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# Analysing structure-boiling point relationships of oxo organic compounds using molecular descriptors

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**Abstract**

In organic chemistry the prefix oxo indicates a double bond between an oxygen atom and carbon atom. The oxo group is present in ketons, estern, carboxilic acids, aldehydes and amids. Topological indices are numerical quantities associated with the molecular graphs. Some of the molecular descriptors have proven their ability in predicting physico-chemical properties certain chemical compounds. In this paper structure boiling point relationships are studied for series of oxo organic compounds by ten molecular descriptors. The QSPR modelling for the oxo organic compounds are presented by the means of linear, quadratic, logarithmic and multilinear analysis. The multilinear analysis model produces a correlation coefficient(r) =0.954 and standard error of estimates $(s) = 17.1902°C$ for the set of 192 oxo organic compounds. Also, the intercorrelation between pair of molecular descriptors is studied. This is validated by Hierarchial cluster analysis. This study helps to classify useful molecular descriptors based on their predicting in structure boiling point of oxo organic compounds.

**Keywords:** Molecular Descriptors, Oxo organic compounds, QSPR-analysis.

## 1. Introduction

Let $G = (V, E)$ be a graph with $|V| = n$ and $|E| = m$. The open neighbourhood of vertex $v \in V$ is $N(v) = \{u|v \in E\}$. The degree of a vertex $v$ denoted by $d(v)$ is $|N(v)|$. The minimum (maximum) degree of graph $G$ is denoted by $\delta(G)(\Delta(G))$, respectively [1].

A Molecular graph is a graph which has vertices corresponds to the atoms and the edge corresponds to the bonds. The chemical graph theory is a branch of mathematical chemistry, concerned with all aspects of the application in mathematical chemistry. The boiling point of compound is an important physical property for the design and optimization of the processing engineering in chemical and petrochemical industries. Therefore, it is important to develop quantitative structure boiling point models for the estimation of boiling points of untested compounds or selection of reliable experimental boiling points of the compounds. Oxo indicates a double bond between an oxygen and carbon atoms. Oxo chemicals are

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intermediate and derivative chemical compounds which are characteristically used in chemical and manufacturing processes of paints, plasticizers, coatings, adhesives and lubricant additives.

Molecular descriptors can be categorised into three types mainly, the degree-based, the distance-based, and the eigenvalue based molecular descriptors. In 1972, Gutman and Trinajsti′c [2], introduced the first degree-based molecular descriptors $M_1(G)$ and $M_2(G)$, called Zagreb indices which are defined as

$$M_1 = \sum_{v \in V(G)} (d(v))^2. \quad (1.1)$$

$$M_2 = \sum_{uv \in E(G)} d(u)d(v). \quad (1.2)$$

In 2004, Milivonic et al. [3] reformulated the Zagreb indices in relating to edge-degrees instead of vertex-degrees. Later in 2012, Ilic and Zhou [4] established a set of bounds for the same, along with an exact formula for the first reformulated Zagreb index in terms of well known degree-based topological indices. Recently, Liu et al. [5] studied the reformulated Zagreb indices and obtained an expression for the first reformulated Zagreb index of the line graph of a graph, which includes both the vertex-degree and edge-degree based indices. In 2014, Furtula et al. [6] studied differences of Zagreb indices and showed that this difference is in close connection with the reduced Zagreb index which is defined over the edge set. In 2013, Shirdel et al. [7] defined the hyper-Zagreb index over the edge set. Mondal et al. [8, 9], introduced some neighbors degree based indices and discussed their mathematical properties.

Till date various molecular descriptors have been studied but the chemical applicability of most of the descriptors is still to be explored. In [10] A. Iqbal et al. developed a mathematical model to study the flow pattern of Lumpy skin disease. The molecular descriptors are the numerical values associated with the corresponding molecular graph. Introducing any molecular descriptors without studying its chemical applicability or predictive power is questionable in chemical graph theory.

Kulli et al. have put forward many degree based molecular descriptors such as Gourava Nirmala Index(GNI) [11], Sombor Leap Index(SLI) [12], Modified Sombor Leap Index(MSLI)[12], Sum Connectivity Gourava Index(SCGI) [13], Product Connectivity Gourava Index(PCGI) [14], Mulltiplicative Atom Bond Sum Conectivity Index(MASCI) [15], Sum Augmented Index(SAI) [16], Revan Sombor Index(RSI) [17] but none of these molecular descriptors are tested for there chemical applicability. In [18] Gutman put forward the Sombor index and studied its molecular geometry, Kulli et.al [19] have studied the Gourava indices of some class of windmill graphs. The modified version of Sombor index was put forward by Kulli [20]. But so far, the chemical applicability of these parameters have not been reported. In this paper the QSPR analysis for these molecular descriptors is conducted to test chemical applicability in predicting boiling points of oxo organic compounds.

The molecular descriptors are defined as below:

**Table 1:** Molecular Descriptors

| | Molecular descriptor | Abbreviation | Mathematical Definition |
|---|---|---|---|
| 1. | Gourava Nirmala Index | GNI | $\sum_{uv\in E(G)} \sqrt{(d(u)+d(v))+(d(u)*d(v))}$ |
| 2. | Sombor Leap Index | SLI | $\sum_{uv\in E(G)} \sqrt{(d(u)^2+d(v)^2)}$ |
| 3. | Modified Sombor Leap Index | MSLI | $\sum_{uv\in E(G)} \frac{1}{\sqrt{(d(u)^2+d(v)^2)}}$ |
| 4. | F-Sombor Index | FSLI | $\sum_{uv\in E(G)} \sqrt{(d(u)^4+d(v)^4)}$ |
| 5. | Modified F-Sombor Index | MFSLI | $\sum_{uv\in E(G)} \frac{1}{\sqrt{(d(u)^4+d(v)^4)}}$ |
| 6. | Sum Connectivity Gourava Index | SCGI | $\sum_{uv\in E(G)} \frac{1}{\sqrt{(d(u)+d(v))+(d(u)*d(v))}}$ |
| 7. | Product Connectivity Gourava Index | PCGI | $\sum_{uv\in E(G)} \frac{1}{\sqrt{(d(u)+d(v))*(d(u)*d(v))}}$ |
| 8. | Mulltiplicative Atom Bond Sum Conectivity Index | MASCI | $\prod_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$ |
| 9. | Sum Augmented Index | SAI | $\sum_{uv\in E(G)} \left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$ |
| 10. | Revan Sombor Index | RSI | $\sum_{uv\in E(G)} \sqrt{(\Delta(G)+\delta(G)-d(u))^2+(\Delta(G)+\delta(G)-d(v$ |

## 2. Data Set

There are 192 oxo chemicals in the data collection, comprising 32 aldehydes, 78 ethers, and 82 ketons (Table 2). The calculated and experimental boiling points are found in [21]. Table 2 also contains values of molecular descriptors of 192 oxo compounds.

