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## Original Research Article

## Gold price dynamics in India: A pre-post-liberalisation comparison

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## ABSTRACT

There are considerable differences in gold price movements in India in the periods of pre-and-post globalised regimes. This is because of a change in the controlled regime in the pre-liberalised to a meticulous dilution in the post-liberalised era. Hence, the liberalised period witnessed an upward trend in price dynamics with only occasional dampening in the price cycles. The jewellery sector in India is not driven by local forces as most of the inputs are imported for production and value-added export. It is revealed that the positive impact is the result of liberalisation and related mechanisation. Gold price shows a kind of co-integration of domestic prices with the global cues. In the pre-post-dichotomy, the post-liberalisation period is more integrated with the global prices than the pre-liberalised.

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## 1. Introduction

The present gold price movements show a stochastic pattern not converging to the usual forms like inflation, interest rates, psychological sentiments and geopolitical uncertainties. The conventional economic theory is handy which purports to explain that the gold price is determined by stock and flows. Unlike other commodities, gold output does not vanish. In this respect the gold stock will either be used for present demand or be stored for future sale. In both the cases price acts as a determining factor. Hence, it all depends on the equi-marginal principle of anticipated return vis-à-vis marginal costs. This will become volatile in unprecedented political and catastrophic situations. This situation is utilised well by the market participants to gain by storing gold.

The gems and jewellery sector are not embedded with local resources, but with imported inputs and hence the economics of this industry is entirely different and

the capitalists playing in the sector is really powerful business groups. They have good knowledge about the local production system and global demand and value of the products. Nonetheless, the gold jewellery sector is connected with a historically important artisan community known as goldsmith and their art and artefacts are popular in global dimensions. But the malady comes in the form of globalisation as the petty home-linked business of jewellery making becomes the arena for big investment for local as well as for export needs with high level of technological change inter alia the beginning of gigantic production and retail showrooms (Krishnakumar R, 2006). Hence, the traditional hand-made jewellery making gives the way for machine made jewellery making.<sup>1,2</sup>

The product market is oscillating with many factors and variables and with this it is trying to reach equipose with factors like price, ability to pay characteristics, design changes, demand volumes, repurchase or exchanges and factors involved in marketing. These forces in a way determine the maximisation principle in business either in the case of craftsmen or in the case of businessmen

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are determined by forces of technology. Technology is considered as the linchpin in all facets of production like, melting, refining, moulding, designing, casting, electroplating, carving, testing and stone fixing. To meet the changes in consumer requirement various software are used to meet the suitability of design. The consumers demand is determined by the quality of the products they purchase and the result of this is the introduction of BIS to give quality assurance to the consumers. Hence, the adoption of new technology in the production and marketing process to a greater extent is useful for sustainable production, consumer confidence and profitability of the producers. Obviously, machineries in the areas of mechanical, electrical, electronic including software applications are essential element for anyone in this market to be sustainable and profitable (Hazra. A and Malakar. M, 2006).

The success of jewellery business is, by and large, based on adoption of the appropriate technology suiting the skills of the artisans in the gems and jewellery sector, which in turn benefits the manufacturer or retailer in the gold business. This is long and cumbersome process and generally it takes at least two years to understand the ins and outs of the technology for using it proficiently. Every type of technology transition needs some kind of cost and the adopter of technology has to meet the cost as the gold and jewellery items have big changes in its prices and the late adoption will be costlier (Pradeep. K. V and Karunakaran. N, 2021). This is a peculiar nature of the gems and jewellery industry in comparison with other resource-based industries or even other types of industries. In this respect, whether it is engaged in traditional manufacturing or trade adoption of technology irrespective of its scale and size have to utilise the best technology available without any delay. The changes in life styles led to concomitant changes in the demand for new design and fashion in gems and jewellery and this is growing at a faster pace and the jewellery manufacturers are well aware of these changes (Madhavi. S and Devi. T. R, 2015). The manufacturers are trying to tap the maximum potential from the global demand in the gems and jewellery products as the international jewellery market is very robust for the Indian products.

## 2. Materials and Methods

The study makes use of secondary data collected from the Report of World Gold Council and the Reserve Bank of India Bulletin. The Compound Annual Growth Rate is used to evaluate the temporal dynamics and growth in gems and jewellery sector in India. The price of gold fluctuates a great deal over time and to evaluate the instability in gold price, Cuddy-Della Index of Instability (CDII) is used. The higher the score, the higher is the instability and vice-versa. The CDII is worked out for both pre and post liberalisation phases and the values are compared to identify any change in the instability score of gold price during the two periods.

The Index is evaluated based on the methodology followed Cuddy and Della (1978).

Cuddy-Della Index of Instability (CDII)

$$CDII = CV \times \sqrt{(1 - R^2)}$$

Where, CV = Coefficient of Variation;  $R^2$  = Coefficient of Determination

## 3. Results, Analysis and Discussions

The dynamics of the sector is not driven by any local issue but is global in nature, which makes the sector always vibrant and this is more so in the post globalised era.

### 3.1. Temporal dynamics in gold price in India: pre-and post-liberalisation period

Temporal dynamics is evaluated with the trend in gold price of India, which is evaluated temporally to work out the growth rate i.e., the annual rate of change in different phases during the pre and post liberalisation periods. The liberalisation in this sector has witnessed a type of co-integration of prices with the international gold price. Though the gold price is on an increase, there are fluctuations. In 2016 onwards, price data show that domestic price of gold was affected by some factors like PAN card regulations, Brexit issue, GST implementation, hike in interest rate in US and demonetisation in India. For a temporal evaluation, the gold price data for India has been classified into two phases, viz. pre and post liberalisation.<sup>3</sup>

#### 3.1.1. Pre-liberalisation phase (1964-90)

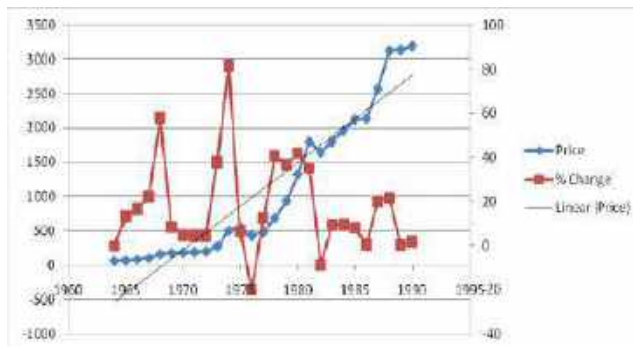
1964-90 period is termed as gold control era. Holding of more than 100g gold by the goldsmith and 2 kg gold by the licensed dealers was prohibited. Forward trading in gold was banned in 1962. The manufacturing of ornaments with more than 14 carat purity was prohibited as per the Gold Control Rules 1963, which was also applicable to the refineries. However, the ban on 14 carat jewellery making was lifted in 1966. As per the Gold Control Act 1968, holding of gold in form other than jewellery was prohibited. The gold bonds which were issued by the government in exchange of gold were also a failure as the women who possessed the lion's share of gold ornaments in the country were unwilling to participate in the scheme. The abolition of Gold Control Act in 1990 was done in tune with liberalisation with the fact that the country had to pledge its gold reserves to the Bank of England due to a foreign exchange default scenario.<sup>4</sup>

The gold price trend during the pre-liberalisation period of 1964-90 is shown in Figure 1. The year 1974 saw an increase in gold price from Rs. 278.5 to Rs. 506 which in percentage terms amounted to 81 percent. The year 1976 saw a fall to Rs. 432. Since 1978, the price of gold has



been increasing rapidly at an average rate of more than 35 percent and reached nearly three times the price of 1978 and in 1981 at Rs. 1800 per 10 grams. But 1982 saw a fall in gold price, after which the price stabilised and showed an increasing trend until 1986. In the years 1987 and 1988 witnessed a sharp increase in the average annual price of gold, after which the price again stabilized. Overall, the price of gold has dwindled during the period. In sub-phase-wise, the first phase 1964-72 witnessed a CAGR of 13.77 percent in price. The second period 1972-80 had a CAGR of 23.29 percent and the phase from 1980-90 realised a CAGR of 8.53 percent.

The impact of the regulations during the pre-liberalisation was manifold, in that it promoted black economy and gold smuggling. While the gold control policy was aimed to curb the purchase of gold by the public, the policy had created reverse effect. The Act was a total failure to curb price rise, control imports and stop black marketing. The jewellery during the period was made using recycled gold or smuggled gold. The jewellery making was the monopoly of the traditional goldsmiths during the period and most of them also started dealing with black marketing.<sup>5</sup>

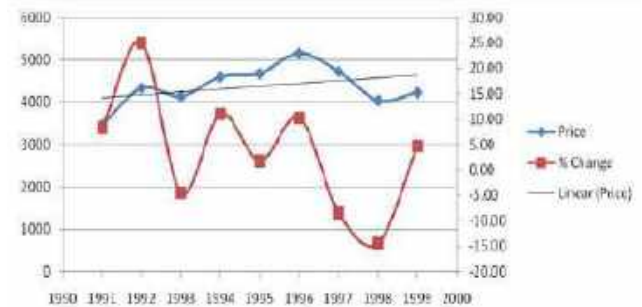


**Fig. 1:** Gold price during Pre-liberalisation period Source: World Gold Council (2018)

### 3.1.2. Post-liberalisation phase since 1991

The 1991 post liberalisation phase started with annulling the gold control act and permitting to hold gold bars and coins. Banks were allowed to import gold in 1997 so as to sell or give loan to jewellers and exporters. Non-resident Indians could now bring gold. Moreover, 100 percent FDI in the sector was also allowed. The liberalisation of the sector and allowing the import facilitated the growth of the sector and integrated the market and price with the international markets. The growth experience in the sector has been immense since globalisation which is evident from the data depicted in the aforementioned sections. The phases during the post-liberalisation are classified into three sub-phases of 9 years duration viz. Phase 1: 1991-99, Phase 2: 2000-08 and Phase 3: 2009-18.<sup>6</sup>

3.1.2.1. Post-liberalisation phase 1 (1991-99). The first sub-phase of post-liberalisation phase witnessed a growth of only 2.25 percent in the gold price (from Rs. 3466 to Rs. 4234 during 1991 and 1999). There were lots of dynamics in price year-wise (Figure 2). The years 1997 and 1998 saw a fall in gold price compared to 1996.



**Fig. 2:** Gold Price 1991-99 Source: World Gold Council (2018)

3.1.2.2. Post-liberalisation phase 2 (2000-08). The second sub-phase (Figure 3) saw a phenomenal increase in the annual price of gold. The price of gold per 10 grams increased from Rs. 4400 in 2000 to 12500 in 2008. The CAGR for the period stood at an impressive value of 12.3 percent. Except for 2001, where there was a slight decline in the gold price, the price has increased during this period and it could be inferred that the trend is going upward. The year-wise growth data also show some fluctuations but an increasing pattern. The period could be termed as one of the important post liberalisation phases. The gold price was impacted due to the domestic growth as well as global factors during this period. The measures taken by government to deregulate the gold industry were showing desired results.<sup>7</sup>

3.1.2.3. Post-liberalisation phase 3 (2009-19). During the start of the period, gold price was Rs. 14500. From 2010-11, there was an increase of 42.70 percent (Figure 4). The price reached a peak of Rs. 31050 per 10 grams during 2012. Afterwards, price started falling and reached a low of Rs. 26344 in 2015. While the trend is positive, the price has shown a decline since 2012. The CAGR for the period is 8.28 percent.

### 3.2. Instability in gold prices: A pre-post liberalisation comparison

Instability in gold prices, particularly inferring pre and post liberalisation has been evaluated using instability index.

It is shown that the p values are significantly related both for pre and post liberalisation phases and the instability value during pre-liberalisation period is less than post-liberalisation score (Table 1); indicates that the liberalisation has increased instability in price of gold in India. The

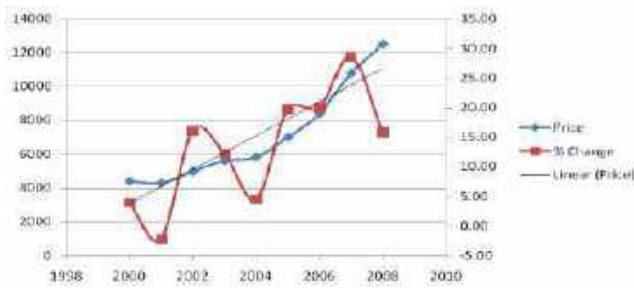


Fig. 3: Gold Price 2000-2008 Source: World Gold Council (2018)

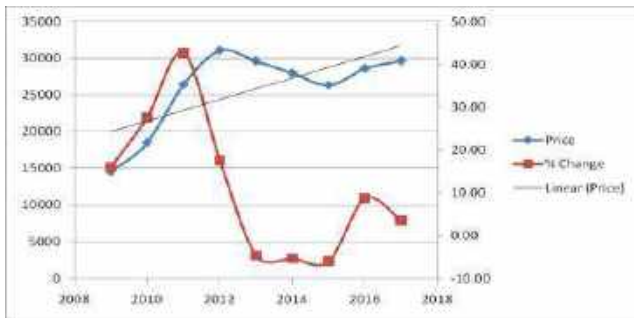


Fig. 4: Gold Price 2009-2018 Source: World Gold Council (2018)

liberalisation has integrated the domestic market with the global market and hence any variation in global gold market affects the domestic market more. Gold is a highly volatile commodity, price of which depends on the demand and supply factors as well as other global and domestic factors. It is evident that the price of gold has been fluctuating more after liberalisation.

Table 1: Instability in gold price

	Pre-liberalisation	Post-liberalisation
R	0.888	0.785
Square		
DW	0.234	0.178
Mean	1109.565	12441.222
SD	1070.663	10346.621
CV	96.494	83.164
T Value	14.057	9.552
P Value	0.000	0.000
C-D	5.404	8.940

### 3.3. Global and domestic gold price: A pre-post liberalisation comparison

Dynamics in gold price is identifiable with respect to stochastic and non-stochastic factors like several government policies, political situations, catastrophic situations, monetary policies of governments, inflation, American bond issues, central banks policies of various

economies and equity markets. Currency volatilities of various countries are also responsible for the gold price as most of the currencies of the world are pegged with dollar. Weak and strong dollar either makes gold price up or down as it becomes cheap or expensive for the foreign purchasers of gold in the international markets.

Even though a change in the global market impacted the domestic price, there was high difference in the price of gold in the global and domestic markets during the pre-liberalisation period. In fact, the domestic price of gold was more than the global price during most of the years of the pre-liberalisation era. The price of gold in India was at least 35 percent more than the international price on an average during the pre-liberalisation period. Only for a brief period of 1979-80 and 1980-81, the difference was minimal (Figure 5). However, the domestic market price is closer with the global price after the liberalisation as the difference has come down and now the average difference during the post liberalisation period is close to 10 percent. The price seems to be more co-integrated with the global market since 2001-02 as the average score is 2.4 percent during the period. However, a close observation of post 2013-14 data shows a higher difference in the gold prices with domestic price of gold higher than the global price. This is due to the increasing duties and introduction of GST on gold from 2017 onwards. Other factors which are influential in the gold price spurt come to be economic slowdown, stock market performance, geo-political tensions, and recently the spread of Covid-19 pandemic.

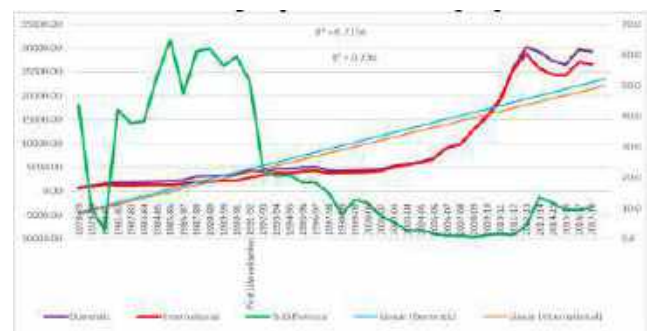


Fig. 5: Domestic and international gold price difference: A pre-post liberalisation comparison Source: RBI (2020)

### 3.4. Factors determining gold price in India

The analysis of the post liberalisation gold data shows that the domestic market price is closely cointegrated with the global market and any decrease or increase in global gold price impacts the domestic market price as well. Though the price of gold in India has increased due to imposition of import duty and other taxes, the prices often move in tandem with the global prices. Gold prices are also determined by dollar exchange rate and stock market performance holding

**Table 2:** Coefficients

Model	Unstandardized Coefficients		Standardized Coefficients	T	Sig.	Correlations			Collinearity Statistics		
	B	Std. Error	Beta			Zero-order	Partial	Part	Tolerance	VIF	
1	(Constant)	1.100	.220		5.001	.000					
	Int	1.102	.064	1.180	17.103	.000	.993	.961	.339	.082	12.122
	Exc	-.286	.104	-.100	-	.011	.798	-.489	-.054	.294	3.397
	Sen	-.092	.056	-.108	-	.115	.934	-.316	-.032	.090	11.144
					2.748						
					1.634						
<b>Model Summary:</b> R=.995; R Square=.991					<b>ANOVA:</b> Sig.= .000; F=840.943						
Predictors: (Constant), Sen, Exc, Int; Dependent Variable: Dom											

other stochastic components are nonacting. To find out which of these have a profound influence on the gold price during the post-liberalisation period, regression inference is used by taking domestic gold price as dependent variable and international gold price, rupee-dollar exchange rate and Sensex rate as independent variables. Model summary shows that the R and R Square values are 0.995 and 0.991 respectively. This is further inferred with the ANOVA result, which is significant (Table 2). To ascertain the validity, multicollinearity is worked out by inspecting the VIF values. VIF value of more than 10 is often considered as a concern and even though international gold price is significant, the concern still exists. Nonetheless the international and domestic gold price move in symmetry, the regression value infers that the dollar rate significantly influences the gold price in India and even negatively correlated.

#### 4. Conclusion

Gold price is always the result of a random ramification and hence is dynamically settled. It is customary to connect the gold price dependency with demand and supply factors; demand is perpetually increasing so also its supply. In this respect nothing makes special, as the quantity is always added up as consumption of gold does not mean that the consumed commodity is exhausted. Instead it is stocked in one form or other. Hence has these incessant dynamics. The dynamics of the sector is not driven by any local issue but is global in nature, which makes the sector always vibrant and this is more so in the post-globalised era or its sub-eras in comparison to the pre-liberalised regime. One reason quite often cited for this positive impact is that the liberalisation and related mechanisation, the prospects of the industry has been elevated and new investors entered into the sector in India with huge capital investment to reap the potential benefit. It is obvious that gold price shows a kind of co-integration of the domestic gold prices with the global prices. But in a pre-post-liberalisation comparison, the post-liberalisation period is more integrated with the global prices than the pre-liberalised. The domestic price

of gold was more than the global price during most of the years of the pre-liberalisation era as the price of gold in India on an average was 30 percent more than the international price. But the caveat in gold liberalisation is that it is integrating the domestic market with the global market and any reverberation in the global gold market has affected the domestic market unequivocally. This is well authenticated with Cuddy-Della Index, regression and correlation inferences all of which show an augmented reality of global integration of prices and its dynamics.

