelligence (AI) methods (Cavaleri *et al.* 2017) in the case when multiple nano-medicine are used for treatment. They concluded that the dose of each medicine could be optimized in an effective way using AI. Rashid *et al.* (2018) presented an experimental evaluations of combination of multiple nano-medicines on mics. They presented a response surface optimization method to acquire the best combination of the drug to improve efficiency of the results. Several studies showed that personalized drug dosing in a must in many cases (Zarrinpar *et al.* 2016, Rashid *et al.* 2018). The possible combination of nanofluidics and artificial intelligence methods was discussed in detail using previously published study by Liu *et al.* (2021d). The design and optimization of drug delivery systems were collected by Serov and Vinogradov (2022). In this review paper, the employment of different machine learning (ML) and artificial neural networks in the field of drug delivery were discussed. There could be found many review articles on the application of AI in nano-medicine, nanotechnology, drug design which are related to the pediatric patients (Casañola-Martin and Pham-The 2019, Adir *et al.* 2020, Singh *et al.* 2020a, b, Hayat *et al.* 2021). Using artificial intelligence and machine learning (ML) methods in cytotoxicity are widely used in the biology and nano-medicine. The toxicity of nano-carriers was gathered in an article by Singh *et al.* (2020b). They presented a roadmap to use AI methods in nano-cytotoxicity. Liu *et al.* (Liu *et al.* 2021e) explored cytotoxicity of metal NPs were using two approaches of ML: random forest and decision tree. They discussed the application ML in improvement of design of drug vehicles. Using the experimental results, Fjodorova *et al.* (2017) evaluated toxicity of metal oxide NPs and presented several effective factors in NPs. Several different

ML models were used by Kar *et al.* (2021) to detect the most toxic metal oxide nanoparticles.

Scaling of nano-medicine is a challenging issue in the therapy of pediatric patients. Dose and type multiple nano-drugs have to be designed using new methods since the conventional methods may not responsive in the case of nano-medicines (Maojo *et al.* 2010). In addition to the dose and type of drug, timing of the drug delivery is another essential parameters in optimizing process (Zarrinpar *et al.* 2016).

In the present study, aspects of the applications and effectiveness of nano-medicine in pediatrics patients are studied. In this regard, using experimental data of previous published researches, combination and dose of nano-medicines are optimized using response surface method (RSM) and adaptive neural-network fuzzy inference system (ANFIS). The input parameters of the selected multiple nano-medicines are dose and type and the output is the effectiveness of the combinations using IC_{50} parameter and A detailed parameter study is presented to observe effects of each inputs on the IC_{50} .

2. Materials and methods

2.1 Experimental data

Experimental data of different nano-medicines is acquired from (Rashid *et al.* 2018) and it is available online from supplementary tables along with the published article. In this article, effects of concentration and type of medicines on the inhibition of some blood cells to 50%, i.e. IC_{50} . The drugs and inhibitors include dactinomycin (Dac), decitabine (Dec), mechlorethamine hydrochloride (Mech), mitomycin C (MitoC) and bortezomib (Bort). Also concentration and combinations of these materials are also considered as effective factors on IC_{50} .

2.2 Response surface method (RSM)

The response surface method provides a platform for fitting the available data using quadratic polynomial function (Adamian *et al.* 2020, Al-Furjan *et al.* 2020a, b, Li *et al.* 2020b, Liu *et al.* 2020c, d, 2021b, Wang *et al.* 2020, Zare *et al.* 2020, Zhou *et al.* 2020, Dai *et al.* 2021a, b, Guo *et al.* 2021a, Habibi *et al.* 2021, He *et al.* 2021, Huang *et al.* 2021a, Shao *et al.* 2021, Wu and Habibi 2021, Zhang *et al.* 2021, Kong *et al.* 2022) to obtain effect of each parameter as well as effects of combinations of factors. The fitted functions are further use to find optimum point of the output, here is minimization of IC_{50} . Moreover, the most effective factor can be achieved using this method.