**Table 2:** Experimental and Calculated BP values and molecular descriptors, [21].

| Compound Name | Exp | Calcd | GNI | SLI | MSLI | FSLI | MFSLI | SCGI | PCGI | MASCI | SAI | SI |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Dimethyl ether | 24.9 | 24 | .47 | .47 | .89 | .24 | 0.48 | .89 | .81 | .33 | 4.0 | .00 |
| Ethyl methyl ether | .4 | .3 | .3 | .3 | .24 | 3.9 | 0.66 | .24 | .06 | .23 | 2 | .07 |
| Methyl propyl ether | 8.6 | 9.3 | 0.12 | 0.12 | .6 | 9.55 | 0.83 | .6 | .31 | .16 | 0 | 0 |
| Diethyl ether | 4.6 | 7.1 | 0.12 | 0.12 | .6 | 9.55 | 0.83 | .6 | .31 | .16 | 0 | 0 |
| Isopropyl methyl ether | 0.8 | 0.1 | 0.84 | 2.16 | .35 | 2.08 | 0.56 | .5 | .16 | .22 | 7.62 | 0.62 |
| Butyl methyl ether | 0.3 | 8.9 | 2.95 | 2.95 | .95 | 5.21 | 1.01 | .95 | .56 | .11 | 8 | 4.14 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ethyl propyl ether | 3.9 | 5.3 | 2.95 | 2.95 | .95 | 5.21 | 1.01 | .95 | .56 | .11 | 8 | 4.14 |
| Ethyl isopropyl ether | 4.1 | 6.5 | 3.67 | 4.99 | .71 | 7.73 | 0.74 | .85 | .41 | .15 | 5.62 | 28.03 |
| Isobutyl methyl ether | 8.6 | 0.2 | 3.67 | 4.99 | .71 | 7.73 | 0.74 | .85 | .41 | .15 | 5.62 | 28.03 |
| Sec-butyl methyl ether | 9 | 7.5 | 3.75 | 4.84 | .76 | 6.99 | 0.79 | .87 | .47 | .14 | 1.25 | 05.54 |
| Tert-butyl methyl ether | 2 | 0.9 | 4.97 | 9.07 | .39 | 8.7 | 0.49 | .71 | .22 | .21 | 4.26 | 108.26 |
| Methyl pentyl ether | 9 | 7.3 | 5.78 | 5.78 | .3 | 0.87 | 1.19 | .3 | .81 | .08 | 6 | 0 |
| Ethyl butyl ether | 2.2 | 2.6 | 5.78 | 5.78 | .3 | 0.87 | 1.19 | .3 | .81 | .08 | 6 | 0 |
| Dipropyl ether | 9.6 | 1.2 | 5.78 | 5.78 | .3 | 0.87 | 1.19 | .3 | .81 | .08 | 6 | 0 |
| Isopropyl propyl ether | 3 | 2.5 | 6.5 | 7.82 | .06 | 9.33 | 1.25 | .21 | .66 | .11 | 3.62 | 44.98 |
| Ethyl isobutyl ether | 2 | 3.9 | 6.5 | 7.82 | .06 | 9.33 | 1.25 | .21 | .66 | .11 | 3.62 | 44.98 |
| Isopentyl methyl ether | 1 | 8.7 | 6.5 | 7.82 | .06 | 9.33 | 1.25 | .21 | .66 | .11 | 3.62 | 44.98 |
| Methyl 1-methylbutyl ether | 1.5 | 4.8 | 6.57 | 7.67 | .11 | 2.65 | 0.97 | .22 | .72 | .1 | 9.25 | 81.37 |
| Methyl 2-methylbutyl ether | 3 | 6.6 | 6.57 | 7.67 | .11 | 2.65 | 0.97 | .22 | .72 | .1 | 9.25 | 81.37 |
| Diisopropyl ether | 9 | 3.6 | 7.21 | 9.86 | .81 | 5.91 | 0.64 | .11 | .51 | .15 | 1.25 | 00 |
| Methyl tert-pentyl ether | 6.3 | 6.1 | 7.95 | 2.66 | .82 | 3.29 | 0.73 | .09 | .55 | .13 | 0 | 250 |
| 1,2-dimethylpropyl methyl ether | 1.3 | 6.3 | 7.36 | 9.57 | .9 | 3.86 | 0.75 | .14 | .59 | .12 | 9 | 60.55 |
| 2,2-dimethylpropyl methyl ether | 0.5 | 0.9 | 7.8 | 1.9 | .75 | 4.36 | 0.66 | .06 | .47 | .15 | 2.26 | 701.96 |
| 1-ethylpropyl methyl ether | 8.5 | 1.9 | 6.65 | 7.52 | .17 | 1.91 | 1.03 | .24 | .77 | .08 | 4.88 | 24.04 |
| Ethyl tert-butyl ether | 3.1 | 6 | 7.8 | 1.9 | .75 | 4.36 | 0.66 | .06 | .47 | .15 | 2.26 | 701.96 |
| Hexyl methyl ether | 25 | 24.5 | 8.61 | 8.61 | .66 | 6.53 | 1.36 | .66 | .06 | .05 | 4 | 8.28 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ethyl propyl ether | 18 | 18.8 | 2.95 | 2.95 | .95 | 5.21 | 1.01 | .95 | .56 | .11 | 8 | 4.14 |
| Butyl propyl ether | 17.1 | 16.4 | 8.61 | 8.61 | .66 | 6.53 | 1.36 | .66 | .06 | .05 | 4 | 8.28 |
| Butyl isopropyl ether | 07 | 07.6 | 9.32 | 0.65 | .41 | 9.05 | 1.09 | .56 | .91 | .07 | 1.62 | 824.28 |
| Isobutyl propyl ether | 06 | 07.6 | 9.32 | 0.65 | .41 | 9.05 | 1.09 | .56 | .91 | .07 | 1.62 | 824.28 |
| Ethyl isopentyl ether | 11 | 10 | 9.32 | 0.65 | .41 | 9.05 | 1.09 | .56 | .91 | .07 | 1.62 | 824.28 |
| Tert-butyl propyl ether | 00 | 00.9 | 0.63 | 4.73 | .1 | 0.02 | 0.84 | .42 | .72 | .1 | 0.26 | 9948.75 |
| Tert-isobutyl propyl ether | 7.6 | 1.8 | 1.34 | 6.77 | .86 | 2.54 | 0.57 | .32 | .57 | .14 | 7.89 | 5983.61 |
| Ethyl 1-ethylbutyl ether | 05.5 | 03.8 | 9.4 | 0.5 | .47 | 8.31 | 1.15 | .58 | .97 | .07 | 7.25 | 644.38 |
| 2,2-dimethylpropyl ethyl ether | 1.5 | 03.4 | 0.63 | 4.73 | .1 | 0.02 | 0.84 | .42 | .72 | .109 | 0.26 | 9948.75 |
| Ethyl 2-ethyl butyl ether | 09.5 | 04.4 | 6.5 | 7.82 | .06 | 9.33 | 1.25 | .21 | .66 | .11 | 3.62 | 44.98 |
| Ethyl tert-pentyl ether | 01 | 9.4 | 7.95 | 1.66 | .82 | 3.29 | 0.73 | .09 | .55 | .13 | 0 | 250 |
| 1,2-dimethylpropyl ethyl ether | 9.3 | 02.3 | 0.19 | 2.39 | .26 | 9.52 | 0.93 | .49 | .84 | .09 | 7 | 019.8 |
| Dibutyl ether | 40.3 | 39.8 | 1.44 | 1.44 | .01 | 2.18 | 1.54 | .01 | .31 | .04 | 02 | 0 |
| Isopentyl propyl ether | 25 | 31.6 | 2.15 | 3.47 | .77 | 4.71 | 1.27 | .91 | .16 | .05 | 9.62 | 159.84 |
| Butyl isobutyl ether | 32 | 30.6 | 9.32 | 0.65 | .41 | 9.05 | 1.09 | .56 | .91 | .07 | 1.62 | 824.28 |
| Butyl sec-butyl ether | 30.5 | 29.8 | 2.23 | 3.33 | .82 | 3.96 | 1.32 | .93 | .22 | .05 | 5.25 | 651.02 |
| Butyl tert-butyl ether | 25 | 24.9 | 3.46 | 7.56 | .45 | 5.67 | 1.02 | .77 | .97 | .07 | 8.26 | 4635.41 |
| Sec-butyl isobutyl ether | 22 | 20.6 | 2.95 | 5.36 | .58 | 6.49 | 1.05 | .83 | .07 | .06 | 2.88 | 605.55 |
| di-sec-butyl ether | 21 | 19.7 | 3.03 | 5.21 | .63 | 5.75 | 1.11 | .85 | .12 | .06 | 8.51 | 250 |
