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Environmental Analysis of Climatic Elements of Ahmednagar District (M.S.)

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Abstract:

Climatic elements are vital in day to day life which affects and determine the behavior of organisms in all eco systems of the world. Present paper focus upon various climatic elements and their distribution in the study area. The main purpose of present study is to investigate and evaluate climatic elements in Ahmednagar District. The temperature of the district is dry and hot. The seasonal variation in temperature is quite high from March to May. The average relative humidity is 35.64% minimum while 76.79% maximum in the district. The average annual rainfall from year 1981 to 2014 in the district is about 527.3 mm. The rainfall in the study region is estimated to be less than 500 mm over a 17-year out of 34 years' period from 1981 to 2014.

Key words: Climate, Eco-system, Rainfall distribution, Variability

Introduction:

Ahmednagar district is a drought-prone area and it is situated in the central part of Maharashtra state. Generally, the study area has hot summer and dry air except monsoon season. Intergovernmental Panel on Climate Change (IPCC). The main purpose of present study is to investigate and evaluate Climatic elements in Ahmednagar District. Many scholars like Singh (1991), Saptarshi (1993), More (2013) etc., have explained that climatic factors are very significant to determine the agricultural land use and agricultural pattern of the region

Study Area:

The present study deals with environmental analysis of climatic elements in Ahmednagar district. Ahmednagar is the largest district of Maharashtra State with a geographical area of 17418 sq. km. which is 5.66% of the area of Maharashtra State. It lies between 18° 2' to 19° 9' N latitude and 73° 9' to 75° 5' E longitude with covering 14 tehsils.

Objectives:

To Study the environmental analysis of climatic elements in Ahmednagar district.

Database and Methodology:

The Climate of the study area is studied on the basis of secondary information gathered from IMD (Pune), District census handbook, District social and economic review.

Tehsil wise temperature variation is presented with the help of table and graph. Average annual rainfall is calculated for the period of 1981 to 2014 with the help of Microsoft excel. Average annual variation of rainfall presented with the help surface trend analysis.

Results and Discussion: For the present analysis, the three elements are selected viz. temperature, humidity and rainfall of the whole district.

1. Temperature: The temperature of the district is dry and hot. The seasonal variation in temperature is quite high from March to May. There is continuous increase in day temperature, nights comparatively remain cool. In the month of May, the temperature remains to its maximum of 38.9°C which occasionally rises to 43°C or 44°C.

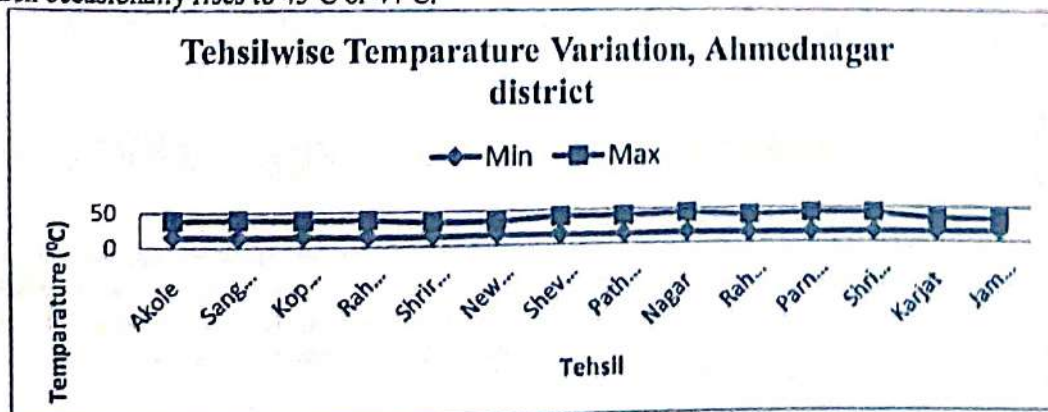


Figure No. 1: Tehsil wise Temperature Variation, Ahmednagar District
 In the month of December, the temperature remains to its minimum of 14.35°C. Occasionally, the temperature drops down to 2°C or 3°C (Figure 1).

2. Humidity:
 The average relative humidity is 35.64% minimum while 76.79% maximum in the district. The maximum humidity is observed in Sangamner, Nagar and Parner tehsils.

Table No. 1: Distribution of Major Climatic Elements, Ahmednagar District

Tehsil	Rainfall		Temperature (°C)		Relative Humidity (%)	
	Rainy Days (No.)	Average Rainfall (mm) (1981 to 2014)	Min	Max	Min	Max
Akole	25	599.3	12	39	25	90
Sangamner	67	413.3	11	40	60	95
Kopargaon	48	429.5	12	39	21	92
Rahata	65	529.8	12	39	30	85
Shrirampur	77	532.4	12	35	21	25
Newasa	77	499.6	12	35	21	25
Shevgaon	33	535.1	11	41	35	78
Pathardi	35	575.2	10	41	35	75
Nagar	42	595	12	44	58	95
Rahuri	67	536	11	40	21	92
Parner	60	507.7	12	43	58	95
Shrigonda	79	502.6	13	43	17	81
Karjat	45	537.7	12	33	55	72
Jamkhed	38	674.5	12	33	42	75
Average	54	527.3	11.7	38.9	35.64	76.79

(Source: Based on Ahmednagar.nic.in & IMD Data, Pune)

3. Rainfall:

Ahmednagar district comes under rain-shadow zone of Western Ghats and hence semi-arid scarcity zone. Annually 75% of the rainfall is received during this period. The average annual rainfall from year 1981 to 2014 in the district is about 527.3 mm. The scale of change in rainfall is large from year to year. The distribution of rainfall is very uneven. The rainfall is higher than any other parts of district in the western part of Akole tehsil near the *Kalsubai* hills. The amount of rainfall decreases from west to east. It can be seen from the table (Table.1) and graph (Figure 2).

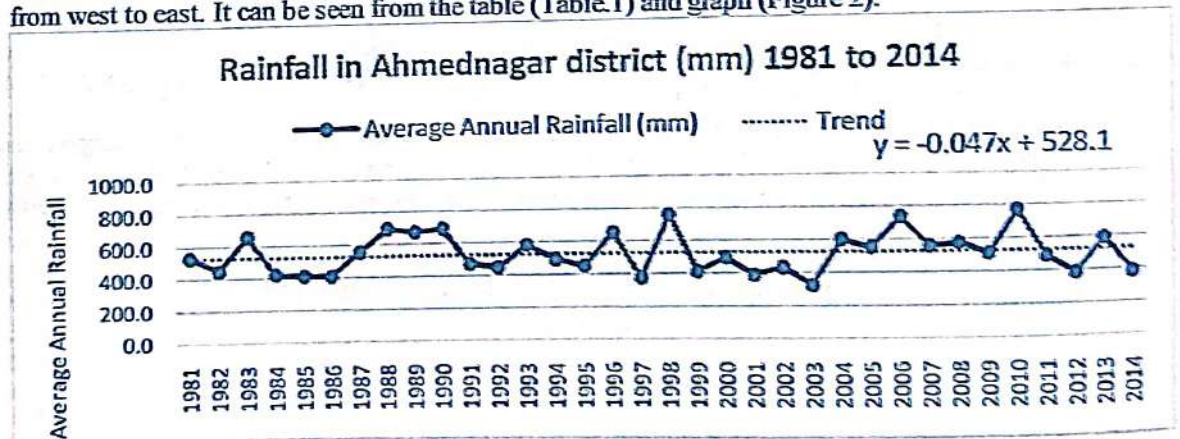


Figure No. 2: Rainfall variation, Ahmednagar District

The number of rainy days is less in Shevgaon, Pathardi, Parner, Jamkhed and Nagar tehsils, which are predominantly rain fed areas. Due to scarcity of water, these areas have limited period of crop cultivation. As there is shortage of water in rabi season during the maturity stage of crops, measures to conserve rainwater are essential. The rainfall is less and erratic, this affects the cultivation & production of crops in the district.

The major rainfall is received during month of June to October. Except Akole tehsil, the entire Ahmednagar district comes under drought prone zone. It is interesting to observe that the district has low rainfall with high variability. The rainfall in the study region is estimated to be less than 500 mm over a 17-year out of 34 years' period from 1981 to 2014.

Conclusion:

There is no uniformity in the climatic elements in overall district. The seasonal variation in temperature is quite high from March to May. The average relative humidity is 35.64% minimum while 76.79% maximum in the district. The average annual rainfall from year 1981 to 2014 in the district is about 527.3 mm. The rainfall in the study region is estimated to be less than 500 mm over a 17-year out of 34 years' period from 1981 to 2014. The scale of variation in rainfall is large from year to year and its distribution is very uneven. However, the trend line neither shows growth or loss in the amount of the rainfall during the 1981 to 2014.

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IMPACT ANALYSIS OF 'JALUKTA SHIVAR' SCHEME: A CASE STUDY OF CHAS VILLAGE IN AHMEDNAGAR DISTRICT

□ Dattatray Sheshrao Ghungarde*
Dr. Jyotiram C. More**

ABSTRACT

The Maharashtra government has launched a water conservation scheme named Jalukta Shivar Abhiyan to make Maharashtra a drought-free state by 2019. The key aim of Jalukta Shivar Abhiyan is to establish a belief in farmer that "every drop of rainwater is owned by me and it should percolate in my land".

'Jalukta Shivar Abhiyan' aims to bring water empowerment to 25,000 drought-affected villages in Maharashtra within next five years. The scheme has been going strong with villages building infrastructure in terms of public participation. The project involves deepening and widening of streams, construction of cement and earthen stop dams, work on nalla's and digging of farm ponds.^[1]

The present research paper attempts to review the work done for water conservation through 'Jalukta Shivar Abhiyan' scheme and its impact on agricultural development in Chas village. The scheme found to have significant impact on Runoff retardation by 916.28 T.C.M. after implementation of 'Jalukta Shivar' scheme in the village. It also has significant impact of the scheme on Agricultural development of Chas village by Increasing NSA by 2.43% and also increment in ground water level by 6 meter for well and 25 meter for bore well.

Keywords: Jalukta Shivar Abhiyan, Earthen stop dams, Agricultural development

➤ Introduction:

Irregular and discontinuous rainfall during crop growth has led to continuous scarcity- conditions in Maharashtra. The last few years have seen a huge impact of these conditions on the agricultural sector. The Rainfed crop production is showing significant fluctuations. This situation is mainly due to scarcity of water. The various measures under water conservation can definitely be planned and implemented to make water available for drinking and sustainable agriculture. To overcome this scarcity situation, the

government of Maharashtra has launched a water conservation scheme named 'Jalukta Shivar Abhiyan' (JSA) in 2015. The slogan 'Water for all-Drought free Maharashtra 2019' has been well announced by this scheme. Various comprehensive watershed development works were done under this scheme.^[2]

The drought stricken village Chas was selected in the year 2015 under this scheme. The village is situated on Nagar-Pune state highway (SH-27). The present research paper attempts to review the work done under 'Jalukta Shivar Abhiyan' scheme and its impact

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on agricultural development in this village.

➤ **Objectives:**

The main objectives of present research paper are;

1. To review of works done under ‘*Jalukta Shivar Abhiyan*’ scheme in the Chas village.
2. To assess the impact of water conservation on General Landuse and Groundwater levels.

➤ **Database and Methodology:**

To fulfil the above objectives, data has been collected from various primary and secondary sources. The primary data is collected through field survey. The secondary data is obtained from various sources viz, Agricultural department of Ahmednagar tehsil, Village *Krushisahayak* and Talathi office etc.

On the basis of the statistical data extracted from the sources referred of Chas village, the comparative study has been carried out before and after implementation of the scheme. The collected data has been processed, tabulated and prepared graphs for the purpose of analysis.

➤ **Study area:**

Chas village is located in Nagar tehsil of Ahmednagar district, Maharashtra. The village is situated on Nagar-Pune state highway (SH-27) and 12 km away from Ahmednagar district headquarters. The Geographical location of the village is $19^{\circ} 1' 59''$ N latitude and $74^{\circ} 38' 54''$ E longitudes. The village has average elevation of 546 m from mean sea level. It lies on the bank of Mendka river which is tributary of Sina river. The total geographical area of the village is 2257.44 hect which is 1.42% of tehsil land. The village receives an average annual rainfall of 533 mm. The minimum and maximum temperature ranges between 14°C to 44°C .

The village has population of 4610 persons of which 2391 are males while 2219 are females as per Population Census 2011. The Sex Ratio of village is 928 ‘F/1000 M’, which

is lower than Maharashtra state average of 929 ‘F/1000 M’.^[3]

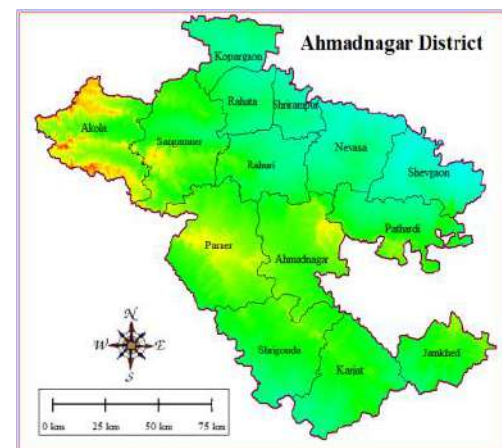
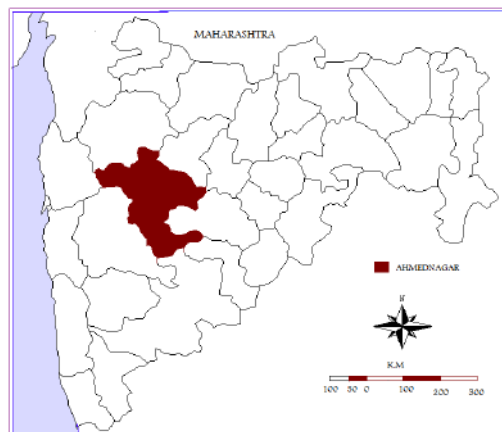
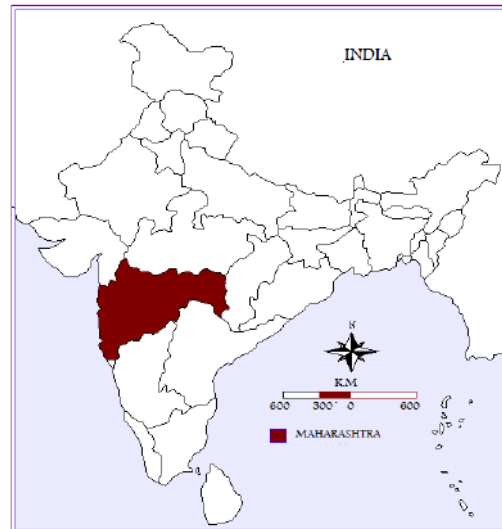


Figure No. 1: Location map of study area

➤ **Result and Discussion:**

1. Water Conservation works carried out under JSA Scheme:

The drought prone village Chas was selected in the year 2015 under the ‘Jalukta

Shivar' scheme. The table (Table No. 1) represents the completed water conservation works before as well as after implementation of this scheme in the village. It also shows the

retarded runoff by respective water conservation work in thousand cubic meter (T.C.M.).

Table No. 1: Water Conservation works and respective retarded runoff before and implementation of JSA Scheme

Sr. No.	Type of Work	Before JSA Scheme		After JSA Scheme		Increment in Retardation of Runoff (T.C.M)
		Number	Retarded Runoff (T.C.M)	Number	Retarded Runoff (T.C.M)	
1	Continuous Contour Trenches	83	12.90	83	12.90	N.C
2	Earthen Nala Bund	60	10	62	150	+100
3	Cement Nala Bund	6	24	11	129	+105
4	Compartment Bunding	95	28.50	81992	519.88	+491.38
5	Farm-ponds	18	2.70	23	12.70	+10
6	Mud removal work	0	0	2	2.80	+2.80
7	Recharging of wells	0	0	2	1.60	+1.60
8	Repairing of K T weirs	0	0	1	40.5	+40.5
9	Repairing of village lake	5	325	5	450	+125
Total		267	403.1	82181	1319.38	+916.28

(Source: Compiled by researcher based on Secondary data)

From the table (Table No. 1), it is observed that total eight types of work were carried out during the course of 'Jalukta Shivar' Scheme in the village. The Mud removal work, recharging of wells and repairing of K T weirs are newly introduced works under this scheme.

Two types of Nala bunds were constructed in Chas village depending upon the type of material used for the construction work, viz, Earthen Nala Bund and Cement Nala Bund. Before JSA scheme, the Earthen bunds were 60 in number, which then increased to 62 while Cement bunds were 6, which then increased to 11 in number after JSA scheme. The retarded runoff by these bunds is increased by 205T.C.M.

The Compartment bunding is a major work carried out under this scheme. They are 81,992 in number after implementation of JSA scheme, while before JSA there were only 95 in number. The highest amount of water (519.88 T.C.M.) is retarded by this structure in Chas village. The Farm-ponds under this scheme are the water harvesting structures constructed on the lower side of the farm to collect runoff water. The constructed farm ponds are increased from 18 to 23 after implementation of JSA scheme, while the retarded runoff is increased by 10 T.C.M. As discussed earlier, the Mud removal work, recharging of wells and repairing of K T weirs are the three newly introduced works under this scheme with retarded runoff of 2.80, 1.60 and 40.5 T.C.M. respectively.

The five village lakes are repaired under JSA scheme which contributed in runoff increment of 125 T.C.M. in the village. As a result, it is recorded that there is increment in Runoff retardation by 916.28 T.C.M. after implementation of 'Jalukta Shivar' scheme in the village.

2. Impact of JSA Scheme on General Landuse:

Agriculture is the main occupation of the people of Chas village. The table (Table No. 2) and figure (Figure No. 2) shows the detailed land use pattern of the Ahmednagar district before as well as after implementation of JSA scheme.

The total geographical area of the Chas village is 2557.44 hect. It is recorded that, there is absence of forest cover in Chas village.

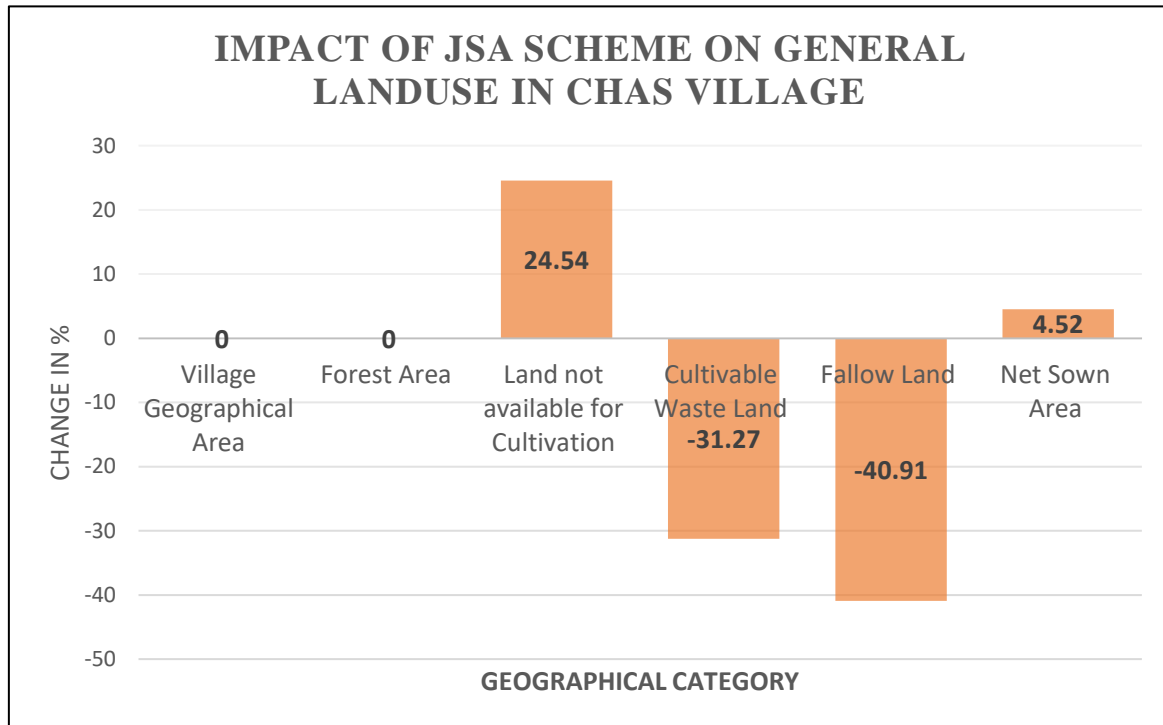


Figure No. 2: Impact of JSA Scheme on General Landuse in Chas village

I. Land not available for cultivation:

The land not available for cultivation is may be described as non-cultivable land. It includes two types of land namely barren and uncultivable land i.e. land of rock, small sand mountains, etc. Area under non-agricultural uses i.e. land under settlement, roads, streams, etc. It reveals that area under this type of land before JSA scheme was 125.6 hect out of the total geographical area. While after implementation of JSA scheme, it is a recorded as 152.65 hect. It is increased by 21.54% per cent. This indicates expansion of settlement, transport etc., due to increasing population and infrastructure facilities.