#### 5. Source of Funding

None.

#### 6. Conflict of Interest

None.

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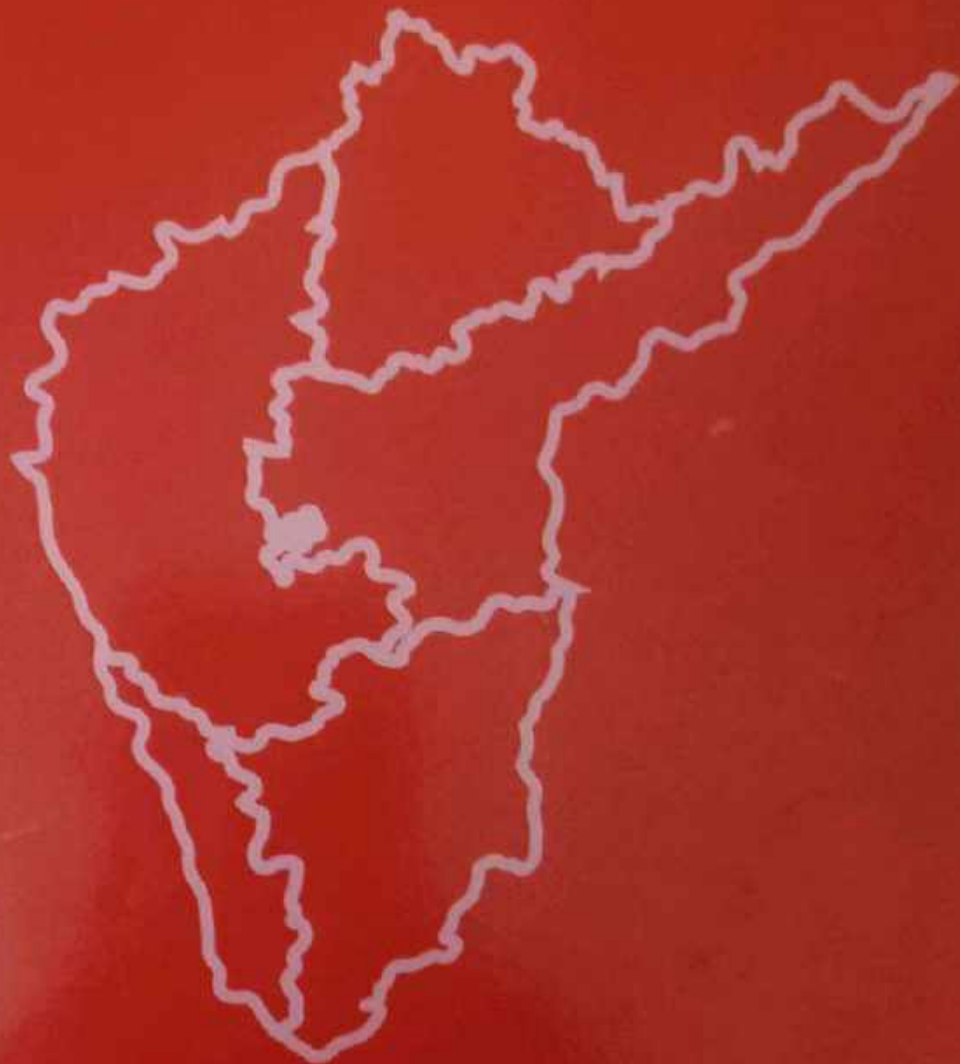
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GULF BOOM IN MALABAR: AN ANALYSIS OF SOCIO CULTURAL AND ECONOMIC FACET IN THE LATE 20<sup>TH</sup> CENTURY KERALAM

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*Abstract*

*The modern era saw a flow of Gulf migration from Kerala to Arabian countries. The discovery of oil in the Gulf region in the 1930s changed the process of migration flows to the region significantly. The discovery of oil had a significant impact on the Gulf countries, and gradually the GCC nations' industrial output increased steadily, resulting in naturally ensuing demands for foreign laborers employed in the oil-induced economic and infrastructure development process. During the last quarter of the twentieth century, gulf migration was the most dynamic factor driving Kerala's economy. When we look at Gulf migration in India as a whole, we see that a large number of people from the Indian state of Kerala went to the Gulf Countries beginning in the 1970s. A large number of migrations began in Kerala, mainly in Malabar. The present paper attempts to focus on the impact of Gulf migration in Kerala. The intensification of Gulf migration resulted in not only great economic prosperity but also radical progress in Malabar society's social and cultural standards. The early stage of migration, which favored mostly Malabar Mappilas, and their subsequent contributions play a significant role in shaping Malabar society's distinct character.*

**Key Words:** Migration-Gulf boom- industrialization- Malabar- Centre for Development Studies- Kerala Economy- Mappilas- Malayalees- Gulf immigrants- Gulf Products- purdha- food habits- Economic opportunity- Educational improvement- consumer culture

India had maintained a significant relation with West Asian countries from the ancient period onwards. Over the years of these maritime trade relations, which benefited India's economic conditions for a long time, the fact was that, during that period, people were not focused on a large level of migration to Gulf countries. The recent era saw a surge in Gulf migration from Kerala to Arabian countries. Kerala, along with Punjab and Goa, became involved in international migration during the Gulf Boom of the mid-1970s<sup>1</sup>. The discovery of oil in the Gulf region in the 1930s changed the process of migration flows to the region significantly<sup>2</sup>. The discovery of oil which was first found in great level in Iran in 1914, in Bahrain in 1932, in Kuwait in 1938, in Abu Dhabi in 1939 and in Iraq in 1939<sup>3</sup>. The oil discoveries were followed by a great level of industrialization throughout the region. It had a significant impact on the Gulf countries, and gradually the GCC nations' industrial output increased steadily, resulting in naturally ensuing demands for foreign laborers employed in the oil-induced economic and infrastructure development process. Kerala, the main source of Indian labor to the Gulf, where six million Indians live, has become reliant on remittances from Gulf migration<sup>4</sup>.

The present study attempts to focus on the diverse levels of impact of Gulf migration in Kerala. During the last quarter of the twentieth century, gulf migration was the most dynamic factor driving Kerala's economy. When we look at Gulf migration in India as a whole, we see that a large number of people from the Indian state of Kerala went to the Gulf Countries beginning in the 1970s<sup>5</sup>. It is estimated that about two third of the Indian employees in the gulf countries were Malayalis. The large number of migrations began in Kerala, mainly in Malabar areas. Accordingly, this paper tries to analyze the cultural uniqueness of Malabar with the emergence of Gulf migration as a great phenomenon, especially in the sphere of the cultural and economic lives of the people. As we know, from the ancient period, Malabar was the centre of Islamic cultural diversities, which played a pivotal role in the formation of Islamic identity in Kerala. The exclusive Islamic cultural



augmentation provided by Gulf contacts is awfully helpful for accelerating the cultural tradition of Kerala Muslims.

In the Malabar region, districts such as Malappuram, Kozhikode, Kannur, and Kasargod had the highest Muslim populations that immigrated to Gulf countries. These emigrants play a decisive role in shaping Kerala society. Large type of migration occurred not only in the Malabar region, but also in the rest of Kerala. One of the facts is that, in Kerala, 52.5% of Muslim households have one or more non-resident Keralites. And in the case of Malappuram district, the percentage is even higher; in Malappuram alone, 71 % of the households have in them either an emigrant or a returnee<sup>8</sup>. The growth of Gulf migration resulted in not only great economic prosperity but also radical progress in Malabar society's social and cultural standards. The early stage of migration, which favoured mostly Malabar *Mappilas*, and their subsequent contributions play an essential role in shaping Malabar society's distinct character.

The Centre for Development Studies (CDS) has conducted numerous studies connected to the impact of Gulf migration in Kerala. One of the significant reports was submitted by K. C. Zachariah, B.A. Prakash, and S. Irudaya Rajan entitled *Gulf Migration Study: Employment, Wages and Working Conditions of Kerala Emigrants in The United Arab Emirates*. The work clearly reflects an assessment of the overall statistical analysis of the migration of Keralites. And the study underscores the contribution of emigrants to the overall development of Kerala.

In addition to various studies have provided different assumptions for the large scale of the migration process. The article written by B.K. Prakash in the *Economic and Political Weekly*, entitled *Gulf Migration and Its Economic Impact The Kerala Experience*. The article analyses the diverse aspects of the reason for the large migration in Kerala, and spot out the prime reason behind those unprecedented economic changes since the mid-1970s in the poor and industrially backward economy of Kerala. And the migration process gives support to emigrants in achieving a high level of income and improving their living conditions.

The significant turning point in the history of migration process in India started from the introduction of Emigration Act of 1983. The government of India introduced Emigration Act of 1983<sup>7</sup>, which increased the systematic flow of migration<sup>5</sup>. Consequently, there was a rapid growth in migration to the Gulf during the first half of the 1990s; the situation has drastically changed since 1996. The Muslim community is more preferred for the first stage of migration to Gulf countries. Later, the migrants became members of almost every social group. The socio-economic conditions of migrant households have improved greatly. Following that, we can see a decline in the course of migration status beginning in 1998. The West Asian political conditions was the central reason for the decline. The large number of emigrants that returned to Kerala from the Gulf between 1996 and mid-1998 was around 3.13 lakh. This unexpected departure of emigrants has created serious economic problems in most of the districts of Kerala<sup>9</sup>.

The northern parts of Kerala, where majority of them are Muslims, were known as the *Mappilas*<sup>10</sup>. With a Muslim population of 68.5 percent in Malappuram district, the majority of them immigrate to the Gulf countries; immigration plays a significant role in shaping Malabar society. The early socio-economic conditions of Malabar were the main reason for the flow of migration. During the time, majority of the peoples of Malabar were unemployed and unable to meet their daily expenses. The situation was more critical at that time and they took advantage of this opportunity. The real fact is that unemployment was the major reason for the increase in emigration.

During the early period, the majority of people were not used to the legal process of migration. Illegal migration was a very common process at that time. During the time the migrants paid some amount of money to illegal organizers, and they used ships, especially merchant ships, also known as *Pathemary*<sup>11</sup> for this illegal process. The migration took place primarily in the Indian Ocean, and it was extremely dangerous at the time<sup>12</sup>. Kerala has a long coastline, which provides many opportunities for Kerala migrants to take this risky route<sup>13</sup>. After some years of effort from recruiting and other agencies, the migration became legalized. But now a day this kind of illegal migration completely impede and people use proper channel.



The flow of immigration had a great impact on the overall development of India's economic structure. The large number of Gulf migrants has resolved the problem of unemployment, especially in Malabar. Gulf migration is a purely temporary one, and the workers have engaged in a labour contract at that time, and they attempt to maximize their savings and remit them to their own homes<sup>14</sup>. The culture of savings among Gulf immigrants and the consequent inflow of remittances is one of the most important factors that have influenced the course of economic development in Kerala over the decades. The government had taken numerous reputable steps to improve the economic situation in the Malabar region. Along with the efforts of the government, the process of Gulf migration has also doubled the benefits of these areas.

The overall impact of Gulf migration is visible in Malabar area. Numerous changes have occurred today as we travel through the Malabar region. The traditional style of houses in these areas is restructured into multiple concrete buildings. Gulf immigrants started various business projects in these areas, and they were ready to invest large amount of money in Kerala. Naturally, the new projects and investments benefited to the improvement of the stability of Kerala economy. The immigrants not only started their projects in Kerala but also established new businesses projects in Gulf countries that gained international recognition. These kinds of networks of businesses were improving our country's economic prosperity. Now the People from Kerala have started a lot of investments in GCC<sup>15</sup> countries.

In one sense this kind of development happened in Kerala. But the real fact is that it has only benefited a small section of the society. Most of immigrants were the common people who are not categorized by this kind of progress. They were engaged in small wage labor works such as building constructions, hotel works, shop employees, drivers, employees in oil companies, etc. Naturally, they received a meager salary. They spent a relatively large proportion of their savings for the construction and renovation of house buildings, repayment of loans, the conduct of marriage of their daughters and relatives, the purchase of consumer durables, gifts, and donations, the purchase and improvement of landed property, the purchase of ornaments, education and medical treatment, financing the emigration of other members of the household, and the purchase of vehicles. The proportion of households that have made investments in businesses or in acquiring financial assets is relatively small. However, the fact is that Kerala's economic equilibrium is entirely dependent on emigrants. Unfortunately, the majority of household savings are spent on non-productive items<sup>16</sup>.

The salient impact of Gulf migration has been a dramatic progress in Kerala's consumption levels. Before the 1970s, the percentage of consumer expenditure in Kerala was lower than that of the all India average. But after the Gulf boom, the per capita consumer expenditure in Kerala, mainly in rural areas, became 20% to 30% higher than the all India average<sup>17</sup>. A Gulf-influenced trend is apparent in the shop selling what *Malayalees* call "Gulf Products." These products are not actually manufactured in the Gulf countries, but are usually imported; Examples of these durable and non-durable goods are: mobile phones, computers, kitchen and cooking devices and so on. The prevalence of a strong consumer culture is linked to the established purchasing power of women.

Influence of Gulf migration in Kerala is not only felt in the economic field but also in social and cultural aspects. When we examine each field, the significant change has been observed in dress pattern. The most important change has been the adoption of *purdah* as a common Muslim dress in Kerala. The introduction of *pardha* is in Kerala as a serious debatable one as to whether it focuses on Muslim identity or as a by-product of cultural integration or a part of new identity crisis. Prior to the 1980s, *pardha* was not the common identity of Kerala's Muslim community. However, due to the influence of Gulf culture, it has become a common Muslim dress in Kerala. In Kerala, for a long time, Muslim women wore their traditional dress, the *kachathuni* (a *mundu* or dhoti), the *pennukuppayam* (a full-sleeved loose blouse), and the *thattom* (long scarf)<sup>18</sup>.

The discourses regarding *purdha* have been raging for about a decade. The multiple levels of arguments are manifested in everyday life. The forces of debate are focused among two groups; such as secularists and Islamic fundamentalists. The secular group promoted a liberal way of approach, and they stand against the Muslim orthodox attitudes, and against to exclude the separate cultural identity. The opposing party refuted the argument. They argue that *pardha* as a part of



adoption of cultural integration in one sense. The modern foreign Arabic cultural integration leaned toward the consumerist. This type of adoption of the *pardha* is related to further rudiments, such as the introduction of different food habits of the nations of Egypt, Saudi Arabia, and Yemen, all of which are available in Kerala restaurants in a society characterized by a strong capability to imbibe foreign elements<sup>19</sup>. The cultural flow is mixed with strong economic inducements that led to successful business enterprises in manufacturing and selling these popular Arab lifestyles<sup>20</sup>.

Each and every society is characterized by ability to induce foreign elements, this adoption of the *pardha* also we can be viewed on this ground. In any way the historical fact is that in the context of Kerala *pardha* was not common dress among the Muslims before 1980's. But after the influence of the Gulf, people used this dress to create a new Islamic identity. Almost all parts of Kerala, the woman either urban or rural accepted *pardha* as a common dress identity for Muslims. But we cannot generalise the fact that some of the Muslim women are still not using *pardha* as own common identity.

Another exemplary change one can perceive is the food habits of Kerala. The appearance of Arabic food is very common in all restaurants in Kerala. Their almost identical menus are comprised of Saudi and Yemeni meat dishes, the most popular food in all restaurants in and around Kerala. Biryani, Arabian Mandi, Khuraishi Mandi, Sufi Mandi, Kabsa, Shwarma, Hummus, Alfaham, Shawai Chicken and various types of grilled chicken are the most popular and appealing foods at weddings, whether Muslim, Christian, or Hindu. The people of Kerala accepted this kind of food as a part of their festivals and other important functions.

Malabar's folklore is composed of hybrid art forms in which indigenous dancing and poetry were fused with Arabic themes. *Duffnattu*, for example, is an art form using the traditional Arabian duff (an Arabic drum). Currently, Muslims stand in a circle singing an Islamic song in Malayalam while playing the Duff. *Oppana*, which is a fusion art form of singing and dancing represented by females during a wedding ceremony. The singing consists of folk *Mappila* (Malabar's Muslim) songs. The *Mappila* songs themselves (in Malayalam, *Mappilapattu*) represent another hybrid form of art. These art forms are now almost entirely found in Islamic school celebrations or on television programming. Malabar wedding is a wonder with music, dancing, or celebration right apart from the incredible amounts of *biryani*, beef curry, and other spicy and delicious food items. The economic prosperity of Malabar as a result of Gulf migration; even the previously low income groups, who have enough money now, are conducting marriage ceremonies like the elite class.

This is not only attributed to consumer goods, but also to the common goal of directing remittance towards building or renovating houses a goal that ended up as a trend. Perhaps what is most significant about this trend is that women's agency and autonomy appear particularly strong. Usually it is the women who are the recipients of money that their husbands send through bank transfers and hence are often solely responsible for all the paper work concerned with obtaining construction permits from the municipality, choosing a design for the house, and managing all construction related steps.

Since the period of the 1980s communication has not been easy. Letter and phone calls were the only way of communication with their own family. Gulf wives, loneliness was one of the foremost problem. More than half the number of young wives considered loneliness as the main problems arising from their husbands' emigration. Loneliness was correlated quantitatively with the length of the period of separation and the frequency of communication between the Gulf wife and her expatriate husband. The longer period of separation affected the communication between wives and husbands leading to loneliness. Similarly, the less frequent the communication between the husband and wife, the higher the degree of loneliness. In the case of about 2.4 percent of the Gulf wives, their husbands had left for the Gulf within days after marriage; almost a-third left within three months of marriage, and about 45 percent left during the first year of marriage. Thus, separation from husbands soon after marriage is indeed a real problem among the Gulf wives, as articulated by them. The situation is much worse among the younger wives, about 2.7 percent of their husbands left for the Gulf immediately after marriage. The problem is partly ameliorated by frequent communication between husband and wife through phone calls and letters. Almost all Gulf

wives communicated with their husbands in one form or another. Nearly 70 percent communicated through letters and phone calls, and 30 percent communicated through letters alone<sup>21</sup>. Almost half of Gulf wives communicated once in every two weeks.