| Diisobutyl ether | 22.2 | 21.3 | 2.87 | 5.51 | .52 | 7.23 | 0.99 | .82 | .01 | .07 | 7.25 | 000 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Isobutyl tert-butyl ether | 11.5 | 15.5 | 4.17 | 9.59 | .21 | 8.2 | 0.74 | .67 | .81 | .1 | 5.89 | 7812.75 |
| di-tert-butyl ether | 07.3 | 09 | 5.48 | 3.68 | .9 | 29.17 | 0.49 | .53 | .63 | .14 | 4052 | 9130 |
| Isopropyl tert-pentyl ether | 14.5 | 13.7 | 4.32 | 9.35 | .28 | 7.13 | 0.81 | .7 | .9 | .08 | 3.63 | 1294.37 |
| Hexyl ethyl ether | 43 | 14 | 1.44 | 1.44 | .01 | 2.18 | 1.54 | .01 | .31 | .041 | 02 | 0 |
| Heptyl methyl ether | 51 | 50.5 | 1.44 | 1.44 | .01 | 2.18 | 1.54 | .01 | .31 | .041 | 02 | 0 |
| 1-ethylpropyl propyl ether | 28.5 | 26.5 | 9.4 | 0.5 | .47 | 8.31 | 1.15 | .58 | .97 | .07 | 7.25 | 655.38 |
| Ethyl 1-methylpentyl ether | 25 | 31.9 | 2.23 | 3.33 | .82 | 3.96 | 1.32 | .93 | .22 | .05 | 5.25 | 651.02 |
| Ethyl heptyl ether | 66.6 | 68.3 | 4.27 | 4.27 | .36 | 7.84 | 1.72 | .36 | .56 | .02 | 10 | 6.56 |
| Butyl isopentyl ether | 57 | 52.8 | 4.98 | 6.3 | .12 | 0.36 | 1.44 | .27 | .41 | .03 | 7.62 | 4594.24 |
| Tert-butyl isopentyl ether | 39 | 37.9 | 7 | 2.42 | .56 | 03.85 | 0.92 | .03 | .07 | .07 | 3.89 | 87705.09 |
| Butyl pentyl ether | 63 | 62.5 | 4.27 | 4.27 | .36 | 7.84 | 1.72 | .36 | .56 | .02 | 10 | 6.56 |
| Isopropyl isopentyl ether | 39 | 43.7 | 2.87 | 5.51 | .52 | 7.23 | 0.99 | .82 | .01 | .07 | 7.25 | 000 |
| Methyl 1-methylheptyl ether | 62 | 60.7 | 5.06 | 6.15 | .17 | 9.62 | 1.5 | .28 | .47 | .03 | 03.25 | 3155.07 |
| Methyl octyl ether | 73 | 75.4 | 4.27 | 4.27 | .36 | 7.84 | 1.72 | .36 | .56 | .02 | 10 | 6.56 |
| 3,5-dimethylhexyl methyl ether | 55.5 | 55.2 | 5.78 | 8.19 | .93 | 2.14 | 1.23 | .19 | .32 | .04 | 0.88 | 0198.03 |
| Ethyl octyl ether | 89.2 | 91.6 | .72 | .81 | .02 | 3.5 | 1.89 | .72 | .81 | .02 | 18 | 0 |
| Ethyl 1,1,3,3-tetramethylbutyl ether | 56.5 | 55.4 | 8.46 | 6.26 | .33 | 33.75 | 0.73 | .91 | .95 | .08 | 0.27 | 88404.94 |
| bis(1-ethylpropyl) ether | 61.5 | 59.1 | 5.93 | 7.89 | .04 | 0.66 | 1.34 | .22 | .42 | .03 | 12.14 | 285.9 |
| bis(1-methylbutyl) ether | 62 | 63.3 | 8.68 | 0.87 | .34 | 7.06 | 1.46 | .56 | .62 | .03 | 04.51 | 6000 |
| Butyl 1-methylpentyl ether | 70 | 73.7 | 7.89 | 8.98 | .53 | 5.28 | 1.68 | .64 | .72 | .02 | 11.25 | 7208.17 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| diisopentyl ether | 72 | 63 | 8.52 | 1.17 | .23 | 8.54 | 1.35 | .52 | .51 | .03 | 3.25 | 2000 |
| dipentyl ether | 86.8 | 83.6 | .72 | .81 | .02 | 3.5 | 1.89 | .72 | .81 | .02 | 18 | 0 |
| Isopropyl heptyl ether | 73 | 76.7 | 7.81 | 9.13 | .47 | 6.02 | 1.62 | .62 | .66 | .02 | 5.62 | 1278.75 |
| heptyl propyl ether | 87 | 86.9 | .72 | .81 | .02 | 3.5 | 1.89 | .72 | .81 | .02 | 18 | 0 |
| Isopentyl pentyl ether | 74 | 73.3 | 7.81 | 9.13 | .47 | 6.02 | 1.62 | .62 | .66 | .02 | 5.62 | 1278.75 |
| methyl 1-methyloctyl ether | 88.5 | 83.8 | 7.89 | 8.98 | .53 | 5.28 | 1.68 | .64 | .72 | .02 | 11.25 | 7208.17 |
| octyl propyl ether | 04 | 08.8 | 9.92 | 9.92 | .07 | 9.15 | 2.07 | .07 | .06 | .01 | 26 | 13.13 |
| Isopropyl octyl ether | 98.5 | 97.8 | 0.64 | 1.96 | .83 | 1.68 | 1.8 | .97 | .91 | .01 | 03.62 | 16753.96 |
| dihexyl ether | 25.7 | 23.3 | 3.34 | 3.34 | .33 | 4.81 | 2.25 | .33 | .15 | .01 | 15 | 01.19 |
| diheptyl ether | 258.5 | 259.2 | 8.41 | 8.41 | 5.13 | 6.12 | .6 | .13 | .81 | .005 | 50 | 20 |
| dioctyl ether | 291.7 | 91.6 | 4.07 | 4.07 | .84 | 7.44 | .95 | .84 | .31 | .002 | 66 | 40 |
| bis(2-ethylhexyl) ether | 69.8 | 68.2 | 5.81 | 7.54 | .57 | 09.52 | .64 | .71 | .22 | .003 | 83.77 | 0816000 |
| acetaldehyde | 0.8 | 9. | .47 | .47 | .89 | .24 | .48 | .89 | .81 | .33 | 4 | |
| propionaldehyde | 8.8 | 0.6 | .3 | .3 | .24 | 3.9 | .66 | .24 | .06 | .23 | 2 | .07 |
| butyl aldehyde | 5.7 | 8.5 | 0.12 | 0.12 | .6 | 9.55 | .83 | .6 | .31 | .16 | 0 | 0 |
| pentaldehyde | 03 | 04.5 | 2.95 | 2.95 | .95 | 5.21 | .01 | .95 | .56 | .11 | 8 | 4.14 |
| 2-methyl butanal | 2.5 | 5.8 | 3.75 | 4.84 | .76 | 6.99 | .79 | .87 | .47 | .14 | 1.25 | 05.54 |
| 3-methyl butanal | 2.5 | 7.1 | 3.67 | 4.99 | .71 | 7.73 | .74 | .85 | .41 | .15 | 5.62 | 28.03 |
| 2,2-dimethyl propanal | 7.5 | 9 | 4.97 | 9.07 | .39 | 8.7 | .49 | .71 | .22 | .21 | 4.26 | 108.26 |
| Hexanal | 28 | 28.9 | 5.78 | 5.78 | .3 | 0.87 | .19 | .3 | .81 | .08 | 6 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-methylpentanal | 17 | 19.6 | 6.57 | 7.67 | .11 | 2.65 | .97 | .22 | .72 | .1 | 9.25 | 81.37 |
| 3-methylpentanal | 18 | 20.6 | 6.57 | 7.67 | .11 | 2.65 | .97 | .22 | .72 | .1 | 9.25 | 81.37 |
| 4-methylpentanal | 21 | 21.6 | 6.5 | 7.82 | .06 | 3.39 | .91 | .21 | .66 | .11 | 3.62 | 44.98 |
| 2-ethylbutaanal | 17 | 17.7 | 6.65 | 7.52 | .17 | 1.91 | .03 | .24 | .77 | .08 | 4.88 | 24.04 |
| heptanal | 52.8 | 51.8 | 8.61 | 8.61 | .66 | 6.53 | .36 | .66 | .06 | .05 | 4 | 8.28 |
| 2-methyl hexanal | 41 | 42.3 | 9.4 | 0.5 | .47 | 8.31 | .15 | .58 | .97 | .07 | 7.25 | 644.38 |
| 3-methyl hexanal | 43 | 43 | 6.57 | 7.67 | .11 | 2.65 | .97 | .22 | .72 | .1 | 9.25 | 81.37 |
| 4-methyl hexanal | 44 | 43.7 | 9.4 | 0.5 | .47 | 8.31 | .15 | .58 | .97 | .07 | 7.25 | 644.38 |
| 5-methyl hexanal | 43.5 | 44.2 | 9.32 | 0.65 | .41 | 9.05 | .09 | .56 | .91 | .07 | 1.62 | 824.28 |