II. Cultivable Waste Land:

Cultivable waste land includes (i) permanent pasture and grazing land (ii) miscellaneous, trees, crops and groves not included in the net sown area. This category of land accounted 18.1 hect. in the village before and 12.44 hect after JSA scheme. During the period of JSA scheme, it has decreased by 31.27%. It shows the impact of JSA, which shows that Cultivable waste land comes under cultivation.

III. Fallow Land:

Fallow lands are divided into two sub types, 1.Current fallow land - means the land fallow during the current years.2. Other fallow

land means the land kept uncultivated one year to five years due to some problems.

Before implementation of JSA scheme, the fallow land in Chas village was 287.34 hect. and it is decreased up 169.79 hect. Throughout the study period, the fallow land has decreased by 40.91%. This means increasing in water availability decreasing drought condition resulted in increased NSA.

IV. Net Sown Area:

The net area sown is the actual area under crops counting areas sown more than once in the same years only once. Earlier, the net sown area was 2126.4 hect. of the total geographical area. After implementation of JSA scheme, it was recorded as 2222.56 hect. It is

increased by 4.52 %, which is a positive indicator of Agricultural development.

3. Impact of JSA Scheme on Groundwater levels:

Groundwater is an important source for irrigation of agriculture as it is one of the reliable and flexible inputs of water. “Use of groundwater can boost agricultural production, improve rural incomes and strengthen farmers’ ability to withstand climate shocks and water variability.” (CGIAR, Research program on Water, Land and Ecosystems).

The table (Table No. 2) represents the Groundwater status of Chas village before as well as after implementation of JSA scheme.

Table No. 2: Groundwater Status of Chas village

Source of Irrigation	Number	Before JSA Scheme (m)	After JSA Scheme (m)	Average Increment in Groundwater Level (m)
Open well	243	12	6	+6
Bore well	439	58	33	+25

(Source: Compiled by researcher based on Secondary data^{[4][5][6]})

The ‘Jalukta Shivar’ scheme have a positive impact on groundwater levels. The average increment in groundwater level for Open well and Bore well are 6 m and 25 m respectively.

➤ Conclusion:

The paper concludes that, Runoff retardation by 916.28 T.C.M. after implementation of ‘Jalukta Shivar’ scheme in the village. Result of retardation is increasing water level of well and Bore well by 6 meter and 25 meter respectively. **“The ‘Jalukta Shivar’ scheme is found to have significant impact on Agricultural development of Chas village by Increasing NSA by 2.43%.** The discussion of general landuse of Chas village clearly indicates that there is decrement in

Cultivable waste land, fallow land and increment in Net sown area; which are good indicators for agricultural development.

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मूल्य : १५० रुपये

या अंकातील लेखकांच्या मताशी संपादक सहमत असतीलच असे नाही. या नियतकालिकास महाराष्ट्र राज्य साहित्य आणि संस्कृती मंडळाकडून अनुदान प्राप्त झाले आहे; परंतु या नियतकालिकात प्रसिद्ध झालेली मते मंडळास मान्य असतीलच असे नाही.

पत्ता : संपादक, तिफण, 'शिवार', श्रीराम कॉलनी, हिवरखेडा रोड,

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दलित साहित्य प्रवाहाच्या निर्मितीची समाजशास्त्रीय चिकित्सा

- डॉ. सहदेव शरद चव्हाण

१९ ६० नंतर दलित साहित्य प्रवाह निर्माण झाला. त्याचबरोबर स्त्रीवादी, ग्रामीण, आदिवासी, विज्ञानवादी यांसारखे वाङ्मयीन प्रवाह सुद्धा निर्माण झाले. दलित साहित्य प्रवाहाची निर्मिती आणि इतर वाङ्मयीन प्रवाहांची निर्मिती यामध्ये वाङ्मयीन, ऐतिहासिक, धार्मिक, भावनिक, मानसशास्त्रीय दृष्टीने मूलभूत फरक आहे. आधुनिक समाजशास्त्रीय सिद्धांत, तत्वे, कसोट्या आणि पद्धती यांच्या आधारे दलित साहित्य प्रवाहाची निर्मिती लक्षात घेणे आवश्यक आहे. विसाव्या शतकात साहित्याच्या समाजशास्त्रीय अभ्यास शाखेचा उदय झाला असला तरी त्यापूर्वी व्हिको यांनी 'New Science' (१७२५) या ग्रंथात तर मादाम दस्ताल यांनी 'De la Literature' या ग्रंथात साहित्य आणि समाज यांचे परस्पर संबंध व प्रभाव यांचा अभ्यास केलेला होता. नंतरच्या काळात तेन या समाजशास्त्रज्ञाने वंश, वातावरण, युगप्रवृत्ती यांचा साहित्यावर होणारा परिणाम सिद्धांताद्वारे दाखविला आहे. अँलन स्विंगवूड यांनी सामाजिक घटक, लेखकाची वृत्ती, सामाजिक बांधिलकीचा परिणाम साहित्याच्या निर्मितीवर होत असतो या विषयीचे विचार मांडले.लेविझ कोझर यांनी 'Functions of Social Conflict' (१९५६) या ग्रंथात समाजाची संरचना टिकून ठेवण्यासाठी कलेचे (साहित्य, नाटक, खेळ) योगदान महत्त्वाचे मानले आहे. 'सामाजिक संरचना दोषयुक्त अन्यायकारी असेल तर त्या संरचनेविरुद्ध साहित्य विद्रोह

पुकारते' हे लेविझ कोझरचे निरीक्षण महत्त्वाचे मानले जाते. डंकन यांनी लेखक, वाचक, समीक्षक यांच्यात होणाऱ्या आंतरक्रियावर आधारित मांडलेला 'सामाजिक आंतरक्रिया दृष्टीकोन' आणि जॉर्ज हूको यांचा सामाजिक संरचनेतील असंतुलन हे लेखकांना लेखनास प्रवृत्त करते हा विचार सांगणारा 'सामाजिक संरचनात्मक दृष्टिकोन' तर लेखकाची जडणघडण आणि वास्तव जीवनानुभव मांडणारा 'सामाजिक प्रक्रिया दृष्टीकोन' आणि जोसेफ रुकेक यांनी 'Social ogy of Literature' या निबंधात, साहित्य निर्मितीत समाज आणि संस्कृती यांचा संबंध कसा येतो याचे विश्लेषण करण्यासाठी स्वीकारलेला 'सामाजिक मूल्यात्मक दृष्टीकोन' हे चारही दृष्टीकोन आणि आधुनिक समाजशास्त्रज्ञांनी मांडलेले सिद्धांत यांचा विचार लक्षात घेऊन दलित साहित्य प्रवाहाचे विश्लेषण करावे लागेल. साहित्याच्या समाजशास्त्रात लेखकाच्या व्यक्तित्वाची जडणघडण, अभिवृत्ती, सामाजिक जाणीव, सामाजिक बांधिलकी, मूल्यनिष्ठा, सामाजिक दर्जा, भाषा, समूह वर्तन, संस्कृती या घटकांचा विचार करणे गरजेचे असते.

दलित साहित्याची निर्मिती १९६० नंतर जोमाने होऊ लागली तरी त्याच्या निर्मितीस त्यापूर्वीच्या अनेक शतकांतील सामाजिक, राजकीय, धार्मिक, भाषिक, ऐतिहासिक, मानसिक वातावरण कारणीभूत आहे. इंग्रजी राजवटीत रेल्वे, रस्ते, दळणवळणाच्या सुविधा निर्माण झाल्या. टपाल खाते, शेती सुधारणा, बंदरांचा विकास यामध्ये कमालीच्या सुधारणा केल्या. कारकून, लष्कर यामध्ये सामान्य लोकांना भरती केले. राज्यकारभार आणि प्रशासनात सुव्यवस्था आणण्यासाठी कायद्याचे राज्य निर्माण केले. त्यामध्ये त्यांना समान वागणूक दिली. लष्करात, रेल्वेत, प्रशासनात नोकर म्हणून नेमणूक करताना जात, वर्ण, धर्म यांना डावलून भरती केली. त्याचा परिणाम तत्कालीन तळगाळातील समाजावर झाला. त्यांनी हिंदू-सवर्णांनी दिलेली सामाजिक वागणूक आणि इंग्रजांनी दिलेली वागणूक यातील फरक अनुभवला. पददलितांना ख्रिस्ती मिशनऱ्यांनी धर्मप्रसारासाठी आणि इंग्रजांनी कारकून निर्माण करण्यासाठी शिक्षण दिले, यापेक्षा दलितांना शिक्षणाची कवाडे मुक्तपणे उघडली याचा दिलासा त्यांना जास्त वाटू लागला. त्यामुळे समाजात साक्षरता वाढू लागली. या सर्व राजकीय घटकांनी समाजात हळूहळू आत्मजागृतीचे भान येऊ लागले.

सवर्ण समाज व्यवस्थेने दलित समाजावर लादलेली अस्पृश्यता म्हणजे सामाजिक, मानसिक गुलामगिरीच होती. सिंधू संस्कृतीतील गणदासप्रथेतून वर्णव्यवस्था निर्माण झाली. त्यातूनच चार वर्णांची निर्मिती झाली. आर्यांच्या वर्णव्यवस्थेतील शूद्र वर्णाला वेदाचा अधिकार नाकारला होता. "शूद्र म्हणजे परगणिय वा अनार्यगणिय ज्यांचा आर्यांच्या पद्धतीने उपनयन संस्कार झालेला नाही."१ यांना शूद्र

असे म्हटले जात होते. या शूद्र वर्णाच्या निर्मितीतून जातीव्यवस्था निर्माण झाली. 'जाती'हा शब्द सर्वप्रथम बौद्ध विनयपिटकात वापरलेला आहे. वैदिक साहित्यात तो केवळ कात्यायन श्रौत सूत्रात आलेला आहे. जाती व्यवसायावरून निर्माण झाल्या. निकृष्ट दर्जाचे काम करणाऱ्या जातींना अस्पृश्य समजण्यात आले."अस्पृश्यतेची चाल सूत्रकाळीच रूढ झाली. मनुष्याचे प्रेत, मृत जनावरे, मलमूत्रादि पदार्थ यांच्याशी संबंध व कुजलेल्या वा कुजविलेल्या पदार्थाशी संबंध ध्वे करणारे लोक अस्पृश्य मानले गेले आहेत."² अस्पृश्यता आणि त्यातून निर्माण झालेली गुलामगिरी टिकवून ठेवण्यासाठी सवर्णांनी त्याला धर्माचा देवदेवतांचा, पाप- पुण्य- पुनर्जन्म यांचा बेगडी आधार दिला. त्यातून दैवभोळेपणा, वैज्ञानिकता, विवेकशून्यता यांनी समाज ग्रासून गेला. समाजाचा बौद्धिक विकास खुंटला. समाजाची अधोगती झाली. त्यामुळे अस्पृश्यतेविरुद्धच्या तीव्र भावना विद्रोहाच्या स्वरूपात दलित साहित्यातून व्यक्त झालेल्या दिसतात.

इंग्रजांनी निर्माण केलेली राजकीय गुलामी आणि सवर्णांनी लादलेली सामाजिक गुलामगिरी यातून स्वातंत्र्यानंतर मुक्तता मिळेल अशी आशा दलितांना वाटत होती. परंतु स्वातंत्र्याने राजकीय गुलामी नष्ट झाली. सामाजिक समता, बंधुता, धर्मनिरपेक्षता मात्र निर्माण होऊ शकले नाही. शिक्षणाची सक्ती आणि मोफत प्रसार, लोकशाहीचे सार्वत्रिकीकरण, सत्तेचे विकेंद्रीकरण, प्रादेशिक असमानता यांच्यातील फोलपणा स्पष्ट दिसू लागला. शिक्षित नवतरुणांमध्ये अस्वस्थता वाढली. विशेषतः शिक्षण घेतलेला दलित तरुण आक्रमकपणे व्यवस्थेला पाश्च विचारू लागला. आपल्या मनातील विचार शब्दशस्त्राद्वारे मांडू लागला. आत्मजागृत झालेला शिक्षित दलित तरुण स्वतःचे, आपल्या समाजाचे, इतिहासातील उपेक्षित कालतत्त्वाचे नव्याने आकलन करू लागला. त्यामुळे दलित लेखकांची मानसिक, बौद्धिक जडणघडण होऊन त्यांच्या लेखणीला नवी वैचारिक दृष्टी मिळाली.

१९६० नंतर दलित लेखकांनी आपल्या समाजाच्या वेदना साहित्यातून व्यक्त केल्या. कारण मराठी साहित्यातील लेखकांच्या भावविश्वाने दलित जीवनाला कधीही आपल्या लेखनाचा विषय बनवले नाही. मध्ययुगीन साहित्य भक्तिरसात गुंतून मोक्षप्राप्तीसाठी लिहिले जात होते. पांडित्य प्रदर्शनातून विद्वत्ता दाखविण्यात पंडिती काव्याने समाधान मानले, तर शाहिरी वाङ्मय स्वामीनिष्ठेसाठी स्तुतिसुमने गात होते. आधुनिक काव्यातील साहित्यिक प्रेम, शृंगार, निसर्गवर्णन यांचे चित्रण करून कलावादाला कवटाळून बसले. समकालीन साहित्याने मध्यमवर्गाचे जीवन, यंत्रयुग, औद्योगिकीकरण, नागरीकरण यांना आपल्या साहित्याचा विषय बनवले. अर्थात याला अपवाद संत चोखामेळा यांचे जातीतील हीनत्व दाखविणारे काव्यलेखन, हरिभाऊ आपटे यांच्या स्त्री दुःखाच्या कहाण्या, वि. स. खांडेकर यांच्या 'दोन मने' मधील चवदार

तळ्याच्या सत्याग्रहाचे केलेले वर्णन, माडगूळकरांनी 'चंदनवाडीत' रेखाटलेले अस्पृश्य जीवन, केशवसुतांच्या काही कविता, 'चक्र' 'माहिमची खाडी' यांच्यातील दलित जीवन यांचा उल्लेख करावा लागेल. श्री. म. माटे, विभावरी शिरूरकर यांच्या लेखनात दलित चित्रण अधिक प्रकर्षाने आलेले आहे. असे असले तरीही तत्कालीन मराठी लेखकांनी मध्यमवर्गाचे चित्रण करण्यातच धन्यता मानली. दलित जीवनातील जाणिव आणि गुलामी त्यांच्या साहित्यात आलेली दिसत नाही. "प्राचीन, अर्वाचीन आणि समकालीन मराठी साहित्यामध्ये दलितांचे वास्तव चित्रण झालेले नाही. म्हणून दलित लेखकांनी मराठी साहित्य परंपरा नाकारलेली आहे दलितांचे वास्तव जीवन चित्रित व्हायचे असेल तर दलित लेखकालाच लिहावे लागणार आहे. तेव्हा आपणच आता दलितांच्या जीवनातील जिवंत अनुभव लिहावेत या हेतूने प्रेरित होऊन दलित लेखकांनी लेखन केलेले आहे."³

दलित साहित्याच्या निर्मितीस दलित चळवळ आणि डॉ. बाबासाहेब आंबेडकरांचे प्रेरणादायी कार्य कारणीभूत ठरलेले दिसते. दलित चळवळीची सुरुवात अनेक अभ्यासक संत चोखामेळा यांच्या साहित्य लेखनापासून मानतात तर काही अभ्यासक ही परंपरा गौतम बुद्ध, श्रीरामानुजाचार्य, कबीर, चक्रधर स्वामी, वारकरी संप्रदायातील काही संत, ज्योतिराव फुले, शाहू महाराज, महर्षी वि. रा. शिंदे यांच्या विषमतेविरुद्ध लढ्याला दलित चळवळीची पार्श्वभूमी मानतात. गोपाळबाबा वलंगकर, किसन फागूजी बनसोड, भाऊ फक्कड, भीमराव कर्डक, केरूबुवा गायकवाड, वामनदादा कर्डक, अर्जुन हरी फडके, अण्णाभाऊ साठे या शाहिरांनी आपल्या शाहिरीतून दलित जाणिवाना प्रकर्षाने मांडले. छत्रपती शाहू महाराज आणि महात्मा फुले यांचे दलितोद्धाराचे प्रयत्न इतर सर्व प्रयत्नांपेक्षा अधिक परिपूर्ण होते. डॉ. बाबासाहेब आंबेडकर उच्चविद्याविभूषित, घटनातज्ञ, कर्ते समाज सुधारक होते. ते स्वतः दलित समाजातील होते. त्यांनी अस्पृश्यता, बहिष्कृतता आणि सामाजिक गुलामी अनुभवलेली होती. त्यामुळे दलितांबद्दलची आत्मीयता त्यांच्या प्रत्येक कार्यातून दिसून येते. दलितांच्या न्याय हक्कांसाठी त्यांनी आग्रही भूमिका घेतली त्यामुळे डॉ. बाबासाहेब आंबेडकर दलित साहित्याची मुख्य प्रेरणा आणि ऊर्जा केंद्र मानले जाते. "डॉ. आंबेडकर यांच्या आंदोलनामुळे वतवज्ञानामधून शोषणाविरुद्ध बंड, विद्रोह, नकार ही सिद्धांत तत्त्वे उदयास आली. अनेक कवी लेखकांच्या मनात स्वतःच्या शोषणाची मीमांसा उदयास आली. ही शक्ती डॉ. आंबेडकरांच्या चळवळीतून व वैचारिक लढ्यातून या लेखकांनी संपादन केली. आपली भावना ते काव्यरूपाने घडवू लागले. त्यामधील दारिद्र्य, दुःख, शोषण हा प्रचंड आविष्कार पाहून दलित साहित्याच्या प्रेरणेचा प्रश्न निर्माण केला. तेव्हा दलित चळवळीतील पहिल्या

पिढीतील लेखकांनी दलित साहित्याची प्रेरणा डॉ. आंबेडकर आहेत हेच मत आग्रहाने प्रतिपादन केले." डॉ. बाबासाहेब आंबेडकर यांच्या विचारांतू शक्ती घेऊन दलित समाजात जागृती झाली. दलित लेखकांना लेखनाची चालना मिळाली. दलित लेखकांच्या व्यक्तिमत्त्वाची जडणघडण बाबासाहेबांच्या कृती आणि उक्तीमुळे झाली.

दलितांचे गावगाड्यातील स्थान कोणते आहे? त्यांचा सामाजिक दर्जा कोणता आहे? गावगाड्याचा दलितांविषयीचा मानसिक दृष्टिकोन कलुषित का आहे? यासारख्या अनेक प्रश्नांची चर्चा शिक्षित दलित तरुण पिढी करत होती. तेव्हा त्यांच्या लक्षात आले की दलितांना गावगाडा तुच्छ लेखतो. त्यांना सार्वजनिक जीवनातील निर्णय प्रक्रियेत, समारंभात, कारभारात कोणतेही महत्त्वाचे स्थान नाही. गावगाड्यातील सण-उत्सव, धार्मिक कार्यक्रमात सहभागी करून घेतले जात नाही. दलित स्त्रीचे अस्तित्व तर नगण्यच होते. गावगाडा चालविणाऱ्या पाटील, कुलकर्णी, देशमुख यांनी बलुतेदारांना विशेषता अस्पृश्यांना अत्यंत तुच्छतादर्शक वागणूक दिलेली होती. या भयानक समाजस्थिती विरुद्ध दलितांच्या मनात चीड, संताप, आक्रोश निर्माण होत गेला. जाणीवपूर्वक निर्माण केलेल्या या विदारक अन्यायकारी गावगाड्याच्या रचनेला, चालीरीतींना, परंपरांना दलित लेखकांनी विद्रोही भूमिका स्वीकारून छेद दिला त्यातून दलित वेदना आणि विद्रोह निर्माण झालेला दिसतो.

समाजशास्त्रीय दृष्टीने साहित्यप्रवाहांचा विचार करताना ज्या भाषेत साहित्य निर्माण झालेले आहे, त्या भाषेची पृथगात्मकता लक्षात घेतली पाहिजे. दलित साहित्याची भाषा जीवनानुभव व्यक्त करणारी आहे. ती गावकुसाबाहेरील व्यथा व्यक्त करणारी बोली आहे. पांढरपेशा मध्यमवर्गीय साहित्यातील गुळगुळीत झालेले शब्द न येता वेदना, विद्रोह आणि संघर्ष व्यक्त करताना जाज्वल रूप धारण करणारी आहे. दलित साहित्याची भाषा स्वानुभवाची आहे. त्यामुळे त्यामध्ये झुंजण्याचे संकेत मिळतात. अस्पृश्य वस्तीतील त्याज्य मानलेले शब्द, शिव्यांचे रूप घेणारे वाकप्रचार आणि म्हणी आलेल्या आहेत. ही भाषा व्यक्तींची नसून समूहाची आहे. दलित साहित्याचे महत्त्वाचे बलस्थान म्हणजे त्या समाजाची अंगभूत असलेली भाषा होय. त्यामुळे भाषिकदृष्ट्या दलित साहित्य वेगळे ठरते.