The majority of those who wrote letters also communicated over the phone. Such frequent communication ameliorated the problem of loneliness to a large extent. The ability to communicate whenever needed was a great help for the wives to unburden on the load of added responsibilities, slightly responsibilities related to financial management. Nearly a-third of the Gulf wives, especially the older ones complained about added responsibilities because of their husbands' migration; responsibilities to take care of the children's education, family finances, family health, and fulfilling family obligations in social, cultural, and religious domains, etc. Taking care of the children's education is a major added responsibility. More than 75 percent of those with children had one child or more in school. As the father is away, the mother is responsible for getting them admission to school, arranging for their transport to school, finding a paid tutor, arranging for transport to the tutor's place, and helping the children with their homework<sup>22</sup>. Only a few of the Gulf wives actually take their children to school, but about eight percent take them to the tuition master, and 75 percent of them help them with their school work. Having gone through the experience of being a Gulf wife, they seem to have second thoughts about their husbands' emigration. It is all right from an economic point of view, but not so if all factors are taken into consideration. Those who have gone through the trauma of separation would prefer that their husbands work at jobs in Kerala, if they could. There is considerable sacrifice involved on the part of migrants, and on the part of the wives and children in Kerala<sup>23</sup>.

The demand for labour in the Gulf countries opened only a window of economic opportunity; however, the *Mappilas* were able to take full advantage of this. Using their strong determination and hard work, they put Malabar Muslims on the path to progress, giving shape to the community compared to the rest of the Indian Muslims. Kerala has seen better days, and though all communities benefited from the economic boom in Gulf, the *Mappilas* of Malabar as a community were the largest beneficiary. Trade was always discussed in an Islamic context with references to Muslim merchants, so trade has been labeled as a Muslim activity because it was mainly conducted by Muslims of the West Asian region. Throughout history, Islamic religious principles have been observed to promote a positive and encouraging attitude towards trade and commerce. Apart from the mutual religious relationship between Islamic principles and trade, Arabs were forced to engage in maritime commerce further into the Indian Ocean. Historical ties, as well as, Malabar Muslims' religious identity has aided in the formation of a bond with Gulf countries. In a nutshell, the gulf is the "golden fortune" of the *Mappilas* of Malabar.

The Gulf dream has also found expression in Malayalam cinema and literature<sup>24</sup>. When we look at the cinemas of 1980s and 1990s some of them were connected to the life of gulf immigrations. M. Mukkundan's "*Daivathinte Vikrithikal*" draws out in detail the socio-economic impacts of Gulf migration on the enclave of Mahe, one of the best examples. The cinema *Pathemari* was written and directed by Salim Ahamed and it sketches the early life of gulf immigrants. The film discusses the early illegal migration to gulf countries. The film draws the risk of the early illegal migration process. The positive and negative impacts of the gulf migration were also discussed in different literary works. Some traditional *Mappila* songs reveal the social status of Gulf immigrants. In the early days, *Mappila Kathu pattukal* had a great influence on the socio-cultural field of Malabar society. The theme of *Kathu pattukal* has centered on the relationship between husband and wife. The song reveals the problems faced by women after getting married. At that time, most of the houses in Kerala, especially in the Malabar area, after marriage to their husband back to the gulf countries the communication was not easy. The letter was the only way to communicate. Once the husband is back in the gulf countries they would return only after a minimum of two or three years. So the wife and husband both faced a lot of mental stress. That kind of issue has also addressed in this *kathu pattukal*.

Educational improvement helped people from Kerala to gain good employment in the Gulf. The economic condition of a number of uneducated families has improved to some extent, but it has



been pointed out by researchers that the community, with an eye on the immediate financial benefits, has ignored its long term interests in human resource development through its preference for Gulf jobs over obtaining adequate educational qualifications<sup>27</sup>. As Miller observed, "The Gulf money, although often wastefully used, provided a means for sympathetic improvements and psychological release from the constant pressure of poverty. Moreover, it had created a kind of economic runway for a *Mappila* flight to a higher level of social achievement. But the plane itself was not aloft. The *Mappila* community now had the opportunity and the means to address its economic and social problems; with the realistic hope that they might be solved and that the community's common life would soar"<sup>28</sup>.

Gulf migration has had a great impact on the socio-cultural milieu of modern Kerala. The discovery of oil in the West Asian countries resulted in a great change in the economic structure. After that, the economic structure of gulf countries reoriented with this oil industry. From the developing processes Gulf countries were demands for foreign laborers employed in the oil-induced economic and infrastructure development process. Kerala is the main source of Indian labor to the Gulf, where six million Indians live, and has become reliant on remittances from Gulf migration. When we look at the Gulf migration in India as a whole, we see a large number of people from the Indian state of Kerala. From the initial stage of the Gulf boom most of the immigration happened is from Kerala, mainly from Malabar areas. The process of Migration witnessed great changes in the political and social sphere of Kerala till 1970. The development of Gulf migration resulted in not only great economic prosperity but also radical progress in Malabar society's social and cultural standards. Gulf money should be seen as a central factor in moving Kerala's economic sector to a great extent. Moreover the Gulf money helped make possible the *Mappila* transition to a new cultural outlook. The immigration process gives support to emigrants in accomplishing a high level of income and improving their living conditions. The process of Gulf migration also became a great part in shaping a new consumer culture even among the common people of Kerala.

## Endnotes

- <sup>1</sup> T.M Thomas Isaac, Economic Consequences of Gulf Migration, K.C Zachariah (ed), *Demographic Transition Developments and Consequences*, 1997, p.270.
- <sup>2</sup> Mehdi Chowdhury and S. Irudaya Rajan, ed., South Asian Migration in the Gulf Causes and consequences, 2018, p.9.
- <sup>3</sup> Roland E Miller, *Mappila Muslims of Kerala*, 1992, p.118.
- <sup>4</sup> Julten Abdelhalim, *Paradoxes of Pardha and Agency Among Muslim Women in Kerala*, p.238, <https://lidemesta.cuni.cz/LM-900-version1-abdelhalim.pdf> last visited on 15-05-2020
- <sup>5</sup> Biju Govind, *GCC Residency cap may force lakhs to Return*, The Hindu, Tuesday, August 19, 2008.
- <sup>6</sup> Julten Abdelhalim, *Paradoxes of Pardha and Agency Among Muslim Women in Kerala*, p.238, <https://lidemesta.cuni.cz/LM-900-version1-abdelhalim.pdf> last visited on 15-05-2020
- <sup>7</sup> According to the Act of 1983 "emigrate" or "emigration" mean the departure of out of India of any person with a view to taking up any employment (whether or not under an agreement or other arrangements to take up such employment and whether with or without the assistance of a recruiting agent or employer) in any or place outside India. For more details of 1983 Acts see: <http://odisha.ipo.iceidcb.gov.in/sites/default/files/Emigration-Act-1983.pdf> last visited on 12-10-2020
- <sup>8</sup> K. C. Zachariah et al, Gulf Migration Study: Employment, Wages and Working Conditions of Kerala Emigrants in The United Arab Emirates, CDS, <https://www.researchgate.net/publication/5127062> last visited on 22-04-2021
- <sup>9</sup> B.A.Prakash, *op.cit.* p.103
- <sup>10</sup> The name "*Mappila*" is transliteration of the Malayalam '*Mappila*'. The transliteration has taken several different forms, the most common being '*Mappila*' and '*Moplah*'. The origin of the term is not yet settled, but it appears to have been basically a title of respect. But recently the term has tended more and more to an exclusive name for Kerala Muslims for more details Roland E. Miller, *Mappila Muslims of Kerala*, 1992, p. 30.
- <sup>11</sup> Large vessels for using for overseas trading, *Pathamari* also known as *Uru* which is constructed in the coastal areas of Malabar especially Beypore.
- <sup>12</sup> A.C.K Nambiar, *The Socio-Economic Conditions of Gulf Migrations*, 1995, P.76.
- <sup>13</sup> *Ibid.*
- <sup>14</sup> T.M Thomas Isaac, *op.cit.* p.271
- <sup>15</sup> The Cooperation Council for the Arab States of the Gulf, also known as the Gulf Cooperation Council, is a regional intergovernmental, political, and economic union comprising Bahrain, Kuwait, Oman, Qatar, Saudi Arabia, and the United Arab Emirates. The council's main headquarters is located in Riyadh, Saudi Arabia

<sup>18</sup> BA. Prakash, *op.cit.*, p.109-111

<sup>19</sup> T.M Thomas Isaac, *op.cit.*, p.290

<sup>20</sup> <https://www.firstpost.com/india/burqa-revolution-in-kerala-was-an-early-sign-of-islam-radicalisation-in-the-state-2887592.html>, last visited on 24-02-2020

<sup>21</sup> Julien Abdelhalim, *Paradoxes of Parda and Agency Among Muslim Women in Kerala*, [www.lidemesta.com](http://www.lidemesta.com) last visited on 21.08.2020

<sup>22</sup> *Ibid.*

<sup>23</sup> Irudaya Raja, *op.cit.*, p.505.

<sup>24</sup> *Ibid.*

<sup>25</sup> *Ibid.*

<sup>26</sup> *Gulf Dream: for Indians The Golden Beaches Still gleam*, MalayalaManorama Year book , 1990,p.15.

<sup>27</sup> U.Muhammed, *Educational Empowerment of Kerala Muslim: A socio-Cultural Perspective*, 2007,p.147

<sup>28</sup> [www.ucl.ac.com](http://www.ucl.ac.com) - last visited on 21.01.2014

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# FACTOR ANALYSIS ON CONSUMER PERCEPTION ON SELECTION OF HOME LOAN AND HFIS

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## Abstract

There is different housing finance institutions offer financial assistance to their customers in a very competitive manner. So the customer's choice is always depends on the various aspects related to their product and services. For this study the 385 samples were selected by random sampling method from selected public and private sector commercial banks. Factor analysis was used to study 29 variables and identified 7 factors. The result indicates that factors like features of the bank, repayment, eligibility, accessibility, loan processing customer care and special attractions provided by the bank were highly influenced the perception of home loan customers while selecting the housing finance agency.

**Keywords:** Home loan, Housing finance institution, Consumer perception, Commercial bank, Investment

## INTRODUCTION

For every person acquiring their own home is the most important milestone and goal in life. Housing is considered as a key sector of the national economy which measures the standard of living and economic condition of the country. Good housing is important for welfare of human being. It gives shelter, safety and privacy .Probably the largest financial investment they make in their lives as well. This financing facility comes with a number of benefits to lure aspiring homeowners. The study focused to analyse the various factors influencing the selection of housing finance agency.

## LITERATURE REVIEW

(Sughana & Sheela, 2021) has studied about the factors influencing the choice of customers while selecting the housing finance institutions in Visakhapatnam City. The study found that the selection of housing finance institutions were depends on the financial benefits and costs of home loan, processing charges, rate of interest, timely sharing of information such as pre-closure charges, income tax enabled services, time for sanctioning of loan and finally, the way customers are being dealt with.

(Kumar & Sudha , 2014) studied - Customer Perspective on Housing Loans in Chennai and found that most of the housing finance companies in India have introduced several new home loan products in order to meet the needs of a wide variety of customers. The customer can choose those schemes which he feels good for him and have the capacity to repay it on that specified time period. The study suggested that the loan providers need to ensure that the procedures followed should not be cumbersome but it should be for the ultimate benefit of loan provider and the customer.

(Vanitha & Kalaivanan, 2015) has studied the factors that influenced the home loan customers of SBI for taking the loan from them. The study found that the factors like low interest rate, no processing fee, lump sum repayment, low margin money ,speedy sanction, no pre closure charge, treatment of staff, easy accessibility un wanted queries, processing of documents , convenient repayment, long repayment and insurance optional that influence the customers to prefer SBI for home loan.

(Jayanthi, Ramya, & Ramya, 2014) observed that minimal formalities and procedures for home loan, low interest rate of flexible repayment system and faster processing were influenced the choice of customers for selecting home loan from HDFC Ltd ,but the bank was failed in proper updating of repayment and not properly conveyed the changes in interest rates.



(Karthikeyan, 2014) observed that the customers prefer the Lakshmi Vilas bank after analyzing the variables like interest rate, income level, repayment facility, loan approval, processing charges etc.

(Narsis, 2016) observed that majority of the customers took home loan for constructing the house and they prefer SBI bank because they offer the home loan at low rate of interest. It also reveals that the procedural formalities of bank were reasonable and customers were well aware about the concerned procedure of getting home loan from SBI.

## OBJECTIVE OF THE STUDY

- To assess the customer perception towards bank loan
- To identify the major influencing factors while selecting the home loan and housing finance agencies by the customers.

## RESEARCH METHODOLOGY

The study is descriptive in nature, it is conducted to know the major factors affecting the selection of housing finance agency. The population consists of home loan customers of selected banks in Kerala. For this study, 385 samples were selected by using simple random sampling method from selected public and private sector commercial banks with special reference to SBI, Canara Bank, Federal Bank and South Indian Bank in Kerala. Factor analysis was used to study 29 variables. Primary data were collected through structured schedule from the respondents.

## FACTORS AFFECTING THE SELECTION OF HOUSING FINANCE AGENCY

In order to identify the factors affecting the selection of housing finance agencies, factor analysis using principle component method and Varimax rotation was applied on the responses of customers on 29 aspects related to services of the banks. The factor analysis extracted 7 factors using the criterion of Eigen values greater than one.

**Table 1.1 Kaiser-Meyer-Olkin Measure of Sampling Adequacy of factor analysis**

KMO and Bartlett's Test		
Kaiser-Meyer-Olkin Measure of Sampling Adequacy.		.840
Bartlett's Test of Sphericity	Approx. Chi-Square	6400.797
	Df	406
	Sig.	.000

The sampling adequacy of factor analysis was moderately sufficient as Kaiser-Meyer-Olkin Measure is 0.840 which is very much close to 1. the significance level of Bartlett's Test of Sphericity is less than 0.05 which indicates that the factor analysis is well fitted to the data and it can be validly used for the study the factors affecting selection of housing finance agency.

**Table 1.2 Components of factor analysis**

	Component						
	1	2	3	4	5	6	7
Amount of loan given by bank	0.317	-0.010	-0.306	0.307	0.373	0.424	0.260
Eligibility criteria for applying loan from bank	0.214	0.052	0.052	0.187	0.792	0.077	0.124
Arranging legal documents for loan	0.048	0.113	0.246	0.183	0.766	0.146	-0.123
Loan to asset value ratio	0.134	0.248	0.141	0.093	0.677	-0.304	0.208
Collateral security requirements	0.287	0.093	0.236	0.203	0.671	0.047	-0.094



Repayment period	0.047	0.045	-0.012	0.774	0.275	0.300	0.049
Rate Interest	0.087	0.053	0.059	0.792	0.238	0.199	0.140
Equated Monthly Installments	0.240	0.070	0.003	0.742	0.044	0.037	0.249
Processing fee	0.129	0.221	0.442	0.625	0.129	-0.128	0.019
Penalty for delay / non- payment	0.153	0.172	0.389	0.545	0.119	0.092	-0.350
Reverse mortgage loan	0.242	0.562	0.279	0.046	0.251	0.147	0.099
Low interest rate for women	-0.016	0.876	0.000	0.078	0.067	0.140	-0.082
Joint home loan account	0.006	0.843	0.103	0.105	0.158	0.012	0.029
Special schemes in the festive seasons	0.250	0.750	-0.103	0.132	-0.100	-0.009	0.217
Balance transfer with top-up loans	0.285	0.765	0.076	0.009	0.115	0.096	0.006
Reputation of Bank	0.169	0.185	0.210	0.185	-0.019	0.811	0.048
Wide Coverage and Branches	0.035	0.154	0.271	0.194	0.086	0.726	0.223
Nearest Location	0.155	0.025	0.195	0.033	-0.042	0.523	0.532
Account within Bank	0.074	0.138	0.144	0.211	0.061	0.179	0.694
Loan processing Procedures	0.385	0.073	0.611	0.044	0.070	0.319	-0.037
Documentation for loan	0.361	-0.055	0.636	-0.003	0.254	0.136	0.017
Timely updating of changes in service	0.235	0.187	0.597	0.212	0.089	0.154	0.071
Sanctioning time for loan	0.312	0.035	0.508	0.202	0.101	0.140	0.445
Timely discharge of loan	0.136	0.003	0.707	0.026	0.226	0.101	0.275
Giving customer's individual attention	0.801	0.108	0.111	0.135	0.092	0.258	0.091
Dealings of employees with utmost care	0.763	0.182	0.116	0.204	0.064	0.119	0.224
Access to top level officials of institution	0.636	0.210	0.269	0.001	0.197	0.042	-0.087
Clearly clarify the doubts	0.699	0.122	0.312	0.159	0.277	-0.070	-0.024
Full disclosure of all information	0.689	0.116	0.266	0.123	0.151	0.020	0.121

By suppressing the factor loading below 0.52, the result of the factors extracted was presented in table.

**Table 1.3 Factor Loadings**

Factors	Variables	Loadings
Customer care	Giving customer's individual attention	0.801
	Dealings of employees with utmost care	0.763
	Clearly clarify the doubts	0.699
	Full disclosure of all information	0.689
	Access to top level officials of institution	0.636
Special Attractions	Low interest rate for women	0.876
	Joint home loan account	0.843
	Balance transfer with top-up loans	0.765
	Special schemes in the festive seasons	0.750
	Reverse mortgage loan	0.562

Loan processing and disbursement	Timely discharge of loan	0.707
	Documentation for loan	0.636
	Loan processing Procedures	0.611
	Timely updating of changes in service	0.597
Repayment Factors	Rate Interest	0.792
	Repayment period	0.774
	Equated Monthly Instalments	0.742
	Processing fee	0.625
	Penalty for delay / non- payment	0.545
Eligibility factors	Eligibility criteria for applying loan from bank	0.792
	Arranging legal documents for loan	0.766
	Loan to asset value ratio	0.677
	Collateral security requirements	0.671
Features of bank	Reputation of Bank	0.811
	Wide Coverage and Branches	0.726
Accessibility	Account within Bank	0.694
	Nearest Location	0.532

The first factor consists of six variables with strongest association to this factor namely giving customers individual attention (0.801), dealing of employees with utmost care (0.763), clearly clarify doubts (0.699), full disclosure of information (0.689) and access to top level officials(0.636). The first factor was named as customer care as the majority of the factors are related to customer centered services provided by the employees and officials of the bank.

The second factor consists of five variables with strongest association to this factor namely low interest rate for women (0.876), joint home loan account (0.843), balance transfer with top-up loans (0.765), special schemes in the festive seasons (0.750) and reverse mortgage loan(0.562). These variables are related to the additional services given by the bank to attract their customers so it is named as special attraction.

There was Four variables were closely associated with the third factor namely timely discharge of loan(0.707),documentation for loan(0.636), loan processing procedures(0.611) and timely updating of changes in service (0.597). The third factor is named as loan processing and disbursement because majority of these variables are closely associated with processing, sanctioning and disbursement of home loan by the banks.