| 2,2-dimethylpentanal | 26.5 | 31.8 | 0.78 | 4.49 | .18 | 8.95 | .9 | .44 | .8 | .09 | 8.009 | 8031.22 |
| 2,3-dimethylpentanal | 41 | 34.1 | 0.26 | 2.25 | .31 | 8.78 | .98 | .51 | .89 | .08 | 2.63 | 19.23 |
| octanal | 71 | 76.6 | 1.44 | 1.44 | .01 | 2.18 | .54 | .01 | .31 | .04 | 02 | 0 |
| 2-ethylhexanal | 60 | 61.1 | 2.31 | 3.18 | .88 | 3.22 | .38 | .95 | .27 | .04 | 10.88 | 192.37 |
| 2-propylpentanal | 60 | 60.2 | 2.31 | 3.18 | .88 | 3.22 | .38 | .95 | .27 | .04 | 10.88 | 192.37 |
| nonanal | 91 | 94.2 | 4.27 | 4.27 | .36 | 7.84 | .72 | .36 | .56 | .02 | 10 | 6.56 |
| 3,5,5-trimethyl hexanal | 70.5 | 66.7 | 7.08 | 2.27 | .62 | 03.11 | .98 | .04 | .12 | .06 | 9.52 | 73361.9 |
| decanal | 08.5 | 13.9 | 7.09 | 7.09 | .72 | 3.5 | .89 | .72 | .81 | .02 | 18 | 2 |
| undecanal | 33 | 32.7 | 9.92 | 9.92 | .07 | 9.15 | .07 | .07 | .06 | .01 | 26 | 13.13 |
| 2-methyl decanal | 29 | 21.7 | 0.72 | 1.81 | .88 | 0.94 | .85 | .99 | .97 | .01 | 19.25 | 05240.6 |
| dodecanal | 54 | 50.6 | 2.75 | 2.75 | .42 | 4.81 | .25 | .42 | .31 | .01 | 34 | 25984 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-methylundecanal | 46 | 39 | 3.55 | 4.64 | .24 | 6.59 | .03 | .35 | .22 | .01 | 27.25 | 97665.36 |
| tridecanal | 67 | 67.8 | 5.58 | 5.58 | .78 | 0.47 | .42 | .78 | .56 | .007 | 42 | 26.27 |
| tetradecanal | 87 | 84.2 | 8.41 | 8.41 | .13 | 6.12 | .6 | .13 | .81 | .005 | 50 | 20 |
| pentadecanal | 04.9 | 99.9 | 1.24 | 1.24 | .49 | 1.78 | .78 | .49 | .06 | .003 | 58 | 52.54 |
| acetone | 6.2 | 7.4 | .93 | .48 | .94 | 7.16 | .33 | .13 | .86 | .35 | 4 | 1.62 |
| 2-butanone | 9.6 | 5.4 | 0.84 | 2.16 | .35 | 2.08 | .56 | .5 | .16 | .22 | 7.62 | 0.62 |
| 2-pentanone | 02 | 00.4 | 3.67 | 4.99 | .71 | 7.73 | .74 | .85 | .41 | .15 | 5.62 | 28.03 |
| 3-pentanone | 01.7 | 8.3 | 3.75 | 4.84 | .76 | 6.99 | .79 | .87 | .47 | .14 | 1.25 | 05.54 |
| 3-methyl-2-butanone | 3.5 | 2.7 | 4.45 | 6.89 | .5 | 8.94 | .52 | .77 | .29 | .2 | 5.375 | 41.42 |
| 2-hexanone | 27 | 25.2 | 6.5 | 7.82 | .06 | 3.39 | .91 | .21 | .66 | .11 | 3.62 | 44.98 |
| 3-hexanone | 23.5 | 22.2 | 6.57 | 7.67 | .11 | 2.65 | .97 | .22 | .72 | .1 | 9.25 | 81.37 |
| 3-methyl-2-pentanone | 18 | 16 | 3.67 | 4.99 | .71 | 7.73 | .74 | .85 | .41 | .15 | 5.62 | 28.03 |
| 4-metyl-2-pentanone | 17 | 17.4 | 7.21 | 9.86 | .81 | 5.91 | .64 | .11 | .51 | .15 | 1.25 | 00 |
| 2-methyl-3-pentanone | 15.5 | 14.5 | 7.36 | 9.57 | .9 | 3.86 | .75 | .14 | .59 | .12 | 9.004 | 60.55 |
| 3,3-dimethyl-2-butanone | 06 | 07.3 | 8.65 | 3.69 | .56 | 4.56 | .46 | .98 | .35 | .19 | 2.63 | 134.64 |
| 2-heptanone | 51.4 | 48.5 | 9.32 | 0.65 | .41 | 9.05 | .09 | .56 | .91 | .07 | 1.62 | 824.28 |
| 3-heptanone | 47 | 45.4 | 7.4 | 0.5 | .47 | 8.31 | .15 | .58 | .97 | .07 | 7.25 | 644.38 |
| 4-heptanone | 44 | 44.4 | 9.4 | 0.5 | .47 | 8.31 | .15 | .58 | .97 | .07 | 7.25 | 644.38 |
| 3-methyl-2-hexanone | 43.5 | 39.5 | 0.19 | 2.39 | .26 | 9.52 | .93 | .49 | .84 | .09 | 7.004 | 019.8 |
| 4-methyl-2-hexanone | 39 | 39.7 | 0.12 | 2.53 | .22 | 0.83 | .87 | .48 | .82 | .09 | 4.88 | 274.75 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 5-methyl-2-hexanone | 44 | 40.5 | 0.04 | 2.68 | .17 | 1.57 | .82 | .46 | .76 | .1 | 9.25 | 414.21 |
| 2-methyl-3-hexanone | 35 | 34.2 | 0.19 | 2.39 | .26 | 9.52 | .93 | .49 | .84 | .09 | 7.004 | 019.8 |
| 4-methyl-3-hexanone | 34.5 | 36.4 | 0.26 | 2.25 | .31 | 8.78 | .98 | .51 | .89 | .08 | 2.63 | 19.23 |
| 5-methyl-3-hexanone | 35 | 37.3 | 0.12 | 2.53 | .22 | 0.83 | .87 | .48 | .82 | .09 | 4.88 | 274.75 |
| 2,2-dimethyl-3-pentanone | 25.6 | 27.4 | 1.55 | 6.37 | .96 | 9.47 | .69 | .35 | .65 | .12 | 6.26 | 2636.15 |
| 2,4-dimethyl-3-pentanone | 25.4 | 28.8 | 0.97 | 4.29 | .05 | 0.73 | .7 | .4 | .71 | .11 | 6.75 | 32.45 |
| 4,4-dimethyl-2-pentanone | 26.4 | 30.6 | 1.34 | 6.77 | .86 | 2.54 | .57 | .32 | .57 | .14 | 7.89 | 5983.61 |
| 2-octanone | 72.5 | 70.7 | 2.15 | 3.47 | .77 | 4.71 | .27 | .91 | .16 | .05 | 9.62 | 159.84 |
| 3-octanone | 67.5 | 67.6 | 2.23 | 3.33 | .82 | 3.96 | .32 | .93 | .22 | .05 | 5.25 | 651.02 |
| 4-octanone | 65.5 | 66.1 | 2.23 | 3.33 | .82 | 3.96 | .32 | .93 | .22 | .05 | 5.25 | 651.02 |
| 2-methyl-4-heptanone | 54 | 57.8 | 2.95 | 5.36 | .58 | 6.49 | .05 | .83 | .07 | .06 | 2.88 | 605.55 |
| 3-methyl-4-heptanone | 53 | 57.2 | 3.09 | 5.07 | .67 | 4.43 | .16 | .86 | .14 | .05 | 0.63 | 600 |
| 3-methyl-2-heptanone | 64 | 61.1 | 3.01 | 5.22 | .61 | 5.17 | .1 | .84 | .09 | .06 | 5 | 884.44 |
| 4-methyl-2-heptanone | 60.5 | 61.6 | 2.95 | 5.36 | .58 | 6.49 | .05 | .83 | .07 | .06 | 2.88 | 605.55 |
| 5-methyl-2-heptanone | 66.5 | 61.9 | 2.95 | 5.36 | .58 | 6.49 | .05 | .83 | .07 | .06 | 2.88 | 605.55 |
| 6-methyl-2-heptanone | 67 | 62.2 | 2.87 | 5.51 | .52 | 7.23 | .99 | .82 | .01 | .07 | 7.25 | 000 |
| 2-methyl-3-heptanone | 58 | 58.3 | 3.01 | 5.22 | .61 | 5.17 | .1 | .84 | .09 | .06 | 5 | 8844.44 |
| 5-methyl-3-heptanone | 61 | 58.6 | 3.03 | 5.21 | .63 | 5.75 | .11 | .85 | .12 | .06 | 8.51 | 250 |
| 6-methyl-3-heptanone | 63.2 | 59 | 2.95 | 5.36 | .58 | 6.49 | .05 | .83 | .07 | .06 | 2.88 | 605 |