एकूणच, समाजशास्त्रीय दृष्टीने दलित साहित्य प्रवाहाच्या निर्मितीची कारणमीमांसा लक्षात घेतल्यास, दमन संस्कृतीचा आग्रह धरणाऱ्या ब्राह्मण्य प्रवृत्तीमुळे शतकानुशतके दलित समाजाच्या शोषणातून निर्माण झालेल्या अनिष्ट रूढी, परंपरा, जातीयता, अस्पृश्यता या घटकांचा विचार करावा लागतो. जातीयतेचा दृष्टिकोन स्वीकारलेल्या या समाज संस्कृती विरुद्धचा शाब्दिक आत्मस्वर दलित साहित्यातून प्रकट झालेला आहे. दलित लेखकाची जडणघडण, त्यांचे संघर्षपूर्ण व्यक्तित्व,

मानसिक आंदोलने, आत्मभानातून आलेली आत्मजागृती याचा साकल्याने परामर्श घ्यावा लागेल. डॉ. बाबासाहेब आंबेडकर यांच्या विचारांनी प्रेरित झाल्यामुळे समाजात वैचारिक, बौद्धिक बदल झाले. इतिहास आणि संस्कृतीच्या पुनर्मांडणीचा आग्रह धरला जाऊ लागला. स्व- मनातील विचारांची, भावनांची मांडणी करण्यासाठी प्रस्थापित रचनाबंधाचे संकेत झुगारून देणारी, अनलंकृत, गावकुसाबाहेरील त्याज्य ठरविलेल्या शब्दांची भाषा वापरली जाऊ लागली. स्वातंत्र्यपूर्व आणि स्वातंत्र्योत्तर काळात या सर्व सामाजिक घटकांविषयीची प्रतिक्रिया म्हणजे दलित साहित्य प्रवाहाची झालेली निर्मिती होय.

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डॉ. शिवाजी हुसे

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● संपादक ●

डॉ. शिवाजी हुसे

● अतिथी संपादक ●

डॉ. युवराज धबडगे प्रा. नागेश बोन्तेवाड

मराठी विभागप्रमुख

मराठी विभाग

दगडोजीराव देशमुख महाविद्यालय, वाळूज, जि. औरंगाबाद

● संपादक मंडळ ●

डॉ. सर्जेराव जिगे

डॉ. ताहेर पठाण

डॉ. ममता इंगोले

डॉ. फुला बागूल

डॉ. वंदना महाजन

डॉ. वामन जाधव

डॉ. अनिल गर्जे

डॉ. रामचंद्र झाडे

डॉ. यशवंत सोनुने

डॉ. संजय सांभाळकर

मूल्य: ३०० रुपये

या अंकातील लेखकांच्या मताशी संपादक सहमत असतीलच असे नाही. या नियतकालिकास महाराष्ट्र राज्य साहित्य आणि संस्कृती मंडळाकडून अनुदान प्राप्त झाले आहे. परंतु या नियतकालिकात प्रसिद्ध झालेली मते मंडळास मान्य असतीलच असे नाही.

पत्ता : संपादक, तिफण, 'शिवार', श्रीराम कॉलनी, हिवरखेडा रोड, कन्नड,
जि. औरंगाबाद - ४३११०३. मो. ९९०४००३९९८

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- डॉ. सहदेव शरद चव्हाण

मराठी विभागप्रमुख

भारतीय जौन संघटनेचे कला,

विज्ञान आणि वाणिज्य महाविद्यालय,

वाघोली, पुणे-412207

लो ककवी, महाकवी, भीमशाहीर, आंबेडकरी विचारकवी या नावाने ओळखले जाणारे वामनदादा कर्डक यांचा जन्म 15 ऑगस्ट 1922 रोजी झाला. सामाजिक गुलामी, अस्पृश्यता, दारिद्र्य आणि आर्थिक चणचण यामुळे त्यांचे बालपण आणि किशोरवयीन जीवनाचा प्रवास अतिशय खडतर झाला. औपचारिक शिक्षणापासून दूर राहिलेले वामनदादा व्यवहारातील शाळेत अनौपचारिकरीत्या शिकले. त्यांनी सभोवतालच्या सामाजिक, राजकीय, धार्मिक परिस्थितीचे आकलन केले. याच काळात डॉ. बाबासाहेब आंबेडकरांचा राजकीय सामाजिक पटलावर झंझावात सुरू झाला. महाड येथील चवदार तळ्याचा सत्याग्रह, काळाराम मंदिर प्रवेशाचा संघर्ष मनुस्मृतीचे दहन, गोलमेज परिषद आणि येवल्यातील धर्मांतराची घोषणा, अस्पृश्य परिषदा, कायदा मंत्री पदाचा काळ, घटना समितीतील अद्वितीय काम, धर्मांतर यासारख्या घटनांचा आंबेडकरी समाजावर फार मोठा परिणाम होत गेला. डॉ. बाबासाहेब आंबेडकरांच्या या संपूर्ण कार्यांचे सुहृदयसाक्षीदार वामनदादा होते. त्यांच्या मनावर बाबासाहेबांच्या विचारांचा संघर्षाचा, लेखनाचा खोलवर परिणाम झालेला होता. वामनदादा कर्डक यांचे आयुष्य बाबासाहेबांच्या विचारांनी उजळून निघाले होते

याच काळात महात्मा फुले यांच्यानंतर सत्यशोधकी जलसे बाळसे धरू लागले समाजात विचारांची पेरणी करण्यासाठी पोवाडे, कलापथके, जलसे यांचा वापर सुरू झाला आंबेडकरी जलसे आणि शाहिरी यांनी तळागाळातील समाजात आत्मभान, आत्मबळ निर्माण केले. या सर्व घटनांमुळे वामनदादांच्या वैचारिक मनोधर्माची मशागत झाली

डॉ. बाबासाहेब आंबेडकर विलायतेतून शिक्षण घेऊन आलेले उच्चविद्याविभूषित कर्ते समाजसुधारक होते. त्यांनी अस्पृश्यांच्या उद्धारासाठी शिक्षणाचा आग्रह धरला. समाजात जागृती घडवून आणण्यासाठी समता, मूकनायक, बहिष्कृत भारत, जनता, प्रबुद्ध भारत यांसारख्या नियतकालिकातून लेखन केले त्यांनी पीपल्स एज्युकेशन सोसायटीचे 1945 साली मुंबईमध्ये सिद्धार्थ कॉलेज तर औरंगाबाद येथे मिलिंद कॉलेज काढले. त्यांच्या लेखणीतून अस्पृश्य समाजाला स्वत्वाची जाणीव होऊन मानसिक, सामाजिक गुलामगिरी तोडण्याची ऊर्जा मिळू लागली. बाबासाहेबांनी दलित तरुणांना शिक्षण घेण्यासाठी आग्रह धरला. समाजाची प्रगती शैक्षणिक प्रगती वरून ठरते, त्यामुळे दलितांनी शिक्षित होऊन शासनकर्ते व्हावे हा त्यांचा दिव्य संदेश तरुणांसाठी मुक्ती मार्ग ठरला वामनदादा कर्डक गायक होते. कवी होते. गीतकार होते. त्यांनी बाबासाहेबांच्या विचारांना गीतातून काव्यातून दलित जनसमूहापर्यंत पोहोचविले. भीमविचार हा त्यांचा श्वास होता. त्यांनी बाबासाहेबांची विचारशक्ती आयुष्याच्या शेवटपर्यंत जोपासली बाबासाहेबांचे शैक्षणिक विचार दलित तरुणांना दलित

स्त्रियांना आणि दलित कामगारांना आपल्या काव्यातून समजून सांगण्यासाठी त्यांनी अनेक कवने लिहिली आहेत.

डॉ. बाबासाहेब आंबेडकरांनी दलित समाजासाठी आयुष्यभर संघर्ष केला अस्पृश्यांच्या शिक्षणाचे महत्त्व व त्यामुळे होणारे सामाजिक परिवर्तन याची जाणीव त्यांनी सरकारला व दलित बांधवांना वेळोवेळी करून दिली डॉ. बाबासाहेब आंबेडकरांमुळेच दलितांना शिक्षणाचा मार्ग मोकळझाला हे सांगताना वामनदादा 'वारसा' या कवितेत म्हणतात,

"जिथे नव्हती तिथे शिक्षणाची
मोकळी वाट केली भीमाने
दीप ज्ञानाची वाट चालताना
हरघडी पालविला भिमाने"¹

अस्पृश्यतेमुळे दलितांना शिक्षणाचा हक्क मिळत नव्हता. सामाजिक बहिष्कार आणि त्यातून निर्माण झालेली गुलामगिरी तोडण्यासाठी बाबासाहेबांनी दलितांना शिक्षणाचा मार्ग दाखविला शिक्षणानेच प्रगती होणार आहे त्यासाठी त्यांनी दलितांचे प्रबोधन केले. दलितांच्या शिक्षणासाठी झगडणाऱ्या बाबासाहेबांविषयी वामनदादांनी अनेक कविता लिहिल्या आहेत. 'जन्मले ज्या कुळी भिमराया', 'तुझीच कमाई', 'भीम गेल्या पाठी', 'भीम धनी', 'तुझे रान भीमा' या कवितांचा त्यामध्ये समावेश होतो.

सर्वसामान्यांच्या न्याय हक्कासाठी, त्यांच्या स्वातंत्र्य समता, बंधुता या मूल्यांसाठी बाबासाहेबांनी आपली लेखणी झिजवली. त्यांनी प्रस्थापितांना चाबूक फटके मारण्यासठी आणि दलितांना अंतर्बाह्य आत्मजागृत करण्यासाठी अनेक ग्रंथ लिहिले. त्यांनी लिहिलेल्या ग्रंथांतून त्यांची तार्किक पण तंत्रशुद्ध संशोधनात्मक मांडणी पाहून त्यांच्या विद्वत्तेची प्रचिती घेत एवढेच नाही तर त्यांनी निर्माण केलेली अमूल्य ग्रंथसंपदा त्यातील विचारांमधून मिळणारी दिव्यदृष्टी ही लोककल्याणाची ज्योत जागवणारी आहे. लोकशाही अभिमुख होत असणारे त्यांच्या ग्रंथातील वैचारिक धन शोषितांच्या उत्थानाचे कार्य करण्यास प्रोत्साहित करते. त्यांची वैचारिक मांडणी अनेक वृत्तपत्रे आणि नियतकालिकांमधून व्यक्त झाली आहे त्यांच्या ग्रंथांचे मूल्य वामनदादांनी शब्दशः व्यक्त केले आहे. दलित तरुणांना त्यांनी बाबासाहेबांच्या ग्रंथांचे वाचन आकलन करून दिव्य दृष्टी प्राप्त करून घेण्यासाठी संदेश दिला आहे. 'कीर्तीला मृत्यू नाही' या कवितेत ते म्हणतात,

"जाहला देहांत तरी ही जिवंत
दिसेल तुला माझा भीम भगवंत
जनहीत ज्यात असे मूर्तिमंत
अमर आहेत त्याचे अनमोल ग्रंथ
दिव्य दृष्टी येई, तू वाचूनिया पाही."²

समाजात शिक्षणामुळेच क्रांती होणार आहे ही बाब वामनदादांनी काव्यातून नेमकेपणाने सांगितलेली आहे बाबासाहेबांची लेखणी वामनदादांची वाणी बनली ते बाबासाहेबांच्या लेखणीसाठी आपली शब्द सुमने वाहतात. 'भीमाची लेखणी', 'भीमाच्या नावा आधी', 'लेखणी' या कवितांमधून वामनदादांनी बाबासाहेबांच्या लेखणीला नमूद करून त्याचे महत्त्व सांगितले आहे. बाबासाहेबांच्या मनातील क्रांतीसाठी लेखणी झिजली होती त्यामुळे वामनदादांना ती जगातली सर्वात सुंदर लेखणी, मनुचा मुडदा पाडणारी समशेरच वाटते त्यामुळे ते 'भीमाची लेखणी' या कवितेत म्हणतात.

"जगातली लेखणी
बाई मी भीमाची लेखणी गं॥
काळ्या मनुचा इमला मी पाडिला
त्यात मनुचा मुडदा मी गाडिला
मुडदा मनुचा मीच पाडला रणीगं
बाई मी भीमाची लेखणी॥"³

मनुस्मृतीमुळे दलितांना शिक्षणाचा अधिकार नाकारला होता त्यामुळे बाबासाहेबांनी मनुस्मृतीचे जाहीर दहन केले

दलितांवर अन्याय करणारी दंडसंहिता नष्ट केली. वामनदादांनी या घटनेचा संदर्भ येथे घेतलेला आहे स्वतः बाबासाहेबांची लेखणी बोलत आहे अशी कल्पना केलेली आहे. "महापुरुषांच्या विचारांवर पराक्रमावर पोवाडे लिहिले गेले. ग्रंथ लिहिले गेले, पण त्यांच्या लेखणीवर ही अशी कविता लिहिण्याची घटना तशी दुर्मिळच म्हणावी लागेल."⁴

दलितांमध्ये शिक्षणाचा प्रसार व्हावा या उद्देशाने बाबासाहेबांनी सिद्धार्थ कॉलेज, मिलिंद कॉलेजची स्थापना केली. अस्पृश्यांसाठी बोर्डिंग काढली. त्यातून अनेक दलित मुले शिक्षण घेऊ लागली. बाबासाहेबांनी शैक्षणिक कार्यासाठी केलेल्या कामाचे कौतुक वामनदादांनी कवितेतून केले आहे 'पराक्रमाची गाथा' या कवितेत चवदार तळ्याचा सत्याग्रह व मनुस्मृतीचे दहन आणि काळाराम मंदिर सत्याग्रहासाठी दिलेला लढा शब्दबद्ध केलेला आहे. बाबासाहेबांच्या लह्याला नवा रंग आला. नवीन सौनिक घडले. नवे धडे गिरवले गेले. ज्ञानमंदिरे उघडली गेली. सिद्धार्थ गौतम बुद्धांच्या नावाने कॉलेज उघडले गेले याची नोंद वामनदादा करतात.

"सिद्धार्थाचे नाव गाजले मुंबईनगरीमधी
वाहू लागली तिथून आता आनंदाची नदी
त्याच नदीचे पाणी प्याले साहेब झाले बडे..."

दलित स्त्रियांच्या मनात शिक्षणाबद्दलची आस निर्माण व्हावी. त्यांनी शिक्षण घ्यावे यासाठी बाबासाहेबांनी मोठ्या प्रमाणावर कार्य केले. 1927 साली महाडच्या सत्याग्रहाला सुरुवात झाली. परंतु काही सनातन्यांनी बाबासाहेबांच्या विरोधात कोर्टात खटला दाखल केला. त्यामुळे त्यांना सत्याग्रह तहकूब करावा लागला त्यावेळी बाबासाहेबांनी 3000 अस्पृश्य स्त्रियांसमोर भाषण करून दलित स्त्रियांना शिक्षणाचे महत्त्व पटवून दिले. त्यांनी आपल्या भाषणात, "स्त्रियांना उच्चवर्णीय स्त्रियांप्रमाणे पोशाख करण्यास सांगितले तसेच मुलांना शिक्षण देऊन सुसंस्कृत करा असा संदेश दिला"

'शिका, संघटित व्हा आणि संघर्ष करा हा दिव्य संदेश बाबासाहेबांनी दलितांना दिला गरीब आईवडिलांनी मुलांना शिकवण्याचा निर्धार केला. स्वतः उपाशी राहून मुलांच्या शिक्षणासाठी कष्ट उपसले मुलांच्या शिक्षणासाठी आईवडिलांनी समाजव्यवस्थेच्या विरुद्ध जाऊन पारंपरिक रूढ संकेत झुगारले वामनदादांनी या परिस्थितीचे वर्णन केले आहे. मुलांनी शिक्षण घ्यावे. उनाडक्या करत हिंडू नये अशी अपेक्षा व्यक्त करणारी आई 'पेंद्याला साळत घाला' या कवितेतून दिसते. या कवितेतील आई स्वतः फाटक लुगडं घालते. दागिन्यांची अपेक्षा ठेवत नाही पण आपला मुलगा शिकला पाहिजे त्याने भिमरायावानी शिक्षण घेतले पाहिजे. वकील झाले पाहिजे. समाजाचे ऋण फेडले पाहिजेत. ही तळमळ व्यक्त करते.

"माझं बर हाय फाटकच लुगडं
बाळ माझं दिसो ना उघड
डागडागिन नको गं मजला
माझ्या पेंद्याला साळत घाला
समाजाचं फेडायया ऋण
बाळ माझं घेईल शिक्षण
व्हईल वकील जयभीमवाला."⁶

शिक्षणाने समाज सुधारला जातो. शासन प्रशासनातील महत्त्वाची अधिकार पदे मिळवता येतात. त्यामुळे शिक्षण घेतले पाहिजे हे दलित समाजाला बाबासाहेबांमुळे कळाले शिक्षण ही आत्मसन्मान मिळविण्याची गुरुकिल्ली आहे याची जाणीव वामनदादा यांनी काव्यातून समाजाला करून दिली. 'फौजदार' कवितेत आईचे दुःख निवारण्यासाठी, कष्ट संपविण्यासाठी तिच्या बाळाने शिक्षण घेतले तर तो फौजदार होईल. तिचा बाळ फौजदार झाला तर तिच्या आयुष्यात सुख येईल. त्यातून संपूर्ण दलित जनतेला तिचा आणि तिच्या फौजदार बाळाचा अभिमान वाटेल् हा आशय व्यक्त झालेला आहे. समाजाची, कुटुंबाची उन्नती करण्यासाठी शिक्षण हाच एकमेव पर्याय आहे, हे वामनदादांनी 'फौजदार' या कवितेतून सांगितले आहे.

वामनदादांनी भावी पिढीने शिक्षण घेतले पाहिजे, शिक्षणाच्या, ज्ञानाच्या बळावर स्वतःचे उत्थान केले पाहिजे असा लोककवी वामनदादा कर्डक : व्यक्ती आणि वाङ्मय / 193

विचार मांडला. त्यासाठी त्यांनी निसर्ग प्रतिमांचा आधार घेतला आहे.

"पोरं आमची शिकू लागली पिकू लागली फळं
पीक हातशी आलं, रस आंब्याचा गळं।।"

बाबासाहेबांनी अस्पृश्यांना शिक्षणाचा अधिकार मिळवून दिला मनुवाद्यांनी अस्पृश्यांच्या ज्ञानावर अधिकारावर गदा आणली होती. ज्ञान वंचित समाजात ज्ञानाचा अंकुर उभे करणे हा चमत्कार बाबासाहेबांमुळे झाला त्यामुळे अल्पावधीतच शिक्षण घेतलेले दलित तरुण मोठमोठ्या हुद्यावर गेले. शिक्षणामुळे दलितांचा भविष्यकाळ निश्चितच उज्ज्वल आहे हे वामनदादा यांना माहीत होते.

"आमच्यासाठी खास आरक्षण
केलं माझ्या भीमानं
करून रक्षण आमचं शिक्षण
केले माझ्या भीमानं"⁷

वामनदादांच्या व्यक्तिमत्त्वावर डॉ. बाबासाहेब आंबेडकरांच्या विचारांचा जसा प्रभाव आहे तसा तथागत गौतम बुद्ध महात्मा फुले, संत कबीर यांचा देखील प्रभाव आहे वामनदादा डॉ. बाबासाहेब आंबेडकर यांची प्रेरणा जशी घेतात तशीच प्रेरणा ते गौतम बुद्धांच्या शिकवणुकीतूनही घेतात ही गुरुशिष्य परंपरा सांगताना वामनदादा म्हणतात

"थोर चेला गुरु गौतमाचा एक भीमराव होऊन गेला
गुरु आणि चेल्याच्या बळाने कोटी कोटींचा उद्धार केला।।"

वामनदादा गौतम बुद्धांना बुद्धीची देवता मानतात ते मानसिक व बौद्धिक दृष्टीने बुद्धांचे आकलन करतात. 'गौतमाचा लढा' या कवितेत ते भीमाचा मळा होऊन मनाची टवटवी फुलवावी आणि गौतमाचा लळा लावून घ्यावा. ज्ञान देणाऱ्या शाळेतल्या लाकडाचा फळा आपण व्हावे, अशी कल्पना करतात.

वामनदादांनी गौतम बुद्धाप्रमाणेच महात्मा फुले यांनी अस्पृश्यांच्या शिक्षणासाठी केलेल्या कार्याचे गुणगान गायले आहे. जोतीराव फुले यांनी स्त्री शिक्षणासाठी, अस्पृश्यांच्या शिक्षणासाठी पुण्यात शाळा सुरू केली त्यांनी तळागाळातील लोकांना शिक्षणासाठी प्रेरित केले. वामनदादांनी त्यांच्या या प्रयत्नांना आगामी झालेल्या महान सामाजिक क्रांतीची नांदी मानली आहे.

"स्त्री जातीच्या मुक्तीसाठी आले महात्मा फुले गं
आले महात्मा फुले, मुलींचे शिक्षण केले
ना ज्ञान मिळाले काही खुले गं त्या दुबळ्या जातींमधी
फुलू लागल्या कळ्या कोवळ्या फुलू लागली फुले गं
ओढ ज्ञानाची लागली, या शाळा पोरांची काढली
तेव्हापासून शिकू लागली अस्पृश्यांची मुले गं"⁸

स्त्रियांच्या शिक्षणासाठी, अस्पृश्यांच्या शिक्षणासाठी जोतीराव फुले यांनी केलेले कार्य वामनदादांनी अद्वितीय मानले आहे त्यांच्या कार्याचे वर्णन करणाऱ्या अनेक कविता त्यांनी लिहिल्या आहेत. जोतीराव फुले वामनदादांना आदरस्थान वाटतात.