The fourth factor consisting of five variables, they were closely associated with this factor namely rate Interest (0.792), repayment period (0.774), Equated Monthly Installments (0.742), processing fee (0.625) and penalty for delay / non-payment(0.545). The fourth factor is named as repayment factors as majority of these factors determine the repayment of home loan.

The fifth factor consists of four variables namely eligibility criteria for applying loan from bank (0.792), arranging legal documents for loan (0.766), loan to asset value ratio (0.677) and collateral security requirements (0.671).Majority of these variables determine the home loan eligibility of the customers; therefore this factor is named as eligibility factors.

Sixth factor consists of two variables namely reputation of bank (0.811) and wide coverage of bank with branches (0.726), they are closely associated to the characteristics of bank. So the fourth factor is named as features of bank. And the seventh factor also consists of two variables namely account within bank (0.694) and nearest location of the bank (0.532) is closely associated with how easily a customer can access the bank for home loan services. So the seventh factor is named as accessibility.

Using the factor loadings the composite variable representing seven factors were estimated and the descriptive statistics of the factors are given in table below.

**Table 1.4 Descriptive statistics of composite variable representing seven factors**

	Customer care	Special Attractions	Loan processing	Repayment Factors	Eligibility factors	Features of bank	Accessibility
Mean	3.67	2.98	3.68	3.80	3.78	3.84	3.77
Median	3.66	3.07	3.65	3.85	3.81	3.89	3.71
Std. Deviation	0.63	0.94	0.54	0.64	0.60	0.60	0.55
Skewness	-0.07	0.00	0.10	-0.76	-0.21	-0.64	-0.18
Kurtosis	-0.52	-0.73	0.15	1.29	-0.12	0.73	0.01
Minimum	2.16	1.21	2.14	1.46	1.83	1.92	2.22
Maximum	5.00	5.00	5.00	5.00	5.00	5.00	5.00

The table shows that mean score of composite variable representing customer care is 3.67 with a standard deviation of 0.63. The median is 3.66 which are very close to the mean and the absolute values of skewness and Kurtosis are very much lower than 2.5 indicating that the score of customer care is all most normally distributed among the sample. The score of customer care ranges from a minimum of 2.16 to a maximum of 5.00.

The mean score of features of bank is found to be 3.84 which are highest score among the factors affecting selection of housing finance agency. At the same time the lowest mean score is obtained for special attractions provided by the bank 2.98. The result indicates that features of the bank is the most influencing factor and special attractions provided by the bank is the lowest influencing factor in the selection of housing finance agency by home loan customers. The second highest mean score is obtained for repayment factors 3.80 and followed by eligibility factors of home loan 3.78, accessibility factors 3.77, loan processing and disbursement 3.68 and customer care factors 3.66. The mean score of these factors are significantly higher than the mean of the response scale namely 3 as the significance level of one-sample t-test with test value 3 is less than 0.05. It indicates that repayment, eligibility, accessibility, loan processing and customer care factors were highly influence the perception of home loan customers while selecting the housing finance agency.

The median values of repayment (M-3.85&  $\bar{x}$ - 3.80), eligibility (M-3.81&  $\bar{x}$ - 3.78), accessibility (M-3.71&  $\bar{x}$ - 3.77) , loan processing and disbursement (M-3.65&  $\bar{x}$ - 3.68) were almost close to the mean . At the same time absolute values of Skewness and Kurtosis are very much lower than 2.5. The result indicates that the score of repayment, eligibility, accessibility, loan processing and disbursement factors influence the perception of home loan customers while selecting the housing finance agency were all most normally distributed among the sample. The score of these variables ranges from a minimum of 2 and above to a maximum of 5.00.

## FINDINGS AND CONCLUSION

The factor analysis extracted seven factors using the criterion of Eigen values greater than one. The reliability statistics for 29 aspects of related to various aspects of home loan indicates high reliability with a KMO value of 0.840, which is very much close to 1. It indicates the sample taken for analysis to be statistically significant. In addition to KMO Bartlett's test of Sphericity chi-square value was 6400.797, the significance level of Bartlett's Test of Sphericity is less than 0.05 which indicates that the factor analysis is well fitted to the data and it can be validly used for the study the factors affecting selection of housing finance agency. By using fixed number of factors, items were subjected to Principal Components Factor Analysis, which are Customer care, Special Attractions, Loan processing and disbursement, Repayment Factors, Eligibility factors, Features of bank and Accessibility factors. The result indicates that features of the bank is the most influencing factor and special attractions provided by the bank is the lowest influencing factor in the selection of housing finance agency by home loan customers. The result also indicated that repayment, eligibility, accessibility, loan processing and customer care factors were highly influence the perception of home loan customers while selecting the housing finance agency.

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**CUSTOMER AWARENESS ON SBI'S GREEN FINANCIAL INITIATIVES-A STEP  
TOWARDS SUSTAINABLE DEVELOPMENT WITH SPECIAL REFERENCE  
TO KERALA**

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**Abstract**

In the present scenario, every industrial and service sector has some responsibility to contribute to fulfilling India's commitment towards the attainment of the SDGs. So banks in India also provide priority for the reduction of pollution and environment protection. Understanding the initiatives of SBI is very important because SBI is India's largest commercial bank. The study focused on understanding the level of awareness of customers about SBI's green financial initiatives and also aims to know the contribution of SBI towards the sustainable development of India. A random sample of 168 SBI customers in Kannur district is considered for the study. The study is both descriptive and analytical in nature. One sample T test and one-way ANOVA have been employed to understand the level of awareness. The study also tested the relationship between educational qualification and level of awareness of customers. It was found that online and offline news and advertisements were the major sources of awareness about the green initiatives of SBI. The awareness level of customers towards sustainability was comparatively low, and the green financial initiatives of SBI were also not very popular among the customers. The study also showed that the qualification of customers influenced their awareness level.

**Keywords** :Customer awareness, Green financial initiatives, sustainable development,

**INTRODUCTION**

Sustainable development means fulfilling the requirements of the present generation without adversely affecting the abilities of future generations. The importance of sustainable development emerges day by day due to increased pollution, climate change, global warming, acid rain, etc. Because of these reasons, everyone in the world starts to think about environment- friendly activities. For economic, social, and environmental growth, 17 sustainable development goals (SDGs) in association with the 2030 Agenda were designed by 193 member states of the United Nations. India also has a commitment to fulfill the SDGs by 2030. All sectors of India need to contribute to fulfill the commitment. Banks take a keen interest in the sustainable development of India. The green financial initiatives of SBI mainly intend to promote individual and industry involvement in environment-friendly activities. The green initiatives of SBI are designed in



such a way to help the nations to attain SDGs goals. This paper intends to understand the awareness levels of customers regarding SBI's initiatives and contributions for the sustainable development of India.

## **LITERATURE REVIEW**

The State Bank of India has undertaken the foremost action towards the attainment of sustainable development in India. Green financial initiatives are offered by SBI by considering sustainability.

(Ajaz & Bhat, 2022) described green banking as one of the sources of sustainable development. It helps the bank, industry and ultimately the environment as well. (Meenakshi & Choubey, 2022) argued that green initiatives of banks help them to restore customers' trust and enhance their green brand image. (Komalpreet & Sandhu, 2019) highlighted the importance of switching from conventional banking to environment-friendly, new digital based methods. In India, the State Bank of India is the foremost institution that has realised the shift from conventional methods. (Neeraja & Joseph, 2021) outlined banks actively contributes towards the sustainable development and argued customers are very familiar with green banking products like mobile and online banking but they are not much aware about green deposits, green CDs and green rewards. (Riya & Shivnani, 2023) pointed out that the awareness level of customers regarding environmental issues is high, but they felt some hindrances while using green banking products. He has suggested establishing help centers under the initiatives of the RBI to clarify the questions of customers about green banking. As per (Prakash & A, 2017) for the sustainability of our nation, the introduction of green banking alone is not enough. Apart from this, banks should concentrate on their lending policies, which help to boost the banking transaction and business transactions of their customers in an environmental friendly manner. Indian banks are engaged in green initiatives, but as compared to global movements, they are lagging. (C.Vijai, 2018) outlined that green banking promotes a greener and cleaner future because it has positively connected with environmental friendly activities. (Hesan Zahid, 2021) mentioned that customers are aware of the environmental consequences of traditional banking, ,so they are trying to change their attitude and support the green initiatives of the bank. (Satheesh, 2017) highlighted to achieve sustainable development in India, the contribution of the Indian banking sector is inevitable.

## **OBJECTIVES OF STUDY**

- To understand the customer awareness on SBI contribution towards sustainable development
- To understand the customer awareness on green financial initiatives of SBI for the sustainable development.
- To Compare the level of customer awareness on the basis of educational qualification and period of service relationship with SBI.

## **RESEARCH METHODOLOGY**

The objectives of the present descriptive and analytical study have been attained through primary data collected from customers of SBI at Kannur district in Kerala. The study is meant to identify the level of awareness of customers on green financial initiatives towards sustainable development. A structured

questionnaire is designed to collect primary data. The questionnaire includes questions regarding the contribution of SBI towards sustainable development and level of awareness of customers on green financial initiatives of SBI. To check the reliability and to refine the questionnaire, a pilot study was conducted. Chronbach’s alpha was used to check the reliability of scaled questions and all the scaled questions have acceptable reliability (Chronbach’s alpha values >0.7). The final questionnaire was distributed among 200 customers of SBI at Kannur in Kerala and 151 fully filled questionnaires have been used for further study. One sample T test, One way ANOVA ,percentage etc. have been employed for analysis with the help of SPSS.

### **GREEN FINANCIAL INITIATIVES OF SBI TOWARDS SUSTAINABLE DEVELOPMENT**

As a responsible bank, SBI significantly contributes towards the attainment of sustainable development goals set up by the United Nations. SBI introduced several green financial products that help the country to fulfil its commitment to sustainability (SBI, 2023)

Name of Green financial initiatives	Purpose
Finance For Biofuel Projects	Loans to corporates for the replacement of existing feedstock to biomass.
Sanjeevani	Financial assistance to manufacture health care products
Stree Shakti Entrepreneur Loan	Institutional credit for women entrepreneurs at affordable interest rate
YONO Krishi Safal Dairy Loan	Intend to meet the dairy farming requirements of farmers
Skill loan scheme	Financial assistance to enhance the skills of an individual.
SBI e-Mudra	Assistance for Micro entrepreneurs to meet their business requirements
Compressed biogas (“CBG”) under SATAT Scheme	Assistance for CBG plants
Green car loan	Financial assistance to promote cleaner mobility
SHG financing	Financial assistance for self help group
Financing polyhouse	Financial assistance for polyhouse farming aims to achieve the SDGs like no hunger, good health ,sustainable production and consumption and climate action
Financing solar photovoltaic pump sets	Financial assistance for the purchase of solar water pumping systems
Grid-connected rooftop solar PV projects	Popularizing renewal energy in industrial buildings and commercial institutions
Healthcare business loan	Financial assistance to boost healthcare facilities in small towns and villages
Affordable Home loan	Financial assistance to accomplish the dream of own house
E-Rickshaw scheme	Financial assistance to encourage the usage of cleaner fuels and promote environmental practice.

**ANALYSIS AND DISCUSSION**

**Table 1: Demographic Variables**

Variables	Description	Frequency	Percentage
Age	25-35	51	30.36
	35-50	42	25.00
	Above 50	6	3.57
	Below 25	69	41.07
	Total	168	100
Sex	Female	84	50.00
	Male	84	50.00
	Total	168	100
Educational Qualification	Below Bachelor's Degree	12	7.14
	Bachelor's degree	51	30.36
	Master's Degree	81	48.21
	Professional degree	12	7.14
	Above Masters Degree	12	7.14
	Total	168	100
Occupation	Govt. Sector	30	17.86
	Private sector	60	35.71
	Self employed	6	3.57
	Others	72	42.86
	Total	168	100

Source: Primary data

Demographic variables in the study showed that the majority of the respondents belonged to the age group below 25, followed by the age group 25–35. The number of males and females was 84 each. 48.21 percent of respondents have a qualification of master's degree. Occupation-wise classification revealed that most of them are distributed under others.

**Table 2: Period of service relationship with SBI**

Variables	Frequency	Percent
Less than 5 years	72	42.9
between 5 to 10 years	63	37.5
More than 10 years	33	19.6
Total	168	100.0

Source: Primary data



The period of service relationship of customers with SBI depicted that the majority of customers have less than 5 years of relationship with SBI, and secondarily, between 5 to 10 years.

**Table 3: Source of awareness on SBI’s Green financial initiatives**

Variable	N	Mean	S.D	t	Sig.
SBI website	168	3.46	1.18	5.08	.000
Friends and Relatives	168	3.41	1.11	4.83	.000
Advertisement	168	3.50	1.12	5.77	.000
Bank employees	168	3.33	1.34	3.27	.001
News ( Online & Offline)	168	3.53	1.16	5.94	.000
Journals & Magazines ( Online & Offline)	168	3.25	1.05	3.05	.003

Source: Primary data

One sample t test was used to check the mean value of the source of awareness. The mean score of the source ‘*News (Online and Offline)*’ (M=3.53, S.D=1.16) was significantly higher than the test value of three,  $t(167)= 5.94, p=0.000$ ). The result indicated that customers get knowledge about the green financial initiatives of SBI mostly from online and offline news. Subsequently, advertisement (M=3.5) played a major role to create awareness among the customers. All other sources like SBI website, friends and relatives, bank employees etc. are significantly higher than the test value three.

**Table 4: Customer’s awareness on SBI’s contribution to Sustainable Development Goals (SDGs)**

Variables	N	Mean	Std. Deviation	t	Sig.
SBI promotes Go Green activities	168	2.60	1.17	-4.32	.000
SBI provides assistance for sustainable projects	168	2.58	1.13	-4.69	.000
SBI provides financial assistance for gender equality and women empowerments	168	2.51	1.12	-5.57	.000
SBI significantly contributes towards the promotion of renewable energy	168	2.55	1.12	-5.16	.000
SBI actively participates for the attainment of SDGs goals	168	2.50	1.05	-6.14	.000
SBI actively participates in Socio Economic Advancement and Empowerment	168	2.55	1.08	-5.32	.000
SBI significantly contributes Employment Generation	168	2.71	1.05	-3.52	.001
SBI supports growth of Affordable Housing and Affordable Infrastructure	168	2.80	1.21	-2.08	.038

Source: Primary data

The result of the one-sample t test revealed that the mean score of all variables of customer awareness of SBI’s contribution to sustainable development was significantly less than the test value three. The result indicated that customers were slightly aware of SBI’s contribution to sustainable development.

**Table 5 : Customer awareness on Green financial Initiatives of SBI**

<b>Variables</b>	<b>Mean</b>	<b>Std. Devia- tion</b>	<b>t</b>	<b>Sig.</b>
Finance for biofuel projects is a loan for replacing feedstock coal with biomass	2.25	1.10	-8.76	.000
Sanjeevani is a SME Loan for Healthcare Sector	2.25	1.07	-9.03	.000
Stree Shakti Entrepreneur Loan is an institutional credit to women entrepreneurs	2.50	1.08	-5.95	.000
YONO Krishi Safal Dairy Loan is designed to meet the needs of dairy farmers	2.53	1.21	-4.96	.000
Status of awareness on Skill loan scheme	2.46	1.03	-6.69	.000
Status of awareness on Green car loan	2.46	1.03	-6.69	.000
Status of awareness on Self Help Group (SHG )financing,	2.78	1.03	-2.68	.008
Compressed biogas (“CBG”) under SATAT Scheme	2.41	1.18	-6.47	.000
Status of awareness onSBI e-Mudra and Healthcare business loan	2.64	1.14	-4.04	.000
Status of awareness on Affordable Home Loan	2.92	1.18	-.78	.434
Status of awareness on E-Rickshaw scheme	2.76	1.22	-2.45	.015
Status of awareness on Financing polyhouse and Grid-connected rooftop solar PV projects	2.46	1.03	-6.69	.000
Status of awareness on financing Purchase, Construction or Renovation of Green Home	2.41	1.11	-6.83	.000

Source: Primary data

The result of the one-sample t test showed that the mean score of affordable housing finance (M=2.92, S.D=1.18) was not significantly lower than the test value of three,  $t(167) = -.78, p=0.434$ ). The result meant that customers have knowledge about affordable housing finance through SBI. The mean score of all other variables of customer awareness of the green financial initiatives of SBI was significantly less than the test value three. The result indicated that customers were comparatively less aware of SBI’s green financial initiatives.

**Table 6: Educational and awareness on SBI’s contribution to Sustainable Development Goals(SDGs)**

Variable		Below	Bach-	Mas-	Pro-	Above	F	Sig.
		Bach- elors De- gree	elor’s de- gree	ter’s De- gree	fes- sional degree	Masters Degree		
SBI promotes Go Green activities	Mean	2.25	2.235	2.778	2.75	3.25	3.047	0.019
	S.D	1.13	0.95	1.26	1.35	0.86		
SBI provides assistance for sustainable projects	Mean	2	2.294	2.778	2.5	3.25	3.465	0.01
	S.D	1.27	0.96	1.23	0.90	0.45		
SBI provides financial assistance for gender equality and women empowerments	Mean	2	2.529	2.556	2.5	2.75	0.79	0.534
	S.D	1.27	0.78	1.20	1.56	1.13		
SBI significantly contributes towards the promotion of renewable energy	Mean	2.5	2.353	2.481	2.75	3.75	4.336	0.002
	S.D	0.90	0.97	1.17	1.35	0.45		
SBI actively participates for the attainment of SDGs goals	Mean	1.75	2.647	2.444	2.5	3	2.587	0.039
	S.D	1.35	0.91	1.14	0.52	0.73		
SBI actively participates in Socio Economic Advancement and Empowerment	Mean	2.25	2.471	2.63	2.5	2.75	0.506	0.731
	S.D	1.35	0.85	1.13	1.56	0.86		
SBI significantly contributes Employment Generation	Mean	2.5	2.706	2.704	2.75	3	0.348	0.845
	S.D	1.16	0.75	1.08	1.86	0.73		
SBI supports growth of Affordable Housing and Affordable Infrastructure	Mean	2	2.941	2.815	2.75	3	1.57	0.185
	S.D	1.27	1.00	1.28	1.35	1.27		

Source: Primary data

One-way ANOVA was conducted to study the relationship between educational qualification and awareness of SBI’s contribution to sustainable development. There was a significant relationship between awareness of SBI’s go green activities and educational qualification  $F(4,163)=3.047, p=0.019$ ). It could be observed from the result that the highly qualified customers were more aware of SBI’s contribution than the less qualified customers. The variables such as awareness of assistance for sustainable projects, contribution towards the promotion of renewable energy, and SBI’s active participation in the attainment of SDGs goals also showed a significant relationship between awareness and educational qualification. All other factors did not possess a significant relationship between awareness and educational qualification.



