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Chemistry

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## Global Journal of Science Frontier Research

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# Cooperativity of Three Fragments: Protonated or Methylated Makaluvamine, Water Molecule and Glutamic Acid Molecule in Twelve Complexes and their Stabilities. A Study Performed at B3LYP/6-31+G(d,p) Level

By Soleymane Koné, Sékou Diomandé & El-Hadji Sawaliho Bamba

*Université Félix Houphouët-BOIGNY*

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*Keywords: makaluvamines, complexes, fragment (body), energy of cooperativity, energy of interaction, hydrogen bond (HB), DFT.*

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Soleymane Koné [α], Sékou Diomandé [σ] & El-Hadji Sawaliho Bamba [ρ]

*Abstract-* Makaluvamines are used by intercalation in the DNA for the treatment of cancer cells such as colon cancer, prostate cancer, breast cancer.... This work studies energetic and geometrical parameters of stability of the 3-body complexes formed by six Makaluvamines, first protonated and then methylated by interactions with a water molecule and a glutamic acid molecule (Glu. Ac), a protein residue of topoisomerase II. This study was carried out by the quantum chemistry method of density functional theory (DFT). Firstly, we determined the energy of each super-molecule, the energies of all units of two fragments and one fragment in the geometries of the complexes. We have also determined the energies of 2-body and 3-body interaction, cooperativity, relaxation and total interaction. The results of these calculations helped to appreciate the rigidity of each fragment between the isolated and complex states. They also allowed knowing the stability of each complex and the contribution of each interaction term to this stability. These calculations were used to consider the form (protonated or methylated) of these Makaluvamines suitable for docking. In a second step, we studied the interactions between the three bodies by using hydrogen bond (HB) parameters. This analysis shows in which cases the hydrogen bonds formed are stronger. All theoretical calculations were performed at B3LYP/6-31+G(d,p). The BSSE correction was taken into account for the total interaction and cooperativity energies of the three fragments.

*Keywords: makaluvamines, complexes, fragment (body), energy of cooperativity, energy of interaction, hydrogen bond (HB), DFT.*

## I. Introduction

In the challenge of fighting cancer, one of the real causes of mortality worldwide [1,2], Makaluvamines represents a "green gold mine" for the scientific community. Indeed, the search for molecules that are "candidates for ideal drugs" against cancer conducted the study of extracts from marine plant organisms. They had found to contain compounds with unique pharmacological properties [3,4]. Makaluvamines are alkaloids extracted from marine algae with anticancer activities [5].

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In previous work, we have studied the hydrogen bond interactions of charged Makaluvamines with an $H_2O$ molecule and with a glutamic acid molecule (Glu Ac.) [6]. This work permitted to elucidate the geometric and energetic parameters of the interactions between two fragments, Makaluvamines charged with an $H_2O$ molecule or with the molecule of Glu Ac. using the density functional theory (B3LYP).

The current study, a continuation of the previous work, focuses on the formation of 3-body complexes between the charged (protonated or methylated) Makaluvamines and the two molecules of $H_2O$ and Glu Ac. Concerning super-molecule with more than two bodies, the cooperativity of the different fragments is very determining for its stability by interactions.

The goal of our study was to determine the energy contributions of each 2-body and 3-body interaction term to the stabilization of super-molecules. It will also allow us to discover in which form, protonated or methylated, the docking of Makaluvamines would give more stable complexes. Moreover, the calculations of the relaxation energies of the different bodies of each complex will allow us to discuss the degree of distortion of the geometry of each fragment between the isolated and complex states. The analysis of the geometric parameters of interactions in these three-body complexes was carried out by applying a hydrogen bond (HB) criteria. All theoretical calculations in this work were done in the gas phase with the B3LYP functional associated with 6-31+G (d,p) basis set.

## II. Studied Makaluvamines and Methods of Calculation

### a) Studied Makaluvamines

This work has focused on twelve three-body complexes: protonated (or methylated) Makaluvamine + one molecule of $H_2O$ + one molecule of Glu Ac. Six Makaluvamines I, A, C, H, O, and N are involved in the formation of the complexes. The protonated ($XH^+$) and methylated ($X^x$) 2D structures of these alkaloids were reported in figure 1.

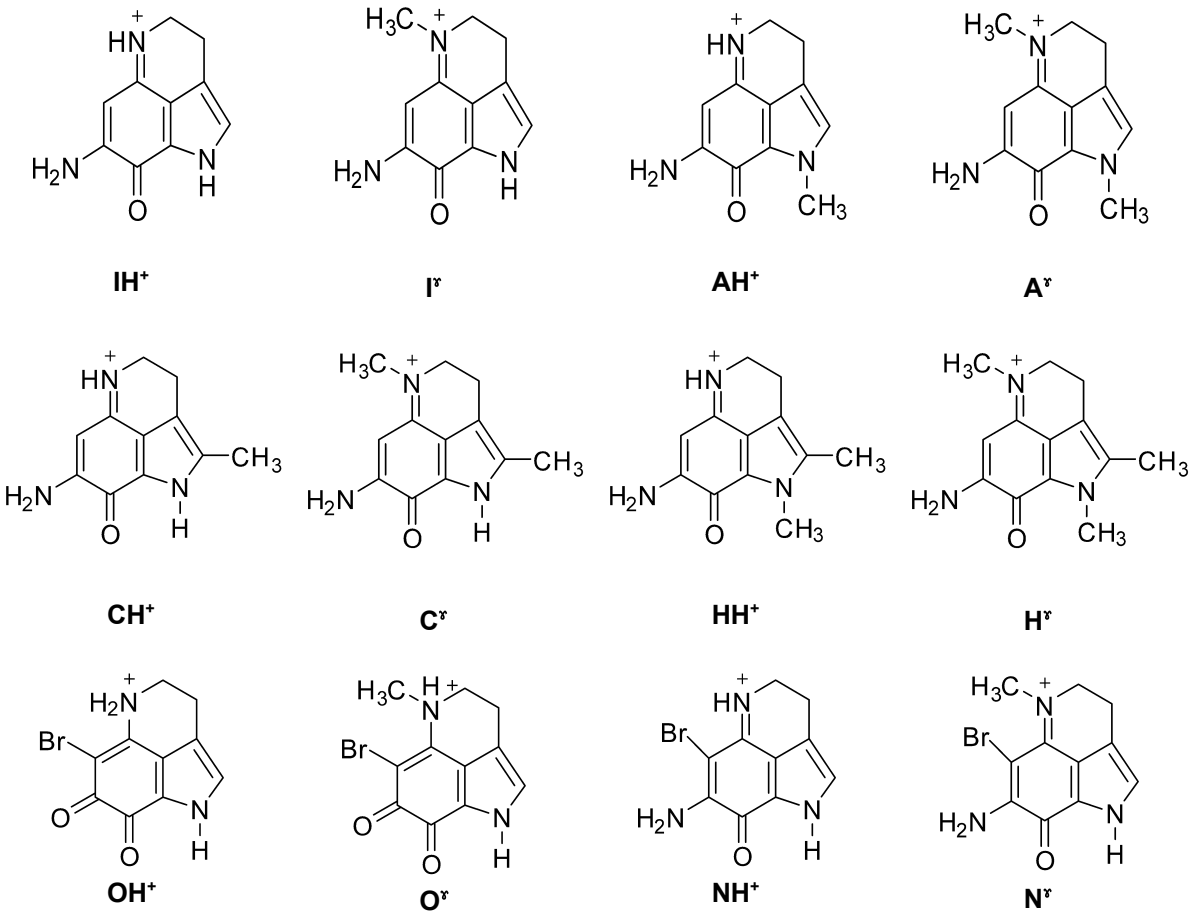



*Figure 1:* 2D structures of studied Makaluvamines in 3-body complexes

*b) Methods of calculation*

Calculations were performed with the Gaussian 09 software [7]. The method used is the density functional theory (DFT) [8]. The hybrid functional B3LYP and others, when combined with an extended base of functions, give a good agreement between experimental and theoretical data of molecular properties [9]. Our choice has focused on the DFT/B3LYP method for all the theoretical calculations. An optimization calculation of the molecular geometry was performed on the twelve structures of figure 1 with one molecule of $H_2O$ and one molecule of Glu Ac. The 2-body and 3-body interaction energies were determined in these complexes. The "super-molecule" approach used here actually leads to an error on the variation of the total energy calculated during the formation of the complex. This error is due to the phenomenon of "Basis Set Superposition Error" or BSSE, which leads to an excessive energetic stabilization of the complex compared to the monomers. In a previous study on 2-body super-molecules of Makaluvamines [10], we have described the procedure for calculating the interaction, relaxation, and BSSE energies. For this work, calculations were performed at B3LYP/6-31+G(d,p) levels.

i. *Estimation of cooperative effects in 3-body complexes*

The stability of a complex is always subject to nature (attractive or dispersive) of the various interactions between the fragments that constitute it. In other words, the interaction between fragments (or the energy of the interaction) is always disrupted by the adding of an additional fragment(s). In our approach, three fragments compose each complex. For example, the first designated A, represents protonated Makaluvamine or methylated Makaluvamine, and the last two fragments, designated B and C, are a molecule of water and a molecule of glutamic acid, respectively. In the approach called "super-molecule" the interaction energy of the formed complexes can also be calculated according to equation 1:

$$\Delta E = \Delta E_{rel}(A) + \Delta E_{rel}(B) + \Delta E_{rel}(C) + \Delta E_{2C}(AB) + \Delta E_{2C}(BC) + \Delta E_{2C}(AC) + \Delta E_{3C}(ABC) \quad \text{(éq. 1)}$$

The relaxation energy, $\Delta E_{rel}$ reflects the distortion of geometry between the isolated and complexed states of a given fragment. The terms $\Delta E_{nC}$ are called n-body energies. Two-body energies are in the majority of cases additive, while three-, four-,

n-body energies are not additive. Indeed, two-body energy derived naturally from the interactions between two neighboring fragments. On the other hand, the interactions existing in the ABC complex (more than two bodies) cannot be expressed as a superposition of two-body interactions, first between A and B, then between B and C, and finally, between A and C. It is the three-body term that reflects cooperative effects, the influence of a fragment C on the interaction between A and B for example. Calculations of the two- and three-body terms are done in equations 2 and 3 respectively below:

$$\Delta E_{2C}(AB) = E_{ABC}^{\alpha\cup\beta}(AB) - E_{ABC}^{\alpha}(A) - E_{ABC}^{\beta}(B) \quad \text{(éq.2)}$$

$$\Delta E_{3C}(ABC) = E_{ABC}^{\alpha\cup\beta\cup\gamma}(ABC) - \left\{E_{ABC}^{\alpha}(A) + E_{ABC}^{\beta}(B) + E_{ABC}^{\gamma}(C)\right\} - \left\{E_{ABC}^{\alpha\cup\beta}(AB) + E_{ABC}^{\beta\cup\gamma}(BC) + E_{ABC}^{\alpha\cup\gamma}(AC)\right\} \quad \text{(éq. 3)}$$

In the end, the corrected cooperativity energy of the BSSE in our complexes was calculated from the following equation 4:

$$E_{coop}(BSSE) = \Delta E_{3C}(ABC) - \Delta E_{2C}(AB) - \Delta E_{2C}(BC) - \Delta E_{2C}(AC) + BSSE \quad \text{(éq. 4)}$$

ii. *Geometric parameters of hydrogen bonds in complexes*

The hydrogen (HB) bond is an attractive interaction between a hydrogen atom of a molecule or molecular fragment X-H in which X is more electronegative than H, and an atom or group of atoms in the same molecule or a different molecule, in which there is evidence of bond formation [11].

The geometric analysis of the HB interactions of Makaluvamines with a molecule of $H_2O$ and GluAc were performed by the recommendations of Desiraju and Steiner [12], including the parameters defined in figure 2.

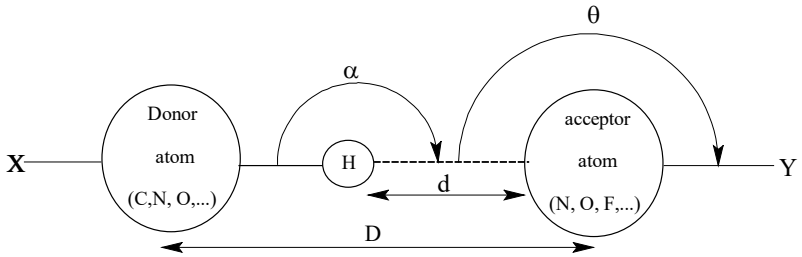



*Figure 2:* Geometric parameters d, D, ∝, and θ describing a hydrogen bond.

In this figure, d is the length of the hydrogen bond expressed about the hydrogen atom (by putting H in the centre of the reference), D is the distance between heavy atoms. The angles α and β describe the linear and directional character of the hydrogen bond.

Figure 3 below shows the numbering of the different atoms of the Makaluvamines and the Ac Glu residue. This numbering permits a more precise description of the interactions by HB between the fragments in the studied super-molecules.