बाबासाहेबांना शैक्षणिकदृष्ट्या अपेक्षित असलेला समाज वामनदादा गीतांतून समजून सांगतात आंबेडकरी समाजाने शिक्षणक्षेत्रात जी गरुडझेप घेतली आहे, स्वतःचे आयुष्य शिक्षणाने समृद्ध केले आहे, हे पाहून वामनदादा कृतकृत्य पावतात. डॉ. बाबासाहेब आंबेडकरांनी अस्पृश्यांना जो शिका, संघटित व्हा आणि संघर्ष करा हा संदेश दिला त्यातून एक मोठा दलित समाज शिक्षित झाला. शब्दशस्त्र हातात घेऊन त्यांनी सामाजिक परिवर्तन घडवून आणले. ही निशस्त्र क्रांती केवळ शिक्षणामुळे झाली. त्याचेच प्रतिबिंब वामनदादांच्या कवितेत उमटलेले आहे "शिक्षणाची महती बाबासाहेबांनी सांगितली आणि दादांनी तो क्रांतीसंदेश खेड्यापाड्यातून गायन करून लोकांच्या काळजापर्यंत पोहोचवला आणि आंबेडकरी समाजात शिक्षणाचे वादळ उठले."⁹ हे यशवंत मनोहर यांचे निरीक्षण अत्यंत उपयुक्त आहे

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एकूणच वामनदादा कर्डक यांनी डॉ. बाबासाहेब आंबेडकर यांच्या शैक्षणिक तत्त्वज्ञानातून प्रेरणा घेऊन आपली शिक्षणविषयक भूमिका तयार केलेली आहे. बाबासाहेबांची लेखणी, त्यांचे ग्रंथ वृत्तपत्रे, नियतकालिकांमधून केलेले लेखन आणि शैक्षणिक संस्था, परिषदा यामधून तयार झालेली शिक्षणविषयक मते वामनदादांच्या काव्यातून व्यक्त झालेली आहेत. वामनदादांच्या शिक्षणविषयक काव्यातून गौतम बुद्धांचे महात्मा फुले यांचे शिक्षणविषयक कार्य प्रसृत झालेले आहे. अस्पृश्य, दलित समाजाला त्यांच्या उन्नतीचा मार्ग शिक्षणाची गंगोत्री पोहोचल्याशिवाय मिळणार नाही. त्यासाठी प्रज्ञासूर्य, ज्ञानवंत डॉ. बाबासाहेब आंबेडकरांचा आदर्श सर्व दलित तरुणांनी ठेवला पाहिजे ही भावना वामनदादा व्यक्त करतात वामनदादा दलित समाजाला जागृत करण्यासाठी शिक्षणाचा मुक्ती मार्ग दाखवतात.

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INDIAN FREEDOM MOVEMENT AND PUNE CITY**Dr. Bhushan Govind Phadtare**

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Abstract

The revolt of Umaji Naik and Vasudev Balwant Phadke posed a challenge to the British rule. Since then, many revolutionaries in the country have taken inspiration from them. Mr. Rand, the British officer, known for his cruelty, was assassinated by the Chafekar brothers. The Chafekar brothers were sentenced to death for this incident. Lokmanya Tilak's editorial in the 'Kesari' newspaper was critical of the British. Lokmanya Tilak was also sentenced to life imprisonment. In 1905, a nationwide anti-secession movement was started against the partition of Bengal. In Pune city, in western Maharashtra, the Holi of foreign clothes was celebrated under the leadership of Savarkar. The mantra of Swadeshi and exclusion was adopted by the people and students. Mahatma Gandhi started a civil disobedience movement by carrying out salt satyagraha at Dandi. The Swadeshi boycott movement was gaining momentum through various organizations in Pune district. Mahatma Gandhi and Dr. Babasaheb Ambedkar signed The Pune Agreement. Hundreds of men and women from western Maharashtra had participated in the individual satyagraha movement. On August 8, 1942, Mahatma Gandhi gave the mantra 'do or die' to the Indian people. The people of Western Maharashtra were overwhelmed by this mantra. On the morning of August 9, the Quit India Movement started across the country. Sixteen year old Narayan Dabhade Dharatirthi sacrificed himself while hoisting the tricolor flag on the Congress Bhavan in Pune. Processions started in Pune district. The underground movement in Pune district was led by Shirubhau Limaye where events like the Capital bomb blast case Dehuroad bomb case, and underground radio are significant. On 15th August 1947, the joy of India's independence was celebrated all over the Country.

Keywords: Revolt, Nationalism, Swadeshi, Commission, Satyagraha, imprison, flag hosting.

The Pune city is considered as an 'intellectual Capital' of the western India. In Pune, the works of Lokhitwadi, Agarkar, Ranade, Bandarkar, Gokhale and Tilak are remarkable. Therefore, the background of the National congress was created in Pune. It was determined that the first convention of the National Congress will be organized in Pune but was finally taken in Mumbai. Nine people from Pune were present at the convention of the first National Assembly held in Mumbai (1885). In 1895, the National Assembly convened in Pune where the chairman was Surendranath Banarjee.¹

Vasudev Balwant Phadake is the first revolutionary of the Modern India. He started revolt against British with the help of Ramoshi and Koli People. The revolt expanded from Pune and when the increasing revolt became harmful to the British Government, Major Henry Williams Denial was appointed to suppress the revolt. Phadake was arrested and imprisoned at Gangapur and impaled. Vasudev Balwant Phadake died in the Eden Jail. The Chaphekar brother and Vinyak Savarkar were inspired by Phadake.

Damodar, Vasudeo and Balkrushna, these Chaphekar Brothers were of the revolutionary thinking. They killed Mr. Rand on 22nd June 1897 at Ganeshkhind in Pune.² The British Government was alarmed by this incident and started oppression to arrest the Chaphekar Brothers.

The martyrdom of Chaphekar brothers inspired Vinyak Damodhar Savarkar of Nationalism and he participated in the freedom movement. The Swadeshi Movement started all over the country against the partition of Bengal. During this movement Vinyak Damodhar Savarkar was taking education at the Fergusson College. Savarkar had burnt the foreign goods at the Deccan Gimkhana and accepted the Swadeshi. This was the first burning of the foreign goods. When, people were accepting the 'Swadeshi all over the country, in Pune there was the direct burning of the foreign goods.' It was a prominent characteristic of the protest in Pune.³ The Samarth School was founded in Talegaon Dabhade to give the education of Nationalism, like Maharashtra school in Pune. The founder of the school was Prof. Vishnu Govind Vijapurkar. In his leadership, the 'Swadeshi Factory' started. Bankimchandra Chaterji's 'vandemataram' and K. P. Khadilkar's drama 'Kichakvadh' played a crucial role in speeding the protest. In the beginning of the 'Vangbhang Protest' Lokmanya Tilak had laid down the program of Swadeshi, National education, Boycott

and Swaraj. At this time, Tilak was imprisoned and sent to the jail of Mandale. While in the Mandale jail, Tilak had written 'Geeta Rahasya'.

The rise of Mahatma Gandhi is in the second decade of the 20th century. His period is known as the Gandhian Period. Namdar Gokhale was the Guru of Mahatma Gandhi. Gokhale had established the institution 'Bharat sevaksamaj' in Pune. Mahatma Gandhi and Lokmanya Tilak met at the Sinhgarh fort near Pune, which was their first and last meeting.

In 1920 the convention of National congress happened in Nagpur. In this convention, the decision of non-cooperation was taken. To make the awareness regarding this movement several meetings held in the Pune region. While disowning the degree Mahatma Gandhi has disowned 'The Kaisar-E-hind'. People had internalized the mantra of 'Swadeshi and boycott' and reflected through their actions. Gents wore the swadeshi Cap and Ladies wore the swadeshi Saree to make the Swadeshi Movement strong. In Pune city, women were in the forefront in popularizing khadi and spinning. The women formed a yarn spinning committee with President Ramabai Biniwale, Vice President Dwarkabai Gujar, Treasurer Ramabai Kuwalekar, and Secretary Andibai Jogalekar.⁴

Apart from this, at Durgabai Kotkar's home the Swadeshi Bangles were stored for sale. L. B. Bhopatkar, a famous lawyer, had boycotted the judicial work. To provide the Swadeshi education, the Tilak Maharashtra Vidyapeeth and Tilak Mahavidyalaya in Pune, Anath Vidyarthi Grahpathshala in Chinchwad and Rasthya Pathshala in Baramati were established. Many of the student participated in the Swadeshi Movement. 'Tilak Swaraj fund' is also important as these funds availed the charakha's to spin the cotton. Khadi became famous all over the country. It was noticeable that women were at the forefront in the cotton spinning. The movement stopped due to the chauri-chaura matter, but there remained the impacts of this movement.

The Simon commission was appointed to understand the demands /changes Indians under the leadership of Sir John Simon. The commission was opposed because there was not a single Indian Person in that commission. When this commission came to Pune, the shopkeepers closed their shops and gave slogans 'Simon go Back'. In the whole country there was an oppose to the Simon commission. But even so, some people in India have testified before the Simon Commission.⁵ So, the British became ready to give colonial freedom to Indians but Pandit Jawaharlal Nehru declared that the Indians want complete freedom. The Republic Day was celebrated on 26th Jan. 1930 as declared by the National Congress.⁶

The 'Savinay Kaydebhang' movement started from the 'Salt Satyagraha' at Dandi. Many people participated in this movement from Pune. Shankarrao Dev & Trimbak Devgirikar were the leaders in salt satyagraha at Shiroda. Apart from this, several groups of Volunteers were created like⁷–

Sr. no	Volunteer Squad	No of Volunteer	Salt Satyagraha Place
1	Swavlamban Rashtriya Pathak (Chinchwad)	11	Vileparle
2	Tilak Maharashtra vidyalaya (Pune)	12	Vileparle
3	Navin Samarth Vidyalaya (Talegaon Dhapbhade)	28	Malwan
4	Chitrashala Pathak (Pune)	17	Pen
5	DeshSevashram Pathak (Pune)	18	Vileparle
6	Talegaon Dhamdhare Pathak (Talegaon Dhamdhare)	18	Vileparle
7	Murali Pathak	11	Malwan

Many of the Volunteers of the groups have taken part in salt Satyagraha and were imprisoned. Like the Salt Satyagraha and were imprisoned. Like the Salt Satyagraha the jungle Satyagraha is also important. Indigenous companies in Pune district gave importance to Swadeshi.⁸

Sr. no	Name of the companies	Goods	Place
1	Deccan Paper Mills company	Paper	Mundwa
2	Paisa Fund Glass Work	Glass	Talegaon Dhabhade
3	Paisa Fund Glass Work	Pot rig	Talegaon Dhabhade
4	Paisa Fund Glass Work	Bracelets	Talegaon Dhabhade
5	Bhagat And Sans	Crayons	Pune City
6	Nadaram Maruti Jadhav	Lantern stand	Rawihar Peth Pune

7	Khunya Murlidhar toy works	Toys	Pune
8	Bharat paper Mint and Company	Paper Mint	Ganesh Peth, Pune
9	R. B. Paranjape	Paper Mint	Sadashiv Peth, Pune
10	Bharath Industrial work	Paper Mint	Sadashiv Peth, Pune
11	D. N. Chandra & Company	Batans	Nana Peth, Pune
12	Sathe Bandu	Biscuit	Pune
13	Caliko Mills shop	Role	Budhawar Chowk, Pune
14	Bhagat & Company	Colour	Pune
15	Parkar Distemper Company	Colour	Sadashiv Peth, Pune
16	Pranjape & sans	Colour	Sukarwar Peth, Pune

In Swadeshi and Boycott movement 51 Businessmen had stressed on selling the swadeshi goods under the Leadership of Desdash Ranade.⁹ Babu Genu died for Swadeshi. Vasudev Balwant Gogate fired Governor Hotson in Fergusson College Library.¹⁰ On January 26, 1932, Sutaram Athavale and Ramchandra Adhav were Sentenced to 6 month imprisonment for hosting a flag on the ground of Ray market.¹¹ In 1940, a meeting was held at Pune of all India Congress Committee to think the over the personal Satyagraha movement. In this meeting it was decided that the personal satyagraha has to be done through the Ahimsa. The first satyagraha was done by Acharya Vainoba Bhave at Pavanar and by Bhalechandra Gupte and Acharya Vishnu Limaye in Pune. Shankarrao Dev was sentenced to one and a half years and Keshavrao Jadhe to one for carrying out personal satyagraha .¹² Inspired by this, many people did the personal Satyagraha.

‘Quit India Movement’ is one of the last remarkable movements in the Indian Freedom Movement. In August 1942 a convention held in Mumbai and for this convention many people with N.V.Gadgil and Keshavrao Jedhe from Pune. In the very opening of the movement Mahatma Gandhi, Pandit Nehru, Sardar Vallabhabhai Patel and Maulana Azad were imprisoned and were taken to Pune. Mahatma Gandhi was beginning at Agakhan palace in Pune. On the first day of the movement Narayan Dabhade, a youth of 16 years old died while hosting the flag of Tiranga on congress Bhavan.¹³ By taking inspiration from Dabhade’s Sacrifice the student of Engineering College, Agriculture College and Fergusson College had marched processions in Pune. The Police had fired on these Processions and several students and people were killed in this incident.¹⁴ Although many people were imprisoned, the intensity of the movement was increasing so, the Government has ordered Curfew. People from Dalit community were involved in the freedom movement in Pune district. E.g. Mahadev Kambel, Datta Kamble, Jandrdhan Waghmare. Apart from this of such castes as potter Dhangar, Shimpi, Gurav and Sonar were also included. Yarawada Jail has records of his imprisonment.

The arson at Bhikardas Police gate¹⁵, the bomb blast at west end & capital the bomb case matter at Dehuroad Depo and the congress radio center all these are the remarkable incident in this movement.¹⁶ The India’s Freedom on 15th August 1947 is the outcome of all these movement. On the 15th August in the morning the flag hosting ceremony was performed by Senapati Bapat at congress Bhavna and by Trimbak Devgirikar at the collector office.¹⁷

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ज्ञान-विज्ञान विमुक्तये

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SYNTHESIS, CHARACTERIZATION AND IN SILICO PREDICTION OF OXIME AND THIOSEMICARBAZONE DERIVATIVES OF HALO HYDROXY NAPHTHOQUINONE AS AN ANTI-VIRAL AGENT AGAINST SARS2 CORONA VIRUS

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Abstract:

Oxime and thiosemicarbazide derivatives of halo juglone synthesized for antiviral activity. Characterization of juglone derivatives are done by IR and NMR Spectroscopy. RM1 –RM6 molecules are selected for in silico study. National Centre for Biotechnology Information server found proteinase (PDB id:2ALV) was found SARS corona virus for serve acute respiratory syndrome. 3 D X-ray crystallographic structure of proteinase (PDB id:2ALV) which was validated on Ramchandran Plot was 99.2% by using PROCHEK server. Auto dock Tools version 1.5.6 was used to optimize 3D module of protein. X-Ray crystal structure as three dimensional coordinate of these target protein was obtained from the research collaborator for structural Bioinformatics (RCSB) protein data bank. Binding pockets has been verified by using PDB sum server. Autocad tools was used for receptor grid calculation. Docked conformation of ligands with 2ALV obtained from Maestro V12.8. Possible ligand binding site in the minimized protein were determined by Computed Atlas of Surface Topography of proteins (CASTp) server. For docking studies, we used the AutoDock Vina 1.1.1, with 1 °A of spacing between the grid points. The PASS server provides all the possible activities of the given halohydroxynaphthaquinone derivatives. Final result was analysed by pymol and lig plot indicate that RM2, RM3 and RM6 showing better activities towards proteinase (PDB id 2ALV) of SARS2.

Keywords: Juglone, Oxime and thiosemicarbazide derivatives, Corona Virus, Silico Prediction

Introduction:

All world experienced covid-19 major outbreak .Coronavirus disease (Covid -19) is an infectious diseases caused by SARS- Cov-2 virus. The corona virus is affecting 221countries in the world, and 237,155,841 people infected all over the world. 4,842,331 death occurs till death due to covid -19 all over the world. There is no successive clinical trial for covid-19. [1]

Ayurveda is great gift for India which is curative and preventive. Juglone which is present in the bark, roots and leaves of Julandiacae family has been used traditionally in ayurvedic medicine for the treatment of anti-inflammatory, antioxidant, antimicrobial, anti-viral and antitumor activities. [2-5]

In pharmacological processes binding of protein with drug is important parameter. Bonding between drug molecule and protein is based on binding energies. Bonding angles, hydrogen bonding, π interactions, Van der Waals interactions are also affecting parameter for bonding between drug molecule and protein. Metabolism between drug molecule and protein impact on therapeutic effects of drug, interaction of drug molecule to protein effects on stereo –chemical changes of proteins. [6]

In silico predication is the first step in drug development. On the basis of literature survey oxime and thiosemicarbazide derivatives of halo-juglone molecular docking have not been reported.

Activity spectra predication done using PASS online module, by way 2 drug server. For the docking study protein was isolated from RCSB online data base. Protein and ligands optimization was done by various software Grid parameter obtained from Cast p server. Actual docking was done using autodoc tools 4.2.

Discovery studio lig plot and maestro used for analysis of protein- ligand complexes. We found that RM2 ,RM3 shows better affinity with the receptor.

Experimental:

Preparation of 2 Chloro Juglone:

Dichloro Juglone derivatives was refluxed in 20 cc ethanol using water bath for 2 hrs after attaining 80 C temperature . The solution was dried in vaccum .The compound containing a mixture of 2 – chlorojuglone and dichlorides. This is tested by TLC using solvent (9:1 n-hexane : ethyl acetate). The product 2-Chloro Juglone purified by column chromatography using silica gel 200 mesh size and 9:1 n -hexane + ethyl acetate mixture as elute. The melting point was 164 C.% yield obtained 42 %.

IR (cm⁻¹):744, 785, 844,909, 1049, 1088, 1193, 1297, 1448, 1587, 1637, 3051,. C¹³NMR:187.311, 181.245, 144.775, 140.96, 134.62, 133.28, 132.211, 131.643, 125.456, 120.629., ¹H NMR(δ):7.94 (s,1H), 7.87 (d,1H), 7.80 (ddd,1H), 7.69 (d,1H) , 2.47(s,1H)

Preparation of 2- Bromo Juglone:

5.00 g of Juglone suspended in 50 ml of glacial acetic acid containing 1.5 ml of bromine was shaken mechanically for 15

minutes. The solution which soon took place was poured with stirring into much cold water. The dibromide separated as a reddish Yellow mass of crystal which is melted at 102°C. The dibromide it was then dissolved in 15 cc of absolute alcohol and heated under reflux condenser for 45 minutes. 6.1 g of monobromo Juglone crystallized in reddish brown plates, the pure product with melting point of 164°C. % yield obtained 36%.

IR (cm⁻¹): 737.57, 871.46, 1129.1, 11199.32, 1245.65, 1580.89, 1639.37, 3060.05., C¹³NMR: 187.494, 181.641, 144.211, 140.283, 135.931, 135.231, 130.691, 127.89, 125.453, 120.999., ¹H NMR(δ): 7.81 (s,1H), 7.67 (d,1H), 7.53 (ddd,1H), 8.69 (s,1H), 2.30(s,1H)

Preparation of 2 Iodo Juglone:

The diiodo product is refluxed in 20 ml ethanol using oil bath for 2 hr after maintaining temperature of 80°C. The solution was dried in vacuum. The compound containing a mixture of 2-iodo juglone and diiodide. This is tested by TLC using solvent (9:1 n-hexane : ethyl acetate). The product 2-iodo Juglone purified by column chromatography using silica gel 200 mesh size and 9:1 n-hexane + ethyl acetate mixture as elute. The melting point was 168°C, yield obtained 55%.