| 3,3-dimethyl-2-hexanone | 51.5 | 50.3 | 4.45 | 9.1 | .36 | 4.8 | .88 | .72 | .93 | .08 | 6.37 | 1000 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4,4-dimethyl-2-hexanone | 54.4 | 51.3 | 0.78 | 4.49 | .18 | 8.95 | .9 | .44 | .8 | .094 | 8.009 | 8031.22 |
| 5,5-dimethyl-2-hexanone | 46 | 52 | 4.17 | 9.59 | .21 | 8.2 | .74 | .67 | .82 | .1 | 5.89 | 7812.74 |
| 2,2-dimethyl-3-hexanone | 46 | 47.8 | 4.38 | 9.2 | .32 | 5.13 | .87 | .7 | .9 | .08 | 4.26 | 3610.67 |
| 2,4-dimethyl-3-hexanone | 45 | 49.3 | 0.26 | 2.25 | .31 | 8.78 | .98 | .51 | .89 | .08 | 2.63 | 19.23 |
| 2,5-dimethyl-3-hexanone | 47.5 | 49.8 | 3.73 | 7.26 | .37 | 7.7 | .83 | .75 | .94 | .08 | 2.63 | 236.06 |
| 4,4-dimethyl-3-hexanone | 48 | 47.7 | 4.53 | 8.95 | .39 | 4.06 | .93 | .73 | .98 | .07 | 2 | 8457.45 |
| 4,5-dimethyl-3-hexanone | 52 | 50.4 | 3.88 | 6.97 | .46 | 5.64 | .94 | .77 | .01 | .07 | 0.37 | 612.45 |
| 5,5-dimethyl-3-hexanone | 46.5 | 48.7 | 4.25 | 9.45 | .26 | 7.46 | .8 | .69 | .87 | .09 | 1.52 | 4432.01 |
| 3-ethyl-3-methyl-2-pentanone | 53.8 | 49.6 | 4.6 | 8.86 | .41 | 3.73 | .94 | .74 | .01 | .07 | 4.12 | 6097.92 |
| 3-ethyl-4-methyl-2-pentanone | 54 | 50.8 | 3.88 | 6.97 | .46 | 5.64 | .94 | .77 | .01 | .07 | 0.37 | 612.45 |
| 2,2,4-trimethyl-3-pentanone | 35.1 | 39.9 | 5.16 | 1.09 | .11 | 06.34 | .65 | .62 | .78 | .11 | 4 | 9650.47 |
| 2-nonanone | 95 | 91.8 | 4.98 | 6.3 | .12 | 0.36 | .44 | .27 | .41 | .03 | 7.62 | 4594.24 |
| 3-nonanone | 90 | 88.8 | 5.06 | 6.15 | .17 | 9.62 | .5 | .28 | .47 | .03 | 03.25 | 3155.07 |
| 4- nonanone | 87.5 | 87.1 | 5.06 | 6.15 | .28 | 9.62 | .5 | .28 | .47 | .03 | 03.25 | 3155.07 |
| 5- nonanone | 88.4 | 86.5 | 5.06 | 6.15 | .17 | 9.62 | .5 | .28 | .47 | .03 | 03.25 | 3155.07 |
| 4-methyl-2-octanone | 84 | 82.6 | 5.78 | 8.19 | .93 | 2.14 | .23 | .19 | .32 | .04 | 0.88 | 0198.03 |
| 5-methyl-3-octanone | 79 | 79.6 | 5.85 | 8.04 | .98 | 1.4 | .28 | .2 | .37 | .04 | 6.51 | 192.38 |
| 7-methyl-3-octanone | 82.5 | 79.6 | 5.78 | 8.17 | .93 | 2.14 | .23 | .19 | .32 | .04 | 0.88 | 0198.03 |
| 3-methyl-4-octanone | 74 | 77.7 | 5.92 | 7.9 | .02 | 0.09 | .34 | .21 | .39 | .04 | 8.63 | 353.91 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2,5-dimethyl-3-heptanone | 66 | 69.8 | 6.64 | 9.94 | .77 | 2.61 | .06 | .12 | .24 | .05 | 6.26 | 700.87 |
| 2,6-dimethyl-3-heptanone | 71.5 | 69.8 | 6.56 | 0.09 | .72 | 3.35 | .01 | .1 | .19 | .06 | 0.63 | 324.55 |
| 3,3-dimethyl-2-heptanone | 73.5 | 71 | 7.28 | 1.93 | .69 | 00.46 | .05 | .07 | .18 | .05 | 4.37 | 16374.67 |
| 4,6-dimethyl-2-heptanone | 73 | 75.8 | 6.49 | 0.23 | .69 | 4.67 | .95 | .09 | .17 | .06 | 8.51 | 905.69 |
| 4,6-dimethyl-3-heptanone | 71.5 | 70.6 | 6.64 | 9.94 | .77 | 2.61 | .06 | .12 | .24 | .05 | 6.26 | 700.87 |
| 7-methyl-4-octanone | 78 | 78 | 5.78 | 8.19 | .93 | 2.14 | .23 | .19 | .32 | .04 | 0.88 | 0198.03 |
| 2,3-dimethyl-4-heptanone | 67.5 | 69.9 | 6.71 | 9.8 | .81 | 1.3 | .11 | .13 | .26 | .05 | 8.37 | 560.7 |
| 2,6-dimethyl-4-heptanone | 69.4 | 69.9 | 6.49 | 0.23 | .69 | 4.67 | .95 | .09 | .17 | .06 | 8.51 | 905.69 |
| 3,5-dimethyl-4-heptanone | 62 | 68.8 | 6.78 | 9.65 | .86 | 0.56 | .17 | .14 | .31 | .04 | 4 | 110.96 |
| 2,2,4,4-tetramethyl-3-pentanone | 52 | 49.2 | 9.36 | 7.9 | .17 | 41.95 | .59 | .83 | .84 | .1 | 1.26 | 09858.01 |
| 2-decanone | 10 | 11.8 | 7.81 | 9.13 | .47 | 6.02 | .62 | .62 | .66 | .02 | 5.62 | 1278.75 |
| 3-decanone | 11 | 09.1 | 7.89 | 8.98 | .53 | 5.28 | .68 | .64 | .72 | .02 | 11.25 | 7208.17 |
| 4-decanone | 06.5 | 07.3 | 7.89 | 8.98 | .53 | 5.28 | .68 | .64 | .72 | .02 | 11.25 | 7208.17 |
| 5-decanone | 04 | 06.4 | 7.89 | 8.98 | .53 | 5.28 | .68 | .64 | .72 | .02 | 11.25 | 7208.17 |
| 2-undecanone | 31.5 | 30.8 | 0.64 | 1.96 | .83 | 1.68 | .8 | .97 | .91 | .01 | 03.62 | 16753.96 |
| 3-undecanone | 27 | 28.4 | 0.72 | 1.81 | .88 | 0.94 | .85 | .99 | .97 | .01 | 19.25 | 05240.63 |
| 5-undecanone | 27 | 25.5 | 0.72 | 1.81 | .88 | 0.94 | .85 | .99 | .97 | .01 | 19.25 | 05240.6 |
| 6-undecanone | 26 | 25.2 | 0.72 | 1.81 | .88 | 0.94 | .85 | .99 | .97 | .01 | 19.25 | 05240.6 |
| 2,2,6,6-tetramethyl-4-heptanone | 85 | 81 | 4.76 | 4.05 | .77 | 57.92 | .8 | .51 | .28 | .06 | 1.78 | 856308.51 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-dodecanone | 46.5 | 49 | 3.47 | 4.79 | .18 | 7.33 | .97 | .33 | .16 | .01 | 11.62 | 30250.07 |
| 2-methyl-3-undecanone | 33.5 | 35.1 | 4.33 | 6.54 | .03 | 7.8 | .81 | .26 | .09 | .01 | 07 | 84604.22 |
| 2-tridecanon | 63 | 66.1 | 6.3 | 7.62 | .53 | 2.99 | .15 | .68 | .41 | .009 | 19.62 | 34031.7 |
| 7-tridecanon | 61 | 60.7 | 6.37 | 7.47 | .59 | 2.25 | .21 | .7 | .47 | .088 | 35.25 | 41924.8 |
| 2-methyl-3-tridecanone | 67 | 68 | 9.99 | 2.19 | .73 | 9.12 | .16 | .96 | .59 | .008 | 23.004 | 476833.8 |
| 7-ethyl-2-methyl-4-undecanone | 52.5 | 55.7 | 5.06 | 0.8 | .64 | 47.43 | .89 | .12 | .63 | .008 | 30.64 | 043598026 |
| 2-pentadecanone | 94 | 98.7 | 8.82 | 9.33 | .006 | 4.3 | .5 | .06 | .69 | .006 | 31 | 9889001.46 |
| 8-pentadecanone | 91 | 93.4 | 2.03 | 3.12 | .3 | 3.56 | .56 | .41 | .97 | .004 | 51.25 | 795938.43 |