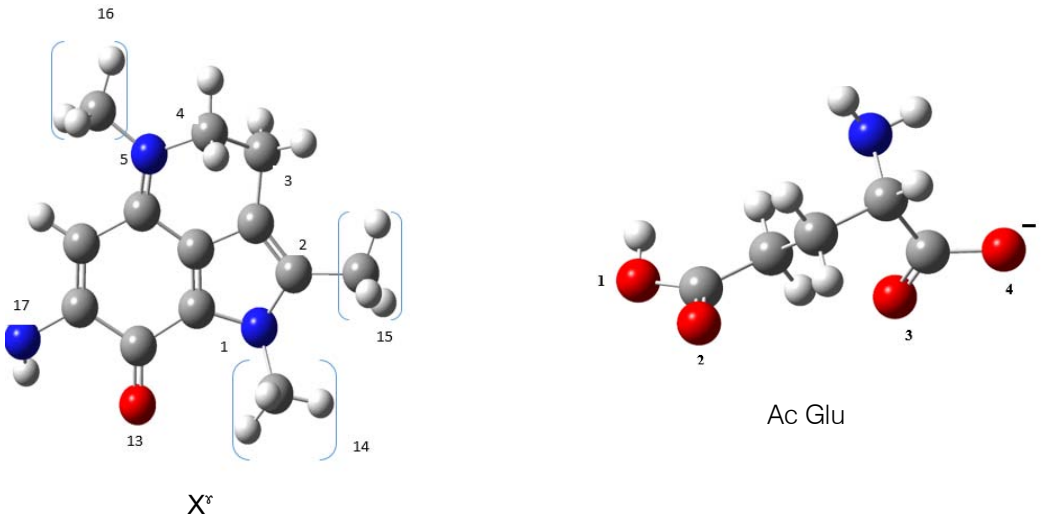



*Figure 3:* Numbering used to describe the interactions (HB) between Makaluvamines and water and glutamic acid molecules. For protonated Makaluvamines $XH^+$, $C_{16}H_3$ was replaced by H.

## III. Results and Discussion

*a) Energy parameters of 3-body complexes*

The geometries of 3-body super-molecules with protonated Makaluvamines ($XH^+$-$H_2O$-Ac Glu) optimized to the level of theory indicated are in Figure 4. The different energy parameters calculated for the six complexes of this figure were presented in table 1.

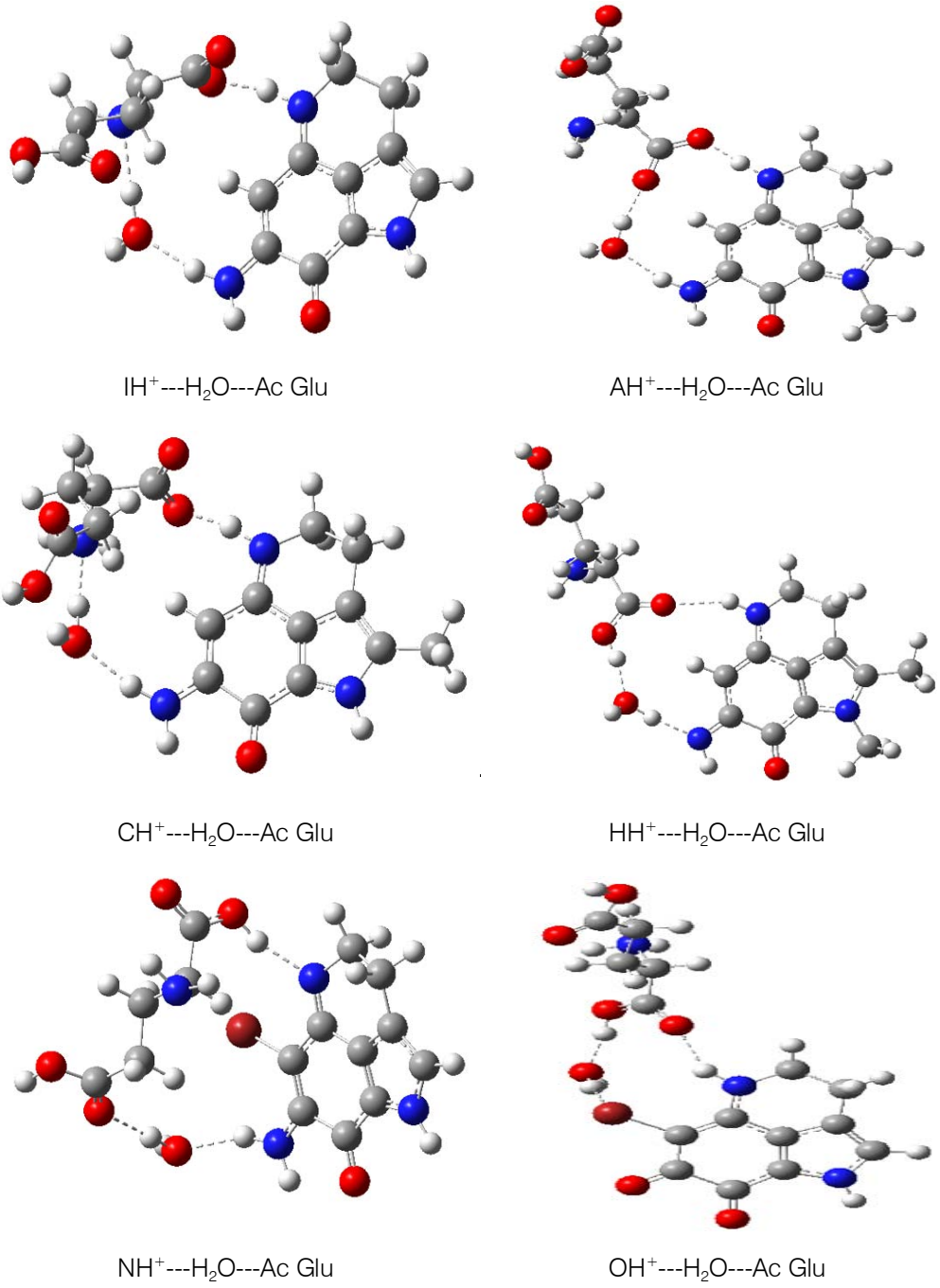



*Figure 4:* Optimized structures of 3-body complexes of a series of protonated Makaluvamines ($XH^+$) with a molecule of $H_2O$ and a molecule of Ac Glu.

All of the structures of the complexes formed are in the form of three-membered ring structures: $XH^+$---$H_2O$---Ac Glu---$XH^+$.

*Table 1:* Energies of the 3-body, 2-body, and 1-body molecular geometries in the geometry of the complex (CPL) $XH^+YZ$. Energies of the $XH^+$, Y, and Z bodies in their geometries (local), $XH^+$, Y, Z bodies relaxation and total relaxation, energies of the 2-body and 3-body interactions. BSSE corrected cooperativity energy. All these energies are in kcal/mol.

| Complexes | BSSE | $E_{XH^+Y\,(CPL)}$ | $E_{YZ\,(CPL)}$ | $E_{XH^+Z\,(CPL)}$ | $E_{XH^+YZ\,(CPL)}$ | $E_{XH^+\,(CPL)}$ | $E_{Y\,(CPL)}$ | $E_{Z\,(CPL)}$ |
|---|---|---|---|---|---|---|---|---|
| $IH^+…H_2O…Ac\ Glu$ | 2.82 | -441058.87 | -393738.52 | -739031.13 | -787006.64 | -393082.02 | -47964.66 | -345850.34 |
| $AH^+…H_2O…Ac\ Glu$ | 2.11 | -465730.80 | -393829.78 | -763701.87 | -811679.08 | -417754.19 | -47964.66 | -345850.78 |
| $CH^+…H_2O…Ac\ Glu$ | 3.11 | -465737.85 | -393828.68 | -763706.67 | -811684.03 | -417761.18 | -47964.66 | -345850.08 |
| $HH^+…H_2O…Ac\ Glu$ | 2.06 | -489985.16 | -394159.19 | -788368.53 | -836351.90 | -442011.19 | -47964.66 | -346179.16 |
| $NH^+…H_2O…Ac\ Glu$ | 7.15 | -2054096.37 | -394166.53 | -2352488.30 | -2400464.31 | -2006118.57 | -47964.66 | -346179.79 |
| $OH^+…H_2O…Ac\ Glu$ | 4.52 | -2066558.46 | -394159.05 | -2364953.91 | -2412929.23 | -2018580.71 | -47964.66 | -346179.16 |

| Complexes | $E_{XH^+\,(local)}$ | $E_{Y\,(local)}$ | $E_{Z\,(local)}$ | $E_{R\,(XH^+)}$ | $E_{R\,(Y)}$ | $E_{R\,(Z)}$ | $\Delta E_{XH^+-Y}$ | $\Delta E_{XH^+-Z}$ | $\Delta E_{Y-Z}$ | $\Delta E_{XH^+-Y-Z}$ | $E_{coop}$ (cor BSSE) | $E_R$ (tot) | $\Delta E_{int}$(tot) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $IH^+…H_2O$ …Ac Glu | -393082.02 | -47980.02 | -345850.44 | 0.00 | 15.36 | 0.10 | -12.19 | -98.76 | -12.91 | 14.24 | 140.91 | 15.46 | -91.34 |
| $AH^+…H_2O$ …Ac Glu | -417754.19 | -47980.02 | -345850.44 | 0.00 | 15.36 | -0.34 | -11.96 | -96.90 | -14.34 | 13.75 | 139.06 | 15.03 | -92.32 |
| $CH^+…H_2O$ …Ac Glu | -417761.18 | -47980.02 | -345850.44 | 0.00 | 15.36 | 0.36 | -12.01 | -95.41 | -13.95 | 13.25 | 137.72 | 15.73 | -89.28 |
| $HH^+…H_2O$ …Ac Glu | -442432.72 | -47980.02 | -345850.44 | 421.52 | 15.36 | -328.72 | -9.31 | -178.18 | -15.37 | 5.97 | 210.88 | 108.17 | -86.66 |
| $NH^+…H_2O$ …Ac Glu | -2006540.57 | -47980.02 | -345850.44 | 422.00 | 15.36 | -329.35 | -13.14 | -189.94 | -22.09 | 23.88 | 256.20 | 108.02 | -86.12 |
| $OH^+…H_2O$ …Ac Glu | -2018961.71 | -47980.02 | -345850.44 | 381.00 | 15.36 | -328.72 | -13.10 | -194.04 | -15.24 | 17.67 | 244.57 | 67.65 | -132.53 |

*Body $XH^+$:* Protonated Makaluvamine; *Body Y:* $H_2O$ and *Body Z:* Ac Glu

The total electronic energies $E_{XH^+YZ(CPL)}$ of the three-body complexes in Table 1 range from -787006.64 kcal.mol$^{-1}$ to -2412929.23 kcal.mol$^{-1}$. These super-molecules are, therefore, very stable, particularly those formed by the protonated Makaluvamines $NH^+$ and $OH^+$. These two complexes are, on average, 3 times more stable than those forming with the protonated Makaluvamines $IH^+$, $AH^+$, $CH^+$, and $HH^+$. The most stable of the structures was obtained with the protonated Makaluvamine $OH^+$. The least stable of these super-molecules is that obtained with the reference Makaluvamine $IH^+$ (absence of substituent on the base skeleton). The introduction of substituents on this reference skeleton further stabilizes these complexes.

The energies of the 2-body fragments in the geometry of the complexes show that for a given structure, the two $XH^+$---Ac Glu fragments are more stable. Their energy is much closer to that of the super-molecule. Secondly, we find the one of the two $XH^+$---$H_2O$ fragments. The energies $E_{XH^+Z(CPL)}$ and $E_{XH^+Y(CPL)}$ respectively of the $XH^+$---Ac Glu and $XH^+$---$H_2O$ fragments depend strongly on the geometry of the super-molecule. Of all the two-body fragments, $H_2O$---Ac Glu has the highest energies ($E_{YZ(CPL)}$). They have the least stable geometries. Their energies seem to depend very little on the geometry of the super-molecule.

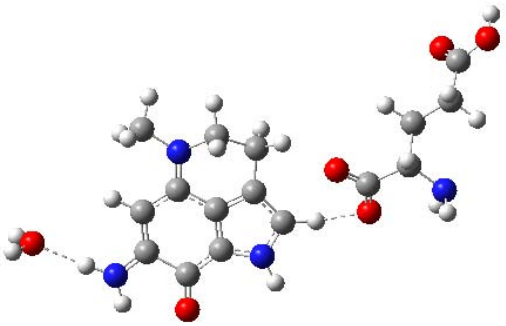
The analysis of the data of the 1-body fragments in the geometries of the complexes clearly shows that the values of the energies $E_{Y(CPL)}$ and $E_{Z(CPL)}$ respectively of the water and Ac Glu molecules are independent of this geometry. Only the $E_{XH^+(CPL)}$ energy of the protonated Makaluvamine is dependent on the geometry of the complex. For a given structure, the sum of the three energy values of the 1-body fragments ($E_{XH^+(CPL)} + E_{Y(CPL)} + E_{Z(CPL)}$) is always higher than that of the super-molecule. This shows that the total electronic energy of a complex is not a direct sum of the energies evaluated at the same level of constituent fragment theory in the geometry of the complex. The terms resulting from interactions must naturally were taken into account.