2.3 Neural fuzzy network

Combination of neural network with fuzzy logic provides a suitable approach for prediction of different responses of a system with a high accuracy and lower computational effort compared to conventional artificial neural networks (ANNs) (Jang 1993). In this type of neural

network, input data (values of each factor) converted to their respective fuzzy values using membership function (Cai *et al.* 2020, Liu *et al.* 2020b, Xiang *et al.* 2021b, 2022a, Lu *et al.* 2022). The effects of all input factors from concentration to the proportion of each drug further combined into one factor using AND statement (Ma *et al.* 2022, Zhao *et al.* 2022, Hou *et al.* 2021, Huang *et al.* 2021b, c, Jiao *et al.* 2021, Liu *et al.* 2021f, Moradi *et al.* 2021, Xu *et al.* 2021, Dong *et al.* 2022, Luo *et al.* 2022a, Michael *et al.* 2022, Wang *et al.* 2022c, Yang *et al.* 2022b, Yu *et al.* 2022):

$$w_i = \prod_{k=1}^N \mu(A_k) \quad (1)$$

where w_i is the combined fuzzy factor of the membership values $\mu(A_k)$ for each effective factor. Each fuzzy value following a rule in which N number of the factors are taken into effect in the rule (Liu *et al.* 2020a, Xiang *et al.* 2021a, 2022b, Xiang 2022). Number of rules in each network are governed by the physics of the problem. The obtained combined fuzzy factor for all rules are normalized according to the below equations (Fan *et al.* 2022, Luo *et al.* 2022b, Michael *et al.* 2022, Wang *et al.* 2022b, c, Yang *et al.* 2022a, Zheng *et al.* 2022):

$$\bar{w}_i = \frac{w_i}{\sum w_j} \quad (2)$$

Membership function has different forms from triangular shape to bell shape functions. In this study, we adopt a triangular shape function for simplicity. This method makes it possible to obtain the values of IC_{50} in the case of new combination of inputs with high accuracy. Since, in contrast to the RSM, in this method correlation factor are very high and the network is evaluated by test data to observe its functionality and efficiency.

3. Results and discussion

3.1 RSM results

The fitted equation in the RSM method are obtained as following:

$$\begin{aligned} IC_{50} = & 202 - 8.05 \text{ concentration} - 202 \text{ Bort} \\ & - 201 \text{ Dac} - 202 \text{ Dec} - 201 \text{ Mech} - 201 \text{ MitoC} \\ & + 0.000321 \text{ concentration} * \text{concentration} \\ & + 0.375 \text{ Bort} * \text{Bort} + 1.130 \text{ Dec} * \text{Dec} \\ & + 8.03 \text{ concentration} * \text{Bort} + 8.03 \text{ concentration} * \text{Dac} \\ & + 8.03 \text{ concentration} * \text{Dec} + 8.01 \text{ concentration} * \text{Mech} \\ & + 8.03 \text{ concentration} * \text{MitoC} \end{aligned} \quad (3)$$

This a simple quadratic equation which can be used to deduce many conclusions. The factors and combination of factors absent in the equations are not influential on the IC_{50} . The importance of each parameters are demonstrated using Poreto chart in Fig. 1. As seen, the most important parameter is square value of concentration of the drugs. The second important factor is the square of the partition of Dec drug in the drug combination. On the other hand, the least important factor is presence of Mech nano-drug in the

Table 1 Optimum values of concentration and drug fraction for minimizing, maximizing the value of IC_{50}

	Concentration [μM]	Bort	Dac	Dec	Mech	MitoC
Max. IC_{50}	100	1	1	1	1	1
Min. IC_{50}	0.0	1	1	1	1	1
$IC_{50} = 0.6$	45.27	0	0	0.5024	0	0.5010

combination which can be a conclusive results. This results can be utilized to design new nano-medicines in the for pediatric cancers.

Difference between RSM output (quadratic fitting) and the actual values of IC_{50} for all data set is plotted in several ways in Fig. 2. It is deduced that the quadratic equations provide an acceptable agreement with actual values since the residuals fall between -0.5 to 0.5. However, it should be mentioned that this is not true for all problems. There are many experimental values which do not follow quadratic equations and the residuals may be extremely large in those cases.

The most powerful aspect of the RSM (Zhu *et al.* 2022) is the prediction of the optimum condition for the output IC_{50} based on the concentrations and fraction of the drugs. Table 1 provides the conditions in which minimum and maximum values of IC_{50} could be obtained. Moreover, the condition of obtaining a desirable value of IC_{50} is also presented. As seen, for maximizing the value of IC_{50} the model predicts, as expected, the concentration of 100 of the drugs. On the other minimum value also obtained for zero concentration. However, for other conditions the optimum value cannot be easily deduced from the data. In this table, the combination condition for $IC_{50} = 0.6$ is also presented which can be used in certain circumstances.