## 3. Results and Discussion

### 3.1. Intercorrelation between molecular descriptors

For 192 oxo chemicals, the logarithmic, linear, quadratic, and multilinear regression models are examined. The intercorrelation between molecular descriptors and boiling points(Exp, Calcd) are recorded below. It is considered that a pair of molecular descriptors with $r \geq 0.97$ are highly intercorrelated, those with $r > 0.9$ appreciably intercorrelated, those with $r < 0.9$ weakly intercorrelated, and molecular descriptors with $r < 0.5$ not intercorrelated, [22]. In the case of Linear, quadratic, and logarithmic regression the model quality was measured by correlation coefficient (r), and in the case of multilinear regression, the model quality was measured by correlation coefficient (r) and standard error of estimate (s).

**Table 3:** Intercorrelation between Molecular Descriptors

| | GNI | SLI | MSLI | FSLI | MFSLI | SCGI | PCGI | MASCI | SAI | RSI |
|---|---|---|---|---|---|---|---|---|---|---|
| GNI | 1 | 0.847 | **0.923** | 0.710 | 0.676 | 0.878 | 0.840 | -0.707 | 0.037 | 0.219 |
| SLI | | 1 | 0.700 | 0.754 | 0.426 | 0.672 | 0.618 | -0.520 | 0.076 | 0.209 |
| MSLI | | | 1 | 0.398 | 0.834 | 0.883 | 0.888 | -0.728 | -0.046 | 0.153 |
| FSLI | | | | 1 | 0.152 | 0.580 | 0.558 | -0.477 | 0.045 | 0.130 |
| MFSLI | | | | | 1 | -0.036 | -0.035 | 0.022 | -0.012 | 0.004 |
| SCGI | | | | | | 1 | **0.993** | -0.828 | -0.019 | 0.185 |
| PCGI | | | | | | | 1 | -0.832 | -0.046 | 0.171 |
| MASCI | | | | | | | | 1 | 0.067 | -0.085 |
| SAI | | | | | | | | | 1 | -0.004 |
| RSI | | | | | | | | | | 1 |

From Table 3 it is observed that

- GNI is appreciably intercorrelated with MSLI and it is weakly intercorrelated with SLI, FSLI, MFSLI, SCGI and PCGI. Further there is no intercorrelation between GNI with MASCI, SAI and RSI.
- SLI is weakly intercorrelated with GNI, MSLI, FSLI, SCGI and PCGI. Further there is no intercorrelation between SLI with MFSLI, MASCI, SAI and RSI.
- MSLI is appreciably intercorrelated with GNI and it is weakly intercorrelated with MFSLI, SCGI and PCGI. Further there is no intercorrelation between MSLI with FSLI, MASCI, SAI and RSI.
- FSLI is weakly intercorrelated with GNI, SLI, SCGI and PCGI. Further there is no intercorrelation between FSLI with MSLI, MFSLI, MASCI, SAI and RSI.
- MFSLI is weakly intercorrelated with GNI, MSLI. Further there is no intercorrelation between MFSLI with SLI, FSLI, SCGI, PCGI, MASCI, SAI and RSI.
- SCGI is Highly intercorrelated with PCGI and it is weakly intercorrelated with GNI, SLI, MSLI, FSLI. Further there is no intercorrelation between SCGI with MASCI, SAI and RSI.
- IPCGI is Highly intercorrelated with SCGI and it is weakly intercorrelated with GNI, SLI, MSLI, FSLI. Further there is no intercorrelation between PCGI with MFSLI, MASCI, SAI and RSI.
- There is no intercorrelation between MASCI and other 9 molecular descriptors.
- There is no intercorrelation between SAI and other 9 molecular descriptors.
- There is no intercorrelation between RSI and other 9 molecular descriptors.

### 3.2. Hierarchial Analysis of Molecular Descriptors

To make our claim much stronger the Hierarchial cluster analysis between these molecular descriptors conducted and it is shown in Figure 1. The dendogram shows that these molecular descriptors are less intercorrelated

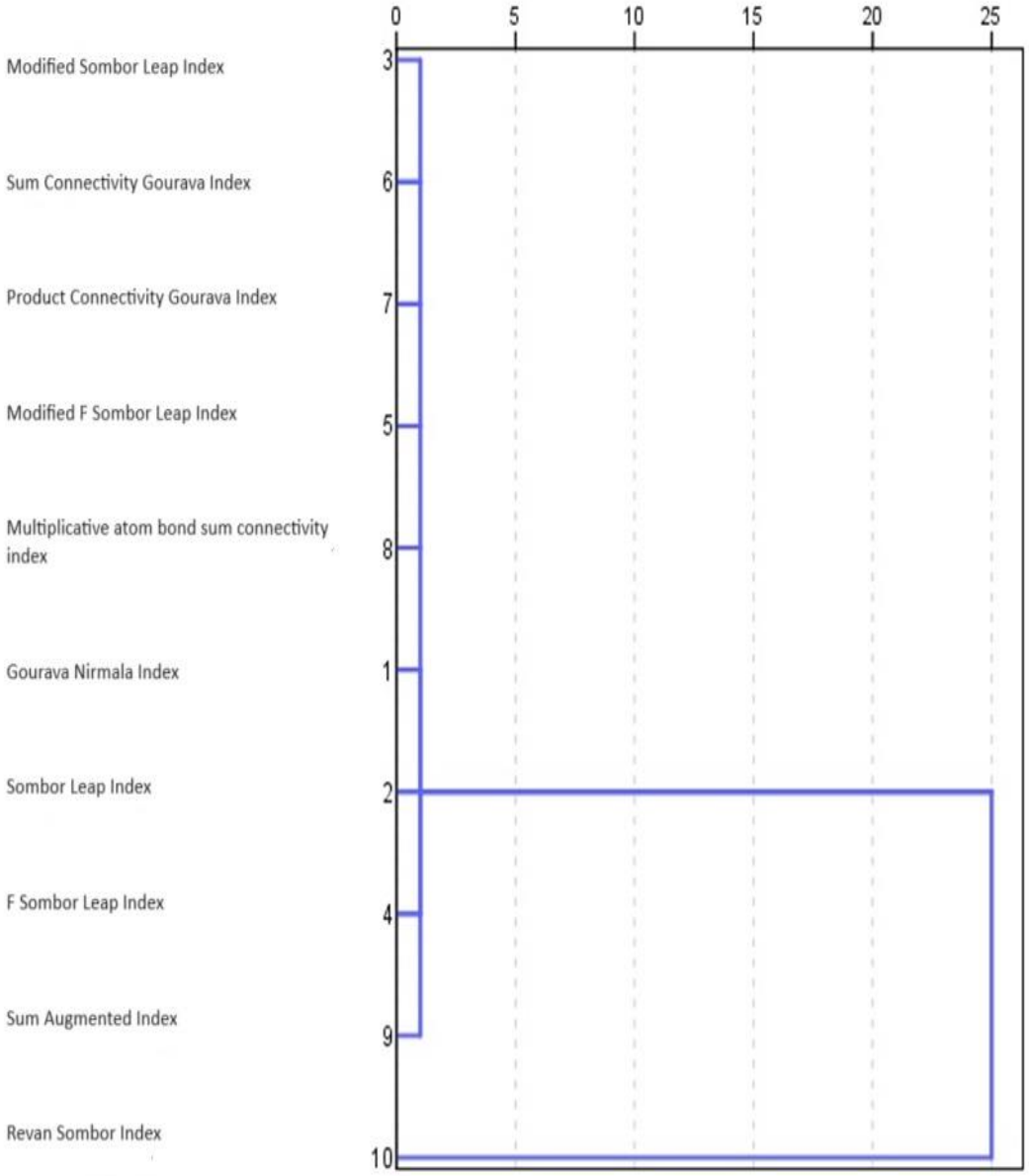


**Figure 1:** Dendograpm of Molecular Descriptors

### 3.3. Intercorrelation between Molecular Descriptors and Boiling Points

**Table 4:** Intercorrelation between Molecular Descriptors and Boiling Points of Oxo-organic compounds

| | GNI | SLI | MSLI | FSLI | MFSLI | SCGI | PCGI | MASCI | SAI | RSI |
|---|---|---|---|---|---|---|---|---|---|---|
| Exp | 0.852 | 0.053 | 0.847 | 0.524 | 0.845 | **0.952** | **0.942** | -0.826 | -0.041 | 0.136 |
| Calcd | 0.853 | 0.048 | 0.846 | 0.529 | 0.852 | **0.952** | **0.942** | -0.826 | -0.039 | 0.140 |

The correlation coefficient for BP(Exp) ranges from -0.826 to 0.952.
The correlation coefficient for BP(Calcd) ranges from -0.826 to 0.952.