The relaxation energy $E_R$ shows that the geometry of the water molecule is subject to the same distortion in all the complexes studied. In the isolated state, this molecule is in a more stable conformation than in the complexed state. As for the fragments of the protonated Makaluvamines $IH^+$, $AH^+$, and $CH^+$, the results indicate that their geometries do not show any deformation from their isolated states to the complexes they form. In the structures of these protonated Makaluvamines, the geometry of the glutamic acid molecule is very little modified compared to its isolated state. Finally, the water molecule is the fragment whose geometry was most modified during the formation of the three-body complexes from the protonated Makaluvamines $IH^+$, $AH^+$, and $CH^+$. The interaction between the water molecule, the glutamic acid molecule, and each of the protonated Makaluvamines $HH^+$, $NH^+$, and $OH^+$ is associated with significant distortions of their geometries about their isolated states. In these complexes, the fragments are in less stable conformations. In these three super-molecules,

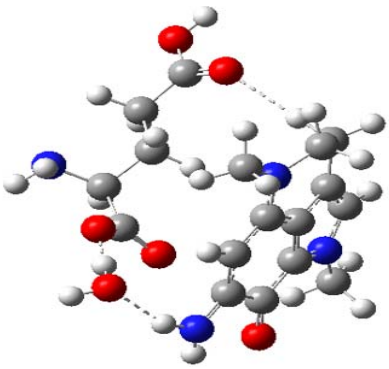
the Ac Glu molecule faces the same relatively important structural distortion. This fragment adopts a lower energy conformation in the complexes than in the isolated state. In general, the Ac Glu fragment tends to take a molecular geometry of low energy in the complexes. The other two bodies ($XH^+$ and $H_2O$), when their geometry is modified, are less stable than in the isolated state. No complex is formed without distortion of at least one fragment, as shown by $E_R(tot) \neq 0$.

The 2-body interaction energies all have a stabilizing character. The terms $\Delta E_{XH^+-Y}$ and $\Delta E_{XH^+-Z}$, correspond respectively to the interactions $XH^+$---$H_2O$ and $XH^+$---Ac Glu. The values of $\Delta E_{XH^+-Y}$ are close to the interaction energies of the 2-body complexes formed by these two fragments [6]. This energy is the weakest contribution to the stabilization interaction in 3-body complexes. The terms $\Delta E_{XH^+-Z}$were compared to the energy of 2-body structures between protonated Makaluvamines and Ac Glu [6]. The interactions between these two fragments are much stronger in 3-body complexes. The difference is apparent in the complexes formed by the protonated Makaluvamines $HH^+$, $NH^+$, and $OH^+$. This 2-body interaction ($XH^+$---Ac Glu) is the main contribution to the stabilization of super-molecules. The third 2-body term, $\Delta E_{Y-Z}$, corresponding to the interaction energy between the water molecule and the glutamic acid molecule is in the range of -12.91 kcal.mol$^{-1}$ to -22.1 kcal.mol$^{-1}$. The 3-body interaction $\Delta E_{XH^+-Y-Z}$ as expected, has a destabilizing character for complexes. This energy ranges from +5.97 kcal.mol$^{-1}$ to +23.88 kcal.mol$^{-1}$. The sum of the 2-body and 3-body terms, the relaxation energies of the individual fragments, and the BSSE correction lead to the total interaction energy between the constituents in the super-molecule. This energy added to the terms of the three 1-body fragments in the geometry of the complex leads to a value that is sufficiently close to the total energy of each structure.

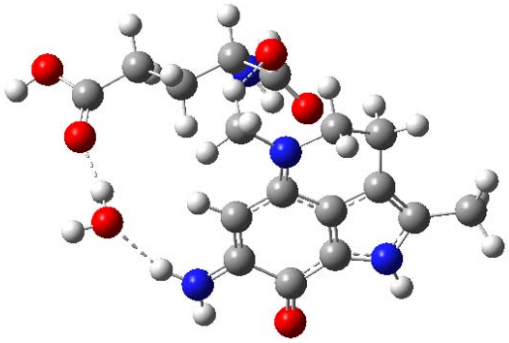
The optimized structures of the six complexes obtained with methylated Makaluvamines ($X^x$-$H_2O$-Ac Glu) were showed in figure 5. Their energy parameters were reported in table 2.



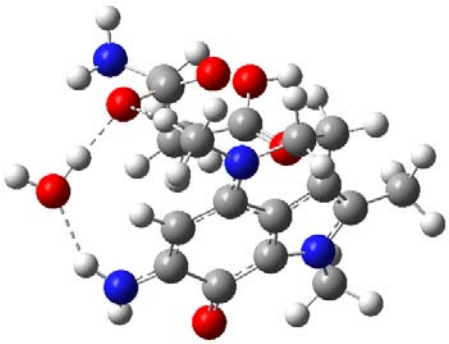
$I^x$---$H_2O$---Ac Glu



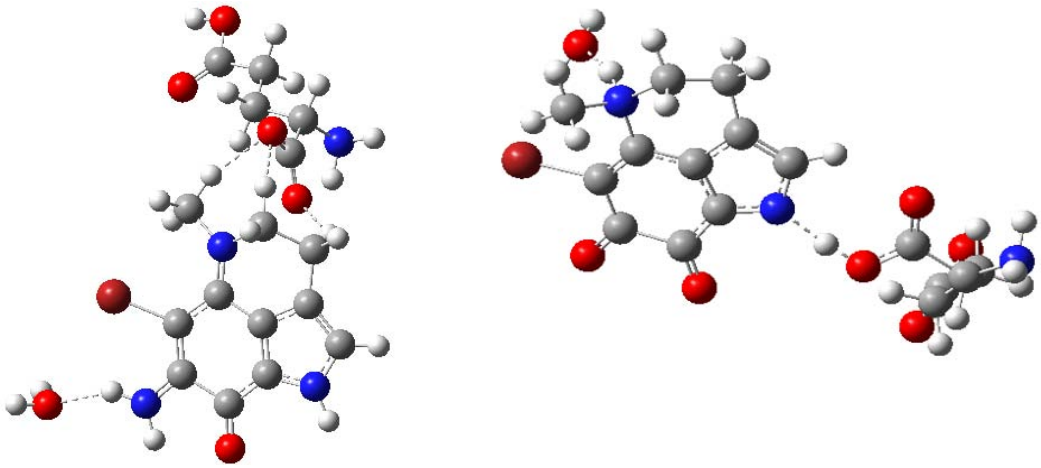
$A^x$---$H_2O$---Ac Glu



$C^x$---$H_2O$---Ac Glu



$H^x$---$H_2O$---Ac Glu



$N^{x}$---$H_2O$---Ac Glu $O^{x}$---$H_2O$---Ac Glu

*Figure 5:* Optimized structures of 3-body complexes of a series of methylated Makaluvamines ($X^{x}$) with a molecule of $H_2O$ and a molecule of Ac Glu.

The structures of the formed complexes are in the form of rings or linear chains.

*Table 2:* Energies of the 3-body, 2-body, and 1-body molecular geometries in the geometry of the complex (CPL) $X^{x}YZ$. Energies of the bodies $X^{x}$, Y, and Z in their geometries (local), $X^{x}$, Y, Z bodies relaxation and total relaxation, energies of 2-body and 3-body interactions. BSSE corrected cooperativity energy. All these energies are in kcal.mol$^{-1}$.

| Complexes | BSSE | $E_{X^{x}Y\,(CPL)}$ | $E_{YZ\,(CPL)}$ | $E_{X^{x}Z\,(CPL)}$ | $E_{X^{x}YZ\,(CPL)}$ | $E_{X^{x}\,(CPL)}$ | $E_{Y\,(CPL)}$ | $E_{Z\,(CPL)}$ |
|---|---|---|---|---|---|---|---|---|
| $I^{x}$…$H_2O$…Ac Glu | 1.73 | -465728.80 | -393812.84 | -763675.89 | -811648.91 | -417752.24 | -47964.66 | -345850.34 |
| $A^{x}$…$H_2O$…Ac Glu | 2.39 | -490400.50 | -393832.98 | -788353.77 | -836337.12 | -442424.19 | -47964.66 | -345850.34 |
| $C^{x}$…$H_2O$…Ac Glu | 2.61 | -490407.69 | -393828.24 | -788362.42 | -836339.19 | -442431.32 | -47964.66 | -345850.34 |
| $H^{x}$…$H_2O$…Ac Glu | 2.88 | -515078.75 | -393831.81 | -813025.74 | -861010.81 | -467102.63 | -47964.66 | -345849.04 |
| $N^{x}$…$H_2O$…Ac Glu | 2.31 | -2079178.53 | -393813.09 | -2377133.16 | -2425104.46 | -2031203.53 | -47964.66 | -345850.34 |
| $O^{x}$…$H_2O$…Ac Glu | 3.17 | -2091182.80 | -394159.15 | -2389571.63 | -2437550.24 | -2043200.92 | -47964.66 | -345850.29 |

| Complexes | $E_{X^{x}\,(local)}$ | $E_{Y\,(local)}$ | $E_{Z\,(local)}$ | $E_{R\,(X^{x})}$ | $E_{R\,(Y)}$ | $E_{R\,(Z)}$ | $\Delta E_{X^{x}\text{-}Y}$ | $\Delta E_{X^{x}\text{-}Z}$ | $\Delta E_{Y\text{-}Z}$ | $\Delta E_{X^{x}\text{-}Y\text{-}Z}$ | $E_{coop}$ (cor BSSE) | $E_{R}$ (tot) | $\Delta E_{int}$(tot) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $I^{x}$..$H_2O$..Ac Glu | -417752.24 | -47980.02 | -345850.44 | 0.00 | 15.36 | 0.10 | -11.90 | -73.31 | 2.16 | -345848.96 | -345764.17 | 15.46 | -345914.81 |
| $A^{x}$..$H_2O$..Ac Glu | -442424.19 | -47980.02 | -345850.44 | 0.00 | 15.36 | 0.10 | -11.65 | -79.24 | -17.97 | -345839.41 | -345728.16 | 15.46 | -345930.43 |
| $C^{x}$..$H_2O$..Ac Glu | -442431.32 | -47980.02 | -345850.44 | 0.00 | 15.36 | 0.10 | -11.71 | -80.75 | -13.24 | -345837.52 | -345729.21 | 15.46 | -345925.15 |
| $H^{x}$..$H_2O$..Ac Glu | -467102.63 | -47980.02 | -345850.44 | 0.00 | 15.36 | 1.40 | -11.47 | -74.07 | -18.12 | -345839.87 | -345733.33 | 16.77 | -345923.87 |
| $N^{x}$..$H_2O$..Ac Glu | -2031203.53 | -47980.02 | -345850.44 | 0.00 | 15.36 | 0.10 | -10.35 | -79.29 | -17.89 | -345828.76 | -345718.92 | 15.46 | -345918.50 |
| $O^{x}$..$H_2O$..Ac Glu | -2043627.25 | -47980.02 | -345850.44 | 426.34 | 15.36 | 0.15 | -17.22 | -520.43 | -344.20 | -345502.81 | -344617.80 | 441.85 | -345939.64 |

*Body $X^{x}$:* Methylated Makaluvamine; *Body Y:* $H_2O$ and *Body Z:* Ac Glu

The values of the terms $E_{X^{x}YZ}(CPL)$ range from -811648 kcal.mol$^{-1}$ to -2437550.24 kcal.mol$^{-1}$. The energy of each $X^{x}$--$H_2O$--Ac Glu complex is at least 24621 to 24659 kcal.mol$^{-1}$ lower than that of the analog $XH^{+}$--$H_2O$--Ac Glu. The 3-body super-molecules formed by the methylated Makaluvamines $I^{x}$, $A^{x}$, $C^{x}$, $H^{x}$, $N^{x}$, and $O^{x}$ with $H_2O$ and Ac Glu are very stable compared to their analogs with the same protonated Makaluvamines. Similar to table 1, structures with the methylated Makaluvamines $N^{x}$ and $O^{x}$ are three times more low than those formed with $I^{x}$, $A^{x}$, $C^{x}$, and $H^{x}$. Analysis of the stability of two-fragment structures in the geometry of the complex shows that the $X^{x}$---Ac Glu fragments are always the most stable. In second place in this classification are the two molecules $X^{x}$---$H_2O$. The energies $E_{X^{x}YZ(CPL)}$ ) and $E_{X^{x}Y(CPL)}$ respectively of the fragments $X^{x}$---Ac Glu and $X^{x}$---$H_2O$ depend strongly on the geometry of the super-molecule. The $H_2O$---Ac Glu fragments have the highest energies ($E_{YZ(CPL)}$) and are, therefore, the least stable. The values of the terms about two fragments depends very little on the geometry of the super-molecule.

The energies $E_{Y(CPL)}$ and $E_{Z(CPL)}$ respectively of the water and Ac Glu molecules (1-body fragments) in the geometries of the complexes clearly show that they do not depend on these geometries. Only the energy

$E_{X^{\gamma}(CPL)}$ of the methylated Makaluvamine is always subject to the complex geometry. The sum of the terms of 1-body fragments ($E_{X^{\gamma}(CPL)} + E_{Y(CPL)} + E_{Z(CPL)}$) in the complex geometry is not equal to the total energy of the complex. The relaxation energy $E_R(X^{\gamma})$ shows that of all the methylated Makaluvamines studied, only the structure of $O^{x}$ was distorted between the isolated state and the complexed state. In this particular case, the Makaluvamine $O^{x}$ is in a lower energy molecular geometry in the uncomplexed state. The geometry of the Ac Glu molecule was slightly distorted between the two states. This fragment is however, more stable in the isolated state. The geometry of the water molecule has the same distortion in all the complexes studied (tables 1 and 3). This fragment is always in a less stable conformation in the super-molecule.