IR (cm⁻¹): 745.45, 832.78, 857.56, 1097.86, 1157.50, 1277.97, 1491.11, 1593.44, 1633.68, 2920.07., C¹³NMR: 190.100, 183.869, 146.76, 139.813, 136.613, 131.610, 124.542, 120.544, 114.240., ¹H NMR(δ): 8.50 (d,1H), 7.87 (ddd,1H), 7.33 (d,1H), 8.57 (s,1H), 2.30(S,1H)

Preparation of 2- bromojuglone mono-oxime (RM1), 2- Iodojuglone mono-oxime (RM2), 2- chloro-juglone mono-oxime (RM3)

0.3 g (2-bromo, 2-iodo, 2-chloro derivative of juglone) dissolved in 10 ml 1 M NaOH solution and 0.1043 g hydroxylamine hydrochloride in 5 ml distilled water. Solution is kept in water bath for 1 hour at 50°C. Then let it cool to room temperature. Solution is then diluted with ice cold water to 50 ml. Add 1Molar HCl to adjust the pH to 5.5. Then solution is kept in ice bath for 2 hours and allowed to precipitate. Precipitate is filtered through Whatmann filter paper and dried completely. Procedure for removal of acid by solvent separation method is carried out, yield obtained 63%, 65% and 54% respectively. [7-12]

RM1: IR (cm⁻¹): 3362, 3155, 1630, 1576, 1293, 1211, 1050, 784, 740,676., C¹³NMR: 182.26, 166.678, 161.275, 147.213, 133.756, 133.0, 132.621, 122.634, 121.802, 120.3., ¹H NMR(δ): 7.4 (d,1H), 7.87 (dd,1H), 7.60 (d,1H), 7.29 (S,1H), 5.31 (S,1H), 8.47(S,1H)

RM2: C¹³NMR: 183.231, 164.693, 162.371, 147.689, 133.987, 132.774, 123.659, 122.731, 121.956, 100.853., ¹H NMR(δ): 7.32(d,1H), 7.57 (dd,1H), 7.42(d,1H), 8.29 (S,1H), 5.41 (S,1H), 2.67(S,1H)

RM3: IR (cm⁻¹): 3341, 3140, 1654, 1545, 1320, 1234, 1065, 952,770, 660., C¹³NMR: 182.313, 166.916, 161.646, 138.790, 133.543, 133.869, 131.537, 124.834, 122.642, 122.93., ¹H NMR(δ): 7.82 (d,1H), 7.54 (dd,1H), 7.12 (d,1H), 7.29 (S,1H), 5.62 (S,1H), 2.37(S,1H)

Preparation of semicarbazide derivatives of 2-bromo Juglone (RM4), 2-iodo Juglone (RM5), and 2-chloro Juglone (RM5)

2 mol of methanolic solution of (2-bromo, 2-iodo, 2-chloro derivative of juglone) is added to 10 ml of 0.2 N NaOH to obtain reddish brown purple solution. 0.02 mol of 50 % methanolic solution of thiosemicarbazone is added drop wise with constant stirring for 3 hours. The solution is neutralized using 10% HCl till precipitation. Then the solution is filtered and recrystallized in methanol. Melting point 135°C, yield obtained 67%, 70% and 63% respectively. [13-18]

RM4: IR (cm⁻¹): 3373, 3270, 3255, 1684, 1620, 1535, 1270, 1023, 778, 654, 590., C¹³NMR: 187.342, 182.881, 165.483, 160.221, 148.195, 133.892, 132.672, 131.324, 129.953, 125.678, 123.692., ¹H NMR(δ): 7.72 (s,1H), 7.64 (d,1H), 7.52 (d,1H), 7.29 (dd,1H), 3.12 (s,1H), 5.34 (s,1H) 2.37(S,2H)

RM5: IR (cm⁻¹): 3356, 3290, 3276, 1679, 1530, 1276, 980, 875, 679, 543., C¹³NMR: 187.342, 184.881, 165.483, 163.221, 146.195, 137.892, 135.672, 133.212, 124.512, 100.2., ¹H NMR(δ): 8.72 (d,1H), 7.64 (dd,1H), 7.59 (d,1H), 7.39 (s,1H), 4.12 (s,1H), 5.34 (S,1H) 2.37(S,2H)

RM5: IR (cm⁻¹): 3300, 3265, 1720, 1656, 1578, 1323, 987, 890, 766, 593., C¹³NMR: 188.312, 186.631, 166.439, 165.384, 155.613, 145.542, 130.617, 131.781, 135.212, 127.684, 121.319., ¹H NMR(δ): 7.67(d,1H), 7.44 (dd,1H), 7.31 (d,1H), 7.19 (1H), 4.11 (s,1H), 5.49 (s,1H), 2.35(s,2H)

Methodology:

Selection of particular Ligands from monooxonaphthalenone derivatives

The important derivatives from synthesized compounds were used in the present investigation for the computational prediction of potential drugs from it by the process of molecular docking against Covi-19.

Biological Activity Prediction

Due to the impossibility of performing a study of the biological activity of a large number of compounds in a short period, it was decided to conduct a preliminary assessment of the potential biological activity of compounds (RM1, RM2, RM3, RM4, RM5 & RM6) using PASS-online modeling. The PASS software product, which predicts more than 300 pharmacological effects and biochemical mechanisms on the basis of the structural formula of a substance, may be efficiently used to find new targets (mechanisms) for some ligands and, conversely, to reveal new ligands for some biological targets. The mean accuracy of prediction with PASS is about 86% in LOO cross-validation. The tool uses the descriptors to predict the activity of a substance. [19-22]

Result:

The prediction of the biological activity spectrum of oxonaphthalenone derivatives **RM1 to RM6** revealed that compounds are

determined as promising SARS coronavirus main proteinase. This indicates that all the three compounds may show good activity against Covid-19 as SARS coronavirus main proteinase is main target for covid treatment.

The 3D SDF structures of the processed six halo hydroxyiminonaphthalenone derivatives **RM1 to RM6** were given as an input for PASS server. The PASS server provides all the possible activities of the given halo hydroxyiminonaphthalenone derivatives as promising SARS coronavirus main proteinase inhibitors. PASS can be effectively applied to predict biological potential of compounds and to analyze large chemical databases. PASS predicted search results show all the available information on the pharmacological and toxicological activity of all the three compounds analysed. Similar observation in accordance with the present study using PASS server was already reported by many researchers. Pa and Pi are the estimates of probability to be active and inactive respectively from the biological activity spectrum. Their values vary from zero to one. Each active compound possesses a number of biological activities. Its specificity of action is always relative and is defined by the peculiarities of object, dose, route, etc. Biological activity spectrum of compound can be predicted on the basis of structure-activity relationships found by the analysis of the known data from the training set. Based on the analysis of large training set consisting of tens of thousands of the known biologically active compounds, computer program PASS provides the means to evaluate any new compound in huge chemical-pharmacological space. On the basis of this study it can be revealed that all the three compounds may show good activity against Covid-19 as SARS coronavirus main proteinase inhibitor.

Molecular Docking Studies:

Target Protein Retrieval and Preparation

On the basis of literature survey we found that SARS coronavirus main proteinase is major target to study anti-covid study. Therefore, fasta sequence of SARS coronavirus main proteinase for Severe acute respiratory syndrome-related coronavirus was retrieved from National centre for biotechnology information server and done Basic Local Alignment Search for regions of similarity between biological sequences available on Protein Data Bank. Then Three-dimensional X-Ray crystallographic structure of SARS coronavirus main protease (PDB id: 2ALV) was obtained from PDB databank which was validated using various parameters like resolution, Mutation and Ramchandran plot.[23-25] Details are as follows.

Table1. Comparison between standard values and retrieved protein for validation of protein selected for docking study

Parameters	Details	Standards
Protein Id and method of experiment	2ALV X-RAY Diffraction	- X-RAY Diffraction
Mutation	No	No
Resolution	1.90 A ⁰	Near about 2.00 A ⁰
Ramchandran Plot (by PROCHECK server) Residues in favoured + Allowed regions	99.2%	>88 %

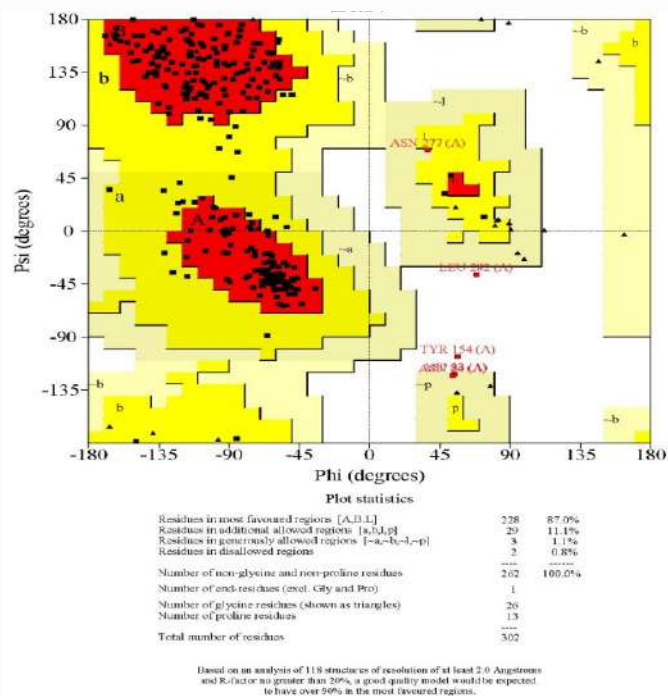


Figure1. Ramachandran Plot 2az5 obtained from PROCHECK server

The preparation of a protein involves importing of the SARS coronavirus main proteinase Protein structure. Binding pocket has been verified using PDBsum server which is a Pictorial database of 3D structures in the Protein Data Bank for interactions of standard inhibitor with protein. The water molecules, unnecessary chains and ligands have been deleted and the protein were retained using Biovia Discovery Studio visualizer V21.1.0.20298. Charges were stabilized, missing residues were filled in and side chains were generated using AutoDockTools v1.5.6 spet_17_14.

The CHIMERA v1.5.3 software was used to minimize the structure of protein, using the Gasteiger charges with 1000 steepest descent steps of minimization.

Grid Generation

AutoDockTools was used for receptor grid identification. The prepared SARS coronavirus main proteinase was displayed in the Workspace. The volume of grid was calculated using dimensions of pocket identified from CASTp server (Computed Atlas of Surface Topography of proteins). The enclosing box was made small so that it will be consistent with the shape and character of the protein's active site and with the ligands that were expected to be docked.[26]

Ligands Preparation

Ligand molecules were designed in MarvinSketch v21.13 and saved in 3D MOL2 format. All the three compounds were processed, and optimized by UCSF Chimera v1.15 using AM1-BCC semi-empirical force field other parameters defaults like steepest descent steps : 1000; Conjugate gradient steps 100, etc.

Molecular Docking of Target Protein with Ligands

After obtaining the ligands and enzymes, their structures were converted to pdbqt format, using the AutoDock Tools 1.5.6 program, in which all the rotatable bonds of ligands were allowed to rotate freely, and the receptor were considered rigid. For docking studies, we used the AutoDock Vina 1.1.1, with 1 Å of spacing between the grid points. The grid box was centred on the active site of the enzyme with high resolution, allowing the program to search for additional places of probable interactions between the ligands and the receptor. Other configurations were considered default. The XYZ coordinates 70.627 X 36.344 X 20.769, and size of the grid box is 24 X 20 X 28 Å⁰. The redockings were performed with the same configurations of the previous performed dockings.

Visualization

Results obtained after Autodock Vina processing were subjected to make a complex using Biovia Discovery Studio visualizer. Interactions and binding energies of test compounds were compared with standard inhibitor.

Result:

All three compounds were prepared to dock with the Crystal Structure of SARS coronavirus main proteinase (PDB id 2ALV). The selected chemical structure of the the important ligands were shown in Figure 2.

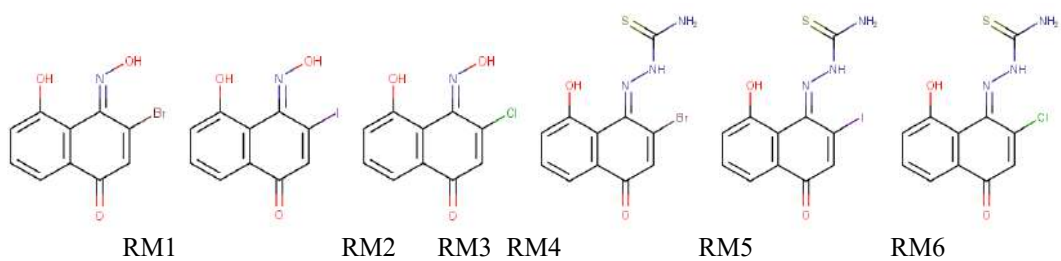
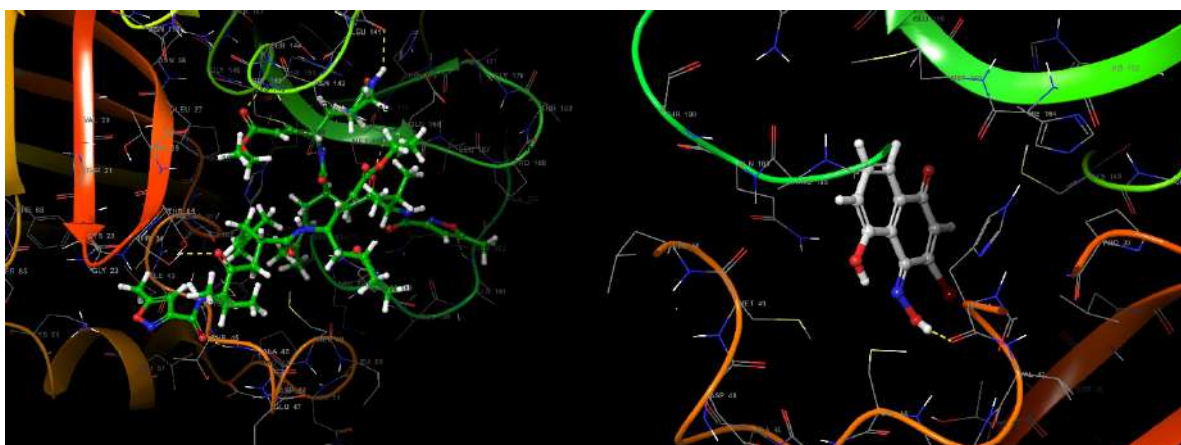
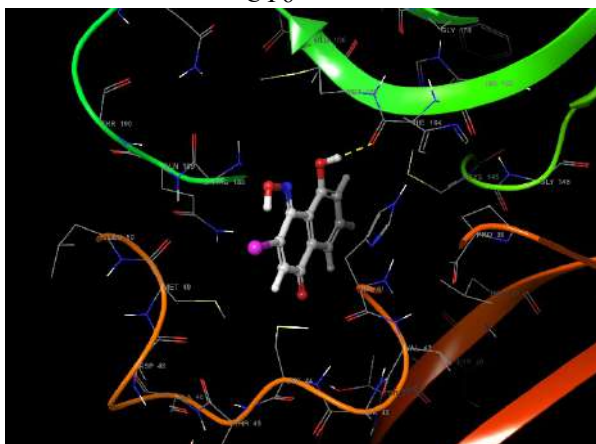


Figure 2. Structure of the Ligands

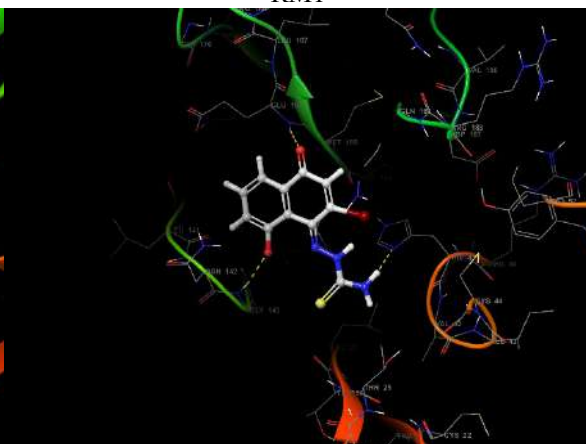


CY6

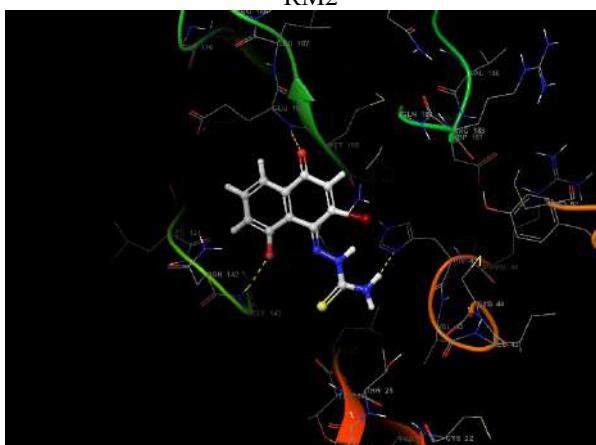
RM1



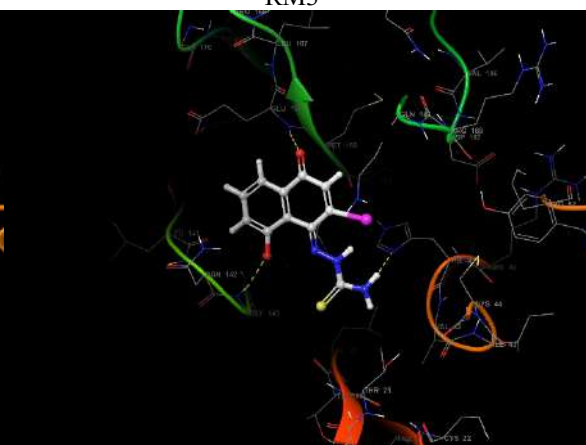
RM2



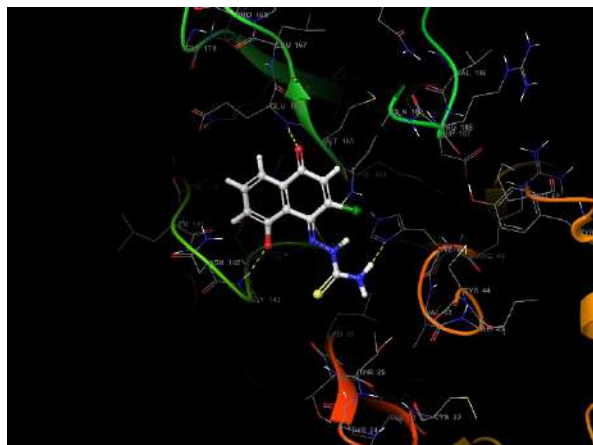
RM3



RM4

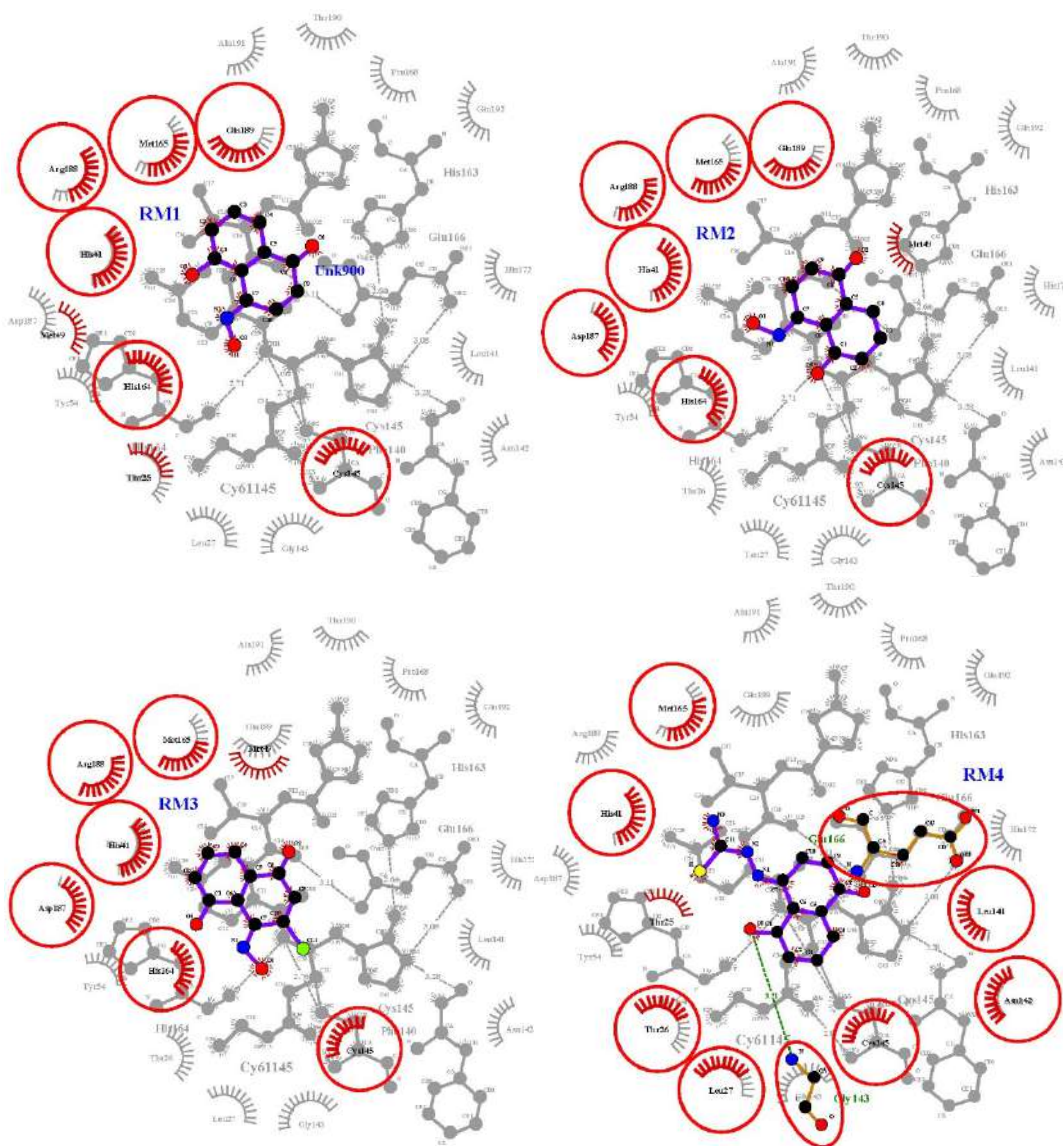


RM5



RM6

Figure 3. Docked conformation of ligands with 2ALV obtained from Maestro V12.8



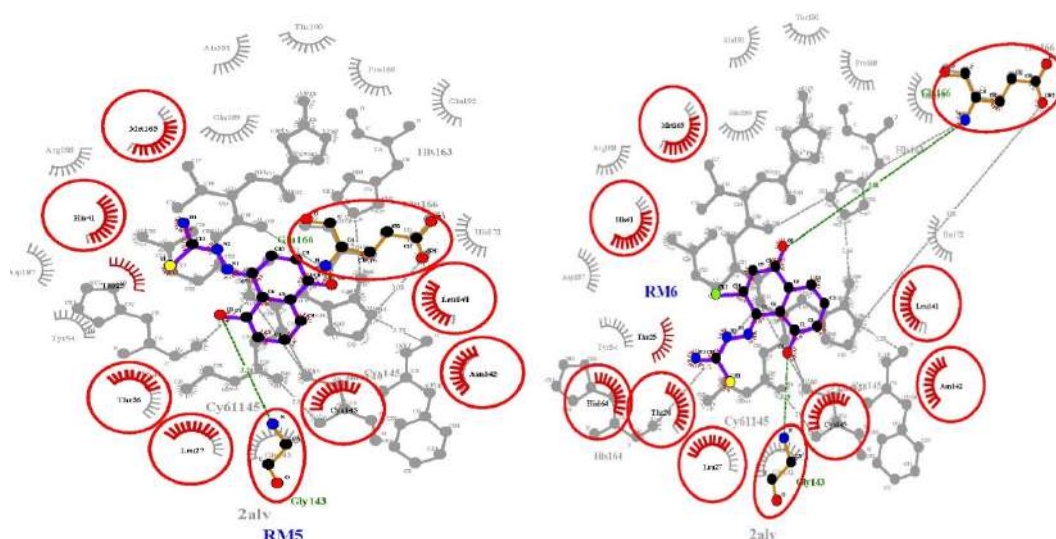


Figure 4. Overlapped 2D interactions images of designed compound compares RM1 to RM6 with standard inhibitor CY6 at binding pocket of SARS coronavirus main proteinase.