**Table 7: Educational qualification and awareness on green financial initiatives of SBI**

<b>Variables</b>		Be- low Bach- elors De- gree	Bach- elor's degree	Mas- ter's Degree	Profes- sional degree	Above Mas- ters Degree	<b>F</b>	<b>Sig.</b>
Finance for biofuel projects is a loan for replacing feedstock coal with biomass.	Mean	1.5	2.35	2.33	2	2.25	1.78	0.135
	S.D	0.52	1.03	1.19	0.73	1.35		
Sanjeevani is a SME Loan for Healthcare Sector	Mean	1.5	2.23	2.37	1.5	3	5.07	0.001
	S.D	0.52	0.88	1.13	0.52	1.47		
Stree Shakti Entrepreneur Loan is an institutional credit to women entrepreneurs	Mean	1.5	2.70	2.51	2	3	4.62	0.001
	S.D	0.52	0.90	1.17	0.73	1.27		
YONO Krishi Safal Dairy Loan is designed to meet the needs of dairy farmers	Mean	2.5	2.82	2.37	2	3	2.18	0.073
	S.D	1.56	1.10	1.25	0	1.27		
Status of awareness on Skill loan scheme,	Mean	1.25	2.94	2.4	2	2.5	8.87	.000
	S.D	0.45	0.94	0.99	0.73	1.16		
Status of awareness on Green car loan	Mean	1.5	2.76	2.33	1.75	3.75	12.85	.000
	S.D	0.52	0.95	1.02	0.45	0.45		
Status of awareness on Self Help Group (SHG )financing,	Mean	1.75	3	2.70	2.5	3.75	7.55	.000
	S.D	0.45	0.97	1.05	0.90	0.45		
Compressed biogas ("CBG") under SATAT Scheme	Mean	1.25	2.88	2.37	1.75	2.5	6.73	.000
	S.D	0.45	1.19	1.19	0.86	0.52		
Status of awareness onSBI e-Mudra and Healthcare business loan	Mean	2.25	2.76	2.55	2.25	3.5	2.76	0.029
	S.D	1.71	1.01	1.07	0.45	1.56		
Status of awareness on Affordable Home loan	Mean	2.5	3.17	2.74	2.5	4	4.71	0.001
	S.D	1.56	1.26	1.11	0.52	0		
Status of awareness on E-Rickshaw scheme	Mean	3	2.94	2.55	2	4	5.74	.000
	S.D	1.27	1.27	1.2042	0.7385	0		
Status of awareness on Financing poly-house and Grid-connected rooftop solar PV projects	Mean	1.75	2.8	2.259	2	3.25	7.65	.000
	S.D	0.45	0.97	1.04	0.73	0.86		
Status of awareness on financing Purchase, Construction or Renovation of Green Home	Mean	1.5	2.64	2.25	2.25	3.5	6.63	.000
	S.D	0.52	1.09	1.18	0.45	0.52		

One-way ANOVA was conducted to study the relationship between educational qualification and awareness of the green financial initiatives of SBI. There was a significant relationship between awareness of the Sanjeevani SME Loan and educational qualification  $F(4,163)=5.07$ ,  $p=0.001$ ). The result meant that the educational qualifications of customers positively influenced their level of awareness. Except for two variables, namely finance for biofuel projects and Yono Krishi, all others have shown a significant relationship between awareness and educational qualification.

## **FINDINGS AND CONCLUSION**

To protect the environment by 2030 from global warming and preserve the environment, banks in India have undertaken various initiatives. SBI, as the largest commercial bank in the banking sector, is a pioneer in this field. The study found that online and offline news and advertisements were the major sources of awareness about the green initiatives of SBI. The awareness level of customers towards sustainability was comparatively low, and the green financial initiatives of SBI were also not very popular among the customers. So the study demands more effective measures to improve the awareness level of customers through the official website and other media. The study also revealed that the qualification of customers influenced their awareness level. In order to achieve the SDGs by 2030, the banking sector in India needs to take a keen interest in green initiatives.

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## Identification of Potent ABL Inhibitors from Coumestrol: An Integrative *In Silico* Approach

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**ABSTRACT:** Chronic Myeloid Leukemia (CML) is known as clonal myeloproliferative disorder resulted by the proliferative and deregulated expression of the BCR-ABL gene. Although targeting the BCR-ABL gene is an effective treatment for CML, the development of drug intolerance and drug resistance is still an issue for BCR-ABL targeted therapy. With an aim to develop novel BCR-ABL inhibitors with fewer side effects, we started with the anti-cancerous natural compound coumestrol as the lead. Chalcone and pyrazole are the well-exploited scaffolds in the anticancer domain; hence, in this work, we designed novel coumestrol derivatives with these structures. In order to quantify the structural changes, we employed *in silico* methods. The new drug leads were compared with the FDA-approved CML drug bosutinib. The molecular orbital analysis of the selected lead compounds was assessed by Density Functional Theory (DFT) approach. Molecular Dynamic (MD) computations were performed on the most promising leads to find the stability. Following which, the pharmacokinetics parameters of the screened compounds were also analyzed to check the drug-like property.

**KEYWORDS:** CML; coumestrol; docking; molecular dynamic simulations; DFT.

### 1. INTRODUCTION

Leukemia, a wide term used to denote the cancer of blood and bone marrow cells, is mainly caused by a combination of genetic as well as environmental factors. The four main types of leukemia include: Acute Lymphoblastic Leukemia (ALL), Acute Myeloid Leukemia (AML), Chronic Lymphoblastic Leukemia (CLL) and Chronic Myeloid Leukemia (CML).<sup>1</sup> CML was the first one probably to be recognized as the distinct one from other leukemias. It is characterized by Philadelphia chromosome, a chromosome formed by the reciprocal fusion of Chromosome 9 and 22 and the consequence of which was the generation of fusion protein BCR-ABL. The bone marrow cells of CML patients showed aberrant expression of the oncogene BCR-ABL.<sup>2–4</sup> Though the function of BCR gene is not yet clear, ABL, the proto-oncogene, is known to encode the nuclear and cytoplasmic tyrosine kinase protein that plays a major role in cell-differentiation,

cell-division and cell-adhesion. ABL protein is found both in the nucleus and cytoplasm and a requisite proapoptotic protein that plays a key role in cellular responses during genotoxic stress.<sup>4</sup> Unlike normal ABL, BCR-ABL protein is exclusively found in cytoplasm and is antiapoptotic.<sup>3</sup> It is known to bring about the various cellular responses like weakening cell adhesion, suppressing apoptosis, promoting cell proliferation by triggering many biochemical signal transduction pathways, which include RAS, mitogen-activated protein kinase pathways, phosphatidylinositol 3 kinase pathways, signal transducers, activators of transcription pathways, Myc pathway, inhibition of apoptosis.<sup>3,5,6</sup> This malignancy transforming property

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of BCR-ABL is thus exploited by the pharmacological field as the drug target; imatinib mesylate being the first drug developed as a BCR-ABL tyrosine kinase inhibitor against CML.<sup>7</sup>

Nilotinib, dasatinib, bosutinib, etc. are the other drugs developed against CML similar to imatinib.<sup>5,7</sup> However, the drug resistance and the over-expression of these drugs have forced the medical field in search of alternative drugs. Uses of natural products are on their rise as effective therapeutic agents; their low-toxicity and cost-effectiveness have gained much advantage over synthetic drugs for treatments of various ailments.<sup>8,9</sup> Many literatures have reported the use of plant secondary metabolites like flavonoids, alkaloids, saponins, phenols, and terpenoids as an effective inhibitor of CML cell lines; quercetin, oroxylin, gallic acid being some of the examples.<sup>1,10</sup>

Coumestrol (Fig. 1), a phytoestrogen belonging to the polyphenols, is mainly found in soybeans, oilseeds legumes, and nuts.<sup>11,12</sup> Coumestrol is known to exhibit a wide range of biological activities that include neuroprotective, antifungal, snake antivenom activity, phytoalexin effects, and antibacterial properties. Likewise, coumestrol has cancer preventive activities, especially for estrogen-responsive carcinoma, they being a structural mimic of mammalian endogenous estrogen (17 $\beta$ -estradiol) that regulates the activities of estrogen receptors (GPER), which helps prevent cardiovascular diseases, osteoporosis, breast cancer, neurological disorders, prostate cancer, and menopausal symptoms. Casein kinase 2, a protein amply expressed in various cancers, is closely associated to inhibition of apoptosis, cell proliferation, and oncogenesis in diverse cancer cell lines like lung, prostate, cervix, and leukemic cells. According to Liu *et al.*, coumestrol reversibly inhibited CK2 as an ATP competitor.<sup>13</sup> As per Lee *et al.*, coumestrol induced the cellular senescence by triggering the production of ROS through p53-p21Cip1/WAF1 signal transduction cascades in colon and breast cancer cells.<sup>14</sup> In addition, Lim and his co-workers reported the chemotherapeutic effects of coumestrol on two prostate cancer cell lines, i.e., PC3 and LNCaP. Also, the inhibitory activity of coumestrol toward the

proliferation of ES2 human epithelial ovarian cancer cells (EOC) via PI3K and ERK1/2 MAPK pathway was reported.<sup>11</sup> According to Zafar and co-workers, coumestrol targeted the elevated copper level, a typical characteristic exhibited by different malignancies in treating human breast cancer. Coumestrol exhibited the cytotoxic action on human breast cancer MCF-7 cells through a copper targeted ROS-mediated p53-dependent mechanism.<sup>12</sup> Motivated by the potent anti-cancer activity of the coumestrol compound, a new series of chalcone and pyrazole-based coumestrol derivatives were designed aiming to produce safer drugs for the treatment of CML.

Chalcones and pyrazole compounds are an important class of chemical compounds widely used as an effective template in medicinal chemistry for the development of various drugs.<sup>15-19</sup> Recently, the practice of combinational therapy is followed to reduce the side effects; hybrid compounds possessing a different mode of action exhibit synergistic action that helps reduce side effects.<sup>20</sup> In this context, chalcones and pyrazole having anticancer effects<sup>15</sup> and numerous prospective effects as a new drug are used to develop coumestrol derivatives.

## 2. COMPUTATIONAL DETAILS

The entire molecular docking, Molecular Dynamics (MD), and ADME analysis were carried out using the Schrodinger suite using the Maestro 11.2 version packages including LigPrep, QikProp, grid generation, Glide XP docking, and MD simulations.<sup>21-23</sup> All Density Functional Theory (DFT) calculations of the ligands were performed by using Gaussian 09 software packages and are visualized using Chemcraft software tool.<sup>24</sup>

### 2.1. Docking study

The molecular docking analysis consists of three major steps; ligand preparation, protein preparation, and ligand docking.<sup>25</sup> The binding affinity of the docked complex was analyzed based on the docking and glide scores, which was compared with the reference drug.<sup>26</sup> The reference standard used in this study is bosutinib, which has been used as CML drug.<sup>27</sup>

#### 2.1.1. Ligand preparation

All the ligand molecules including the natural compound coumestrol and its modified compounds, and the reference drug bosutinib were prepared using the

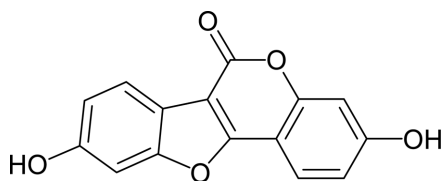


Fig. 1. Chemical structure of coumestrol.

LigPrep's ligand preparation protocol of the Schrödinger software.<sup>28</sup> LigPrep generates several structures from each input structure with various ionization states, tautomers and stereoisomers of the ligands using Epik module. The OPLS-2005 force field was used for optimization, which produces the low-energy conformer of the ligands. Finally, all the prepared ligands were subjected to molecular docking with the target ABL kinase using Glide.<sup>23,26</sup>

### 2.1.2. Preparation of protein target structure

In this study, the crystal structure of human BCR-ABL kinase in complex with nilotinib (PDB ID: 3CS9)<sup>29,30</sup> was obtained from the Protein Data Bank (PDB) and imported to maestro work environment. Further, the protein was prepared by using "protein preparation wizard", which is available in Glide module of the Schrödinger software.<sup>31</sup> The "protein preparation wizard" has two components, namely "preparation" and "refinement".<sup>32,33</sup> After ensuring chemical accuracy, the preparation component adds hydrogen atoms and neutralizes side chain that is neither close to the binding cavity nor involved in the formation of salt bridges. Protein preparation also implicated the removal of bad contacts, optimization of bond lengths, capping of protein terminals. Prepared structure of ABL kinase was used for the grid generation using Glide. The OPLS-2005 force field was used for this purpose, and then the active site of protein was refined. Glide used OPLS-2005 force field at an intermediate docking stage and is disclaimed to be more sensitive to geometrical detail compared to other docking algorithms.<sup>23,31</sup>

### 2.1.3. Molecular docking simulation

A glide grid was generated on the prepared target protein by trapping the native ligand. Docking was performed using extra-precision (XP) glide docking method, which docks the ligands flexibly. During the ligand docking process, the epic state penalties were added to the docking score. The force-field used in this study is OPLS-2005. The docked poses were scored and ranked according to their Glide XP scores.<sup>23</sup> Glide score is an empirical scoring function that predicts the strength of the non-covalent interaction between the receptor and the ligands; in terms of its binding affinity, more negative values represent the tighter binders. The Glide score (G Score) is calculated by using the following equation:

$$\begin{aligned} \text{Glide Score} = & 0.065 * \text{vdW} + 0.130 * \text{Coul} + \text{Lipo} \\ & + \text{Hbond} + \text{Metal} + \text{BuryP} + \text{RotB} \\ & + \text{Site}, \end{aligned}$$

where vdW represents the van der Waals energy, Coul is the Coulomb energy, Lipo denotes the lipophilic contact term, Hbond denotes the hydrogen-bonding term, Metal represents the metal binding term, BuryP is the penalty for buried polar groups, RotB is the penalty for freezing rotatable bonds and Site is the polar interactions at the active site.<sup>34</sup>

## 2.2. Electronic structure calculations

The reference compound bosutinib and the molecules selected from the docking study were carried for electronic feature calculations using DFT method with B3LYP (Becke's three-parameter exchange potential and the Lee-Yang-Parr correlation functional) and using the basis set 6-31G\* level. B3LYP/6-31G\* has been commonly employed to examine the electronic properties of donor-acceptor molecular system and determine the corresponding energies. It is also suitable for studying geometry optimization.<sup>35</sup> All DFT calculations were carried out using Gaussian 09 software packages.<sup>36</sup> The molecular frontier orbitals (FMOs) and MESP<sup>37</sup> of the selected molecules were also calculated in this study and are visualized in chemcraft software.<sup>38</sup> The FMOs of the molecules provide information about the ability of the molecule to transmit its energy from the HOMO to a LUMO, which can act as an electron donor and acceptor, respectively. The color-coded isosurface of the MESP maps affords the overall molecular size and the negative and positive electrostatic potential regions of the molecules.<sup>39</sup>

## 2.3. Molecular dynamic analysis

MD simulations were computed to the ABL kinase and the interaction mode of ABL kinase complex with high scored compounds, which provide information regarding the time-dependent behavior of any molecular system by integrating Newton's equation of motion. All MD simulations were performed for a period of 100 ns by using the Desmond module of the Schrödinger with an OPLS-2005 force field.<sup>40,41</sup> The selected ligand-receptor complex was centered in a cubic box and filled with TIP4P water molecules and is neutralized using an appropriate number of counter ions and 0.15 M of salt concentration. The systems were equilibrated using the default protocol provided in Desmond. The equilibrated systems were further carried to perform MD simulations at a constant temperature of 300 K and the constant pressure of 1 atm under certain periodic boundary conditions. RMSD plots for the backbone atoms for both protein (ABL kinase) and the high

scored ligand-bound protein complexes were generated to understand the relative stability of the ligand inside the ATP binding pocket of the ABL kinase.<sup>42</sup>

#### 2.4. ADME predictions and toxicity estimation

QikProp program of the Schrodinger software is performed for all the chemically modified coumestrol compounds, which predicts the pharmaceutically relevant properties and physically significant descriptors of the possible drug compounds. QikProp also provides ranges for comparing particular molecule's properties with those of 95% of known drugs.<sup>43</sup>

### 3. RESULTS AND DISCUSSION

#### 3.1. Analysis of the ABL kinase receptor and their active site (3CS9)

Human ABL kinase in complex with nilotinib (PDB ID: 3CS9) has been taken as the target receptor. Crystal structure resolution of 3CS9 is 2.21 Å and a grid was generated around the same interacting region of the receptor. The most important residues namely Phe382, Leu248, Tyr253, Val256, Leu370, Phe317, Met318, Thr315, Asp381, Glu286, and Val289 are present in the active site. Of these, it is reported that the formation of at least one H-bond interaction with the hinge region residue Met318 of ABL kinase is essential for the inhibition of kinase activity<sup>44,45</sup>

#### 3.2. Binding mode analysis of reference drug bosutinib with ABL kinase

In our quest to search for novel inhibitors against the ABL kinase, bosutinib (4-anilino-3-quinolinecarbonitrile) was used as the reference to compare the effect of the novel derivatives. Bosutinib is an ATP-competitive second-generation ABL kinase inhibitor, currently available in the market as a CML drug<sup>46,47</sup> Additionally, it has shown activity against Src family kinases including Src, Lyn, and Hck, platelet-derived growth factor and vascular endothelial growth factor.

Upon a closer examination of the docking result, bosutinib displayed two H-bond interactions (amino group and the methoxy group of the bosutinib with the residues Thr315 and Asp381, at a distance of 1.84 Å and 2.25 Å, respectively), one  $\pi$ - $\pi$  interaction (terminal aromatic ring of the bosutinib with Tyr253, at a distance of 5.43 Å), and one  $\pi$ -cation ( $\text{NH}^+$  of the piperazine with Asp381, at a distance of 4.03 Å) interaction with the amino acid residues of the

receptor with the docking score of  $-10.70$  kcal/mol (Fig. 2).

#### 3.3. Binding mode analysis of chalcone and pyrazole-based coumestrol derivatives with ABL kinase

The designed chalcone and pyrazole-based coumestrol derivatives were docked into the ATP binding site of the target receptor to explore the binding and interaction mode between them (Fig. 3). The docked poses of the modified compounds were scored and ranked based on their docking and glide scores, which are tabulated in Table 1.