Apart from the term $\Delta E_{Y-Z}$ corresponding to the interaction between the fragments $H_2O$ and Ac Glu in the complex $I^{x}$--$H_2O$--Ac Glu, the 2-body interaction energies all have a stabilizing character. The interaction energies $\Delta E_{X^{\gamma}-Y}$ between the fragments $X^{\gamma}$ (methylated Makaluvamines) and the H2O molecule are always close to the interaction energies of the 2-body complexes formed by these fragments [6]. It is the lowest energy of the stabilization interaction in the complexes in Table 3. The interaction energies $\Delta E_{X^{\gamma}-Z}$ between the methylated Makaluvamines $X^{\gamma}$ and Ac Glu are higher in 3-body complexes than in 2-body complexes [6]. Exceptionally, this interaction is four times stronger in the $O^{x}$--$H_2O$-Ac Glu complex than in the $I^{x}$---Ac Glu complex. It is still the energy $\Delta E_{X^{\gamma}-Z}$ that constitutes the most important 2-body interaction for the stabilization of these 3-body complexes. The third 2-body term, $\Delta E_{Y-Z}$ , indicates a strong interaction between the $H_2O$ molecule and the Ac Glu molecule in the complex $O^{x}$--$H_2O$--Ac Glu (-344.20 kcal.mol$^{-1}$). The energy of this interaction ranges from -13.24 kcal.mol$^{-1}$ to -17.89 kcal.mol$^{-1}$ for the complexes $A^{x}$--$H_2O$--Ac Glu, $C^{x}$--$H_2O$--Ac Glu, $H^{x}$--$H_2O$--Ac Glu and $N^{x}$--$H_2O$--Ac Glu. The 3-body interaction $\Delta E_{X^{\gamma}-Y-Z}$, unexpectedly, has a stabilizing character in these six complexes. It ranges from -355502.81 kcal.mol$^{-1}$ to -345848.96 kcal.mol$^{-1}$. This energy reflects the strong global interaction $\Delta E_{int}(tot)$ between all the fragments of these complexes. This global interaction $\Delta E_{int}(tot)$ is estimated to range between -345914.81 kcal.mol$^{-1}$ and -345939.64 kcal.mol$^{-1}$. The 3-body interaction $\Delta E_{X^{\gamma}-Y-Z}$ doesn't contribute to the calculation of total energy of the complex, although it is stabilizing. Indeed, the total energy of each complex ($E_{X^{\gamma}YZ}(CPL)$) was obtained with a good approximation by summing the energies of the 1-body fragments in the geometry of the complex ($E_{X^{\gamma}}(CPL) + E_{Y}(CPL) + E_{Z}(CPL)$) and the terms of 2-body interaction energies ($\Delta E_{X^{\gamma}-Y} + \Delta E_{X^{\gamma}-Z} + \Delta E_{Y-Z}$). Since all 2- and 3-body interactions are stabilizing in these super-molecules with an exceptionally important contribution of the 3-body terms, we can affirm that the three fragments $X^{x}$, $H_2O$, and Ac Glu cooperate very well in these complexes. The high values of $\Delta E_{X^{\gamma}-Y-Z}$ confirm this result.

In the final analysis, we note that for the six Makaluvamines studied, the 3-body complexes of the methylated forms are at least 24600 kcal.mol$^{-1}$ more stable than those obtained with the protonated forms.

For a given protonated or methylated form, Makaluvamines O and N lead to the most stable complexes, the complex with Makaluvamine H has a low energy than those obtained with Makaluvamines A and C having close stabilities. Makaluvamine, I form the least stable complex. The total energy of interactions in these 3-fragment complexes is also at least 345800 kcal.mol$^{-1}$ lower with methylated Makaluvamines. There is also better cooperativity of these in these complexes. All these results would indicate that the structures of the methylated Makaluvamines are more favorable for forming complexes by docking compared to those of the protonated Makaluvamines.

*b) Geometrical parameters of interactions in 3-body complexes*

These geometrical interaction parameters analyzed according to the H-bond approach are reported in Table 3 for the six structures in figure 4 and Table 4 for the complexes in figure 5.

*Table 3:* Geometrical parameters of HB determined at B3LYP/6-31+G(d,p) level in complexes of protonated Makaluvamines interacting with an $H_2O$ molecule and an Ac Glu molecule.

| Complexes | Interactions | $\alpha$ (°) | $\theta$ (°) | $d$ (Å) | $D$ ( Å) |
|---|---|---|---|---|---|
| $IH^{+}$-$H_2O$-Ac Glu | $N_5H\ldots O_4C_5H_9N$ | 163.25 | 105.59 | 1.55 | 2.60 |
| | $N_{17}H\ldots OH_2$ | 168.35 | 127.20 | 1.86 | 2.87 |
| | $OH_2\ldots NH_2$(Ac glu) | 175.93 | 110.91 | 1.79 | 2.79 |
| $AH^{+}$-$H_2O$-Ac Glu | $N_5H\ldots O_4C_5H_9N$ | 175.71 | 126.71 | 1.52 | 2.61 |
| | $N_{17}H\ldots OH_2$ | 165.93 | 114.48 | 1.87 | 2.88 |
| | $OH_2\ldots O_3C_5H_9N$ | 170.67 | 175.49 | 1.75 | 2.72 |
| $CH^{+}$-$H_2O$-Ac Glu | $N_5H\ldots O_4C_5H_9N$ | 164.81 | 115.24 | 1.50 | 2.57 |
| | $N_{17}H\ldots OH_2$ | 169.52 | 121.10 | 1.84 | 2.86 |
| | $OH_2\ldots NH_2$(Ac glu) | 179.82 | 104.57 | 1.85 | 2.85 |
| $HH^{+}$-$H_2O$-Ac Glu | $N_5H\ldots O_3C_5H_9N$ | 151.63 | 165.91 | 2.21 | 3.15 |

| | | | | | |
|---|---|---|---|---|---|
| | $N_{17}H\ldots OH_2$ | 173.97 | 106.71 | 1.01 | 2.73 |
| | $OH_2\ldots O_3C_5H_9N$ | 165.08 | 114.98 | 1.01 | 2.63 |
| $NH^+$-$H_2O$-Ac Glu | $N_5H\ldots O_4C_5H_9N$ | 159.43 | 114.52 | 1.00 | 2.76 |
| | $N_{17}H\ldots OH_2$ | 156.74 | 115.20 | 1.92 | 2.89 |
| | $OH_2\ldots O_2C_5H_9N$ | 177.44 | 136.09 | 1.87 | 2.84 |
| $OH^+$-$H_2O$-Ac Glu | $N_5H\ldots O_3C_5H_9N$ | 142.91 | 161.46 | 2.06 | 2.94 |
| | $OH_2\ldots O_4C_5H_9N$ | 171.04 | 112.05 | 1.00 | 2.67 |
| | $OH_2\ldots BrOH^+$ | 168.08 | 112.58 | 2.40 | 3.36 |

Each fragment of these complexes establishes two interactions. As expected, $XH^+$ protonated Makaluvamines interact by preferred hydrogens (sites), namely $N_5H$ and $N_{17}H$ [6]. Ac Glu binds preferentially by its oxygen atoms $O_3$ and $O_4$ on $HN_5$ to the protonated Makaluvamine. The water molecule is binding to the $XH^+$ hydrogen $HN_{17}$ through its oxygen. In the interaction between the Ac Glu and $H_2O$ fragments, water is frequently the donor and glutamic acid the acceptor. All the geometrical parameters of these interactions show values that are very favorable to the formation of H-bonds. The linearity angle α ranges from 143° to 180°. On average, this angle is 167°. The directionality parameter θ, varies between 105° and 176°, with an average of 125°. This angle is suitable for forming H-bonds. Also, all the distances d between hydrogen and the acceptor atom are shorter than the sum of their Van Der Waals radii. The values are between 1.00 Å and 2.06 Å. Thus, strong H bonds were established in these complexes between the different fragments.

*Table 4:* Geometrical parameters of HB determined at B3LYP/6-31+G(d,p) level in complexes of methylated Makaluvamines interacting with a molecule of $H_2O$ and a molecule of Ac Glu.

| Complexes | Interactions | $\alpha$ (°) | $\theta$ (°) | $d$ (Å) | $D$ (Å) |
|---|---|---|---|---|---|
| $I^x$-$H_2O$-Ac Glu | $C_2H\ldots O_4C_5H_9N$ | 167.30 | 105.67 | 1.85 | 2.93 |
| | $N_{17}H\ldots OH_2$ | 175.58 | 122.60 | 1.94 | 2.95 |
| $A^x$-$H_2O$-Ac Glu | $OH_2\ldots O_4C_5H_9N$ | 176.94 | 130.34 | 1.59 | 2.60 |
| | $C_3H\ldots O_2C_5H_9N$ | 177.21 | 141.45 | 2.41 | 3.51 |
| | $N_{17}H\ldots OH_2$ | 150.24 | 98.59 | 1.80 | 2.79 |
| $C^x$-$H_2O$-Ac Glu | $C_{16}H\ldots O_4C_5H_9N$ | 130.33 | 125.47 | 2.20 | 3.03 |
| | $N_{17}H\ldots OH_2$ | 160.97 | 119.40 | 1.89 | 2.88 |
| | $OH_2\ldots O_2C_5H_9N$ | 169.59 | 151.62 | 1.83 | 2.80 |
| $H^x$-$H_2O$-Ac Glu | $C_{16}H\ldots O_4C_5H_9N$ | 151.22 | 97.54 | 2.35 | 3.35 |
| | $N_{17}H\ldots OH_2$ | 146.04 | 117.86 | 1.95 | 2.86 |
| | $H_2O\ldots O_3C_5H_9N$ | 173.42 | 138.75 | 1.67 | 2.67 |
| $N^x$-$H_2O$-Ac Glu | $C_{16}H\ldots O_4C_5H_9N$ | 160.05 | 98.34 | 2.05 | 3.10 |
| | $N_{17}H\ldots OH_2$ | 149.95 | 123.79 | 2.00 | 2.92 |
| | $C_3H\ldots O_3C_5H_9N$ | 135.33 | 113.33 | 2.22 | 3.10 |
| | $C_4H\ldots O_4C_5H_9N$ | 146.47 | 107.13 | 2.18 | 3.15 |
| $O^x$-$H_2O$-Ac Glu | $N_1H\ldots O_4C_5H_9N$ | 173.80 | 115.45 | 1.07 | 2.58 |
| | $OH_2\ldots N_5H$ | 159.11 | 135.08 | 1.62 | 2.64 |

All interactions established to form these complexes were performed on privileged electrophilic (hydrogen) sites identified in the structures of the methylated Makaluvamines $X^x$ [6].

The angular parameters satisfy the conditions for the formation of H-bonds. Indeed, the angle of linearity α is wide open, on average 159°, indicating an appropriate alignment of the donor, hydrogen and acceptor atoms. Also, it was noted that the directionality angle θ defined between the one next to the acceptor and the hydrogen involved in the interaction is well above its lower limit, which is 90°. The spacing of the donor and acceptor atoms, D, is between 2.58 Å and 3.51 Å. It is, therefore, suitable for the formation of H bonds. The distances d between hydrogen-acceptor in the $X^x$---$H_2O$---Ac Glu complexes shown in table 4 range 1.07 Å to 2.41 Å. Compared to those established in the $XH^+$---$H_2O$---Ac Glu complexes in Table 2, they are longer. It can, therefore, was said that the H bonds in the $X^x$---$H_2O$---Ac Glu structures are generally weaker than those in the $XH^+$---H2O---Ac Glu complexes. In contrary to 2-body super-molecules, in 3-body complexes, multicentric interactions are rarely observed. Only one case was observed, the $N^x$---$H_2O$---Ac Glu complex.

## IV. Conclusion

This study revealed that the complexes between the methylated Makaluvamines and the two fragments $H_2O$ and Ac Glu are very clearly more stable, by at least 24800 $kj.mol^{-1}$ than those formed between these two fragments and the protonated Makaluvamines. Two Makaluvamines N and O are distinguished for the stronger stability of their complexes. Their energies are at least three times lower than those of each of the super-molecules with Makaluvamines I, A, C, and H. The study of cooperativity confirms as expected that all 2-body interactions in the twelve complexes contribute

to stabilizing them. However, it has shown that the interaction between the three bodies is destabilizing during complex formation with protonated and stabilizing Makaluvamines when methylated Makaluvamines were used. In complexes with methylated Makaluvamines, there is better cooperativity of the three fragments. The total interaction energy in these complexes is at least 345800 kcal.mol$^{-1}$ lower than in complexes with protonated Makaluvamines. No super-molecule is formed without distortion of at least one fragment, as shown by $E_R(tot) \neq 0$. In these complexes, the H-bonds between the methylated Makaluvamines, water, and glutamic acid are more long than those in the structures of protonated Makaluvamines, water, and glutamic acid.

