S/N	Questions answered from research paper	First Research Paper Used: Mahmud, A. W., Shallangwa, G. A., & Uzairu, A. (2020). QSAR and molecular docking studies of 1,3-dioxoisoindoline-4-aminoquinolines as potent antiplasmodium hybrid compounds. Heliyon, 6(3), e03449. https://doi.org/10.1016/j.heliyon.2020.e03449	Second Research Paper Used: Pingaew, R., Prachayasittikul, V., Worachartcheewan, A., Thongnum, A., Prachayasittikul, S., Ruchirawat, S., & Prachayasittikul, V. (2022). Anticancer activity and QSAR study of sulfur-containing thiourea and sulfonamide derivatives. Heliyon, 8(8), e10067. https://doi.org/10.1016/j.heliyon.2022.e10067	Third Research Paper Used: Zięba, A., Laitinen, T., Patel, J. Z., Poso, A., & Kaczor, A. A. (2021). Docking-Based 3D-QSAR Studies for 1,3,4-oxadiazol-2-one Derivatives as FAAH Inhibitors. International journal of molecular sciences, 22(11), 6108. https://doi.org/10.3390/ijms22116108
1	What is the dependent variable?	Activities in pIC50 were taken as the dependent Variable.	pIC50 values were assigned as dependent variable.	The pIC50 of each compound were treated as dependent variables.
2	What are the independent variables?	The descriptors were assigned as independent variables.	Descriptor values were assigned as independent variables.	The Comparative Molecular Similarity Indices Analysis (CoMSIA) fields were used as independent variables.
3	How were the independent variables selected?	Genetic Function Algorithm (GFA) was used to select descriptors and build the model.	Multiple Linear Regression (MLR) algorithm was selected as a machine learning algorithm for the QSAR modeling in this study due to its interpretable characteristic.	The Leave-One-Out (LOO) approach was used to select the best out of the established models and generate the cross-validated value of R^2 (Q^2) and the optimum number of components.
4	What statistical method was used?	The model generated was assessed using Friedman formula.	Reliability of the constructed models was assessed by statistical parameters calculated by average values of several rounds of the sampling. Two aspects of the model performance were considered by calculated correlation coeffificient (R) and root mean square error (RMSE) values to reflect the predictive performance and predictive errors of the built models, respectively.	The Partial Least Square (PLS) analysis was performed for the optimum number of components to determine correlation coeffificient R^2, standard error of prediction, and F-value.
5	What calculator was used in the generation of independent variables?	Molecular descriptors of the optimized molecules of 1,3-dioxoisoindoline-4-aminoquinolines derivatives were computed with PaDEL-Descriptor software version 2.20	Waikato Environment for Knowledge Analysis (WEKA) version 3.4.5 was used to generate independent variables.	In order to examine the correctness of the utilized docking procedure, the RMSD value was calculated in Yasara (v20.1.2.24, CMBI, Radboud University Nijmegen, The Netherlands). The CoMFA analysis was carried out using the QSAR module available in Sybyl-X (v2.1., Tripos Inc., St. Louis, MO, USA).