Docking and glide scores of all the chalcone and pyrazole-based coumestrol derivatives are found better as compared to the reference drug bosutinib ( $-10.70$  kcal/mol), which indicates that these compounds can have more potent inhibitory action against the target ABL kinase (Table 1). Among the designed coumestrol compounds, chalcone-based compounds A01 and pyrazole-based B01 showed the best docking scores of  $-13.28$  kcal/mol and  $-13.37$  kcal/mol, respectively (Fig. 4). Both ligands (A01 and B01) fit into the same binding site of the ABL kinase (PDB ID: 3CS9). These two high scored compounds are selected for further *in silico* investigations.

From Fig. 4(a), it is exposed that four amino acid residues such as Met318, Tyr253, Thr315, and Lys271 are seen as important key players in binding to A01. Two H-bond interactions are observed in the complex with Met318, and Thr315 and the bond lengths are 1.75 Å and 1.85 Å. Tyr253 makes one strong  $\pi$ - $\pi$  stacking interaction (4.68 Å), and Lys271 (5.05 Å) exhibits one  $\pi$ -cation interaction with A01. Also, amino acid residues Met290, Ala380, Phe382, Val256, Tyr253, Leu248, Met318, Phe317, Leu370, Val299, Ala269, Ile313, and Val270 of target ABL kinase formed hydrophobic interactions with the ligand (A01).

In the case of pyrazole incorporated compounds, B01 shows that the best potential (docking and glide scores are of  $-13.37$  kcal/mol and  $-13.77$  kcal/mol, respectively) is to be developed into an ABL kinase inhibitor. This potential is due to the existence of two H-bonds with the receptor, one is between the hydroxyl group of the coumestrol moiety with Gly249 ( $\text{NH}_2\text{-OH}$ , bond distance of 2.08 Å) and the remaining is between the carbonyl group of the coumestrol with Met318 ( $\text{CO-HN}$ , bond distance of 1.55 Å) of the ABL kinase (Fig. 4(b)). Additionally, two  $\pi$ - $\pi$  stacking interactions are also noticed between the pyrazole ring

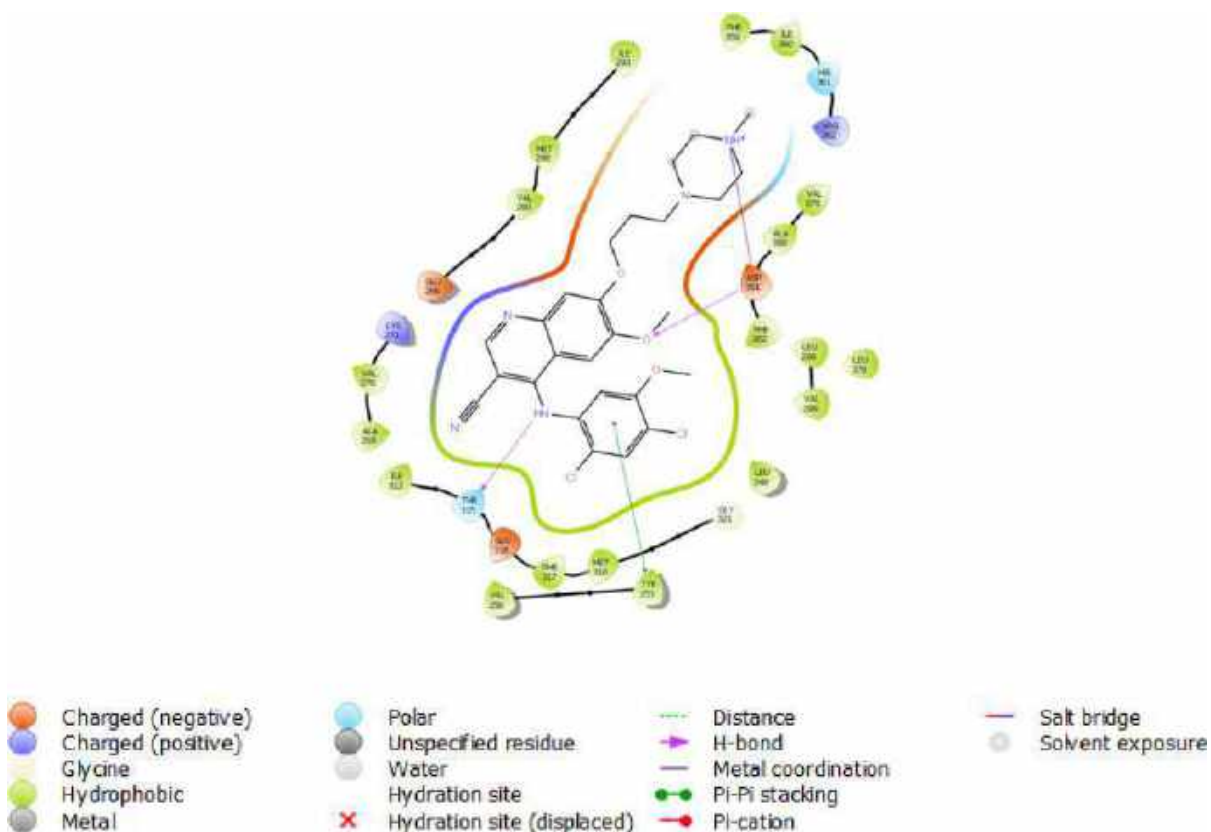


Fig. 2. (Color online) Binding interaction diagram of bosutinib with 3CS9.

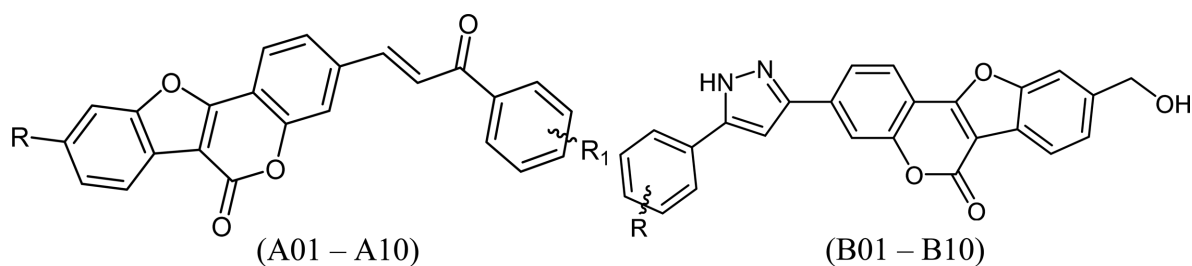


Fig. 3. Design of chalcone and pyrazole-based coumestrol derivatives as novel ABL kinase inhibitors.

Table 1. The structure, docking and glide scores (kcal/mol) of the coumestrol derivatives.

Compounds	R	R1	D Score	G Score	Compounds	R	D Score	G Score
A01	CH <sub>3</sub>	2-hydro	-13.28	-13.32	B01	3-dimethyl amino	-13.37	-13.77
A02	OH	2-hydro	-13.24	-13.29	B02	3-methyl	-13.19	-13.60
A03	H	2-hydro	-13.24	-13.28	B03	3-chloro	-13.18	-13.59
A04	OH	3-amino	-13.22	-13.22	B04	4-methoxy	-13.11	-13.52
A05	CH <sub>2</sub> OH	2-hydro	-13.19	-13.24	B05	3-methyl amino	-13.05	-13.44
A06	OH	3-hydro	-13.13	-13.14	B06	4-amino	-13.01	-13.38
A07	NHCOCH <sub>3</sub>	3-hydro	-13.12	-13.16	B07	3-methoxy	-12.92	-13.33
A08	NO <sub>2</sub>	3-hydro	-12.94	-12.98	B08	3-amino	-12.79	-13.18
A09	OH	3-dimethyl amino	-12.53	-12.53	B09	3-hydroxy	-12.78	-13.21
A10	OH	H	-12.35	-12.35	B10	3-nitro	-12.66	-13.07



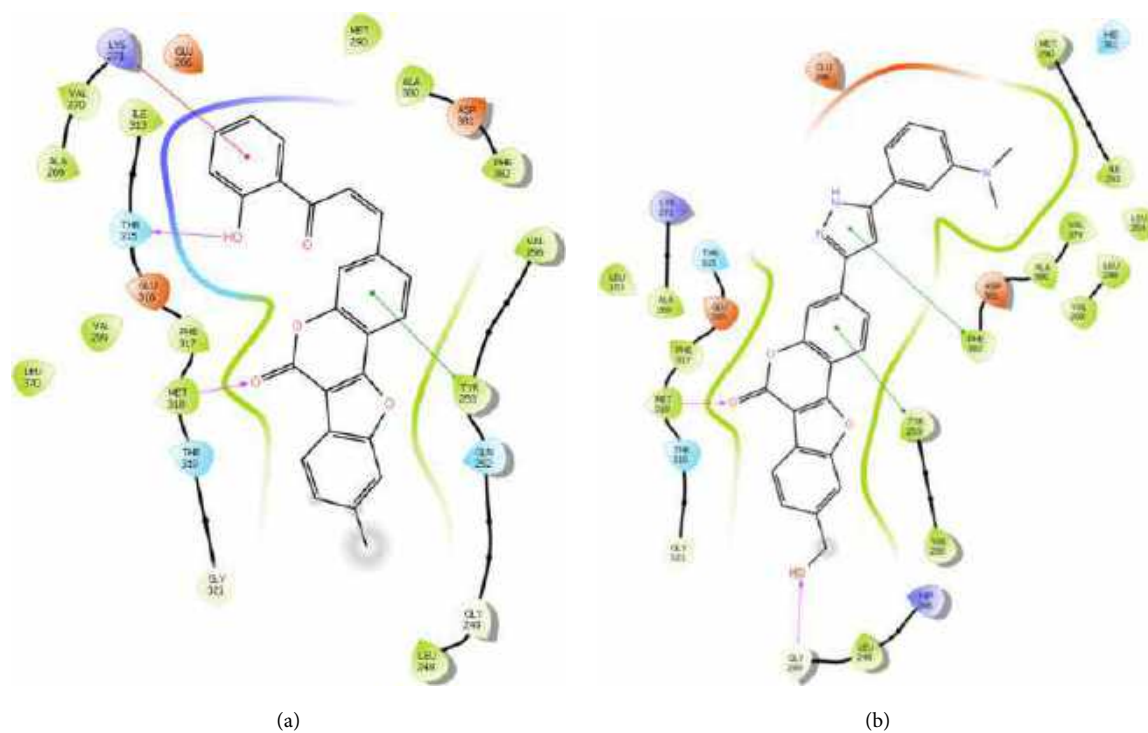


Fig. 4. (Color online) Binding interaction diagram of (a) A01 and (b) B01 with 3CS9.

and aromatic ring of the coumestrol with the residues Phe382 and Tyr253 of the targeted receptor (5.03 Å and 5.29 Å). Amino acid residues Met290, Ile293, Leu354, Val379, Leu298, Ala380, Val299, Phe382, Tyr253, Val256, Leu248, Met318, Phe317, Ala269, and Leu370 of the target receptor show hydrophobic interaction with the ligand (B01).

The key interacting residues Met318, Thr315, Lys271, Phe382, Gly249, and Tyr253 were conserved within the ATP binding site of the receptor and contributed to the efficient and more potent binding affinity of these two (A01 and B01) top ranked compounds for ABL kinase. Most of these residues have also been reported for compounds having strong interactions with ABL kinase. Among which, the interaction with Met318 (a residue in the hinge region of the ABL) is remarkably conserved in both the complexes. It is known that a bond with Met318 is a characteristic feature of the binding mode of the ABL kinase inhibitors. But it is not observed in bosutinib–ABL kinase complex. Importantly, these two compounds (A01 and B01) made strong hydrophobic contacts with the hydrophobic region present at the ATP binding region of the BCR-ABL. These preliminary results suggest that the binding of A01 and B01 to the ATP binding pocket not only disrupts the auto-phosphorylation of ABL kinase in

CML cells but also more effective than the reference drug.

Due to the variations of substituents in both scaffolds, some of the effective interactions with important active site residues such as Met318, Thr315, Tyr253, and Lys271 of the targeted ABL kinase are missed. Interactions with these residues are essential for inhibiting ABL kinase and most of the existing CML drugs also have this with ABL kinase. The compounds A04–A10 not showing interaction with the Thr315 and Lys271 are an example.

### 3.4. Molecular electrostatic potential profiles

The reference compound bosutinib and the high scored compounds of each type, A01 and B01, were taken for electronic structure analysis. The result shows that all these three compounds share specific electronic properties (Fig. 5). In the molecular electrostatic potential (MESP) profiles, the electropositive and electronegative potential regions are indicated in blue and red color, respectively. It is obvious from these results that the reference drug bosutinib gives more contracted negative electrostatic potential regions and hence it can mainly act as H-bond donor with the amino acids of the partner receptor. In the case of A01 and B01, the distributions of ESP are found to be different from the

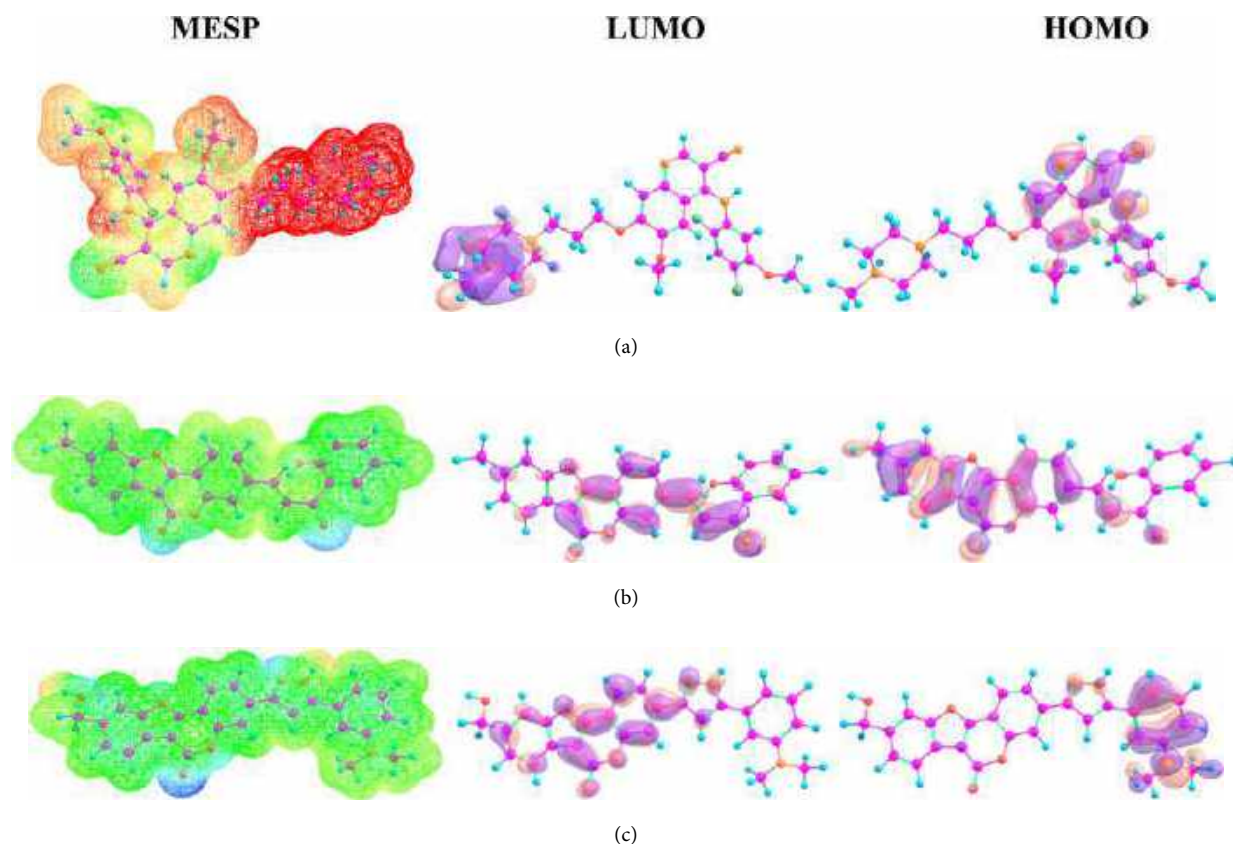


Fig. 5. (Color online) MESP, LUMO and HOMO profiles of (a) bosutinib, (b) A01 and (c) B01.

bosutinib. In A01, large electropositive regions of ESP are found at the carbonyl groups of the coumestrol and chalcone ring. While in the case of B01, the electropositive regions are concentrated on the oxygen atom and carbonyl groups of the coumestrol and the nitrogen atom of the pyrazole ring. The electronegative regions of the B01 are concentrated on the NH group of the pyrazole ring and the CH<sub>2</sub>OH group of the coumestrol moiety. Generally, appearance of both most electronegative and electropositive regions of the ligands illustrates that these regions can act as electron donors or acceptors to the active site of the targeted receptor, thus making these compounds very reactive,<sup>48</sup> especially the carbonyl group of the coumestrol ring interacts with the Met318 residue of the ABL kinase.

The distribution of HOMO and LUMO, corresponding energies, and the energy gap values of the two best hit compounds (A01 and B01) and the reference drug bosutinib were computed (Fig. 5). The LUMO of the compounds directly associated with the “electron affinity” and the tendency to accept an electron from the partner, whereas the HOMO related to its “ionization potential” and the tendency to donate an electron. The energy gap between HOMO and LUMO

determines the chemical stability of the compounds. The calculated HOMO and LUMO orbital energies of A01 are found to be  $-6.09$  eV and  $-2.70$  eV, respectively; for B01, the respective energies are  $-5.38$  eV,  $-1.63$  eV. Comparing these values with bosutinib ( $E_{\text{HOMO}} = -7.33$  eV,  $E_{\text{LUMO}} = -3.45$  eV) reveals that  $E_{\text{HOMO}}$  of both the molecules are higher; hence these two molecules have higher H-bond donor capability<sup>49</sup> with their partner than the reference drug bosutinib. The lowest energy gap between HOMO and LUMO of the A01 and B01 (3.39 eV and 3.75 eV) discloses its bioactive nature.