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# Alcohol Disinfection Liquid Vaporization and Inhalation Applied in Vivo Antiseptic and Sterilization Treatment Method

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*Abstract-* The use of ethanol has low toxicity, is almost harmless to the human body, and has the characteristics of quickly absorbing the water in viruses and bacteria, causing the protein to dehydrate and freeze, leading to the rapid death of viruses and bacteria; it is directly vaporized with anhydrous ethanol, mixed with air, and modulated An appropriate concentration of therapeutic gas mixture is used to allow patients to inhale the respiratory tract or fasting digestive tract for direct disinfection and sterilization; it is used to treat all respiratory or digestive tract infectious diseases caused by viral and bacterial infections containing protein structures.

*Keywords:* *alcohol vaporization, respiratory and digestive tract, direct sterilization.*

*GJSFR-B Classification:* *FOR Code: 040399*


*Strictly as per the compliance and regulations of:*

# Alcohol Disinfection Liquid Vaporization and Inhalation Applied in Vivo Antiseptic and Sterilization Treatment Method

Huang Zhenqiang

*Abstract-* **The use of ethanol has low toxicity, is almost harmless to the human body, and has the characteristics of quickly absorbing the water in viruses and bacteria, causing the protein to dehydrate and freeze, leading to the rapid death of viruses and bacteria; it is directly vaporized with anhydrous ethanol, mixed with air, and modulated An appropriate concentration of therapeutic gas mixture is used to allow patients to inhale the respiratory tract or fasting digestive tract for direct disinfection and sterilization; it is used to treat all respiratory or digestive tract infectious diseases caused by viral and bacterial infections containing protein structures.**

*Keywords: alcohol vaporization, respiratory and digestive tract, direct sterilization.*

## I. Introduction

For patients with various respiratory and digestive tract infections caused by bacterial viruses, it has a new method of non-toxic side effects and broad-spectrum in vivo disinfection and sterilization.

Existing domestic and foreign health and epidemic prevention systems are available. For a variety of patients with respiratory and digestive tract infections caused by bacterial viruses, there is no complete set of simple, general and rapid treatment methods. A variety of broad-spectrum antibiotics and anti-inflammatory and antipyretic drugs or targeted antibiotics or specific drugs are mainly used to treat various infectious diseases infected by bacteria. A variety of targeted vaccines or specific drugs are used to treat various infectious diseases infected by the virus. For various infectious diseases infected by bacteria, due to the long-term use of various antibiotics in the medical community, the resistance of many bacteria has gradually increased, and the efficacy has decreased. For infectious diseases infected by the virus, the development and production of various targeted vaccines and specific drugs, including animal experiments and clinical tests, require a lot of time and human and material resources. As a result, the ability of all humans to prevent and control newly-infected viral infectious diseases is seriously lagging behind, and the near-expensive vaccines or potent drugs also make patients sick. Therefore, for a sudden new large-scale acute infectious disease with a high mortality, such as SARS virus in the past ten years is a coronavirus, it should be transmitted to humans through an animal host, which is highly toxic. MERS, which occurred in the Middle East, is the second most coronavirus, and this time Wuhan's new coronavirus is the third. Both cause regional or global panic.

Aiming at the existing human treatment methods for patients with various respiratory and digestive tract bacterial and viral infections. All have the disadvantages of poor curative effect, long time and high cost. The alcohol disinfection solution of the present invention is directly vaporized and mixed with air (and oxygen) to prepare a therapeutic mixture gas containing an appropriate ethanol concentration. The treatment method applied to the internal suction respiratory tract and digestive tract for direct contact anti-virus sterilization may have the advantages of good curative effect, short time, low cost, and easy popularization. This will be described in further detail below.

## II. Principles of Vaporization and Internal Absorption of Alcohol Disinfectant Applied to in Vivo Antiseptic and Sterilization Treatment

First, the pneumonia epidemic caused by the new coronavirus infection in Wuhan has exploded and formed a sudden global public health event. What is worth looking forward to: The National Health and Medical Commission's "New Coronavirus Infected Pneumonia Diagnosis and Treatment Program" clearly states that "new coronavirus is sensitive to ultraviolet and heat, 56 ° C for 30 minutes, ether, 75% ethanol, chlorine-containing disinfectant, per oxygen Lipid solvents such as acetic acid and chloroform can effectively inactivate the virus, and chlorhexidine cannot effectively inactivate the virus."

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*Table 1:* Experimental results of the action time required for different concentrations of alcohol to kill bacteria

| 酒精浓度 Alcohol concentration | 大肠杆菌 Escherichia coli | 金黄色葡萄球菌 Staphylococcus aureus | 绿脓杆菌 Pseudomonas aeruginosa | 溶血性链球菌 hemolytic streptococcus |
|---|---|---|---|---|
| 100% | 24 小时 hour | 7 天 Day | 2 小时 hour | 15 分钟 minute |
| 90% | 15 小时 hour | 30 分钟 minute | 5 分钟 minute | 5 分钟 minute |
| 80% | 1 小时 hour | 2 分钟 minute | 2 分钟 minute | 10 秒 second |
| 70% | 30 秒 second | 5 分钟 minute | 1 分钟 minute | 10 秒 second |
| 60% | 20 秒 second | 30 分钟 minute | 30 秒 second | 10 秒 second |
| 50% | 20 秒 second | 30 分钟 minute | 30 秒 second | 20 秒 second |
| 40% | 22 分钟 minute | 4 小时 hour | 2 分钟 minute | 2 分钟 minute |
| 30% | 2 分钟 minute | 4 小时 hour | 30 分钟 minute | 30 分钟 minute |
| 20% | | | 24 小时 hour | 24 小时 hour |

Further analysis of the sterilization and disinfection mechanism of 75% ethanol disinfectant, we searched the following results from the Internet:

Alcohol can kill the virus because it can dissolve the "lipid envelope" of the virus, so it must be a virus with an envelope (including a protein shell) like "coronavirus" in order for alcohol to be effective to play a role. 75% alcohol can absorb the water in the protein of bacteria and virus shell, make it dehydrate, denature and solidify, so as to achieve the purpose of killing bacteria and viruses. If a higher concentration of alcohol is used, the bacterial virus protein is dehydrated too quickly, so that the surface protein of the bacterial virus is denatured and coagulated first, forming a solid envelope, but the alcohol cannot penetrate into the inside of the bacterial virus well, which will affect its killing bacteria The ability of the virus. 75% alcohol is close to the osmotic pressure of the bacterial virus. It can gradually infiltrate into the bacterial vision before the surface protein of the bacterial virus is not denatured, so that all proteins of the bacterial virus are dehydrated, denatured and coagulated, and eventually kill the bacteria and virus. Below 75%, the ability to kill bacteria and viruses is also affected due to reduced permeability. Many scholars have done comparative experiments in this regard, and the results are shown in Table 1.

From the experimental results in Table 1, it can be seen that for different bacteria, the alcohol concentration is different, and the time required to kill the bacteria is also different. However, the general trend is that the alcohol concentration of 50% to 80% can kill all kinds of bacteria as quickly as possible. Therefore, the theoretical basis for the effective treatment of the new coronary pneumonia epidemic designed by the present invention can be summarized as follows: The National Health and Medical Commission's "Pneumonitis Diagnosis and Treatment Program for New Coronavirus Infection" has confirmed that 75% alcohol disinfectant can kill the new coronary virus.

## III. Detailed Description

According to Table 1 of the above experimental results, we can preliminarily imagine that if the 75% alcohol disinfectant is directly vaporized and then mixed with air (and oxygen) to prepare a therapeutic mixture with an appropriate ethanol concentration, it will be applied to the inhaled internal respiratory and digestive Internally, as the therapeutic gas mixture spreads, it is a new treatment method that directly contacts the inner wall of the organ for disinfection and sterilization. As long as viruses such as "coronavirus" have a "lipid envelope" and all proteins containing protein most bacteria, viruses ... can be effectively disinfected within seconds to minutes.

There are about 50 trillion cells in our body, and the total amount of microorganisms parasitizing in our body should be incompletely estimated to be more than 10 times the number of human cells, at least 500 trillion. The total number of genes of these microorganisms is about 200 times that of human genes, and the number of genes in the human genome is about 20,000. Please note: Microbial cells are usually small, only one-tenth to one-hundredth of the cell size of human organs and tissues. However, due to their large number, their total weight is only about one-third of the adult's weight.

Distribution of microorganisms (bacteria) in the human body. The gastrointestinal tract bacteria associated with this article vary by site. Due to the bactericidal effect of gastric acid, the stomach and jejunum of healthy people are generally free of bacteria. If infected by a bacterial virus, related viral bacteria and inflammation will occur. If gastric dysfunction, such as reduced gastric acid secretion, especially in gastric cancer, sarcoma, lactobacilli, bacillus ... Adults have few or even aseptic bacteria in the upper jejunum and ileum, and bacteria in the lower intestine gradually increase. The large intestine accumulates food residues, and has a suitable acidity, suitable for bacterial reproduction,

and the amount of bacteria accounts for about 1/3 of feces. There are many types of microorganisms in the large intestine, mainly including E. coli, Bactericides fragile, Bifidobacterium, anaerobic cocci, etc. Others include Lactobacillus, Staphylococcus, Pseudomonas aeruginosa, Proteus, fungi, etc.

Bacteria in the respiratory tract, staphylococcus, diphtheria... On the throat and tonsil mucosa, Streptococcus aureus and catarrhal is predominate. In addition, there are often potentially pathogenic microorganisms such as pneumococcus, influenza, streptococcus... The bronchi and alveoli of normal people are sterile. Of course, if the respiratory tract is infected with related bacteria or viruses, the related bacteria or viruses and various corresponding inflammations or lesions will naturally occur.

The main ingredient of human daily drinking beverages is water alcohol with different concentrations. According to statistics, the average lethal dose of ethanol for adults is 250 to 500 grams. Even drunks who are drunk because of greed and anger, most of them will vomit out excessive alcohol and food in time to save their lives through the natural emergency response of the body. After ethanol enters the body, 70% is absorbed through the stomach, 25% is absorbed through the duodenum, and a small amount is absorbed in the remaining small intestine. When there is no content in the stomach, the alcohol in the blood reaches its peak within 30 to 90 minutes. Acute toxicity toxicology experiments show: LD50 7060mg / kg (rat oral); 7340 mg / kg (rabbit percutaneous); LC50 37620 mg / $m^3$, 10 hours (rat inhalation); human inhalation 4.3 mg / L L) (the same below) × 50 minutes, head and face fever, cold limbs, headache; human inhalation 2.6 mg / L × 39 minutes, headache, no after effects.

Further, we can imagine that if a human inhales 2.6 mg / L × 39 minutes, headache and no after-effect are the upper limit of the medicinal dose safety. Then, when the inhalation time is shortened by about 40 times, the ethanol concentration can be increased by about 40 times! Reached 0.1g / L * 1 minute! Alternatively, reduce the concentration and dose by half and take 0.05g / L * 2 minutes as the reference dose for inhalation and disinfection in general adults. As for the specific time for inhalation, it can be based on the type of infectious disease and the actual needs of the patient. It usually takes 20 seconds to 2 minutes. If the effect is insufficient, you can continue after proper rest.

Because the air comes with some moisture, expressed as humidity. At normal temperature, it is about 0.01g / L. The inner wall of the human's respiratory tract and digestive tract naturally also has a layer of moisture-protective film. Therefore, it is recommended to directly use the micro-boiling method of anhydrous alcohol to modulate the therapeutic mixture. When the therapeutic mixture is inhaled into the human's respiratory tract or digestive tract, the vaporous ethanol molecules rapidly diffuse and dissolve into the aqueous protective film on the inner surface of the organ. With continuous breathing, the ethanol concentration in the aqueous film gradually increases... When the ethanol concentration reaches 50% to 80%, the virus bacteria and the infected cells that adhere to the inner wall of the organ will naturally perform a rapid and efficient anti-virus sterilization. As the water and bacteria in the inner wall of the organ and proteins in infected human cells continue to be absorbed, the ethanol concentration gradually decreases. At this time, the ethanol concentration in the aqueous membrane is replenished by continuous breathing, thereby maintaining the concentration balance and the function of disinfection and disinfection.

The density of ethanol liquid is 0.789g / $cm^3$, the density of ethanol gas is 1.59g / L, and the boiling point is 78.2 ° C. Body temperature of healthy people is 36 ～ 37 ℃, fever is 37 ～ 41 ℃. Under standard conditions (25 ° C, one atmosphere), the density of air is 1.29kg / m3 = 1.29g / L. It is about 25 times as much as a therapeutic gas mixture that can be safely used with an ethanol concentration of <0.05g / L! Therefore, the temperature of the prepared mixed gas is close to that of air.

Please note: The microbial cells in the human body are bacteria, and they are generally 0.2 to 100 microns in size, which is only one-tenth to one-hundredth the size of the cells of human organs and tissues. Most viruses are generally 2 nanometers to 100 nanometers in size, and they are only about one to one thousandth of the size of bacteria. Compared with the experimental results in Table 1, the general bacteria can be killed within seconds to minutes in a concentration of 50% to 80% alcohol disinfectant. Then, a virus that is only about one-thousandth to one-thousandth of the size of a bacterium can be killed in seconds.

From the comparison of the size of human cells, bacteria and viruses, it can be known that the therapeutic gas mixed with the ethanol gas with a concentration of 0.05g/L and air (or a certain percentage of oxygen) is cytotoxic to human organs and tissues. And killing effects are small. Even if some cells on the inner surface of each organ are killed by bacterial virus infection, they can still be repaired quickly by the automatic response system of each organ and cell's own emergency response system.