### 3.4. Regression models for experimental data

The Linear regression model is formulated as

$$\boldsymbol{PP = a(MD) + b}.$$

The Quadratic regression model is formulated as

$$\boldsymbol{PP = a(MD)^2 + b(MD) + c}.$$

The Logarithmic regression model is formulated as

$$PP = aln(MD) + b.$$

The Multilinear regression model is formulated as

$$PP = a_0 + a_1(MD_1) + a_2(MD_2) + \cdots + a_n(MD_n)$$

The best Linear Correlation for exp is obtained by Sum Connectivity Gourava Index (SCGI).

$$exp = +61.001(SCGI) + (-28.645) \quad (2.1)$$
$$n = 192 \qquad r = 0.951 \qquad F = 1814.004.$$

The Quadratic correlation with Sum Connectivity Gourava Index gives most improoved model

$$exp = -4.465(SCGI)^2 + 90.153(SCGI) + (-71.930) \quad (2.2)$$
$$n = 192 \qquad r = 0.956 \qquad F = 1010.513.$$

The Logarithmic correlation with Sum Connectivity Gourava Index gives most improoved model

$$exp = 172.372(SCGI) + (-26.894) \quad (2.3)$$
$$n = 192 \qquad r = 0.943 \qquad F = 1542.852.$$

The Multilinear regression is

$$exp = 0.203(GNI) + (-43.075)(MFSLI) + 11.415(SCGI) + 97.552(PCGI) + (-46.310) \quad (2.4)$$
$$n = 192 \qquad r = 0.954 \qquad s = 17.5867 \qquad F = 463.646.$$