Effects of different individual effective factors are presented in this section. Fig. 3 shows the effect of Bort inhibitor fraction on the IC_{50} as predicted by RSM. It is observed that increasing Bort fraction cause decrease in IC_{50} and hence improvement in inhibition of the cell. However, caution must be taken when using these results since they are only a fitted result from experiment which may not follow a quadratic curve. It is also seen, increase in concentration of the nano-medicine dramatically reduces IC_{50} as expected in the absent of other drugs. On the other hand, combination of only two nano-medicine Bort and Dac results in improvement in inhibition of cancer cells.

Fig. 4 demonstrates effect of nano-medicine concentration on the IC_{50} for different Bort fraction in combination with other nano-medicine. It can be seen that with only Bort as drug in the combination at concentration = 24 μM the best results are obtained in terms of minimizing IC_{50} regardless of the fraction of the nano-medicine. In lower concentration, increase in the Bort fraction results in significant drop in IC_{50} . But in the Bort fraction equal to unity there observed slight increase in the IC_{50} and in the concentrations above 24 μM for Bort fraction of unity, increase in concentration cause inverse results. In this figure it is also depicted combination of Bort with only one other drug in various concentration. The general theme of the graph is the appearance of minimum point in the IC_{50} -

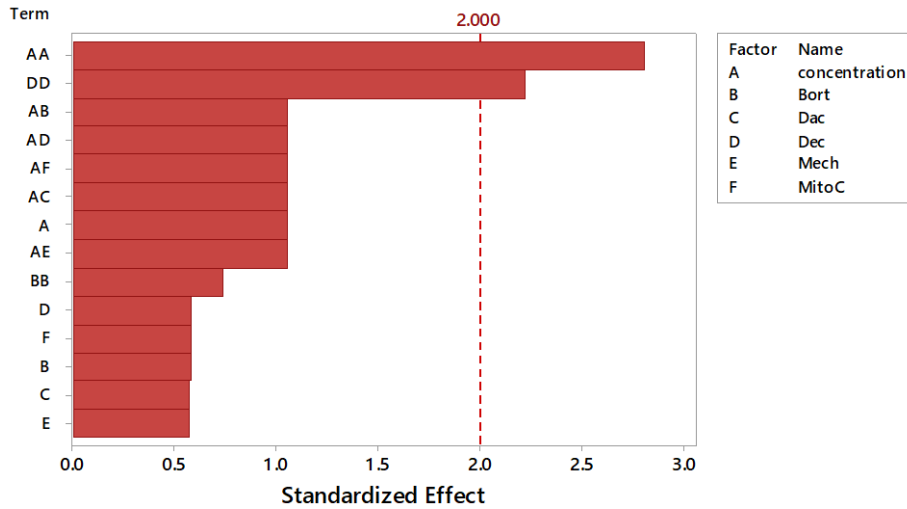


Fig. 1 Importance of different input factors of nano-medicines on IC_{50}

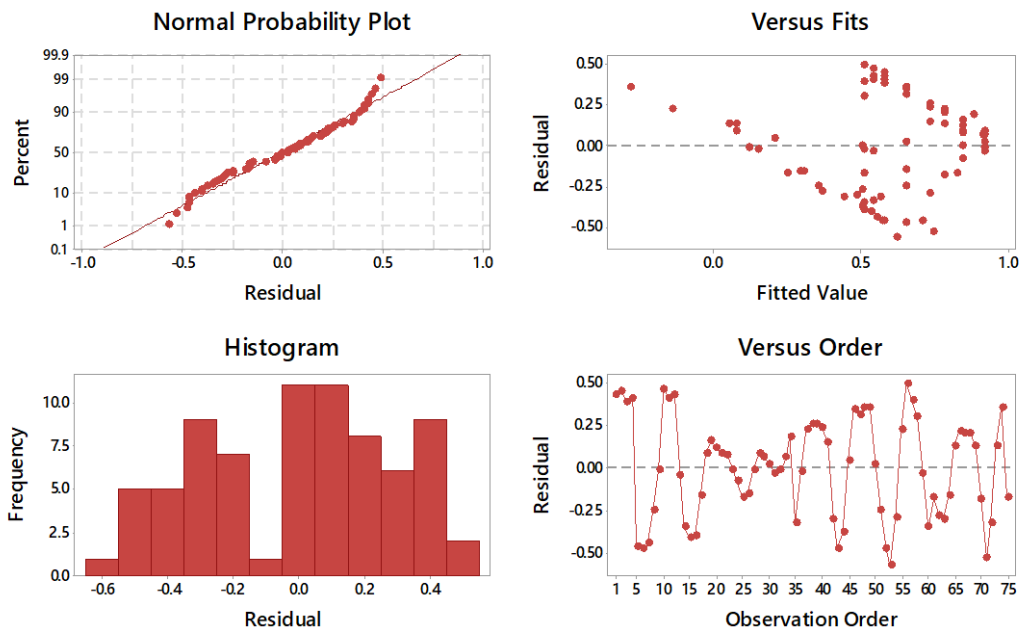


Fig. 2 Representation of residuals of the fitted quadratic functions in comparison to actual IC_{50}

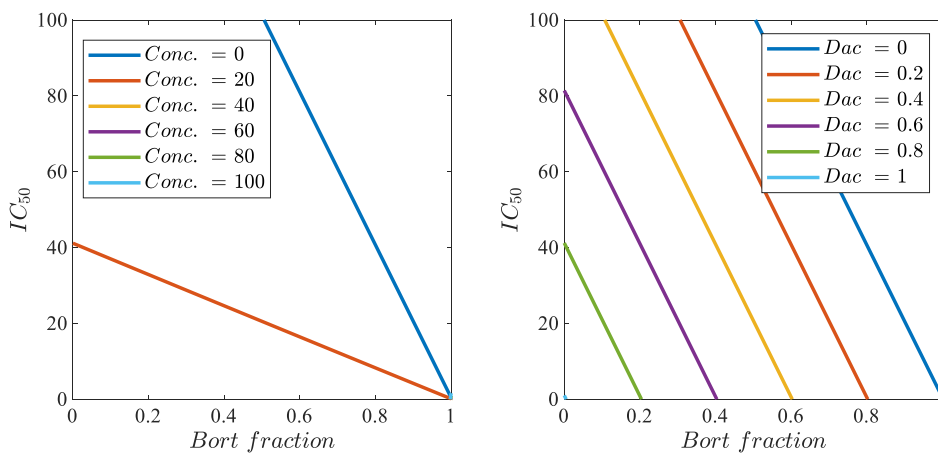


Fig. 3 Effect of Bort fraction on the IC_{50} for different values of concentration and Dec fraction in the absent of other nano-medicines