Table 2. Docking Score and intermolecular interactions of ligands against SARS coronavirus main proteinase (PDB id 2ALV) using LigPlot v1.4.5, PLIP server, Maestro V12.8 and Biovia Discovery studio visualizer.

Name of compound	Binding energy	Type of interaction	Residue id	Distance (in Å ⁰)
CY6 (standard)	-7.1	Hydrophobic	THR25A HIS41A PHE140A GLN189A	3.77 3.45 3.55 3.7
		Hydrogen bond	ASN142A GLY143A HIS163A GLU166A GLN189A GLN192A	2.34 3.08 3.56 3.44 3.31 3.14
RM1	-6.3	Hydrophobic Interactions	MET165A GLN189A	3.75 3.75
		Hydrogen bond	HIS41A	1.77
		π -Cation Interactions	HIS41A	3.80
RM2	-6.3	Hydrophobic Interactions	HIS41A	3.85
		Hydrogen bond	HIS164A ASP187A	2.81 3.62
		π -Stacking	HIS41A HIS41A	4.36 4.23
RM3	-6.3	Hydrophobic Interactions	HIS41A	3.80
		Hydrogen bond	HIS164A HIS164A	1.91 3.33
		π -Stacking	HIS41A	4.04
RM4	-6.2	Hydrophobic Interactions	GLU166A	3.67
		Hydrogen bond	HIS41A HIS41A GLY143A	2.85 2.08 2.23

			GLU166A	2.00
RM5	-6.2	Hydrophobic Interactions	GLU166A	3.68
		Hydrogen bond	HIS41A	2.94
			HIS41A	2.15
			GLY143A	2.25
GLU166A	2.00			
RM6	-6.1	Hydrophobic Interactions	GLU166A	3.74
		Hydrogen bond	HIS41A	2.81
			HIS41A	2.09
			GLY143A	2.21
			GLU166A	2.07

All the Six compounds were found to be binding with the SARS coronavirus main proteinase (PDB id 2ALV) and were used for further docking studies. The binding energy, type of interaction and their distances, interacted residues of protein with docked compounds are exhibited in Table. Compound id RM1, RM3 & RM6 exhibited good binding energy (-6.3) and formed H-bond with target as compared to standard inhibitor CY6 (-7.1) forming six hydrogen bond with five residues present in binding pocket of SARS coronavirus main proteinase (PDB id 2AZ5). The other three compounds RM2, RM4 and RM5 also having good binding affinity with protein -6.2, -6.2 and -6.1 respectively. From the above results it has been confirmed that all compounds have good affinity for SARS coronavirus main proteinase.

Molecular docking studies:

Molecular docking studies were performed to provide a theoretical perspective for possible molecular interactions of AB-series compounds and reference/ standard (CY6) molecules with the target proteins. The theoretical binding affinities were determined by energy minimization from docking calculation results. Molecular docking calculations were performed on Autodocktools version 4.2. energy minimization done using chimera, and molecular visualization of docking results were carried out by using the maestro.

Preparation of AB-series (ZG 1-7) and model inhibitor molecules for molecular docking was performed with MarvinSketch software. Before the docking process, the drawing and editing of the novel AB-series compounds in SD File format was done with the MarvinSketch suit program. These molecular structures have been protonated, added charges, and conformation minimization was performed with the root mean square gradient (RMS 0.001 kcal/mol/Å²) by using the MMFF94 Forcefield parameters, which can be accessed in Energy Minimization protocols of these software.

Docking studies of AB-series compounds were carried out for important target structure named SARS-COV main protease from corona virus. The X-ray crystal structures as three-dimensional coordinates of these target proteins was obtained from the Research Collaboratory for Structural Bioinformatics (RCSB) Protein Data Bank. For use in docking calculations, structures with PDB ID 2ALV was chosen as crystal structure model corresponding to target protein. Structural defects in target protein were eliminated automatically with the DeepView - Swiss-Pdb Viewer V 4.1 software provided by the SIB Swiss Institute of Bioinformatics. Then interactions of standard inhibitor supplied by depositor with protein were checked using PDBsum (Pictorial database of 3D structures in the Protein Data Bank) online server of European Bioinformatics Institute, UK from where position of ligand was noted. Other unnecessary entries present in pdb file were removed manually using textpad 8 software.

AutodockTools version 1.5.6 was used to optimize 3D module of protein. Then energy minimization of the system was performed with UCSF Chimera 1.12 using AMBER FF14SB by considering 1000 steepest descent steps & 100 conjugate gradient steps. Possible ligand binding site in the minimized protein were determined by Computed Atlas of Surface Topography of proteins (CASTp) server.

Molecular docking studies of selected compounds into protein targets were carried out using AutoDock Vina. Docking studies were conducted on SARS-CoV-2 main protease. For docking studies, proteins were pre-processed by removal of all water and addition of kollman charges. Hydrogen bond (H-bond) optimization was done and Gasteiger charges were added to it using AutoDock MGL tools 1.5.6. A receptor grid-box was generated by AutoGrid4 with grid box dimensions of 60 Å × 80 Å × 60 Å with spacing of 1 Å centering around hotspot residues Lys31, Glu35, Asp38, and Lys353 for ACE2 protein. Grid box for S-RBD was also set with spacing of 0.442 Å and dimensions of 62 Å × 82 Å × 82 Å centering around residues Leu455, Phe486, Asn487, Gln493, and Ser494. Lamarckian Genetic Algorithm (GA) in combination of grid based energy evaluation method was used for docking. The program was run for a total number of 50 Genetic algorithm runs. Other parameters were set as default and the final result obtained was analyzed manually by PyMol and LigPlot.

Docking of AB-series compounds and model inhibitors to the active site of these targets proteins was performed via AutodockTools 4.2 using the default docking calculation parameters. The average score of the top 10 final docking poses defined by the binding minimum energy (kcal/mol) for each compound was used as the final molecular docking score results. London dG scoring function was used for docking calculations. The London dG scoring function estimates the free energy of binding the ligand at a particular pose in a target structure. This scoring function is explained in detail in the user manual of the MOE software. After the initial scoring function for the obtained docking poses, the GBVI/WSA ΔG scoring function was used as the final docking

scoring methodology. The GBVI/WSA dG is a force field-based scoring function, which estimates the free energy of binding of the ligand from a given pose [42]. This scoring function is explained in detail in the user manual of the MOE software.

Conclusion:

Interaction between Proteinase (PDB id: 2ALV) of corona virus and RM1 to RM6 studied by molecular docking. Negative value of ΔG indicates all compounds forms stable complexes with proteinase. RM1, RM2, RM3 shows better binding energy. It shows that changing halogen group does not showing any effects on complexation with proteinase. Oxime derivatives forms better complexes with proteinase than semicarbazide derivatives. Hydrogen bonding, electrostatic interactions, hydrophobic and van der Waals interactions are studied.

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INSILICO PREDICTION OF NOVEL HALOSUBSTITUTED HOMOISOFALAVONOID DERIVATIVES AS AN ANTI-INFLAMMATORY AGENTS

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Abstract:

Flavonoids are class of organic compounds derived from families of plants like Hyacinthaceae, Fabaceae, Asparagaceae. These compounds are phenolic secondary metabolites having skeleton C6-C3-C6 and have 15 carbon atoms containing aromatic rings. Homoisoflavonoids are small group of natural flavonoids containing 3-benzyl-4-chromanones reported to occur mainly in the genera in in Hyacinthaceae. In the present study, we have synthesized hydroxy and nitro derivatives of chloro substituted homo isoflavonoids. The structures of of synthesized compounds were confirmed by H1 NMR and IR spectral techniques. Naturally occurring homoisoflavonoids are extensively used in medication and their biological activities are reported such as antiinflammatory obtaining antioxidant, antifungal and anticancer drugs. In our work we have synthesized novel synthetic hydroxy and nitro derivative of chloro substituted homoisoflavonoids and their insillico anti-inflammatory activities are studied and compared using molecular docking.

Introduction:

In ancient time humans use medicinal plants and there extract in the form of of tinctures and lotions for medication purpose. Plants produce primary and secondary metabolites. Secondary metabolites include alkaloids, glycosides, amines, steroids and flavonoids. Recently the secondary metabolites homoisoflavonoids is small subclass from class of flavonoids widely used in in drug medication. Homoisoflavonoids are generally known to contain 3-benzyl-4-chromanones backbone. These compounds are widely used studied as a anti-inflammatory drugs and for different biological activities. The Anti-inflammatory activities of novel hydroxy and nitro derivatives of chloroisoflavonoids can be predicted insillico study by molecular docking. Activity spectra prediction is done using pass online module of "Way to drug" server.

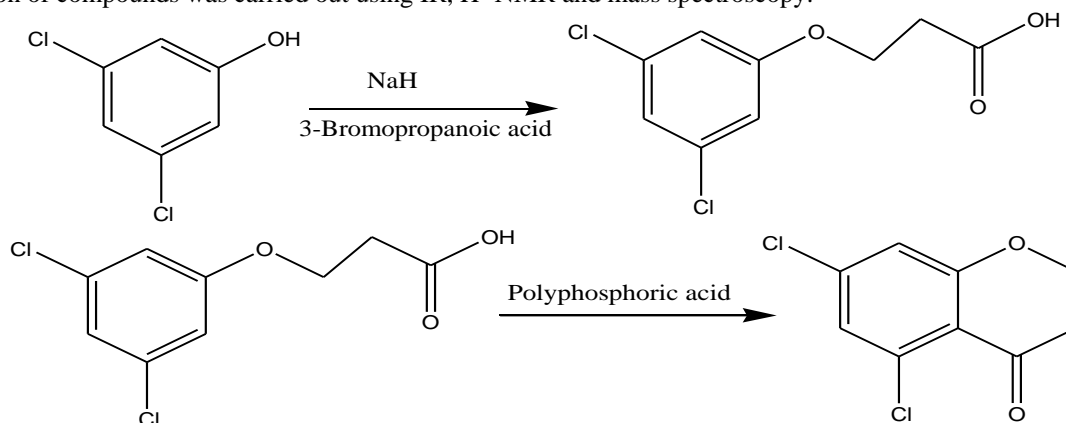
For docking study protein was isolated from Research collaborator for Structural Bioinformatics (RCSB) online database. Then protein and ligands optimized using various softwares. Grid parameters obtained from Cast- P –server.

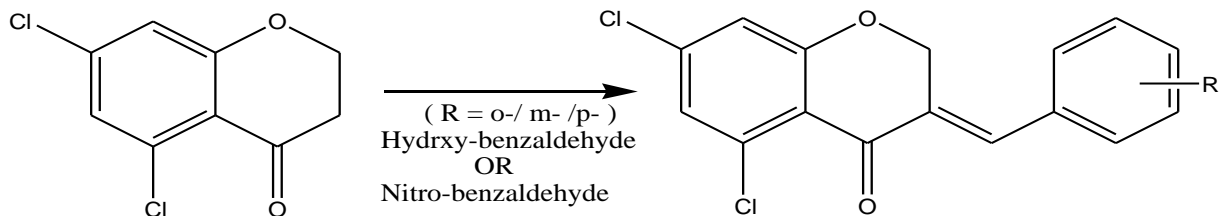
Actual docking one using Auto.Doc tools 4.2. Analysis of protein ligand complex obtained by docking using "Discovery studio "lig plot and Maestro. On the basis of comparative anti-inflammatory study, H- bond and other electrostatic forces forming compounds shows better affinity towards receptor.

Experimental

Synthesis of homoisoflavonoids

The compound 3-(3,5-dichlorophenoxy) propanoic acid(A) is synthesized from 3,5-Dichlorophenol by the action of NaH and 3- Bromopropanoic acid in DMF. Further in step -2 compound (A) is treated with polyphosphoric acid to give 5,7-dichloro-2,3-tetrahydro-4H-chromen-4-one. In step-3 compound B is treated with -ortho, -meta and -para hydroxyl and nitro benzaldehyde to get hydroxyl and nitro substituted chlorohomoisoflavonoids. The purity of compounds were checked using TLC. The characterization of compounds was carried out using IR, H¹ NMR and mass spectroscopy.





Methodology, Result and Discussion

Selection of particular Ligands from Homoisoflavonoids derivatives

The important derivatives from synthesized compounds were used in the present investigation for the computational prediction of potential drugs from it by the process of molecular docking against COX-2 isoenzyme as an anti-inflammatory agent.

Biological Activity Prediction

Due to the impossibility of performing a study of the biological activity of a large number of compounds in a short period, it was decided to conduct a preliminary assessment of the potential biological activity of compounds (DG1, DG2, DG3, DG4, DG5 & DG6) using PASS-online modelling. The PASS software product, which predicts more than 300 pharmacological effects and biochemical mechanisms on the basis of the structural formula of a substance, may be efficiently used to find new targets (mechanisms) for some ligands and, conversely, to reveal new ligands for some biological targets. The mean accuracy of prediction with PASS is about 86% in LOO cross-validation. The tool uses the descriptors to predict the activity of a substance.

Result

The prediction of the biological activity spectrum of homoisoflavonoid derivatives DG1 to DG6 revealed that compounds are determined as promising selective cox-2 inhibitors. This indicates that all the compounds may show good anti-inflammatory activity as selective COX-2 inhibitor.

The 3D SDF structures of the processed six Homoisoflavonoid derivatives RM1 to RM6 were given as an input for PASS server. The PASS server provides all the possible activities of the given Homoisoflavonoid derivatives as promising COX-2 inhibitors. PASS can be effectively applied to predict biological potential of compounds and to analyze large chemical databases. PASS predicted search results show all the available information on the pharmacological and toxicological activity of all the three compounds analysed. Similar observation in accordance with the present study using PASS server was already reported by many researchers. Pa and Pi are the estimates of probability to be active and inactive respectively from the biological activity spectrum. Their values vary from zero to one. Each active compound possesses a number of biological activities. Its specificity of action is always relative and is defined by the peculiarities of object, dose, route, etc. Biological activity spectrum of compound can be predicted on the basis of structure-activity relationships found by the analysis of the known data from the training set. Based on the analysis of large training set consisting of tens of thousands of the known biologically active compounds, computer program PASS provides the means to evaluate any new compound in huge chemical-pharmacological space. On the basis of this study it can be revealed that all the three compounds may show good anti-inflammatory activity.

Molecular Docking Studies

Target Protein Retrieval and Preparation

On the basis of literature survey we found that COX-2 isoenzyme is major target to study anti-inflammatory study. Therefore, fasta sequence of cyclooxygenase-2 (Prostaglandin-endoperoxide synthase 2) for Homo sapiens was retrieved from National centre for biotechnology information server and done Basic Local Alignment Search for regions of similarity between biological sequences available on Protein Data Bank. Then Three-dimensional X-Ray crystallographic structure of COX-2 (PDB id: 5F1A) was obtained from PDB databank which was validated using various parameters like resolution, Mutation and Ramchandran plot. Details are as follows.

Table 1. Comparison between standard values and retrieved protein for validation of protein selected for docking study

Parameters	Details	Standards
Protein Id and method of experiment	5F1A X-RAY Diffraction	- X-RAY Diffraction
Mutation	No	No
Resolution	2.38 Å ⁰	Near about 2.00 Å ⁰
Ramchandran Plot (by PROCHECK server)		
Residues in favoured + Allowed regions	100 %	>88 %

The preparation of a protein involves importing of the Prostaglandin-endoperoxide synthase 2 Protein structure. Binding pocket has been verified using PDBsum server which is a Pictorial database of 3D structures in the Protein Data Bank for interactions of standard inhibitor with protein. The water molecules, unnecessary chains and ligands have been deleted and the proteins were

retained using Biovia Discovery Studio visualizer V21.1.0.20298. Charges were stabilized, missing residues were filled in and side chains were generated using AutoDockTools v1.5.6 spet_17_14.

The CHIMERA v1.5.3 software was used to minimize the structure of protein, using the Gasteiger charges with 1000 steepest descent steps of minimization.

Grid Generation

AutoDockTools was used for receptor grid identification. The prepared Prostaglandin-endoperoxide synthase 2 was displayed in the Workspace. The volume of grid was calculated using dimensions of pocket identified from CASTp server (Computed Atlas of Surface Topography of proteins). The enclosing box was made small so that it will be consistent with the shape and character of the protein's active site and with the ligands that were expected to be docked.

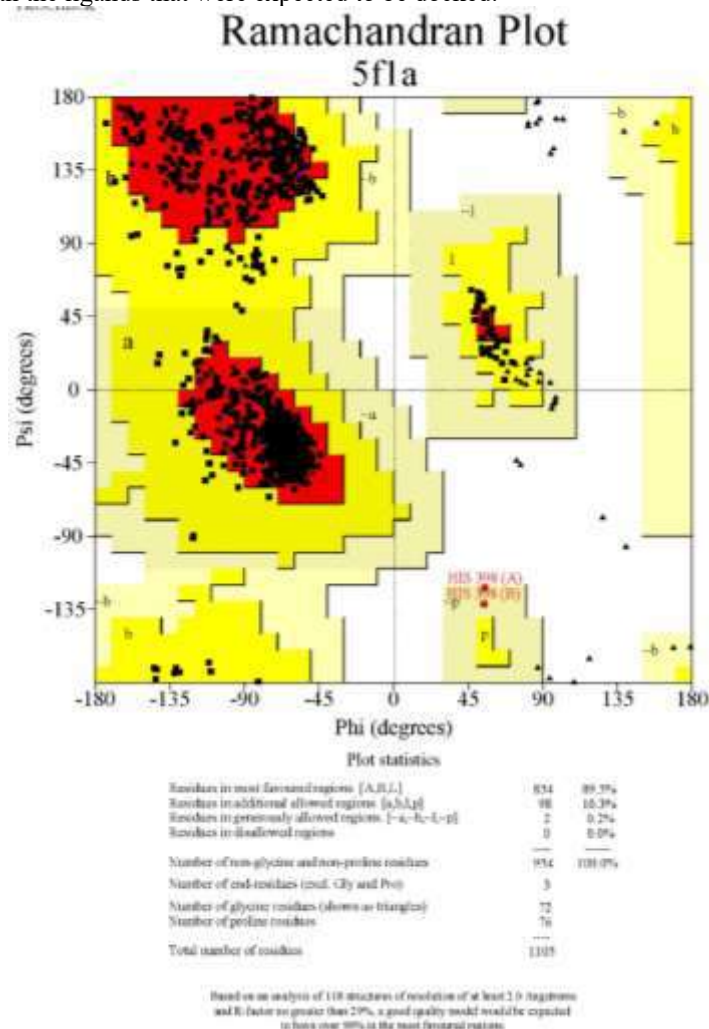


Figure 1. Ramachandran Plot 5F1A obtained from PROCHECK server

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Ligand molecules were designed in Marvin Sketch v21.13 and saved in 3D MOL2 format. All the three compounds were processed, and optimized by UCSF Chimera v1.15 using AM1-BCC semi-empirical force field other parameters defaults like steepest descent steps : 1000; Conjugate gradient steps 100, etc.

Molecular Docking of Target Protein with Ligands

After obtaining the ligands and enzymes, their structures were converted to pdbqt format, using the AutoDock Tools 1.5.6 program, in which all the rotatable bonds of ligands were allowed to rotate freely, and the receptor were considered rigid. For docking studies, we used the AutoDock Vina 1.1.1, with 1 °A of spacing between the grid points. The grid box was centred on the active site of the enzyme with high resolution, allowing the program to search for additional places of probable interactions between the ligands and the receptor. Other configurations were considered default. The XYZ coordinates 41.81 X 23.95 X 240.11, and size of the grid box is 20 X 20 X 20 A⁰. The redockings were performed with the same configurations of the previous performed dockings.

Visualization

Results obtained after Autodock Vina processing were subjected to make a complex using Biovia Discovery Studio visualizer. Interactions and binding energies of test compounds were compared with standard inhibitor.