According to the distribution characteristics of bacterial viruses in the respiratory tract and digestive tract of healthy people and patients infected with bacterial viruses. You can directly let the patient selectively inhale the therapeutic mixture into the respiratory tract or fasting digestive tract, and breathe at a smaller (or half) frequency than normal breathing. Each treatment lasts from 20 seconds to 2 minutes. The surface layer and the superficial layer of the inner wall tissue of the organ infected by the bacterial virus are

disinfected by direct contact with the gas diffusion in the body of the treatment mixed gas. Such a therapeutic mixture will not only have negligible toxic and side effects on the human body, but may also have an immediate antibacterial and sterilizing effect on the surface and superficial layers of tissues and cells in the inner wall of the respiratory or digestive system of the patient. That is to say, the relatively cheap alcohol disinfectant commonly used in the medical field is prepared by treating the mixed gas with the method of gas diffusion inside the body and directly contacting the method of disinfection and sterilization. It may become a new method to treat almost all respiratory and digestive tracts of all human beings caused by bacterial and viral infections, and all of them have good efficacy, short time, low cost, and very easy to popularize. .

The current situation of epidemic prevention and control is grim, and saving people is like fighting fire. It is recommended that the medical community choose a suitable model from the existing ventilator, and then ration the vaporized anhydrous alcohol gas into the air intake. Experts are invited to conduct clinical trials as soon as possible to evaluate the efficacy.

## IV. In Summary

We can conclude that the use of ethanol has low toxicity, is almost harmless to the human body, and has the characteristics of rapidly absorbing water in the proteins of viruses and bacteria, dehydrating and solidifying proteins, resulting in rapid death of viruses and bacteria. The treatment method is to directly vaporize anhydrous ethanol and mix it with air to prepare a therapeutic gas mixture with an appropriate concentration to allow patients to inhale the respiratory tract or fasting digestive tract to directly perform anti-virus and sterilization. The methods used to treat all respiratory or digestive tract infections caused by viral and bacterial infections containing protein structures are worthy of clinical examination.

If clinical trials prove effective, they can be expanded further. The use of ethanol has low toxicity, is almost harmless to the human body, and has the characteristics of quickly absorbing the water in the proteins of viruses and bacteria, dehydrating and solidifying the proteins, leading to the rapid death of viruses and bacteria. For other viral and bacterial infectious diseases of the non-respiratory and digestive tracts, an appropriate concentration of ethanol solution can be used to directly perform a needle-injection anti-virus sterilization treatment method for viral and bacterial infections in various organs inside the body or tumor masses Worth clinical examination.

Father, like son. Traditional Chinese medicine can effectively cure new coronary pneumonia, but the effect is still slow. Western medicine does not currently have related vaccines and specific drugs. Experts and patients are waiting for the pricey vaccines or special effects that monkeys can only get when they do not know the monkeys and monkeys, watching death step by step, it's better to try this straightforward, simple and feasible method that is likely to be efficient and fast and low-cost cure?

If patients are eager to seek medical treatment, they can conduct simple clinical trials by themselves. The design scheme is as follows: 1. Use a glass bottle or glass test tube with a capacity of about 100 ~ 200 ml, punch two holes in the lid, one hole is connected with a two-way knob switch, and one hole is connected with a plastic tube; 2. Pour the white wine into the height 5 ~ 10 ml, put it in the hot water cup, the hot water temperature must be higher than the boiling point of alcohol (78.2 ℃); 3. Hold the plastic tube with the mouth, adjust the knob switch, adjust the mixing ratio of alcohol vapor and air, and change the alcohol vapor Modified with a proper amount of air to cure the mixed gas, just breathe in the respiratory tract or digestive tract; 4. The proportion of mixed gas and the inhalation time are completely controlled by your own feelings, and gradually recommended to the patients after the test. Once the test is successful, you will immediately became an expert with real talents.

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# The Results of Ecological Variety Trial of Varieties and Hybrids of Spring Rapeseed in the Conditions of Western Siberia

By Kuznetsova G. N. & Polyakova R. S.

*Abstract-* In 2017-2019, the ecological trial was conducted on the experimental fields of the Siberian experimental station, branch of VNIIMK. The study object was varieties and hybrids of spring rapeseed of breeding of VNIIMK, VNIIR and other breeding institutions which are presented by 17 samples of 15 varieties: Yubileyny – standard, Kupol, Granit, 55 region (the Siberian experimental station, branch of FSBSI FSC VNIIMK), Tavrion, Viking, Ruyan, Amulet (FSBSI FSC VNIIMK), Forward, Flagman, Antares, Sirius (FSBSI VNIIR), Highlight, Kampino, Hunter (Germany) and 2 hybrids: Ozorno, Salsa (Germany). The goal of research is to study the biological potential of spring rapeseed varieties and hybrids in the conditions of Western Siberia; on the basis of field experiments and laboratory analyzes, to identify the highly productive varieties and hybrids suitable for cultivation in the Siberian region.

*Keywords: variety, hybrid, spring rapeseed, ecological trial, yield, oil content, oil yield, glucosinolates, fatty-acid composition.*

*GJSFR-B Classification: FOR Code: 039999*

# The Results of Ecological Variety Trial of Varieties and Hybrids of Spring Rapeseed in the Conditions of Western Siberia

## РЕЗУЛЬТАТЫ ЭКОЛОГИЧЕСКОГО ИСПЫТАНИЯ СОРТОВ И ГИБРИДОВ РАПСА ЯРОВОГО В УСЛОВИЯХ ЗАПАДНОЙ СИБИРИ

Kuznetsova G. N. [α] & Polyakova R. S. [σ]

***Абстрактный-*** **На экспериментальных полях Сибирской опытной станции-филиала ВНИИМК в 2017-2019 гг. проводилось экологиче- ское сортоиспытание. Объектом исследований послужили сорта и гибриды рапса яровогоселекции ВНИИМК, ВНИИР и других научных учреждений, которые представлены семнадцатью образцами из них 15 сортов: Юбилейный-стандарт, Купол, Гранит, 55регион (СОС-филиал ФГБНУ ФНЦ ВНИИМК), Таврион, Викинг, Руян, Амулет (ФГБНУ ФНЦ ВНИИМК), Форвард, Флагман, Антарес, Сириус (ФГБНУ ВНИИР), Хайлайт, Кампино, Хантер (Германия) и два гибрида: Озорно, Сальса (Германия). Цель исследований: изучить биологический потенциал сортов и гибридов масличных культурв условиях Западной Сибири; на основании полевых опытов и лабораторных анализов выявить высокопродуктивные сорта и гибриды рапса ярового пригодные для возделывания в Сибирском регионе.Сорта (Хайлайт, Кампино) и гибриды (Озорно, Сальса) зарубежной селекции в среднем за три года выделены с высокой урожайностью семян (2,45-2,57 т/га). В условиях Западной Сибири наибольший интерес по урожайности и масличности семян представляют сорта селекции Сибирской опытной станции-филиала ВНИИМК: Гранит (2,33 т/га, 51,2%), Купол (2,43 т/га, 51,7%) и 55регион (2,36 т/га, 52,1%), которые вполне конкурируют с сортами и гибридами зарубежной селекции. Сорта Антарес,Хайлайт, Хантер отличаются коротким периодом вегетации (80-81 суток), что важно при создании нового исходного материала в условиях Западной Сибири. Содержание глюкозинолатов в семенах у всех изучаемых сортов и гибридов соответствует межгосударственным стандартам. Сорт Амулет отличается улучшенным жирно-кислотным составом масла (содержание олеиновой кислоты 75,2-77,5%).**

*Ключевые слова: сорт, гибрид, рапс яровой, экологическое испытание, урожайность, масличность, сбор масла, глюкозинолаты, жирно-кислотный состав.*

***Abstract-*** **In 2017-2019, the ecological trial was conducted on the experimental fields of the Siberian experimental station, branch of VNIIMK. The study object was varieties and hybrids of spring rapeseed of breeding of VNIIMK, VNIIR and other breeding institutions which are presented by 17 samples of 15 varieties: Yubileyny – standard, Kupol, Granit, 55 region (the Siberian experimental station, branch of FSBSI FSC VNIIMK), Tavrion, Viking, Ruyan, Amulet (FSBSI FSC VNIIMK), Forward, Flagman, Antares, Sirius (FSBSI VNIIR), Highlight, Kampino, Hunter (Germany) and 2 hybrids: Ozorno, Salsa (Germany). The goal of research is to study the biological potential of spring rapeseed varieties and hybrids in the conditions of Western Siberia; on the basis of field experiments and laboratory analyzes, to identify the highly productive varieties and hybrids suitable for cultivation in the Siberian region. Varieties (Highlight, Kampino) and hybrids (Ozorno, Salsa) of foreign breeding were selected wit high seed yield (2.45-2.57 t/ha) on the average for three years. In the conditions of Western Siberia, the breeding varieties of the Siberian experimental station are the most interesting in terms of yield and oil content of seeds: Granit (2.33 t/ha, 51.2 %), Kupol (2.43 t/ha, 51.7 %), and 55region (2.36 t/ha, 52.1 %), which compete well with varieties and hybrids of foreign breeding. Varieties Antares, Highlight, Hunter are characterized by a short growth season (80-81 days), which is important for the development of new parent material in the conditions of Western Siberia. The content of glucosinolates in the seeds of all studied varieties and hybrids meets the requirements of interstate standards. Variety Amulet is characterized by the improved fatty-acid composition of oil (the content of oleic acid is 75.2-77.5 %).**

*Keywords: variety, hybrid, spring rapeseed, ecological trial, yield, oil content, oil yield, glucosinolates, fatty-acid composition.*

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## I. Введение

Рапс – потенциально высокопродуктивная культура. Однако ее урожайность сильно зависит от почвенно-климатических условий и уровня культуры земледелия. Успешное выращивание высоких урожаев маслосемян определяется использованием лучших гибридов и сортов рапса, приспособленных к тем или иным конкретным условиям региона. Правильный выбор сорта – малозатратный и весьма эффективный агроприём[1].

Одним из основных факторов развития отрасли рапсоводства являются современные сорта и гибриды рапса, которые должны обеспечивать высокую и стабильную урожайность в зоне районирования. [2].

Рапс – вторая масличная культура в мире, занимающая 36,4 млн га с валовым сбором 71,9 млн т в

2017 г., уступающая лишь сое (126,1 млн га и 347,9 т соответственно) и опережающая подсолнечник (25,8 млн га и 46,3 млн т). Рост посевных площадей культуры сопровождается увеличением сортимента, представляемого на рынки селекционными учреждениями, лишь при условии реализации механизма возврата средств, вкладываемых в селекцию, то есть расширенного воспроизводства [3].

Современное рапсовое масло, как и масла ряда других капустных культур, уникально и разнообразно как по составу жирных кислот, так и по областям его применения. Широкому использованию рапсового масла на пищевые цели положило начало создание в 60-70-х годах прошлого века в Канаде безэруковых сортов. Сэтого момента культура получила второе название –canola, подразумевающее содержание эруковой кислоты в масле менее 2% в сочетаниис низким содержанием в семенах нежелательных глюкозинолатов.С начала 90-х годов прошлого века и по настоящее время усилия селекционеров направлены на увеличение доли олеиновой кислоты в рапсовом масле (не менее 75%), что позволит значительно повысить его потребительские характеристики. Оксистабильностьвысокоолеинового масла в 3 раза выше, чем у масла с традиционным жирно-кислотным составом [4]. Во ВНИИМК работы по созданию высокоолеинового селекционного материала рапса ярового начаты в 2006 г [5].

Селекционная программа Сибирской опытной станции-филиала ВНИИМК осуществляется по следующим направлениям: семенная продуктивность (урожайность, сбор масла, скороспелость, содержание жира (масличность), качество (жирно-кислотный состав, глюкозинолаты). При реализации селекционных программ по выведению высокоурожайных, устойчивых к абиотическим и биотическим факторам среды, с высоким качеством масла и жмыха сортов и гибридов рапса, большое значение уделяется изучению генофонда, его постоянному пополнению новыми образцами. В рамках научного сотрудничества между селекционными учреждениями происходит постоянный обмен селекционным материалом и его широкая агроэкологическая оценка [6].

Большинство районов Западной Сибири благоприятны для возделывания рапса ярового. По агроклиматическим условиям территория Западной Сибири делится на степную, лесостепную черноземную, лесостепную солонцеватую, подтаежную и таежную зоны. Черноземная лесостепная зона занимает обширные пространства в Омской, Новосибирской, Кемеровской, Тюменской областях и в Алтайском крае. Для нормальной жизнедеятельности растений рапса необходима влага и только при наличии влаги в оптимальном количестве идут нормальные процессы роста, развития репродуцирования растений. Дефицит влаги замедляет и угнетает органогенез растений [7]. Для Сибири с её специфическими особенностями климата нужны сорта рапса равномерно созревающие, технологичные в уборке, засухоустойчивые, устойчивые к основным патогенам. При этом очень важно использовать сорта хорошо проверенные, разрешенные к выращиванию в данной зоне. Завозимые иностранные сорта должны предварительно пройти государственное и производственное испытания [8].