The HOMO and LUMO distributions are plotted onto the surface of the two best hit compounds (A01 and B01), and the reference drug bosutinib is displayed in Fig. 5. Analysis of LUMO maps of A01 illustrates that LUMO concentrated on both coumestrol and chalcone moiety, and the HOMO concentrates mainly on the coumestrol moiety of the A01. In the case of B01, the LUMO orbitals are located on the coumestrol and pyrazole moiety, and the HOMO concentrates on the dimethyl-aniline ring of the compound. Thus, the distributions of HOMO and LUMO onto the surface of the A01 and B01 shed some insight on steric and

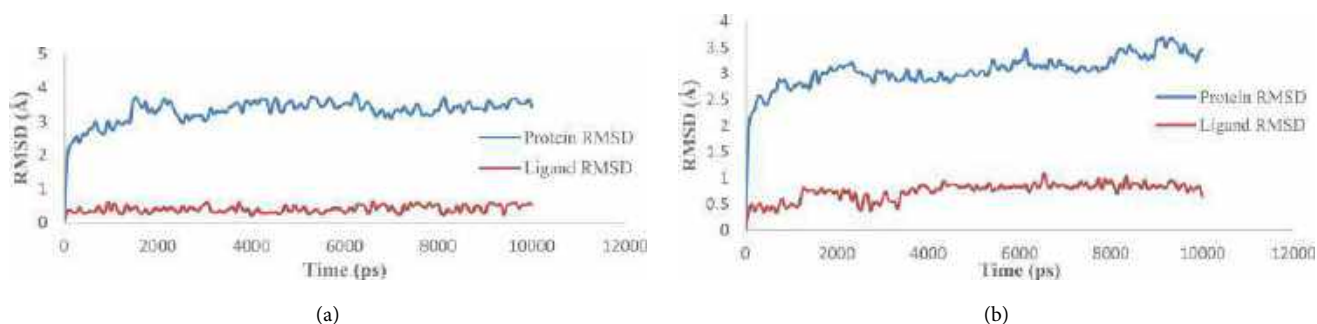


Fig. 6. (Color online) RMSD plots of (a) A01 and (b) B01 complexed with 3CS9.

electronic complementarities of these molecules to the targeted receptor. The comparison of the DFT and docking results of the top hit compounds A01 and B01 revealed that the carbonyl group of the compounds involved in the formation of the essential H-bond interactions with the Met318 residue of the targeted receptor.

### 3.5. Molecular dynamic simulations

To assess the binding stability and the flexibility of the A01 and B01 with the target ABL kinase (PDB ID: 3CS9), we performed MD simulations using Desmond module of the Schrödinger over a period of 100 ns by applying OPLS-2005 force field. MD simulation results were analyzed in terms of their stability (RMSD), flexibility (RMSF), and ligand-interaction profile of the

ligand–receptor complex. In the presence of ligands A01 and B01, the protein back bone RMSD values were comparable to that of the protein only (Fig. 6). Even though the RMSD values of A01 and B01 initially rise to 2 Å from their initial coordinates, their fluctuations are very less after that. This can be suggestive of the stable complexation of the ligands inside the cavity of the protein.

After MD simulations, the final ligand–protein complex structures of A01 and B01 are analyzed to assess their binding or interaction stability with the target ABL kinase (Fig. 7). The H-bond network profiles of A01 show two H-bonds interactions with the protein. One H-bond interaction formed between the hydroxyl group of the A01 with the residue Thr315 and the second H-bond formed between the carbonyl group of the A01 with the Met318 (hinge region) of the

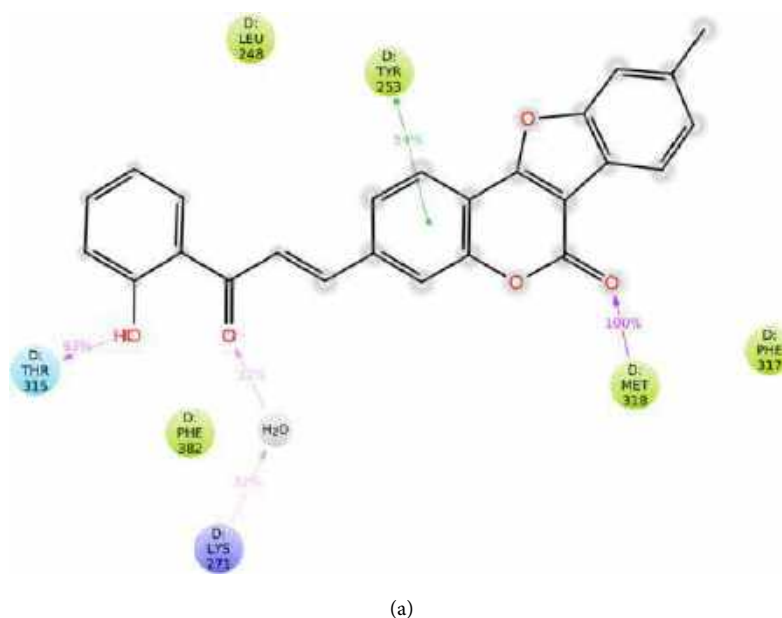
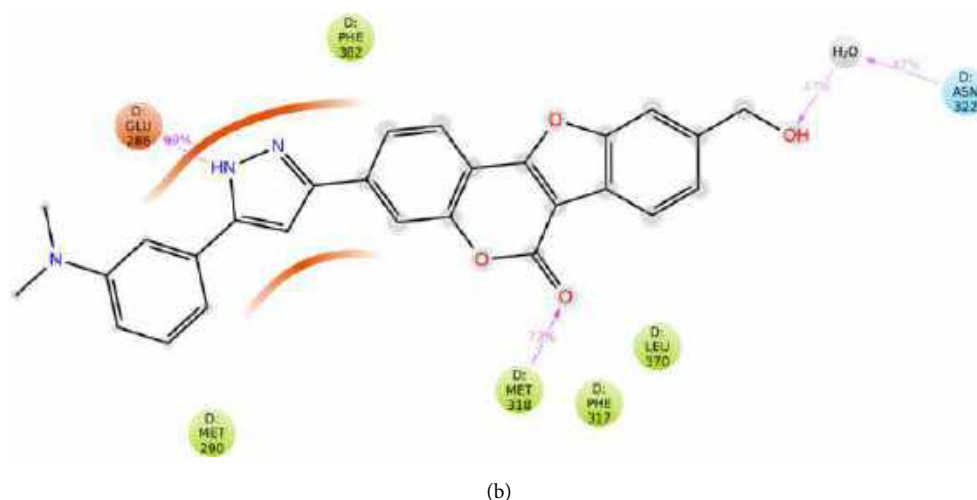


Fig. 7. (Color online) P-L contacts of (a) A01 and (b) B01 with 3CS9 evolved during MD simulation.



(b)

Fig. 7. (Continued)

protein. The calculated % H-bond occupancy of Thr315 and Met318 is found to be 63% and 100%, respectively. In addition, A01 makes one  $\pi$ - $\pi$  stacking interaction with Tyr253 (55%) and several hydrophobic (Leu248, Tyr253, Met318, Phe317, and Phe382) interactions with the receptor. The 100% H-bond occupancy of A01 with the hinge region residue Met318 confirmed that the proposed chalcone-based coumestrol derivative can disrupt the effector function of the ABL kinase.

The evaluated H-bond network profile of B01 during the MD simulation reveals that B01 makes three H-bond interactions with the ABL. One H-bond formed between the pyrazole NH group of the B01 with the ABL residue Glu286 (99%), second bond formed between the carbonyl group of the coumestrol ring in B01 with Met318 (72%) of the protein. A third H-bond is formed between the CH<sub>2</sub>OH group of the ligand with Asn322 residue through a water bridge, indicating high-affinity binding. In addition, B01 shows some

Table 2. Results of ADME prediction by QikProp.

Compounds	MW	Volume	HBD	HBA	HOA	QPlogP <sub>0</sub> /W	QPlogHERG	QPPCaco	QPPMDCK
A01	396.39	1210.54	0	4.75	3	4.39	-7.05	414.58	191.00
A02	398.37	1173.16	1	5.5	3	3.48	-7.01	125.58	52.28
A03	382.37	1150.41	0	4.75	3	4.07	-7.14	414.56	191.00
A04	397.38	1182.20	2.5	6.75	3	2.64	-6.96	76.08	30.56
A05	412.39	1233.26	1	6.45	3	3.43	-7.09	124.82	52.18
A06	398.37	1175.38	2	6.5	3	2.83	-6.96	88.72	36.08
A07	439.42	1319.09	1	7.25	1	3.59	-7.39	113.00	46.86
A08	427.36	1221.73	0	5.75	3	3.32	-7.04	52.06	20.28
A09	425.44	1308.34	1	6.75	1	3.99	-7.13	274.46	122.29
A10	382.37	1152.75	1	5.75	3	3.55	-7.09	290.82	130.19
B01	451.48	1371.85	2	6.7	1	4.26	-7.19	276.43	123.24
B02	422.44	1276.34	2	5.7	1	4.12	-7.10	293.57	131.53
B03	442.85	1260.64	2	5.7	1	4.31	-7.10	293.24	323.88
B04	438.44	1291.45	2	6.45	1	3.92	-7.09	293.74	131.61
B05	437.45	1310.87	3	6.7	1	3.59	-7.17	177.02	76.13
B06	423.42	1246.16	3.5	6.7	3	2.86	-7.06	76.17	30.60
B07	438.43	1291.21	2	6.45	1	3.91	-7.08	293.25	131.37
B08	423.42	1245.98	3.5	6.7	3	2.86	-7.06	76.42	30.71
B09	424.41	1239.22	3	6.45	3	3.06	-7.06	89.10	36.24
B10	453.41	1288.78	2	6.7	1	3.12	-7.10	35.15	13.26



hydrophobic interaction (residues: Phe381, Met290, Met318, Phe317, and Leu370) with the receptor (Fig. 7). In summary, the MD simulation analysis reveals that the chalcone-based A01 and pyrazole-based B01 coumestrol derivatives are stable throughout the simulation period and are making critical H-bond interactions with the conserved hinge region residue Met318 of the ABL.

### 3.6. ADME prediction

The designed chalcone and pyrazole-based coumestrol derivatives were subjected to pharmacokinetics descriptor analysis to check the drug-likeness properties by QikProp module of the Schrodinger (Table 2).<sup>50</sup> The descriptors such as molecular weight of all compounds are below 500 with < 4 H-bond donors and < 8 H-bond acceptors, which are satisfied with the Lipinski's rule of five. The average of partial coefficient (QPlogP<sub>0</sub>/W) of the chalcone and pyrazole-based coumestrol derivatives is 3.52 and 3.60, respectively, and is the critical parameter for the absorption and distribution of drugs. Cell permeability (QPPCaco) is another important factor regulating the drug metabolism and its transport across membranes, which is in the acceptable ranges of all compounds. The obtained log IC<sub>50</sub> values for the blockage of HERG K<sup>+</sup> channels (QPlogHERG) of both scaffolds are in the range of < -6. The cell permeability through MDCK cells (QPPMDCK) of all the compounds except A08 and B10 is in the acceptable ranges, which are considered to be the excellent mimic for the blood-brain barrier of the drug. The total volume of the compound enclosed by solvent-accessible molecular surface (Volume); Vmol in all compounds are within the range (500–2000). The computed values of the physiochemical properties and ADMET parameters of the designed chalcone and pyrazole-based coumestrol compounds lying in the acceptable range defined for human use confirm that they can be considered as drug candidates for further studies.

## 4. CONCLUSION

Aberrant activity of the non-receptor tyrosine kinase BCR-ABL causes leukemogenesis and consequently CML in bone marrow cells. Patients with CML are currently administered synthetic drug imatinib, nilotinib, bosutinib, ponatinib, etc.; the longer treatment duration of these drugs results in non-hematological toxicities and induces various side effects. Therefore, in this study, we sought to identify alternative CML drugs

from an anti-cancerous natural product coumestrol. The molecular docking and MD analysis of the chalcone and pyrazole-based coumestrol derivatives were analyzed to determine their suitability as drug molecules for treating CML. All of the designed compounds exhibited effective docking and glide scores with good binding affinities. The conclusion drawn from this docking is that the chalcone ring incorporated coumestrol derivative A01 and pyrazole incorporated B01 showed superior docking scores to that of other docked molecules and the reference compound bosutinib against ABL. Our observation on the docked complexes suggests that the top-scored compounds have a maximum level of binding affinities with a favorable H-bond,  $\pi$ - $\pi$  stacking interactions, and hydrophobic interaction with the receptor. Mainly, it can be found that the top-scored A01 and B01 compounds have a critical interaction with the hinge region residue Met318 of the ABL kinase, which is essential for the inhibition of ABL kinase.

Furthermore, the MD simulation analysis supports that the complex formations between the inhibitors A01 and B01 with the effector protein ABL are highly stable compared to free ABL. Specific electronic properties such as HOMO and LUMO of the A01 and B01 indicate that both these compounds are very reactive and information regarding the electrostatic features of both compounds are obtained from the MESP maps. The ADME properties of all coumestrol derivatives (chalcone and pyrazole-based) were predicted, and the scores are found well within the recommended ranges. Therefore, the overall results obtained from the computational approach will be helpful for the structure-based lead optimization and development of potent ABL inhibitors. The chalcone and pyrazole-based coumestrol derivatives reported here for the first time are said to have anti-cancer activity; further studies are required to delineate the exact mechanism of action.

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## CONFLICTS OF INTEREST

The authors have no conflicts of interest to disclose.

## PUBLISHER'S NOTE

In the original submitted and accepted manuscript, Karakkad P. Sajesh (K.P.S.) was not included in the

author list. It was conveyed to the Publisher post-acceptance that this was an unintentional omission, and that K.P.S. had performed the docking of two compounds in this research work. All other authors declared individually to the Publisher that they agree to the addition of K.P.S. to the author list, and the Publisher hereby accepts this change.

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## Tailoring Structural and Optical Properties of Cu Doped Chemically Deposited ZnSe Nanostructured Thin Films

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## Tailoring Structural and Optical properties of Cu Doped Chemically Deposited ZnSe Nanostructured Thin Films

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Chemical bath deposition has been used for depositing undoped and copper doped ZnSe thin films at 343 K temperature. Growth of the thin film requires zinc sulphate cation and sodium selenosulphate anion. The preparative parameters are optimized with an aim to obtain high quality thin films. Three different concentrations of Cu source are used. XRD pattern indicates the incorporation of copper in to polycrystalline cubic ZnSe in doped thin films and is confirmed by EDAX spectrum. SEM micrographs indicate that ZnSe dispersion in the films is homogeneous. UV-visible transmission spectra of the thin films have put into evidence that the dispersion of ZnSe nanocrystals in the thin film is improved their optical transmission. Room temperature PL spectra have shown that the addition of Cu into ZnSe enhanced the emission with additional green peak other than blue band edge emission. Electrical conductivity also modified on addition of Copper.

### Introduction

The binary chalcogenide II-VI group semiconducting thin films are potential candidates in short wavelength optoelectronic devices like photovoltaic cells, lasers and light emitting diodes due to their novel physical properties (1-3). Metal selenides find various applications in light emitting devices, photovoltaic cells, optical sensors and optical recording materials (4-7). Zinc selenide has benign optical and luminescent properties with attractive characteristics which makes it promising candidate for optoelectronic applications (3, 8). It is an n-type wide band gap semiconducting material having direct band gap energy 2.7eV with unique physical properties such as high refractive index, low optical absorption and dispersion and high transmission in the visible and infra-red spectral region (9-10). ZnSe films find several applications in optoelectronic devices (11-12), optical coatings, thin film transistors, window material in hetero junction solar cells (13, 14) and photo electrochemical applications (15). Polycrystalline ZnSe thin films have been reported suitable device applications in optoelectronics like non-toxic buffer layer for Cu (In,Ga) Se<sub>2</sub> based photovoltaic cell, LED, blue green laser diodes (4-5, 16).

A vast variety of techniques are available for deposition of polycrystalline ZnSe thin films like Chemical Bath Deposition (CBD) (15-19), electrodeposition (20),

Solvothermal (21), hydrothermal (22), Successive Ionic Layer Adsorption and Reaction (SILAR) (12, 23-24) and Photo assisted Chemical Deposition (PCD) (25-27). In this work we report the investigation of effect of Cu doping on structural, morphological, optical and electrical properties of nano structured ZnSe thin films synthesized through typical chemical bath deposition (CBD).

### Experimental Details

The chemicals used were ZnSO<sub>4</sub>, Na<sub>2</sub>SO<sub>3</sub>, selenium powder, Triethanol ammine (TEA), trisodium citrate (TSC) and NaOH. For the preparation of aqueous chemical bath 20 ml 0.25 M Zinc sulphate solution was taken. Under constant stirring, 30 drops TEA was added in to it. The resultant solution becomes milky turbid indicating the formation of Zn(OH)<sub>2</sub>. Addition of sufficient amount of 4M NaOH dissolved the turbidity and the solution became transparent. Then 5 ml 0.1M TSC was added to the bath, followed by 20 ml 0.25 M freshly prepared anionic source sodium selenosulphate (Na<sub>2</sub>SeSO<sub>3</sub>) solution. The Na<sub>2</sub>SeSO<sub>3</sub> solution was prepared by refluxing 2gm Selenium powder and 6gm Sodium sulphite (anhydrous) in 40 ml water at 343 K for 5 hours under constant stirring.

Sodium seleno sulphate releases Se<sup>2-</sup> ions through hydrolysis in aqueous alkaline medium (28-29). Microscopic glass substrates of dimensions 75x25x2 mm<sup>3</sup> were placed vertically in the chemical bath at 343 K for 1.5 hours. The properties of substrate affect the quality of thin films and hence substrates were well cleaned and ultrasonicated in distilled water prior to the deposition process. The final pH of the solution was maintained at 12.25. The deposition is based on slow release of Zn<sup>2+</sup> and Se<sup>2-</sup> ions in the solution which condense on the substrate surface. ZnSe deposition occurs when the ionic product of Zn<sup>2+</sup> and Se<sup>2-</sup> exceeds the solubility product of ZnSe (14).

After the deposition, the samples were thoroughly washed in distilled water, dried in air and annealed at 373 K for 30 minutes. This work describes the synthesis and characterizations of copper doped ZnSe thin films with three different weight percentages of dopant such as 2%, 4% and 6%. The source of dopant, Copper sulphate solution was added into the zinc sulphate solution. The undoped sample was named as ZS and the doped samples with increase in copper concentration were named ZCU1, ZCU2 and ZCU3 respectively.

### Results and Discussion

The undoped and doped films appear well adherent, uniform and pale yellow in colour. The thickness of the samples having mass ‘m’ is estimated using the equation

$$t = \frac{m}{\rho A} \quad [1]$$

where ‘ρ’ represents the bulk density of ZnSe 5.27x10<sup>3</sup> Kg/m<sup>3</sup> and ‘A’ represent the deposited area of the film. It is seen from Table I. that the thickness decreases with increase in copper concentration.

## Structural Properties

The structural properties of the thin films are studied from the X-ray diffraction patterns in the range  $20^{\circ}$  to  $80^{\circ}$  and shown in Figure 1.