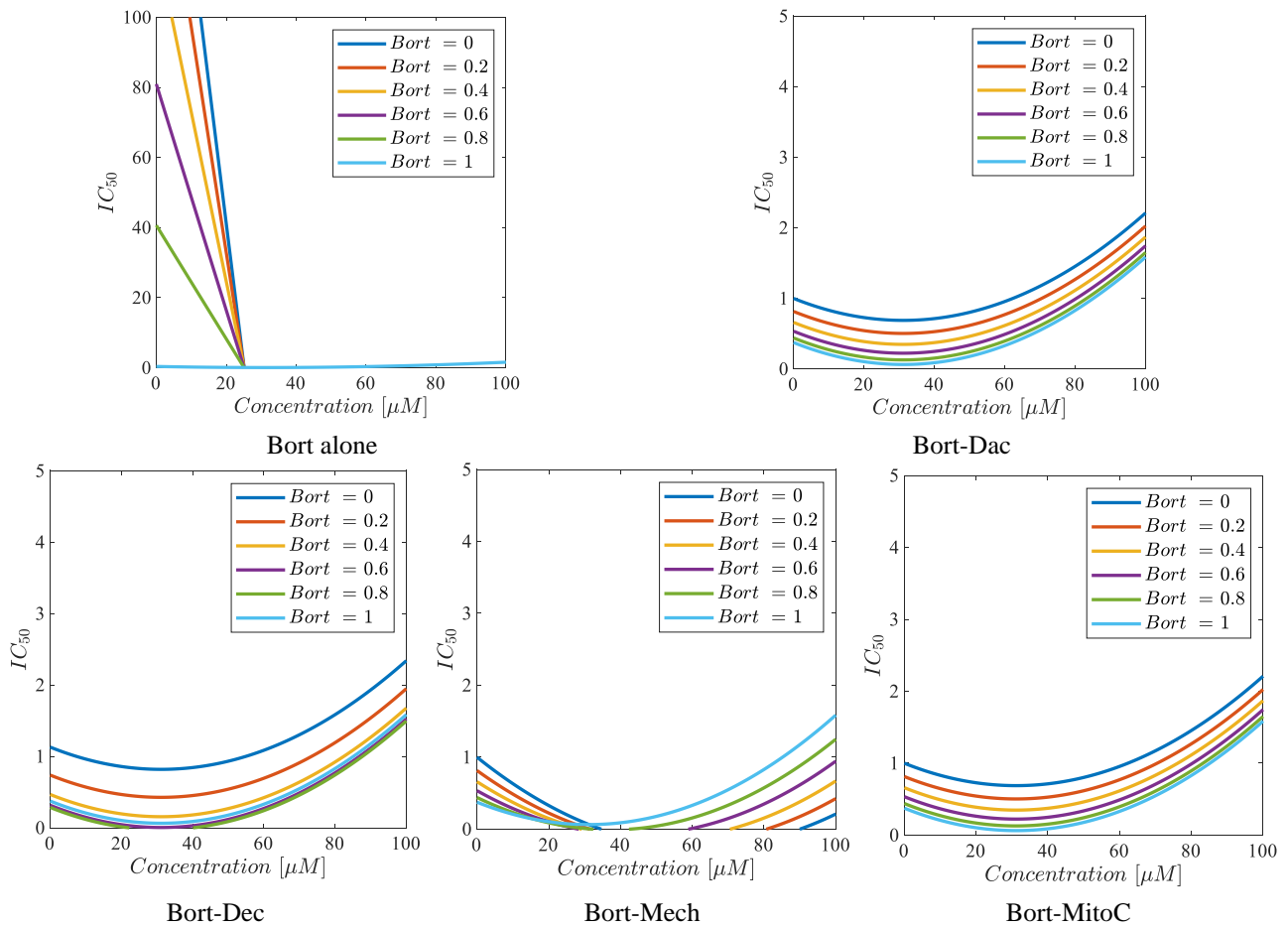


Fig. 4 Effect of the concentration and combination of nano-medicine with Bort on the IC_{50}

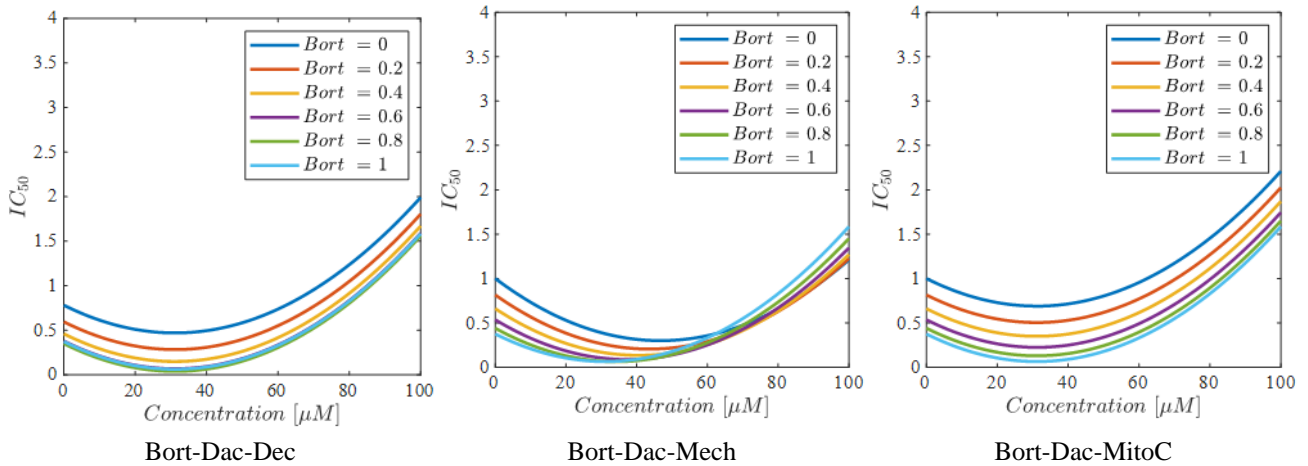


Fig. 5 Effect of Bort fraction on the IC_{50} for different values of concentration and Dec fraction in the absent of other nano-medicines