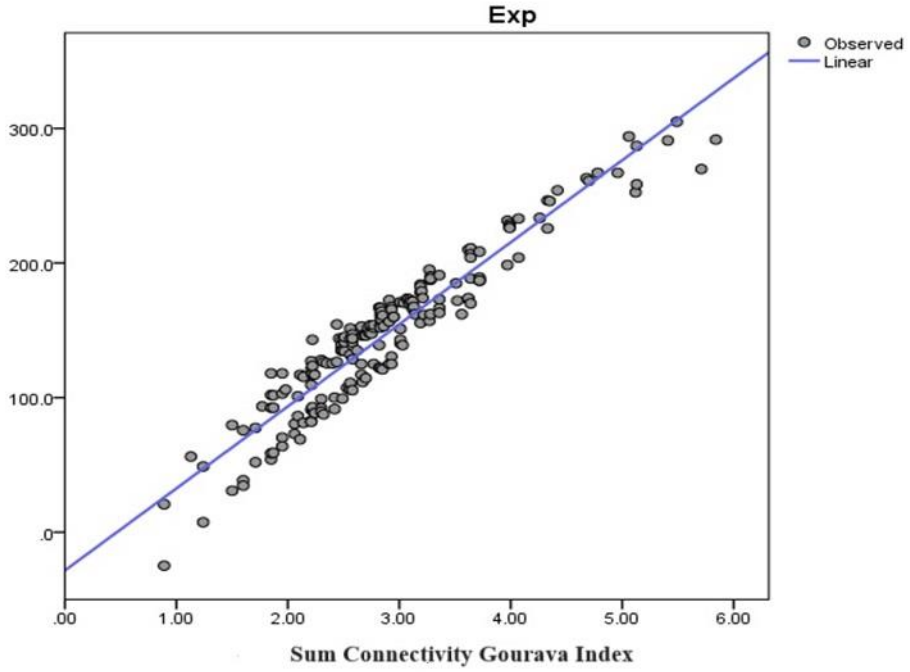


**Figure 2:** Linear regression for experimental boiling point

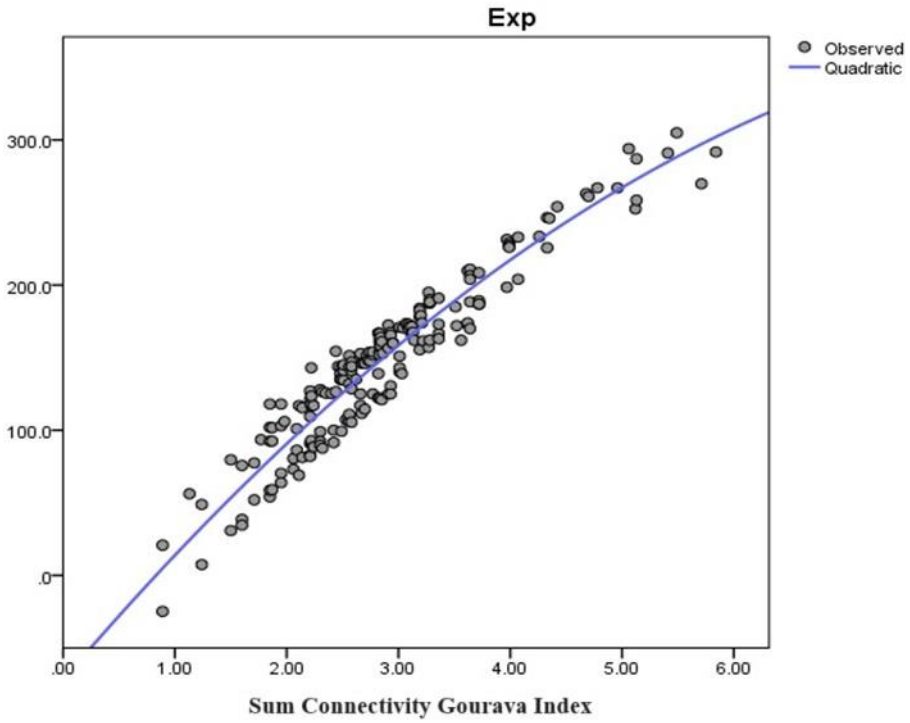


**Figure 3:** Quadratic regression for experimental boiling point

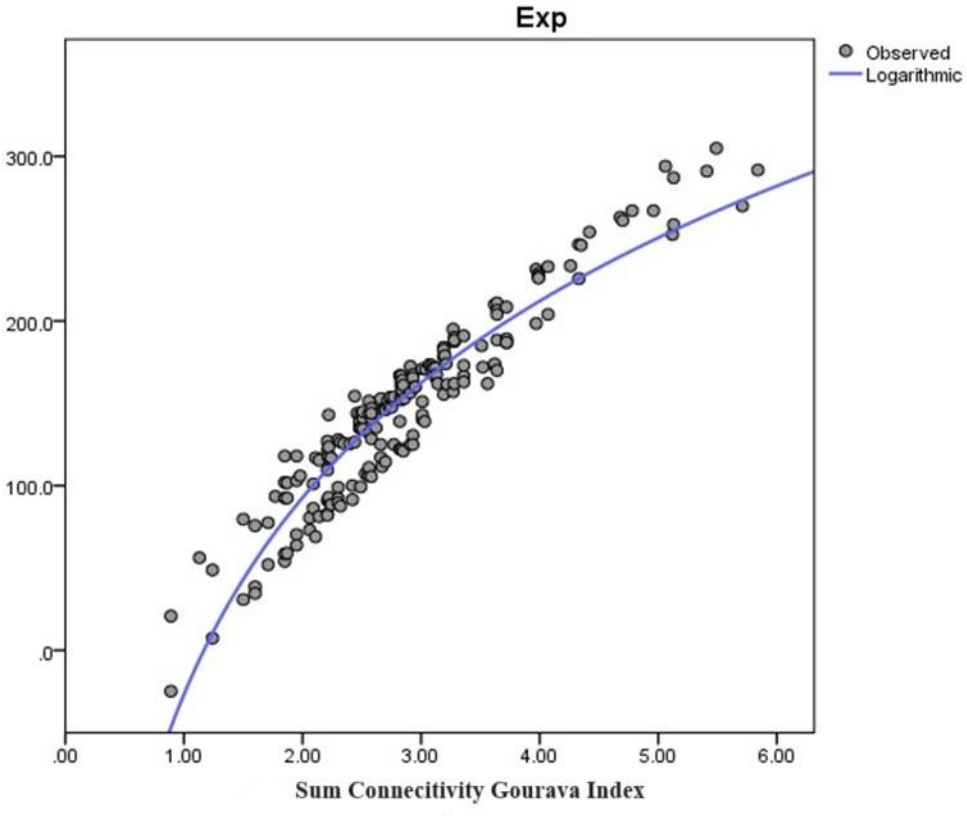


**Figure 4:** Logarithmic regression for experimental boiling point

### 3.5. Regression models for calculated data

The best Linear Correlation for calcd is obtained by Sum Connectivity Gourava Index

$$calcd = 61.021(\pm 1.431)(SCGI) + (-28.916) \quad (2.5)$$
$$n = 192 \qquad r = 0.951 \qquad F = 1817.978.$$

The Quadratic correlation with Sum Connectivity Gourava Index gives most improoved model

$$calcd = (-4.486)(SCGI)^2 + 90.312(SCGI) + (-72.408) \quad (2.6)$$
$$n = 192 \qquad r = 0.956 \qquad F = 1014.004.$$

The Logarithmic correlation with Sum Connectivity Gourava Index gives

$$calcd = 172.490(SCGI) + (-27.227) \quad (2.7)$$
$$n = 192 \qquad r = 0.944 \qquad F = 1556.094.$$

The multilinear Regression

$$calcd = 0.220(GNI) + (-34.399)(MFSLI) + 24.942(SCGI) + (-110.193)(MASCI) + 63.826(PCGI) + (-15.952). \quad (2.8)$$
$$n = 192 \qquad r = 0.956 \qquad s = 17.1902 \qquad F = 389.972.$$

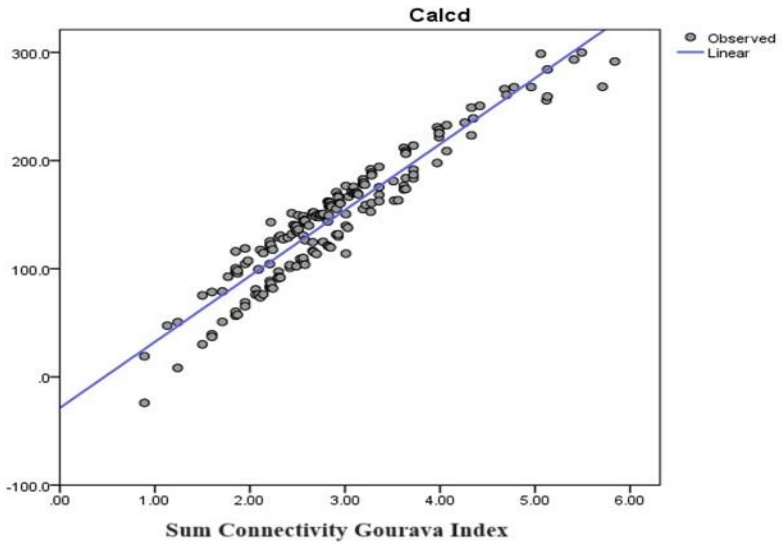


**Figure 5:** Linear regression for calculated boiling point

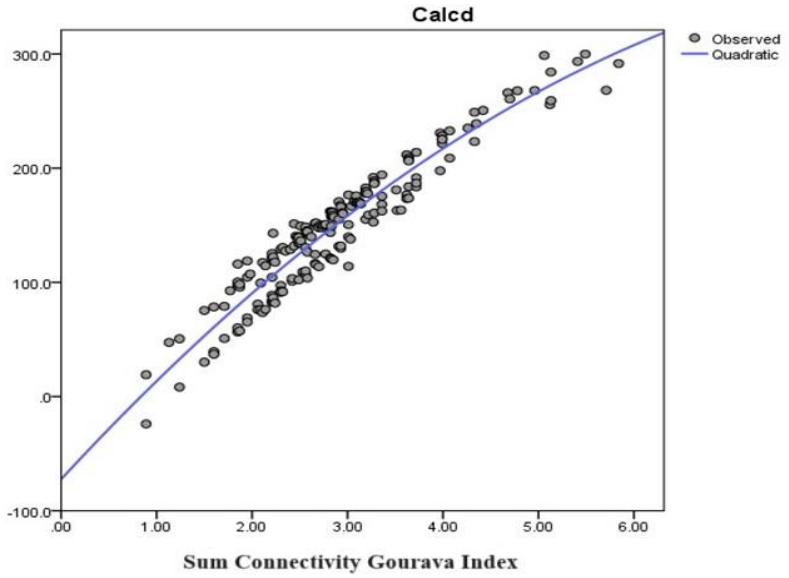


**Figure 6:** Quadratic regression for calculated boiling point

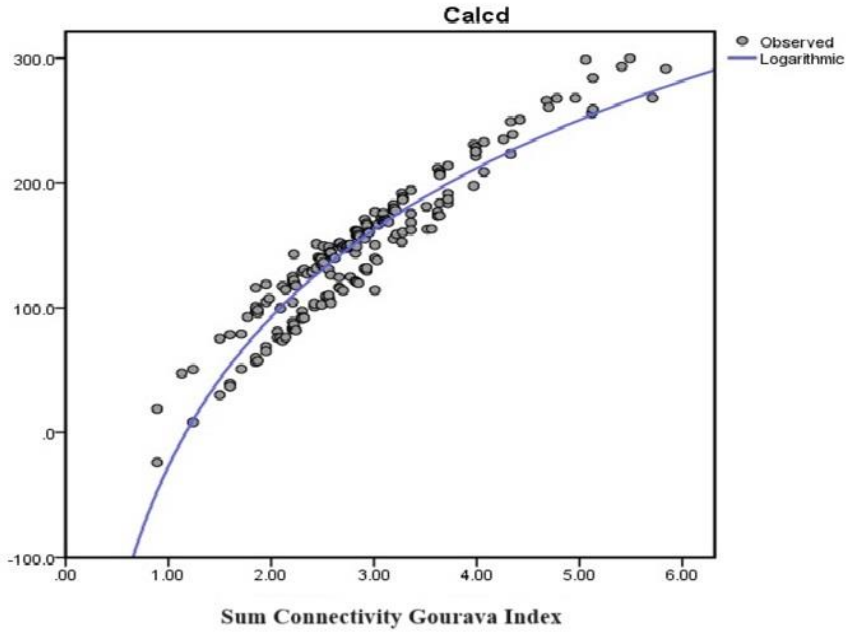


**Figure 7:** Logarithmic regression for calculated boiling point

## 4 Conclusions

It is found in this study that the molecular descriptor Sum Connectivity Gourava Index (SCGI) has finest linear, multilinear, quadratic, logarithmic models with the calcd boiling point of oxo organic compound with correlation coefficient 0.951, 0.956, 0.956, 0.944, respectively. This molecular decriptor (SCGI) has best linear, multilinear, quadratic and logarithmic model for exp boiling point with correlation coefficient 0.951, 0.954, 0.956, 0.943, respectively.

The study of intercorrelation between molecular descriptors shows that Sum Connectivity Gourava Index and Product Connectivity Gourava Index are highly intercorrelated with correlation coefficient r=0.993.

Thus the final conclusion of the study is that molecular descriptor Sum Connectivity Gourava Index quality exceeds in comparison with other 9 molecular descriptors, Sum

Augmented Index and Revan Sombor Index are not suggested for this analysis as their correlation coefficient is very low with calcd and exp boiling point

## 5 Data and Software Availability statement

For this study we have user IBM-SPSS software which is available at https://www.ibm.com/spss. The data set used in this work is presented in the form of Table 1 and 2, also the regression model figures are obtained from the same software.

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