Result

All three compounds were prepared to dock with the Crystal Structure of Prostaglandin-endoperoxide synthase 2 (PDB id 5F1A). The selected chemical structures of the three important ligands were shown in Fig.

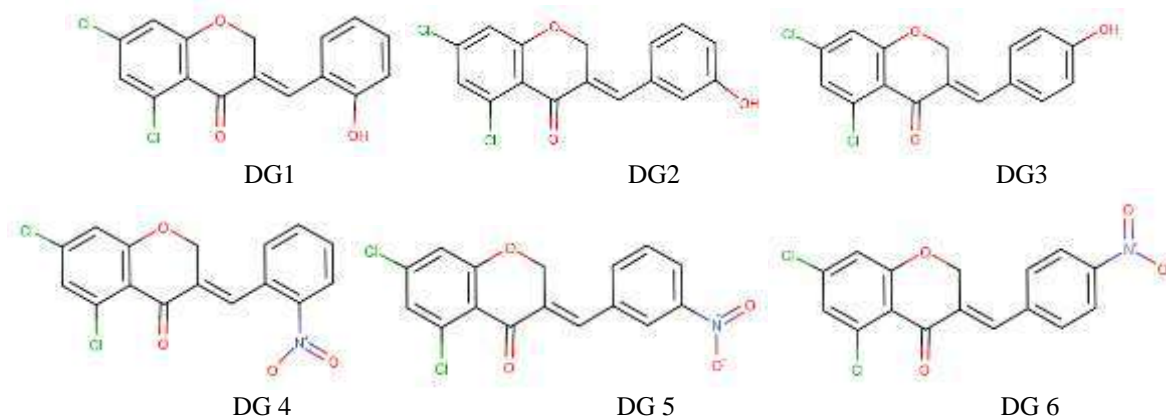
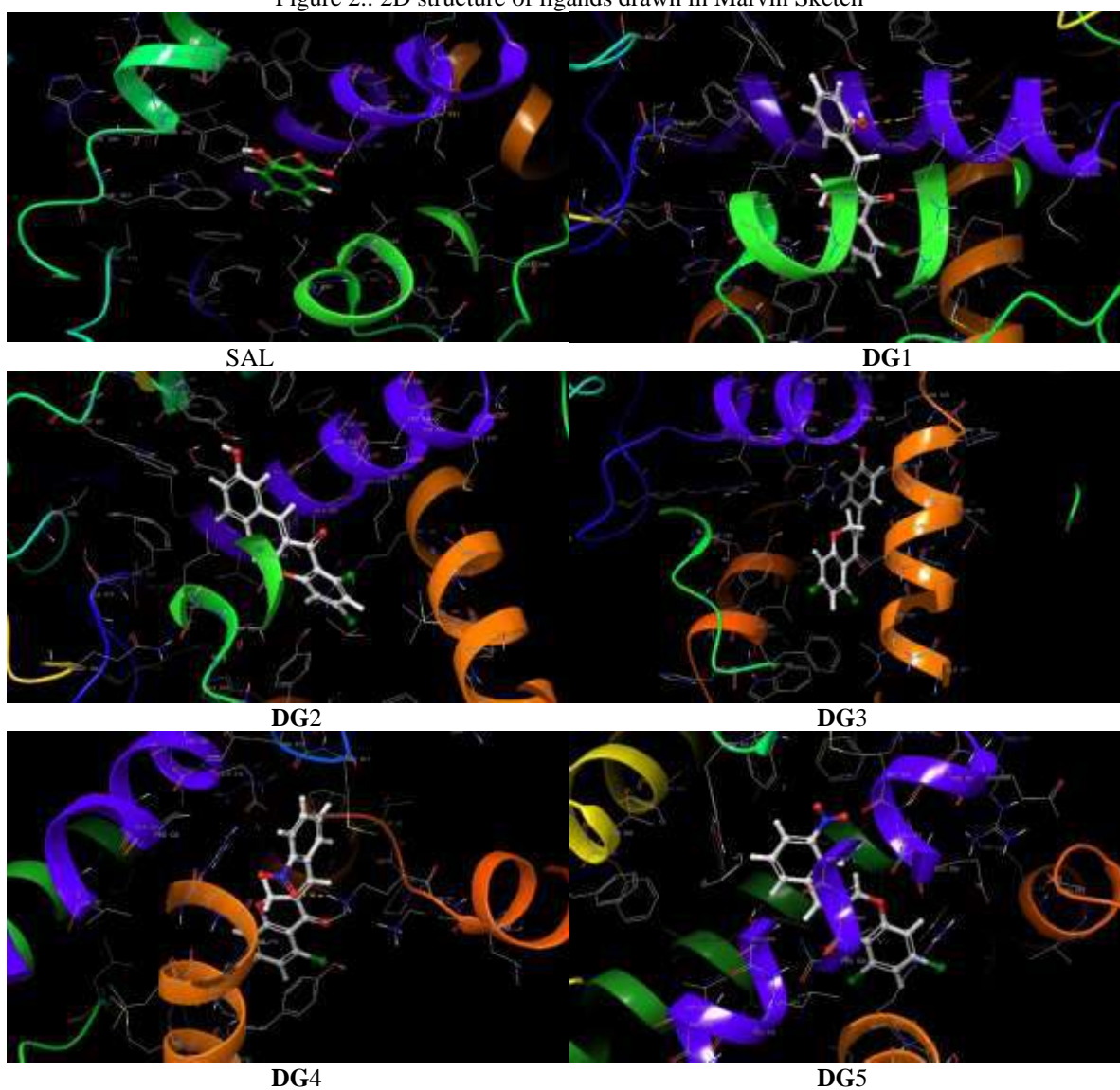
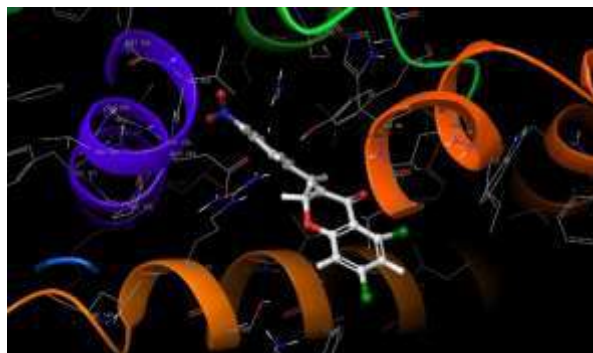


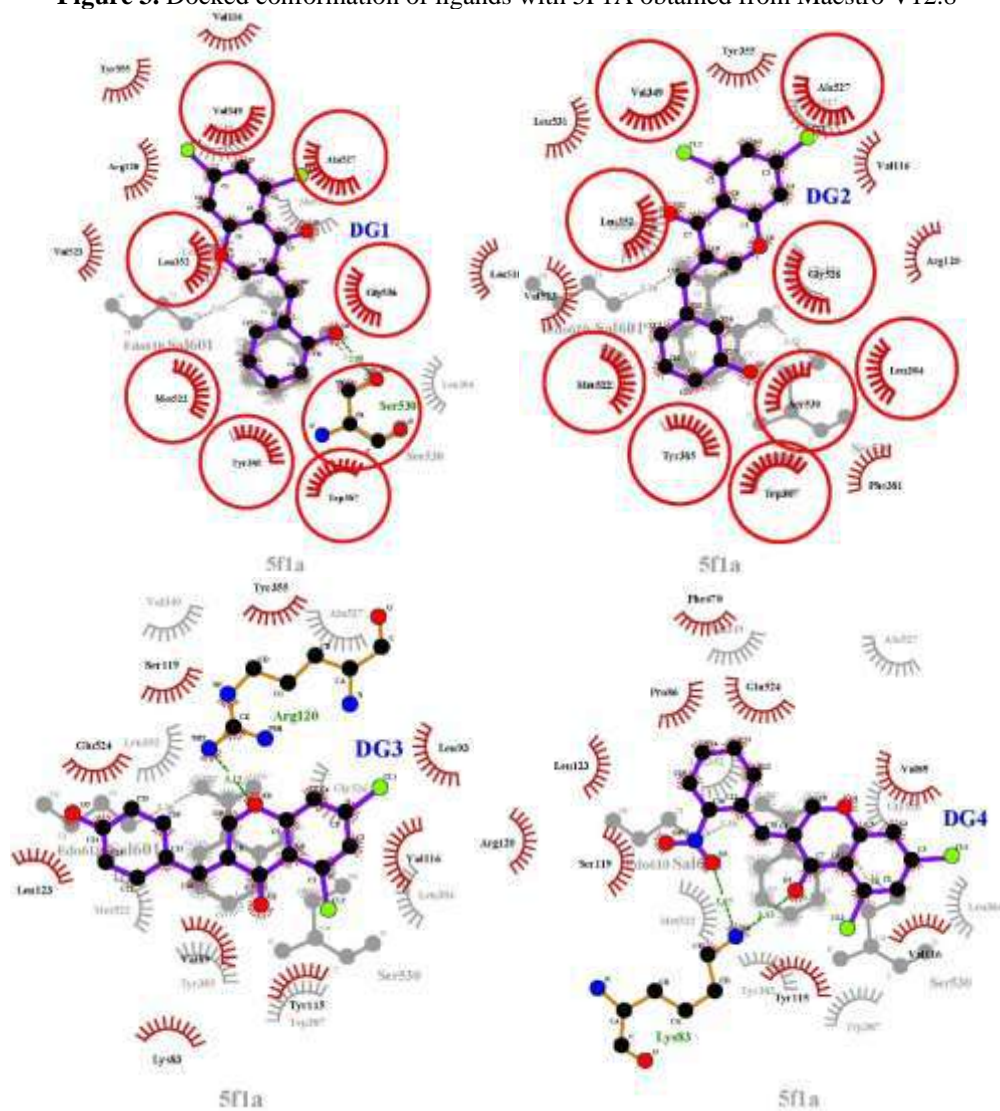
Figure 2.: 2D structure of ligands drawn in Marvin Sketch





RM6

Figure 3. Docked conformation of ligands with 5F1A obtained from Maestro V12.8



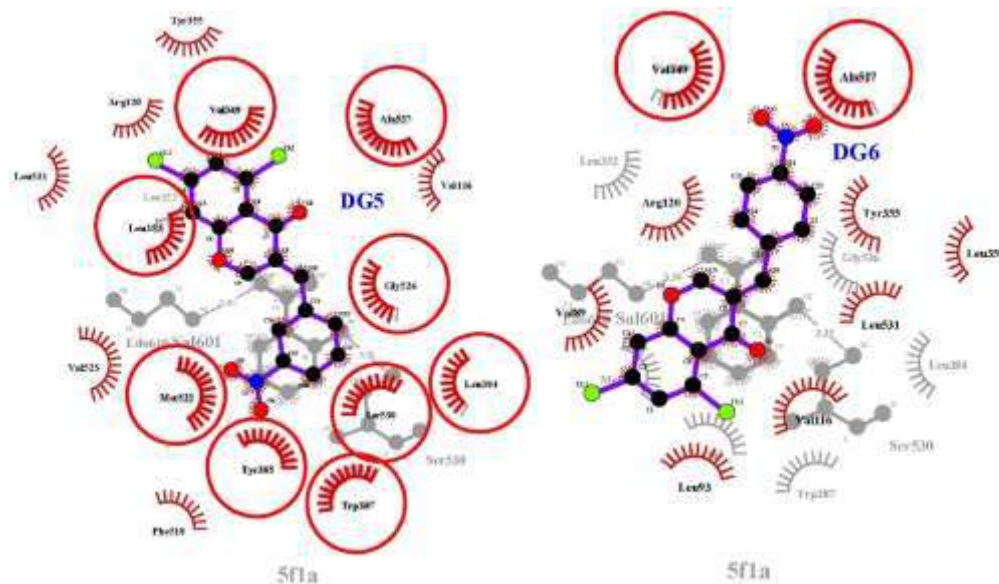


Figure 4. Overlapped 2D interactions images of designed compound compared DG1 to DG6 with standard inhibitor SAL at binding pocket of Prostaglandin-endoperoxide synthase 2

Table 2. Docking Score and intermolecular interactions of ligands against Human Cyclooxygenase-2 (PDB id 5F1A) using LigPlot v1.4.5, PLIP server, Maestro V12.8 and Biovia Discovery studio visualizer

Name of compound	Binding energy	Type of interaction	Residue id	Distance (in Å ⁰)
SAL (standard)	-6.935	Hydrophobic	LEU 352A TRP 387A PHE 518A	3.54 3.63 4.00
		Hydrogen bond	TYR 385A SER 530A	1.94 1.78
DG1	-7.414	Hydrophobic Interactions	VAL 116A VAL 349A TRP 387A TRP 387A ALA 527A	3.27 3.43 3.61 3.80 3.25
		Hydrogen bond	TYR 355A TYR 385A TYR 385A SER 530A	3.48 3.30 3.14 1.94
DG 2	-7.505	Hydrophobic Interactions	VAL 116A LEU 352A TRP 387A ALA 527A	3.31 3.94 3.52 3.33
DG 3	-4.463	Hydrophobic Interactions	VAL 89A TYR 355A	3.68 3.83
		Hydrogen bond	ARG 120A ARG 120A PHE 470A	3.13 2.69 2.74
		π -Cation Interactions	ARG 120A ARG 120A PHE 470A	3.13 2.69 2.74
DG 4	-5.074	Hydrophobic Interactions	PRO 86A LEU 93A TYR 115A VAL 116A LEU 123A	3.58 3.96 3.74 3.61 3.69

			LEU 472A	3.98
		Hydrogen bond	LYS 83A	2.45
DG 5	-6.533	Hydrophobic Interactions	VAL 116A	3.26
			VAL 349A	3.90
			VAL 349A	3.39
			LEU 352A	3.94
			TYR 385A	3.86
			TRP 387A	3.49
		ALA 527A	3.27	
		Hydrogen bond	TYR 355A	3.49
DG 6	-4.363	Hydrophobic Interactions	VAL 116A	3.10
			VAL 349A	3.52
			TYR 355A	3.25
			LEU 359A	3.69
			ALA 527A	3.24
			LEU 531A	3.35
				Hydrogen bond
			ARG 120A	3.25

From All the Six compounds were found to be binding with the Human Cyclooxygenase-2 (PDB id 5F1A) and were used for further docking studies. The binding energy, type of interaction and their distances, interacted residues of protein with docked compounds are exhibited in Table 2 Compound id DG1 & DG2 exhibited good binding energy and intermolecular interactions with respect to standard inhibitor Salicylate. The other four compounds DG3, DG4, DG5 & DG6 also having moderate binding affinity with protein. From the above results it has been confirmed that compounds with meta-hydroxy and ortho-hydroxyl derivatives of homoisoflavonoids have good affinity for Prostaglandin-endoperoxide synthase 2. We can conclude from docking study that homoisoflavonoids with Electron donating groups has good binding affinity than electron withdrawing groups.

Acknowledgment

The authors are thankful to SPPU, Pune, department of Chemistry, BJS College, Wahgoli, Pune, B R Gholap College, Sangavi, Pune for allowing the facilities to do research work

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SYNTHESIS, CHARACTERIZATION AND MOLECULAR DOCKING OF CONDENSED MOLECULES OF HALOGEN DERIVATIVES OF SOME NATURALLY OCCURRING QUINONES AND PHENYLENE DIAMINES

Rajendra T. Jagtap Pimpri Chinchwad College of Engineering, Nigdi.

Sanjay. D. Gaikwad BJS college of Arts, Science and Commerce, Wagholi.

Abstract:

Naphthoquinones are natural pigments and widely distributed in nature and having interesting co-ordination, analytical and biological activities. Lawsone (2-hydroxy,1-4 naphthoquinone), its halogen derivatives and their synthetic polymeric molecules with phenylene diamine, have propitious potential for treatment of many diseases because of their ant seborrhic, anticancer, antituberculosis, antifungal, antibacterial and uninflammatory effects. The present communication deals with synthesis of condensed polymeric molecules of -chloro lawsone with para phenylene diamine and their characterization using IR, H1 NMR. These molecules are subjected for molecular docking or modeling technique is used to predict how a protein (enzyme) interacts with small molecules (ligands). It allows prediction of molecular interactions that hold together a protein and a ligand in the bound state.

Keywords: Lawsone, Chlorolawsone, Condensed Molecules, Phenylene Diamine, Molecular Docking.

Introduction:

Lawsone (2-hydroxy,1-4 naphthoquinone) is naturally occurring pigment extracted from Henna plant (*Lawsonia inermis*). As already reported in literature, Lawsone shows antiseptic, antipyretic and astringent properties [1]

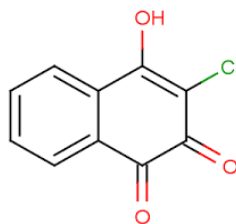
The synthesis and characterization of lawsone derivatives is carried out. All chemicals used were of A.R. grade. Solvents used were purified by methods given in literature. Ligands are purified by column chromatography using silica gel (100-200 mesh). Ligands like chlorolawsone were synthesized on laboratory scale following literature reported procedures. Lawsone (2-hydroxy-1,4-naphthoquinone), dichlone (2,3-dichloro-1,4-naphthalenedione) and 2-methyl-1,4-naphthalenedione were obtained from Merks laboratory. All compounds were characterized by their identical TLC behavior with the standard and authentic samples. Melting points were obtained with paraffin oil bath. The elemental analysis for the percentage of hydrogen and carbon were performed in the micro analytical laboratory using a Hosli C,H micro analysis instrument.

Experimental

Chloro derivative of lawsone, namely 3-chlorolawsone were synthesized from dichlone and lawsone.

Synthesis of chlorolawsone [2,3]: In a 100 ml beaker, a slurry of 1 gm of dichlone solution was prepared using 20 ml methyl alcohol. Then 4M aqueous solution of potassium hydroxide solution was added drop by drop with constant stirring. The entire mass was warmed on a water bath at 60°C until a red crystalline paste was formed. After about 1 hour of heating, a solution of hydrochloric acid (6M) was added dropwise to the above paste with constant stirring. This acidification converted the red paste in to bright yellow precipitate of 3-chlorolawsone (Figure 1). The precipitate was filtered under suction and washed repeatedly with cold distilled water and dried in vacuum over fused calcium chloride. The crude product was purified by column chromatography using chloroform as an eluent.

Figure 1. Chlorolawsone



Synthesis of Condensed molecules of chloro lawsone and phenylene diamine [4]

1) 0.001 mole (0.20865 gm) of chloro lawsone was dissolved in 20 ml pure ethanol and a solution of 0.001 mole (0.10810 gm) ortho phenylene diamine in 10 ml ethanol is added dropwise with constant stirring at room temperature. An intense brownish precipitate was obtained, after evaporation of all solvent content. The precipitate was washed with distilled water and dried under vacuum. It is then purified by column chromatography using chloroform solvent. Its purity was checked by TLC using mixture of

20 ml ethyl acetate and 80 ml n-hexane, where a single spot was obtained.

2) 0.001 mole (0.20865 gm) of chloro lawsone was dissolved in 20 ml pure ethanol and a solution of 0.001 mole (0.10810 gm) meta phenylene diamine in 10 ml ethanol is added dropwise with constant stirring at room temperature. A brown blackish precipitate was obtained, after evaporation of all solvent content. This precipitate was washed with distilled water and dried under vacuum. It is then purified by column chromatography using chloroform solvent. The purity was checked by TLC using mixture of 20 ml ethyl acetate and 80 ml n-hexane, where a single spot was obtained.

3) 0.001 mole (0.20865 gm) of chloro lawsone was dissolved in 20 ml pure ethanol and a solution of 0.001 mole (0.10810 gm) para phenylene diamine in 10 ml ethanol is added dropwise with constant stirring at room temperature. A brownish precipitate was obtained after evaporation of all solvent content. The precipitate was washed with distilled water and dried under vacuum. It is then purified by column chromatography using chloroform solvent. Its purity was checked by TLC using mixture of 20 ml ethyl acetate and 80 ml n-hexane, where a single spot was obtained.