*Цель работы:* изучить биологический потенциал новых сортов и гибридов масличных культур селекции ВНИИМК и других научно-исследовательских учреждений в условиях Западной Сибири; на основании полевых опытов и лабораторных анализов выявить высокопродуктивные сорта и гибриды рапса ярового пригодные для возделывания вСибирском регионе.

## II. Объекты и Методы Исследований

Объектом исследованийв 2017-2019 гг. на экспериментальных полях Сибирской опытной станции ВНИИМК были сорта и гибриды рапса яровогоселекции ВНИИМК, ВНИИР и других селекционных учреждений, которые представленышестнадцатью образцами из них 15 сортов: Юбилейный-стандарт, Купол, Гранит, 55регион (СОС-филиалФГБНУ ФНЦ ВНИИМК), Таврион, Викинг, Руян, Амулет (ФГБНУ ФНЦ ВНИИМК), Форвард, Флагман, Антарес, Сириус (ФГБНУ ВНИИР), Хайлайт, Кампино, Хантер (Германия) и 2 гибрида: Озорно, Сальса (Германия).

Опыт закладывался по типу питомника конкурсного сортоиспытания, площадьучетной делянки составляла 23 кв.м., в 3-х кратной повторности, размещение делянок – рендомизированное. Общая площадь опыта 1104 кв.м. Способ посева сплошной (сеялкой – СС-11), междурядье 15 см. Норма высева– 1,75 млн. всхожих семян на гектар. В качестве стандарта использовали сорт Юбилейный.Почва опытного участка – чернозём обыкновенный среднемощный, среднегумусный, характеризуется средней обеспеченностью фосфором и высокой – калием. Предшественник – чёрный пар. Технология возделывания общепринятая, согласно рекомендациям Сибирской опытной станции ВНИИМК [9]. В течение вегетации проводились фенологические наблюдения, в ходе которых, отмечались даты: всходы; цветение; созревание (желто-зелёный стручок).

Погодные условия в период испытания были контрастными (табл. 1).

*Таблица 1:* Характеристика погодных условий вегетационного периода

| Годы | Температура воздуха, $^0$C | | | | Количество осадков, мм | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | май | июнь | июль | август | май | июнь | июль | август | сумма |
| 2017 | 12,9 | 19,1 | 20,9 | 19,6 | 12 | 76 | 102 | 29 | 219 |
| 2018 | 13,1 | 19,3 | 18,1 | 17,9 | 57 | 24 | 89 | 14 | 184 |
| 2019 | 7,3 | 17,9 | 22,6 | 16,6 | 73 | 48 | 71 | 101 | 293 |
| ср. мн. | 11,7 | 17,5 | 19,5 | 17,1 | 29 | 53 | 56 | 49 | 187 |

В целом по температурному режиму вегетационный период 2017 г. характеризовался повышенными среднесуточными температурами воздуха. Отклонения от среднемноголетних значений составляли от +1,2 до +2,5°C. При этом наблюдался дефицит увлажнения в мае и августе – 41 и 59% от многолетней нормы. В июне и июле месячная сумма осадков составила 76-102 мм – 102-182% от нормы.

Начало вегетационного периода 2018 г. было благоприятным для развития растений рапса. Отмечалось избыточное увлажнение в мае (196% от нормы) и июле (159% от нормы). Среднемесячные температуры воздуха при этом были в среднем выше нормы (+0,8…+1,8°C). По количеству своевременно выпавших осадков и среднесуточной температуры воздуха 2018 год оказался более благоприятным для роста и развития рапса.

Метеорологические условия вегетационного периода 2019 г. характеризовались резкими отклонениями основных показателей по декадам от многолетних значений, хотя средние значения температуры воздуха по месяцам (кроме мая и июня) находились на уровне нормы или близки к ней. Май характеризовался неустойчивой и холодной погодой, поэтому сроки посева рапса были передвинуты на 8-10 дней. Обильные осадки составили 250% от нормы. Среднемесячные температуры воздуха в июне, июле и августе была на уровне среднемноголетних показателей или чуть выше. В августе в первой декаде была благоприятная погода, что позволило провести уборку рапса в сжатые сроки.

Исследования проводились в лабораториях селекции, семеноводства и агротехники капустных культур и в лаборатории агробиохимии. Масличность семян определяли на ЯМР – анализаторе АМВ-1006М, жирно-кислотный состав масла методом газожидкостной хроматографии (Кристалл-2000), содержание глюкозинолатов в семенах рапса ярового на фотометре фотоэлектрическом КФК-3-01. Полученный урожай переведен к 100% чистоте 10% влажности, проведена статистическая обработка данных [10].

## III. Результаты и Обсуждения

Экологическое испытание позволяет в одной почвенно-климатической зоне сравнить сорта и гибриды по основным хозяйственно ценным признакам.

Анализируя урожайные данные по годам в 2017г. урожайность семян рапса в среднем составила 2,23т/га с минимальными показателями (1,85 т/га) у сорта Антарес, и максимальными (2,57 т/га) у сорта Хайлайт при среднем показателе изменчивости признака CV – 10,5 % (табл. 2).

*Таблица 2:* Урожайность сортов и гибридов рапса ярового экологического сортоиспытания

| Сорт, гибрид | Урожайность семян, т/га | | | Среднее | Откло-нениеот стандарта | CV, % |
|---|---|---|---|---|---|---|
| | 2017 | 2018 | 2019 | | | |
| Юбилейный –ст. | 2,23 | 2,61 | 1,83 | 2,22 | - | 17,5 |
| Купол | 2,41 | 2,70 | 2,19 | 2,43 | +0,21 | 10,5 |
| Гранит | 2,29 | 2,74 | 1,96 | 2,33 | + 0,11 | 16,8 |
| 55 регион | 2,31 | 2,72 | 2,07 | 2,36 | + 0,14 | 13,9 |
| Таврион | 2,17 | 2,49 | 1,82 | 2,16 | – 0,06 | 15,5 |
| Руян | 2,07 | 2,39 | 2,03 | 2,16 | – 0,06 | 9,1 |
| Амулет | 2,10 | 2,21 | 2,09 | 2,13 | – 0,09 | 3,1 |
| Форвард | 2,05 | 2,41 | 2,14 | 2,20 | – 0,02 | 8,5 |
| Антарес | 1,85 | 2,51 | 2,14 | 2,17 | – 0,05 | 15,3 |
| Сириус | 1,95 | 2,20 | 2,04 | 2,06 | – 0,16 | 6,1 |
| Озорно ($F_1$) | 2,33 | 2,60 | 2,33 | 2,42 | + 0,20 | 6,4 |
| Сальса ($F_1$) | 2,56 | 2,45 | 1,93 | 2,31 | + 0,09 | 14,6 |
| Хайлайт | 2,44 | 2,30 | 2,03 | 2,26 | + 0,04 | 9,2 |
| Хантер | 2,22 | 2,45 | 2,08 | 2,25 | +0,03 | 8,3 |
| Среднее | 2,23 | 2,51 | 2,02 | - | - | - |

| | | | | | | |
|---|---|---|---|---|---|---|
| CV, % | 10,5 | 6,8 | 6,6 | - | - | - |
| $НСР_{05}$ | 0,17 | 0,12 | 0,15 | - | 0,19 | - |

В 2018 году максимальная урожайность получена у сортов Гранит и 55регион (2,74 и 2,72 т/га соответственно), при среднем показателе 2,51 т/га, наблюдалась незначительная изменчивость признака CV – 6,8 %. Избыточное переувлажнение почвы в 2019 году привело к снижению урожайности рапса (средний показатель 2,02 т/га). Наименьшая урожайность отмечена у сортов Таврион и Юбилейный (1,82 и 1,83 т/га), а максимальная (2,33 т/га) у гибрида Озорно, CV – 6,6%.

В среднем за три года испытаний достоверно превысили по урожаю семян сорт-стандарт Юбилейный сорта Купол, Кампино и гибрид Озорно имея разную степень изменчивости по годам по этому признаку. В зависимости от года испытания, урожайность семян в сортах рапса ярового: Юбилейный, Купол, Гранит, 55регион, Таврион, Викинг, Антарес, и гибрид Сальсаменялась в средней степени изменчивости признака от –10,5 % (Купол) до 18,7 % у Викинга. Незначительное варьирование этого признака 3,1 – 9,2% по годам отмечено в сортах Руян, Амулет, Форвард, Сириус, Хайлайт, Хантер. В условиях Западной Сибири по урожаю семян сорта Амулет, Сириус, Руян, Антарес в среднем за три года исследований уступали сорту-стандарту Юбилейный на 0,05-0,16 т/га

Вегетационный период изучаемых сортов и гибридов в среднем за 3 года составил 80-89 суток. С более коротким вегетационным периодом (80-82 суток) отмечены сорта селекции ВНИИМК (Таврион, Амулет), ВНИИР (Антарес), а зарубежной селекции (Хайлайт и Хантер). Сорта селекции ФГБНУ СОС-филиала ВНИИМК: Юбилейный, Купол, Гранит и 55регион имеют более продолжительный период вегетации (86-89 суток), при этом полностью реализуют высокий потенциал продуктивности: урожайность семян (2,22-2,43 т/га), масличность семян (50,0-52, 1 %) и сбор масла (999- 1131 кг/га), уступая лишь по семенной продуктивности сортам Хайлайт – (2,57 т/га), Кампино (2,49 т/га) и гибридам (Озорно – 2,52 т/га, Сальса – 2,45т/га) зарубежной селекции (табл. 3).

*Таблица 3:* Характеристика сортов и гибридов рапса ярового экологического сортоиспытания

| Сорт, гибрид | Вегетаци-онный период, сутки | Маслич-ность, семян, % | Сбор масла, кг/га | Масса 1000 семян,г | Глюкози-нолаты, мкмоль/г | Олеино-вая кислота, % |
|---|---|---|---|---|---|---|
| Юбилейный | 88 | 50,0 | 999 | 3,5 | 11,9 | 63,99 |
| Купол | 89 | 51,7 | 1131 | 3,6 | 14,3 | 65,14 |
| Гранит | 86 | 51,2 | 1074 | 3,6 | 11,4 | 64,75 |
| 55регион | 89 | 52,1 | 1107 | 3,7 | 9,8 | 64,10 |
| Таврион | 81 | 48,5 | 943 | 3,5 | 11,4 | 65,14 |
| Руян | 84 | 50,3 | 977 | 4,1 | 10,5 | 66,81 |
| Амулет | 82 | 50,4 | 966 | 3,7 | 9,2 | 75,20 |
| Форвард | 85 | 49,4 | 978 | 3,9 | 13,5 | 64,82 |
| Антарес | 80 | 49,9 | 988 | 4,0 | 14,7 | 66,00 |
| Сириус | 85 | 48,7 | 889 | 3,9 | 13,2 | 66,12 |
| Озорно ($F_1$) | 83 | 50,4 | 1143 | 4,1 | 13,5 | 63,64 |
| Сальса ($F_1$) | 84 | 50,3 | 1109 | 3,5 | 8,8 | 64,52 |
| Хайлайт | 81 | 49,1 | 1136 | 3,6 | 12,0 | 63,28 |
| Хантер | 81 | 49,3 | 998 | 3,7 | 13,5 | 63,83 |

В среднем за три года с более коротким вегетационным периодом (81-84 суток) отмечены сорта селекции ВНИИМК: Таврион, Викинг, Руян, Амулет с урожайностью 2,13-2,20 т/гасемян и масличность семян 48,5-50,4 %. С масличностью 48,7-49,9 % и урожайностью семян 2,03-2,20 т/га представлены сорта селекции ВНИИР, при этом более высокое содержание глюкозинолатов в семенах (14,7-15,0 мкмоль/г) отмечено в сортах Флагман и Антарес. По крупности семян 4,0-4,1 г выделены новые сорта Руян, Антарес и гибрид Озорно.

Проведя оценку по испытанию сортов и гибридов рапса ярового различного эколого-географического происхождения, было установлено большое генетическое разнообразие по хозяйственно ценным признакам. В среднем за годы изученияСортазарубежной селекции Хайлайт, Кампино и гибриды Озорно,Сальса выделены с более высокой урожайностью семян (2,45-2,57 т/га). Наибольший интерес в условиях Западной Сибири по урожайности и масличности семян представляют сорта селекции Сибирской опытной станции ВНИИМК: Гранит (2,33 т/га т/га, 51,2%), Купол (2,43

т/га, 51,7%) и 55регион (2,36 т/га, 52,1%) и вполне конкурируют с сортами и гибридами зарубежной селекции.

Сорта Антарес,Хайлайт, Хантер отличаются коротким периодом вегетации (80-81 суток), что важно при создании нового исходного материала в условиях Западной Сибири. Содержание глюкозинолатов в семенах у всех изучаемых сортах и гибридах соответствует межгосударственным стандартам (8,8-15,0 мкмоль/г).

## IV. Заключение

Таким образом, проведенное экологическое испытание сортов и гибридов рапса яровогопоказало, что почвенно-климатические условия Западной Сибири подходят для возделывания этой культуры и каждый новый,районированный сорт или гибрид имеет свои достоинства и может быть использован в качестве ценного материала.