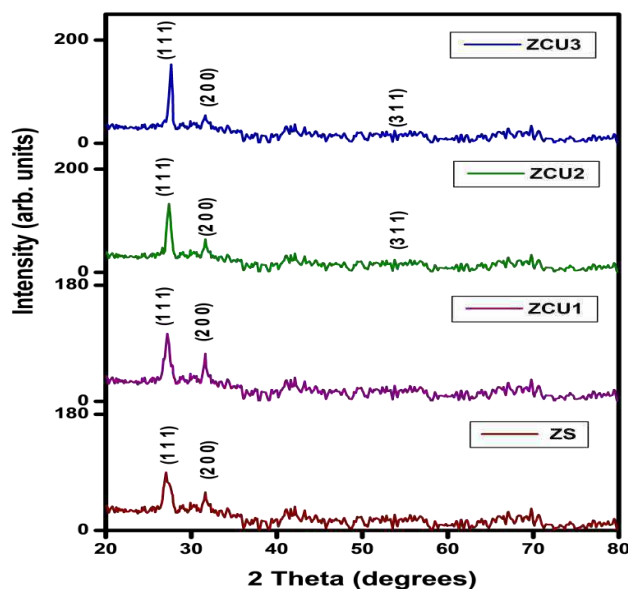


Figure 1. XRD spectra of undoped and Cu doped ZnSe thin films

The diffraction spectra of all the samples display the polycrystalline cubic zinc blende phase of ZnSe with lattice constant  $5.618 \text{ \AA}$  (JCPDS card No: 80-0021) (30). Two diffraction peaks are observed along directions (111) and (200) for all samples. Some samples possess orientations along (311) direction also. The intensity of the peak (111) increases with increase in doping concentration which indicates the preferred direction of orientation.

**TABLE I.** Structural Properties of ZnSe thin films prepared via CBD.

Sample	Thickness (nm)	Grain size (nm) from		Micro strain ( $\times 10^{-3}$ )	Dislocation density ( $\times 10^{15}$ lines/m)
		W-H plot	FWHM		
ZS	505	26.3	28.4	5.4	1.1
ZCU1	483	26.9	29.3	4.3	1.07
ZCU2	459	28.8	30.1	4.27	1.01
ZCU3	411	31.5	32.5	3.8	0.95

The peaks become sharper with increase in copper concentration represents enhancement of clusters and hence better crystallinity in doped films. The peaks are gradually shifted to higher  $\theta$  values with increase in impurity concentration designating adhesion of Cu in to the ZnSe lattice. As a result the lattice is under compressive strain. The grain size D can be evaluated using Debye-Scherrer Equation (31-32)



$$D = \frac{k\lambda}{\beta \cos\theta} \quad [2]$$

where 'k' is the shape factor (k=0.94)  $\lambda$  the wavelength of X-ray used for diffraction, ' $\beta$ ' the FWHM of the XRD signal with peak position ' $\theta$ '. The average grain size is found to increase with increase in copper concentration. The grain size is also evaluated from the reciprocal of y-intercept of the W-H plot. The plot is shown in Figure 2. The values obtained from the two methods are comparable. The negative slope of W-H plots confirms the compressive nature of residual strain in the doped and undoped thin film lattice.

According to Williamson and Hall the FWHM ( $\beta$ ) of the XRD peaks can be expressed as a linear combination of micro strain ( $\varepsilon$ ) and particle size (D) given by (33)

$$\frac{\beta \cos\theta}{\lambda} = \frac{1}{D} + \frac{\varepsilon \sin\theta}{\lambda} \quad [3]$$

The slope of the plot of  $(\beta \cos\theta)/\lambda$  versus  $(\sin\theta)/\lambda$  gives the residual strain and the reciprocal of Y-intercept gives the average grain size of the sample. The micro strain can be determined using the tangent formula (34)

$$\varepsilon = \frac{\beta}{4 \tan\theta} \quad [4]$$

Dislocation density is a function of grain size and is given by the equation (35-36)

$$\delta = \frac{1}{D^2} \quad [5]$$

The micro strain and dislocation density values are found to decrease with the doping concentration. This represents the improvement in crystallinity in doped films. The estimated values are tabulated in Table I.

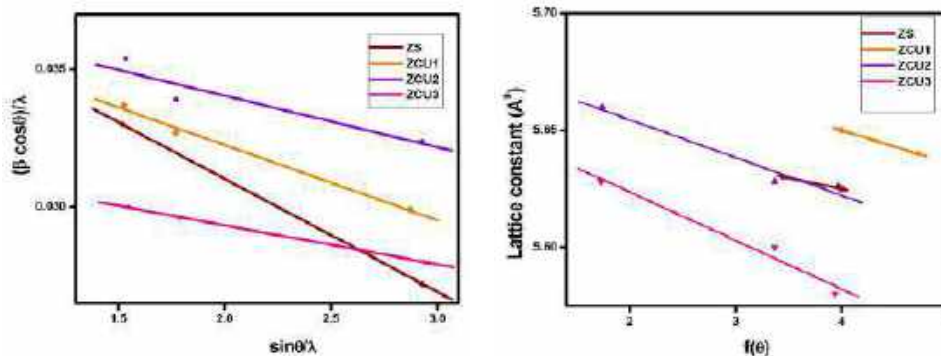


Figure 2. W-H plot and Figure 3. Nelson-Riley plot of Cu doped ZnSe thin films

The lattice parameter ‘a’ can be calculated for cubic crystal from the interplanar spacing ‘ $d_{hkl}$ ’ corresponding to the Miller indices h, k and l value obtained from XRD spectra using the relation (31)

$$d_{hkl}^2 = \frac{a^2}{[h^2+k^2+l^2]} \quad [6]$$

The corrected values of lattice parameter are estimated from the Nelson-Riley plot between calculated lattice parameters for different planes and the error function (37)

$$f(\theta) = \left(\frac{\cos^2 \theta}{\sin \theta}\right) + \left(\frac{\cos^2 \theta}{\theta}\right) \quad [7]$$

‘a’ can be determined by extrapolating the plot to  $\theta=90^\circ$  or  $f(\theta)$  to zero. The N-R plot is shown in Figure 3. and the obtained values are tabulated in Table II. The lattice parameters are found to approach the ideal value with rise in copper concentration and show slight variation in doped thin films. The deviations in lattice parameter cause stress and strain in the lattice.

**TABLE II.** Lattice parameters of undoped and Cu doped ZnSe thin films

Sample	Ideal	ZS	ZCU1	ZCU2	ZCU3
Lattice constant ( $\text{\AA}$ )	5.618	5.63	5.653	5.64	5.613
form	W-H plot	5.652	5.678	5.673	5.653

### Morphological and compositional properties

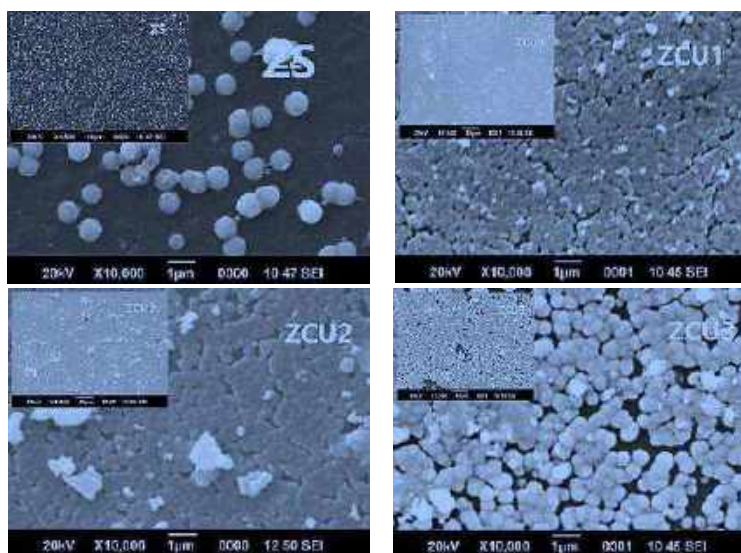


Figure 4. SEM micrographs of undoped and Cu doped ZnSe thin films (inset x1500)

The morphological aspects of the thin films are studied from the SEM micrographs. Figure 4 shows the obtained SEM images of the samples with two different magnifications. The film grows in two dimensions resulting in homogeneous deposition over the substrate surface. Uniform round shaped agglomerations without cracks are distributed on smooth background. The introduction of copper in to the ZnSe lattice considerably increased the density. The smooth background may possess amorphous phase of ZnSe film (38). Doping caused the fusion of spherical aggregates with increased density of agglomerations on the film surface, which may be a reason for variations in optical and transport properties of doped films.

The elemental composition of copper doped Zinc selenide thin films are studied from the EDAX spectra. A representative EDAX spectrum of 4% Cu doped ZCU1 is shown in Figure 5. The spectrum contains peaks corresponding to Zn, Se and Cu. The additional peaks like O, Si, C, Na and Ca are associated with the composition of the soda lime glass substrate (39-40). The inset shows the pie diagram showing the contributions of Zn, Se and Cu. The obtained atomic percentages of Cu in various doped samples are depicted in Table III. The observed doping concentrations are in agreement with the expected values.

**TABLE III.** Weight percentage of copper in ZnSe thin films

Sample	ZS	ZCU1	ZCU2	ZCU3
Weight % of Cu	0	1.91	3.75	5.6

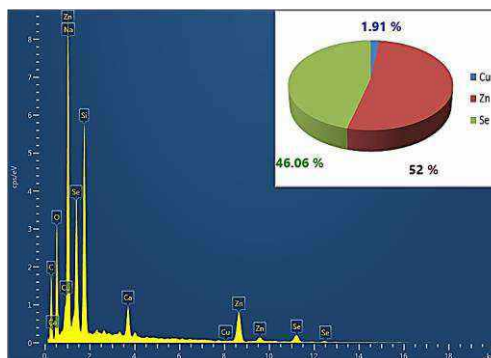


Figure 5. Representative EDAX spectrum of ZCU1

### Optical Properties

The UV-visible absorption and transmission spectra of the undoped and copper doped ZnSe thin film samples are shown in Figure 6 and Figure 7 respectively. Absorption of the samples are very low towards the visible and IR region. The samples possess sharp absorption edges indicating direct transition taking place within the sample. The doped samples possess very low absorbance which is further reduced with increase in copper concentration.

All samples possess uniform optical transmission values and are found to increase with increase in dopant concentration. The thin films doped with 4% and 6% copper have a uniform transmission greater than 90%. This implies that a minimum amount of copper

doping is required to enhance the transmission. The uniform transmission may be due to the increased crystallinity and uniformity on doping. Optical transmissions at 600 nm are depicted in Table IV.

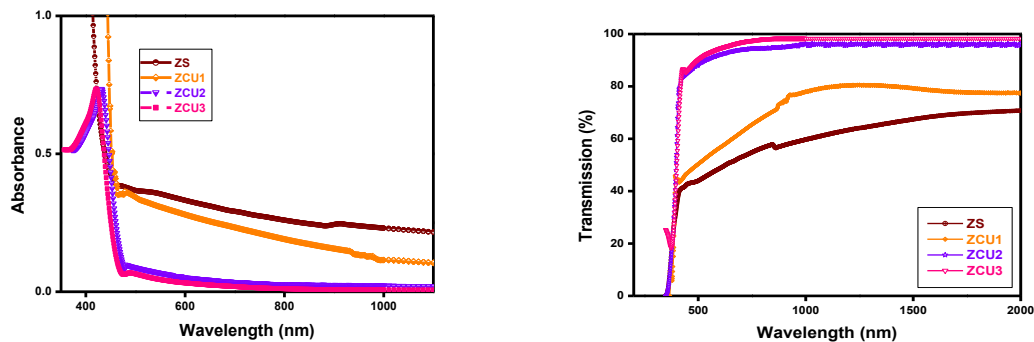


Figure 6. Absorption spectra Figure 7. Transmission spectra of Cu doped ZnSe thin films

The optical band gap values of the thin film samples are related to the optical absorbance values through the Tauc relation given by the relation (41)

$$\alpha = \frac{A(h\nu - E_g)^n}{h\nu} \quad [8]$$

$$\alpha = \frac{2.303Abs}{t} \quad [9]$$

where  $h\nu$  is the photon energy  $E_g$  is the band gap energy,  $A$  and  $n$  are constants.  $A$  depend on transition probability, temperature phonon energies. For allowed direct transition  $n=1/2$ . The Tauc plot is depicted in Figure 8.

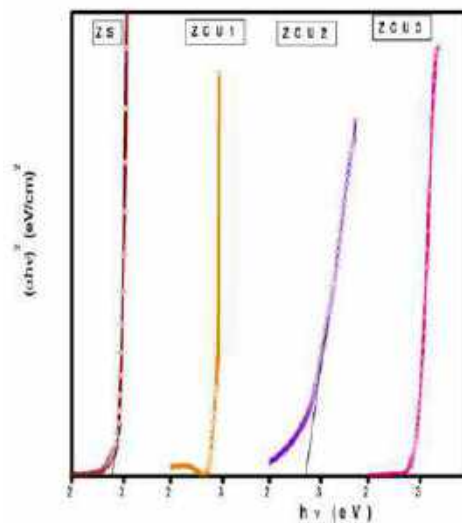


Figure 8. Tauc plot of undoped and Cu doped ZnSe thin films



It can be seen that the plot varies linearly above the band gap value. The band gap energies are evaluated from plot by extrapolating the linear portion of the graph towards the X-axis. The linear nature of plot confirms the direct transition from valence band to conduction band in the thin film. The optical band gap value is found to decrease on the introduction of Cu in to the ZnSe thin films. Further increase in copper concentration enhances the optical band gap energy. The decrease in band gap on the introduction of copper may be attributed to increased lattice scattering due to defects and sudden increase may be caused by the improved crystallinity. The obtained band gap energies are depicted in Table IV.

**Table IV.** Optical characteristics of Cu: ZnSe thin films

Sample	Band gap (eV)	Transmission at 600 nm (%)	PL peaks (nm)
ZS	2.78	51.4	458
ZCU1	2.69	59.6	437,524
ZCU2	2.72	93.4	456,515
ZCU3	2.77	95.9	433, 528

### Photoluminescent Properties

The room temperature PL spectra of copper doped zinc selenide samples excited with electromagnetic radiation of wavelength 350 nm are shown in Figure 9.

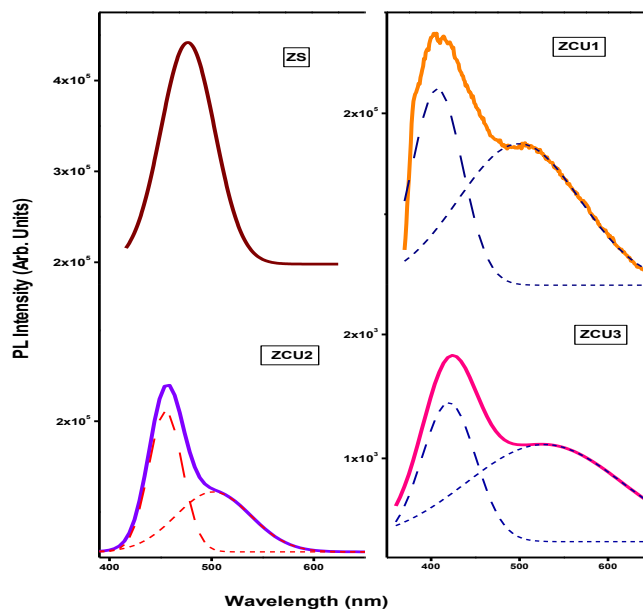


Figure 9. PL spectra of undoped and Cu doped ZnSe thin films

The PL spectra of all samples indicate emission peak near 450 nm resulting in the band to band transition of ZnSe (42). In the Cu doped samples, an additional peak related to Cu impurity near 520 nm in green region is also present. It is reported that the peak around 520 nm is attributed to trap states (43-45). For Cu: ZnSe, two copper acceptor centres have reported, one at 0.4 eV above VB (530 nm) and other 0.7 eV above VB (620nm) involved in red emission (46-47). The observed green emission may be resulted from transition of electrons from CB or surface states to the  $^2T_2$  acceptor level of  $Cu^{2+}$ , which is a deep level transition (48). For deep transition states, emission indicates a small

shift as the transition is from deep levels. This may be the reason for slight shift in wavelength of peak for various samples. The observed peak and EDAX spectra confirm the doping of copper impurity in the ZnSe crystal.

### Electrical properties

Electrical conductivity of the films is enhanced for the doped films. The room temperature electrical properties of the thin film samples are analysed by the Keithly two probe set up. According to Ohm's law, electrical resistance is proportional to sample's length 'L', and resistivity 'ρ' and inversely proportional to sample's cross sectional area 'A' given by product of the film thickness and the width of the film. The equation for resistivity is given by

$$\rho = \frac{RA}{L} \quad [10]$$

The estimated values are depicted in Table V. The resistivity increases on the introduction of copper initially. The increased concentrations of copper impurity further reduced the resistivity considerably. The resistivities of all samples are of the order of  $10^4$  Ω-cm. The increased resistivity on doping may be due to the lattice scattering occurred on the introduction of Cu impurity. The further decrease may be attributed to the improvement in crystallinity, which reduced the grain boundaries.

**Table V.** Electrical properties of Cu: ZnSe thin films

Sample	ZS	ZCU1	ZCU2	ZCU3
Resistivity ( $\times 10^4$ Ω cm)	2.86	7.25	3.62	1.94

### **Conclusion**

Nano structured polycrystalline Cu: ZnSe thin films prepared through CBD technique. The effects of addition of copper impurity into crystal lattice on various physical properties of the ZnSe thin films were analysed. The undoped and doped samples crystallized in to cubic zinc blende crystal structure. Doping slightly enhanced the crystallinity. The thickness and crystal imperfections like micro strain were found to decrease on doping and grain size increased. The lattice parameters of the unit cell were estimated and found to approach the bulk ZnSe lattice parameters on increased concentration of copper.

The morphology shows that doped films are more densely packed than undoped films. The elemental composition one of the doped samples was confirmed by EDAX spectra. The doped samples with 4 and 6 weight percentages showed very high transmission above 90%. These properties make the samples a potential candidate for window and buffer layer applications in photovoltaics.

The optical band gap energies were first found to decrease on doping which further increased with copper concentration. These properties make the samples a potential

candidate for window and buffer layer applications in photovoltaics. The PL spectra of the doped sample showed an additional peak corresponding to impurity level of copper in addition to the band to band transition. The PL emission intensity can be tuned by controlling the amount of copper in the reaction bath. This may be the reason for slight shift in wavelength of peak for various samples. The electrical conductivity of the samples found to decrease on introduction of dopant which further increased with copper concentration. The tunable band gap, increased electrical conductivity and induced green emission on copper doping and enables ZnSe thin films to find application in optoelectronic devices.

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