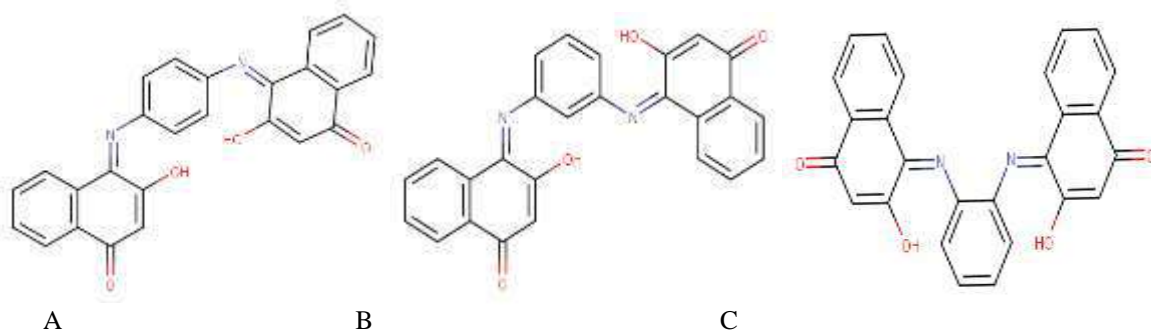


Figure 2. Condensed molecules

A is condensed molecule of chlorolawsone and o-phenylene diamine

B is condensed molecule of chlorolawsone and m-phenylene diamine

C is condensed molecule of chlorolawsone and p-phenylene diamine

UV Spectral Study

Table 1. Significant UV absorptions

Compound	$\Pi - \Pi^*$ transition		n - Π^* transition
	BET	QET	
Clorolawsone	299	334	457
A	299	--	490
B	290	353	457540
C	---	--	--

Visible spectrum of 2-hydroxy,1,4 naphthoquinone in DMSO is recorded and studied. In this spectrum, prime transitions are observed in 296,339,415 and 448 wavelengths. The best commonly transitions are n to pi star and pi to pi star. Here because of conjugation, absorption shifted to longer wavelength and also pi to pi star transitions are more intense than n to pi star transitions.[5] The electronic spectra of the lawsone and condensed molecules are done in ethyl alcohol. The spectra has intense band at 230 – 245 nm and at 345 – 460 nm are due to $\Pi - \Pi^*$ transition. The first band is due to benzenoid electron transfer, while the second band is due to quinonoid electron transfer. The band at low intensity is observed in the spectra of lawsone is due to n - Π^* transition. The new broad band with low intensity is observed at 500 – 600 nm in the spectra of the polymer, it may be due to increase in the chromophoric length of the polymers. In case of B the absorption is less than C, it is due to less planarity of the polymer.[6]

IR Spectral Study

In the IR spectra of the parent compound lawsone the frequency observed at 3300 cm^{-1} , it is attributed to $\nu(\text{O-H})$. It is shifted to higher frequency by ~ 30 to 75 cm^{-1} , it is due to polymerization and are in conjugation. This peak is also broadened and its high intensity get reduced and it is merged in broad peak of N-H. The $\nu(\text{C=O})$ stretching frequency is assign for the carbonyl group present in lawsone at 1 and 4th position. [7]. This peak is not observed in the spectra of all polymers. The broad peak is observed at 3421 cm^{-1} is assign to $\nu(\text{N-H})$ vibrations. It is not observed in lawsone. The broadness and shifting to higher frequency may be due to polymerization and in conjugation. The sharp band observed at 1629 cm^{-1} in all polymer spectra, it is attributed for $\nu(\text{C=N})$ stretching frequency. Similarly the another stretching frequency at $\sim 1135\text{ cm}^{-1}$ in all the polymers is observed, it is assign for the $\nu(\text{C-N})$. IR studies showed that 3170 (stretching O-H which overlaps the C-H vibrations), 1681 and 1640 (stretching C=O,

such splitting is due to presence of internal hydrogen bonding), 1578 and 1592 (C=C vibrational bands of naphthalene ring) and 1214 (stretching for C-O)[8]

Table 2, Significant peaks in Infrared Spectra (all frequencies are in cm^{-1})

Assignment	Lawsone	A	B	C
N-H	---	3421	3421	
C=O	1680	---	---	
C=N	---	1629	1630	1632
C-N	---	1135	1138	1139
O-H	3300	3360	3375	3367
Aromatic Stretching.	1617	1617	1617, 1560	1594, 1503

^1H NMR (FT-250 MHz, DMSO- d_6) showed δ : 7.78-8.01(m, 4H of aromatic ring) and 6.17(s, 1H).

Methodology, Results and Discussion [13]

Selection of particular Ligands from oxonaphthalenone derivatives

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The prediction of the biological activity spectrum of oxonaphthalenone derivatives RJ1, RJ2, RJ3 revealed that compounds are determined as promising TNF- α inhibitors. This indicates that all the three compounds may show good activity against Psoriasis as TNF alpha is main target for psoriasis treatment.

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Table 3. Comparison between standard values and retrieved protein for validation of protein

Parameters	Details	Standards
Protein Id and method of experiment	2AZ5 X-RAY Diffraction	- X-RAY Diffraction
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Ramchandran Plot (by PROCHECK server)		
Residues in favoured + Allowed regions		>88 %

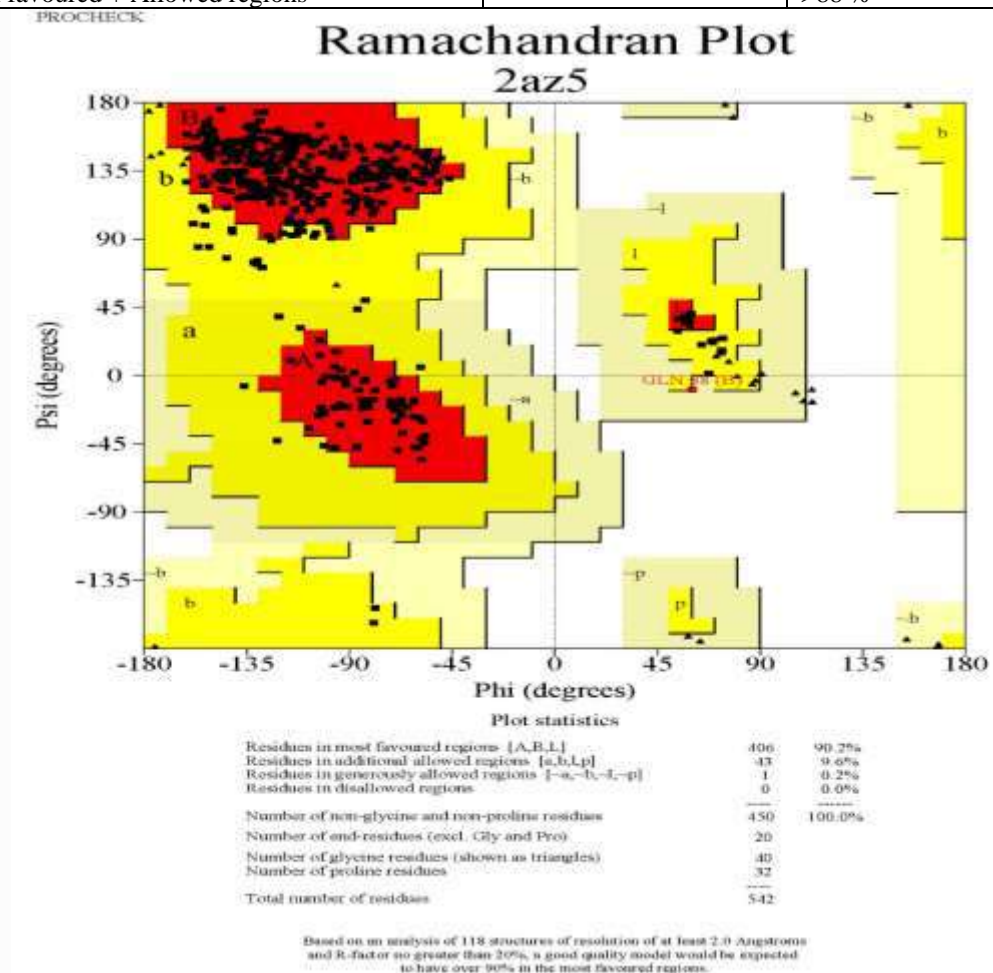


Figure 3. Ramchandran Plot 2az5 obtained from PROCHECK server

The preparation of a protein involves importing of the TNF-alpha Protein structure. Binding pocket has been verified using PDBsum server which is a Pictorial database of 3D structures in the Protein Data Bank for interactions of standard inhibitor with protein. The water molecules, unnecessary chains and ligands have been deleted and the protein were retained using Biovia Discovery Studio visualizer V21.1.0.20298. Charges were stabilized, missing residues were filled in and side chains were generated using AutoDockTools v1.5.6 spet_17_14.

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Results obtained after Autodock Vina processing were subjected to make a complex using Biovia Discovery Studio visualizer. Interactions and binding energies of test compounds were compared with standard inhibitor.

Result:

All three compounds were prepared to dock with the Crystal Structure of TNF-alpha (PDB id 2AZ5). The selected chemical structure of the three important ligands were shown in Fig.

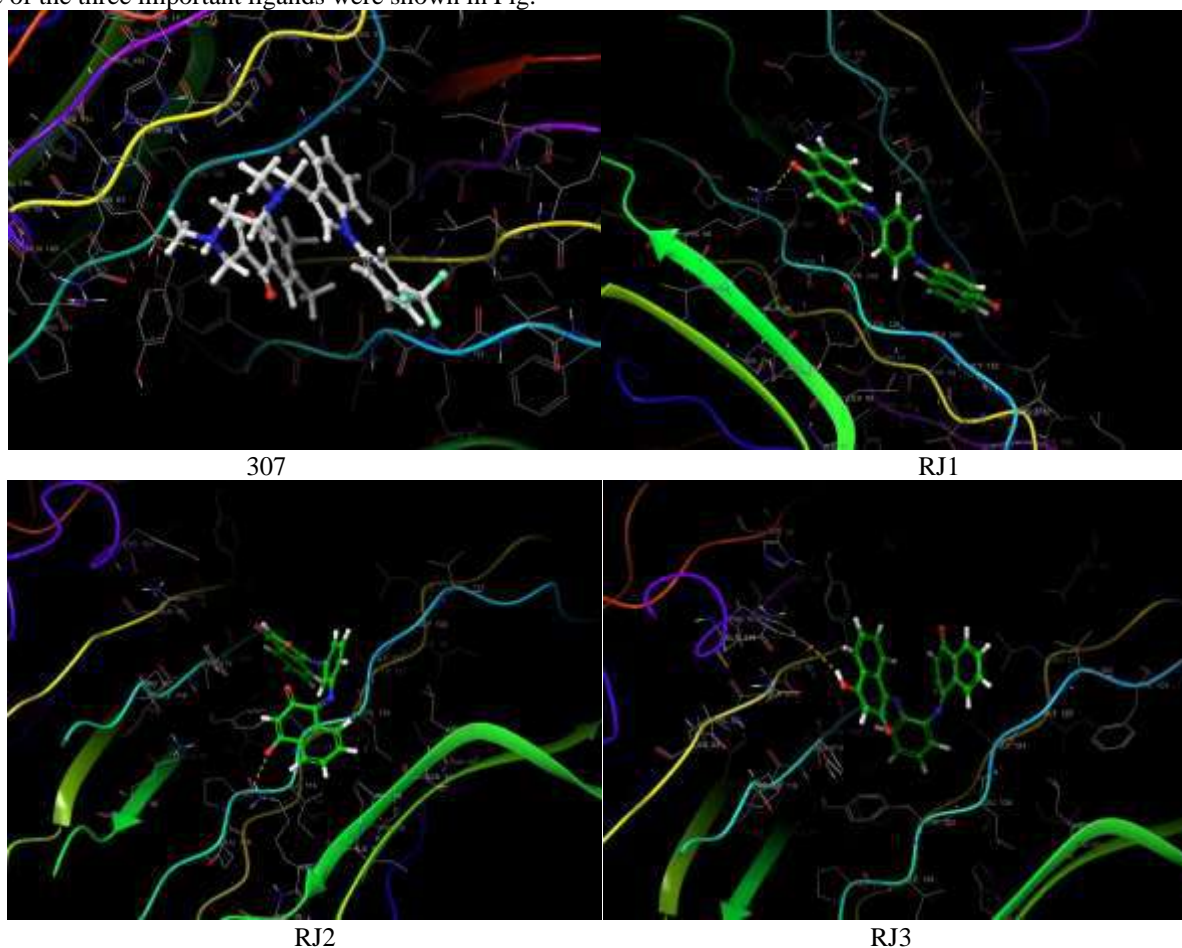


Figure 4. Docked conformation of ligands with 2AZ5 obtained from Maestro V12.8

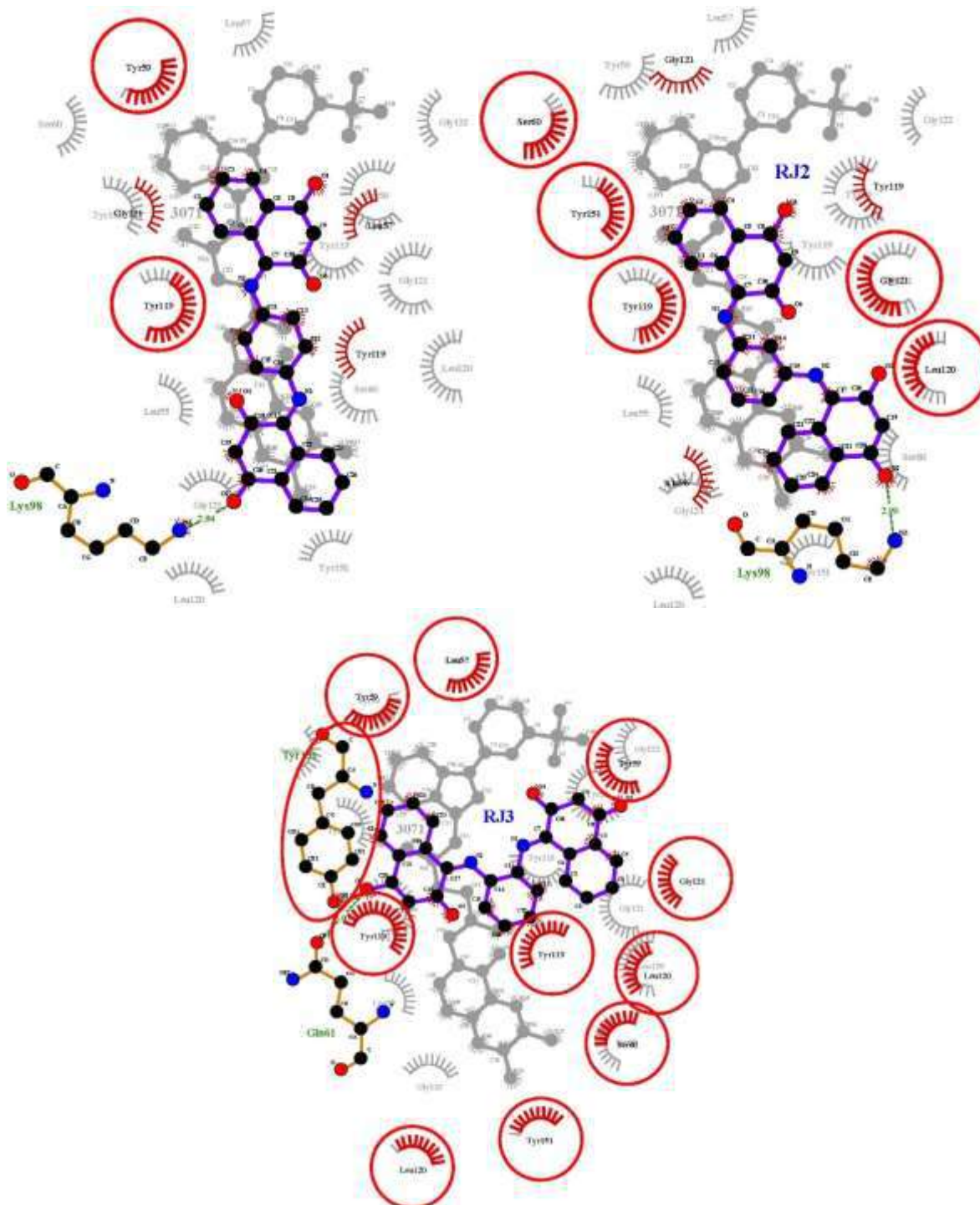


Figure 5. Overlapped 2D interactions images of designed compound compares RJ1, RJ2, RJ3 with standard inhibitor 307 at binding pocket of TNF- α .

Table 4. Docking Score and intermolecular interactions of ligands against TNF- α (PDB id 2AZ5) using LigPlot v1.4.5, PLIP server, Maestro V12.8 and Biovia Discovery studio visualizer..

Name of compound	Binding energy	Type of interaction	Residue id	Distance (in A ⁰)
307 (standard)	-6.772	Hydrophobic	LEU57A	3.52
			LEU57B	3.9
			LEU57B	3.77

			TYR59A	3.89
			GLN61B	3.93
			TYR119B	3.93
			TYR119B	3.62
			TYR151B	3.4
		Hydrogen bond	TYR151A	2.45
		π -Stacking	TYR119B	5.44
		Π -Cation Interactins	TYR59A	4.58
RJ1	-4.6	Hydrophobic Interactions	TYR59B	3.45
			TYR59B	3.63
			TYR119A	3.6
			TYR119A	3.77
			TYR119B	3.48
		Hydrogen bond	LYS98B	2.84
RJ2	-5.418	Hydrophobic Interactions	TYR59B	3.99
			ALA96B	3.76
			TYR119B	3.89
			TYR151B	3.77
		Hydrogen bond	LYS98B	2.98
		Pi-Pi stacking	TYR119A	5.32
RJ3	-6.408	Hydrophobic Interactions	LEU57B	3.97
			LEU57B	3.6
			TYR59A	3.45
			TYR59A	3.88
			TYR59B	3.75
			TYR119A	3.52
		TYR119B	3.67	
		Hydrogen bond	TYR151A	3.25

All the three compounds were found to be binding with the TNF- α (PDB id 2AZ5) and were used for further docking studies. The binding energy, type of interaction and their distances, interacted residues of protein with docked compounds are exhibited in Table. Compound id RJ3 exhibited good binding energy (-6.408) and formed 1 H-bond with target as compared to standard inhibitor 307 (-6.772) forming hydrogen bond with same residue (TYR151A) of TNF- α (PDB id 2AZ5). The other two compounds RJ1 and RJ2 also having moderate binding affinity with protein -4.6 and -5.418 respectively. When compared hydrogen bonds RJ1 and RJ2, first having strong interactions than second as distance of bond is smaller in RJ1. From the above results it's confirmed that the compound RJ3 was found to be best among the three compounds selected for the study, as it recorded the formation of one hydrogen bond and also exhibited a good binding energy.

Molecular docking studies :

Molecular docking studies were performed to provide a theoretical perspective for possible molecular interactions of AB-series compounds and reference/ standard (lawsone) molecules with the target proteins [12].

The theoretical binding affinities were determined by energy minimization from docking calculation results. Molecular docking calculations were performed on Autodocktools version 4.2. energy minimization done using chimera, and molecular visualization of docking results were carried out by using the maestro.

Preparation of AB-series (ZG 1-7) and model inhibitor molecules for molecular docking was performed with MarvinSketch software. Before the docking process, the drawing and editing of the novel AB-series compounds in SD File format was done with the MarvinSketch suit program. These molecular structures have been protonated, added charges, and conformation minimization was performed with the root mean square gradient (RMS 0.001 kcal/mol/A²) by using the MMFF94 Forcefield parameters, which can be accessed in Energy Minimization protocols of these software[11]

Docking studies of AB-series compounds were carried out for important target structure named SARS-COV main protease from corona virus. The X-ray crystal structures as three-dimensional coordinates of these target proteins was obtained from the Research Collaboratory for Structural Bioinformatics (RCSB) Protein Data Bank. For use in docking calculations, structures with PDB ID 2ALV was chosen as crystal structure model corresponding to target protein. Structural defects in target protein were eliminated automatically with the DeepView - Swiss-Pdb Viewer V 4.1 software provided by the SIB Swiss Institute of Bioinformatics. Then interactions of standard inhibitor supplied by depositor with protein were checked using PDBsum (Pictorial database of 3D structures in the Protein Data Bank) online server of European Bioinformatics Institute, UK from where position of ligand was

noted. Other unnecessary entries present in pdb file were removed manually using textpad 8 software.

AutodockTools version 1.5.6 was used to optimize 3D module of protein. Then energy minimization of the system was performed with UCSF Chimera 1.12 using AMBER FF14SB by considering 1000 steepest descent steps & 100 conjugate gradient steps. Possible ligand binding site in the minimized protein were determined by Computed Atlas of Surface Topography of proteins (CASTp) server.

Molecular docking studies of selected compounds into protein targets were carried out using AutoDock Vina. Docking studies were conducted on SARS-CoV-2 main protease. For docking studies, proteins were pre-processed by removal of all water and addition of kollman charges. Hydrogen bond (H-bond) optimization was done and Gasteiger charges were added to it using AutoDock MGL tools 1.5.6. A receptor grid-box was generated by AutoGrid4 with grid box dimensions of 60 Å × 80 Å × 60 Å with spacing of 1 Å centering around hotspot residues Lys31, Glu35, Asp38, and Lys353 for ACE2 protein. Grid box for S-RBD was also set with spacing of 0.442 Å and dimensions of 62 Å × 82 Å × 82 Å centering around residues Leu455, Phe486, Asn487, Gln493, and Ser494. Lamarckian Genetic Algorithm (GA) in combination of grid based energy evaluation method was used for docking. The program was run for a total number of 50 Genetic algorithm runs. Other parameters were set as default and the final result obtained was analyzed manually by PyMol and LigPlot.

Docking of AB-series compounds and model inhibitors to the active site of these targets proteins was performed via AutodockTools 4.2 using the default docking calculation parameters. The average score of the top 10 final docking poses defined by the binding minimum energy (kcal/mol) for each compound was used as the final molecular docking score results. London dG scoring function was used for docking calculations. The London dG scoring function estimates the free energy of binding the ligand at a particular pose in a target structure. This scoring function is explained in detail in the user manual of the MOE software. After the initial scoring function for the obtained docking poses, the GBVI/WSA ΔG scoring function was used as the final docking scoring methodology. The GBVI/WSA dG is a forcefield-based scoring function, which estimates the free energy of binding of the ligand from a given pose [42]. This scoring function is explained in detail in the user manual of the MOE software.

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