concentration curve between 20 to 40 μM . Therefore, regardless of the combinations of the nano-medicine against cancer cells, the concentration of the drug should keep between 20-40 μM . The specific value for each drug combination must be determined in each case. Among different combination of Bort nano-medicine with other drugs, the best results is obtained for Bort fraction = 0.6 and Mech fraction = 0.4 at 2-60 μM concentration which

minimizes the value of IC_{50} . In other cases, except for combination of Bort and Dec, the best results are obtained when Bort fraction is maximum or unity. However, and interesting results is obtained when Bort nano-medicine combined with Dec. In this case best results are at Bort fraction 0.8 and Dec fraction 0.2. In this case the IC_{50} curve is lower than all other fractions of these two nano-drugs.

Combinations of 3 nano-medicines are also possible in pediatric cancer therapy. In Fig. 5 the combination of Bort and Dec nano-medicine are depicted with only on another drug. The fraction of Dec and the third drug kept equal in these graphs. In the case of Bort-Dac-Dec the best results in terms of minimizing IC_{50} is obtained when Bort fraction equals to 0.8 and, consequently, the other two nano-medicine fraction equal to 0.1 each. In Bort-Dac-Mech combination, there is seen a turning point around 60 μM concentration in all combinations depicted. Prior to this value increase in Bort fraction cause deterioration of the drug efficacy. However, in the higher concentrations, the reverse effect is observed. The combination of Bort-Dac-MitoC effect is similar to combination of two medicine of Bort-Dac and Bort-MitoC in which maximum value of Bort gives the best results.

The above RSM results show the importance of nano-medicine design in terms of combination and concentration which hardly obtained from conventional methods.

3.2 ANFIS results

The ANFIS model described in Section 2 is employed to train a neural network capable of prediction of IC_{50} value in different nano-medicine combination and concentration. For this purpose, among total 75 set of experimental data 60 set is randomly selected to train the network and 15 set is used to test the model. The results of predicted values of IC_{50} and the actual measured values in different condition is shown in Figure 6. The correlation between data from trained network and the provided data for training is 0.921 after 50 epochs. At the same time the time the test set of input data is fed in the trained network to observe the differences between predicted IC_{50} and the actual measured value. The trained model satisfactorily predicts results with correlation equal to 0.892 which is regarded a high value.

The above results are obtained with time and computational effort much lower than RSM and experimental methods. The high correlation coefficients ensures us about the reliability of such methods. Therefore, artificial intelligence method have a great potential to be used alongside experimental methods to avoid some tedious experiments and scaling of nano-medicine in pediatric patients.

4. Conclusions

In the present study, aspects of the applications and effectiveness of nano-medicine in pediatrics patients were studied. Using experimental data of previous published researches, combination and dose of nano-medicines were optimized using response surface method (RSM) and adaptive neural-network fuzzy inference system (ANFIS). The input parameters of the selected multiple nano-medicines were dose and type and the output is the effectiveness of the combinations using IC_{50} parameter and A detailed parameter study is presented to observe effects of each inputs on the IC_{50} . The main outcome of the study can be encapsulated in the below:

- The most important parameter is square value of concentration of the drugs and the least important factor is presence of Mech nano-drug in the combination.
- The condition of obtaining a desirable value of IC_{50} can be calculated using RSM.
- Regardless of the combinations of the nano-medicine against cancer cells, the concentration of the drug should keep between 20-40 μM .
- With only Bort as drug in the combination at concentration = 24 μM the best results are obtained in terms of minimizing IC_{50} .
- When Bort nano-medicine combined with Dec, best results is at Bort fraction 0.8 and Dec fraction 0.2.
- Artificial intelligence method have a great potential to be used alongside experimental methods to avoid some tedious experiments and scaling of nano-medicine in pediatric patients

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