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# Accusteel – Acoustic Computer Control System for EAF and BOF Steelmaking Process - Technology of XXI Century

By O. Shlik & A. Shlik

*Abstract-* The result of analysis of data from computer systems which used on BOF and EAF furnaces is proved that the main technological parameters (the temperature, the chemical composition of the melt in the end of melting process) are incorrect.

The Accusteel acoustic computer system is proposed as an alternative to existing certified computer complexes and systems. It is proved that the Accusteel computer system uses the method of determining of mass-average temperature, chemical composition of the melt in real time and has confidence which determined the correlation coefficient 0.97-0.99.

*Keywords:* *acoustics, system, thermocouple, correlation, computer.*

*GJSFR-B Classification:* *FOR Code: 670801*


*Strictly as per the compliance and regulations of:*

# Accusteel – Acoustic Computer Control System for EAF and BOF Steelmaking Process - Technology of XXI Century

O. Shlik [α] & A. Shlik [σ]

*Abstract-* The result of analysis of data from computer systems which used on BOF and EAF furnaces is proved that the main technological parameters (the temperature, the chemical composition of the melt in the end of melting process) are incorrect.

The Accusteel acoustic computer system is proposed as an alternative to existing certified computer complexes and systems. It is proved that the Accusteel computer system uses the method of determining of mass-average temperature, chemical composition of the melt in real time and has confidence which determined the correlation coefficient 0.97-0.99.

*Keywords: acoustics, system, thermocouple, correlation, computer.*

## I. Introduction

Acoustic systems for the slag control and management by the noise of BOF melting process were widely used in the 1960s [1-2].

Accusteel - acoustic computer system - provides control of the BOF or EAF process in real time by the noise of smelting. The algorithm's simplicity [3] and reliability of acoustic computer system allows us control of the mass-average temperature, chemical composition and slag formation in the melt by noise of the process. Testing and improvement of the system's algorithm was held since 1992 to 2014 on BOF and EAF furnaces with a charge of 15 – 350 tons on steelmaking plants in Israel, Italy, Spain, Japan, China, Ukraine, Russia, USA, Brazil. More than one hundred thousand heats were made, the data of which was used in the comparative evidence-based analysis.

It was recognized that certified computerized process control and management systems can control the process only at the end of smelting. The correlation of these temperatures and chemical composition is determined by a correlation coefficient of 0.2–0.5.

Consider the experience of using the Accusteel system at one of the US companies, the company Nucor. It was DC electric arc furnace with charge 150 tons. The smelting process was controlled by the robotic complex. Where the temperature was measured out by a thermocouple and carbon percentage %C was calculated using temperature data.

The results of statistical analysis of 151 heats (the main technological parameters of smelting: temperature T°F and carbon percentage %C) in 150t. DC electric arc furnace are presented in table 1.

*Table 1:* Statistics of technological parameters of EAF heats

| | T1°F | Ta1°F | T2°F | Ta2°F | %C1 | %Ca1 | %C2 | %Ca2 |
|---|---|---|---|---|---|---|---|---|
| Count | 148 | 151 | 99 | 113 | 142 | 146 | 99 | 119 |
| Average | 2990 | 2973 | 2953 | 2969 | 0.036 | 0.035 | 0.036 | 0.035 |
| St. Dev. | ±41 | ±27 | ±59 | ±30 | ±0.003 | ±0.004 | ±0.003 | ±0.005 |

There is a statistical data analysis of 151 heats, main technological parameters: T1°F and T2°F - temperatures measured by thermocouple, Ta1°F and Ta2°F - temperatures determined by the computer system Accusteel in the moment of thermocouple measurement. The chemistry: the concentration of carbon in the melt %C1 and %C2 was determined by the plant's computer system that allows to determine the carbon percentage by the temperature mesured by thermocouple. The carbon percentage %Ca1 and %Ca2 which determined by the Accusteel system in the moment of the carbon percentage determination %C1 and %C2 are the same in absolute value to %C1 and %C2. The average mathematically expected temperatures are slightly varied within 5-17°F. Standard deviation of the temperatures of the melt determined by the thermocouple is twice the standard deviation of the temperatures determined by the Accusteel system.

The result of the correlation data analysis of determined temperatures and melt chemistry is presented in Table 2.

*Table 2:* Correlation analysis of technological parameters of heats

| Function | T1°F (T2°F) | Ta1°F (Ta2°F) | %C1%(C2) | %Ca1%(Ca2) |
|---|---|---|---|---|
| Coefficient | 0.72 | 0.98 | 0.22 | 0.99 |

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From Table 2 it can be seen that the correlation coefficient of temperatures measured by thermocouple and carbon percentage determined by the local method is low compared with the data of the Accusteel system, requires graphic confirmation.

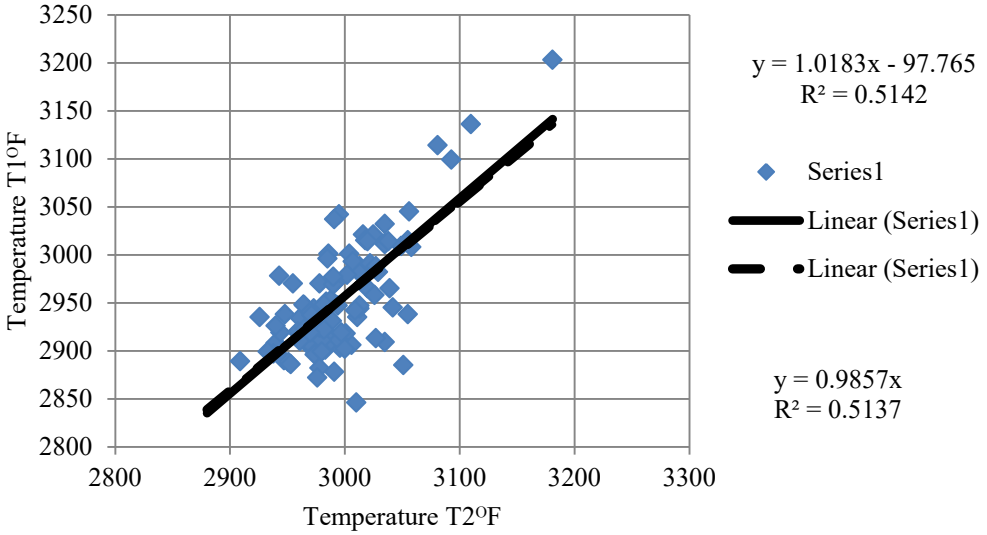


*Fig. 1:* Correlation function T1°F (T2°F) of temperatures determined by the local method of the thermocouple measurement

Fig.1 shows that the temperature data determined by the local method of the thermocouple measurement have a data spread with square deviations $R^2 = 0.51$. The temperature data determined by the computer control system was showed high reliability for local random variables, the information obtained confirmed by a correlation coefficient of 0.72.

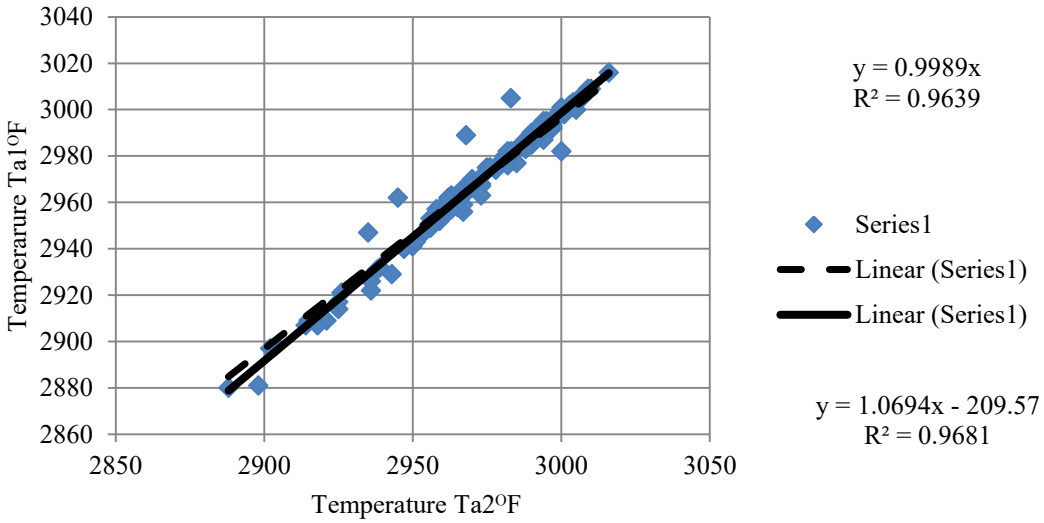


*Fig. 2:* Correlation function Ta1°F (Ta2°F) of mass average temperature determined by the Accusteel system

Fig. 2 shows that the data with great reliability describe straight lines, as evidenced by $R^2 = 0.96$ of quadratic deviations of the function describes of the data distribution. Mass-average temperatures of the melt determined by the Accusteel system have a correlation coefficient of 0.98.

One of the main technological parameters is the percentage of %C carbon in the melt. The control of carbon concentration in the melt on the furnace was made by a computer system on the basis of measured local random temperatures by the thermocouple system.

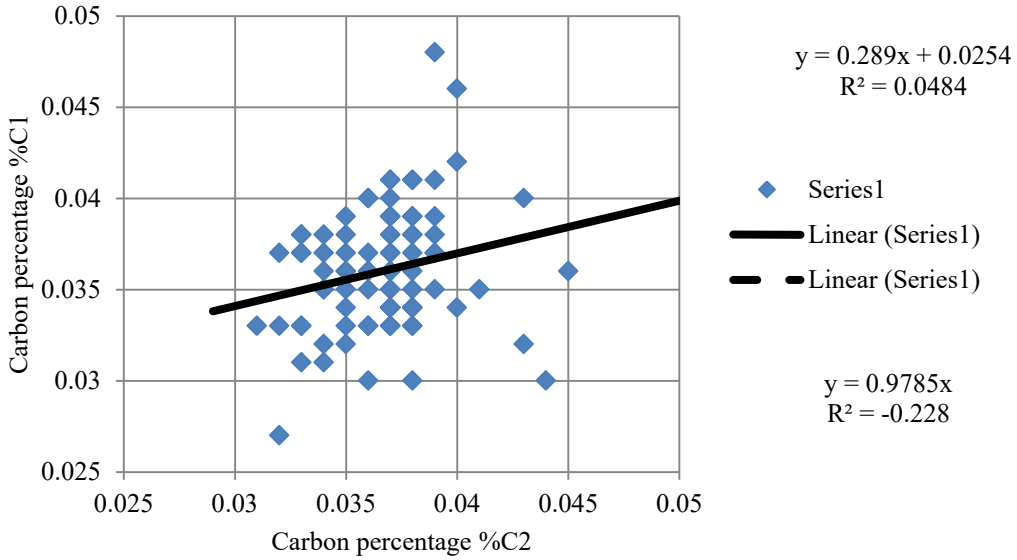


*Fig. 3:* Correlation function %C1(%C2) of the carbon percentage determined on the temperature measured by the thermocouple system

Fig. 3 shows that the data have a large spreading as evidenced by the low correlation coefficient of 0.22. The low reliability of data about the carbon percentage %C is result of using by computer system in the calculation algorithm locally randomly determined physical temperatures by the thermocouple system.

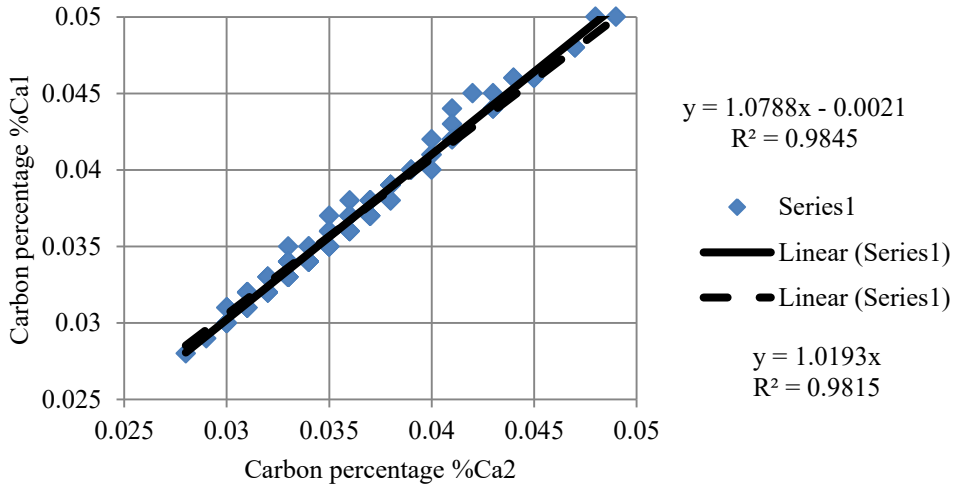


*Fig. 4:* Correlation function %Ca1(%Ca2) of the carbon percentage determined by the Accusteel computer system on the basis of temperatures Accusteel

Fig. 4 shows high reliability of determining the carbon percentage in the melt based on the temperature data determined by the Accusteel system. The high reliability of the mass-average temperatures determination by the Accusteel system allows us to determine with high confidence the data on the percentage of chemical elements in the melt. What indicates the correlation coefficient 0.99.

Improving the technological process. Figure 5 shows the diagram of visualization of technological parameters of the smelting process in EAF furnace with a charge of 150 tons.

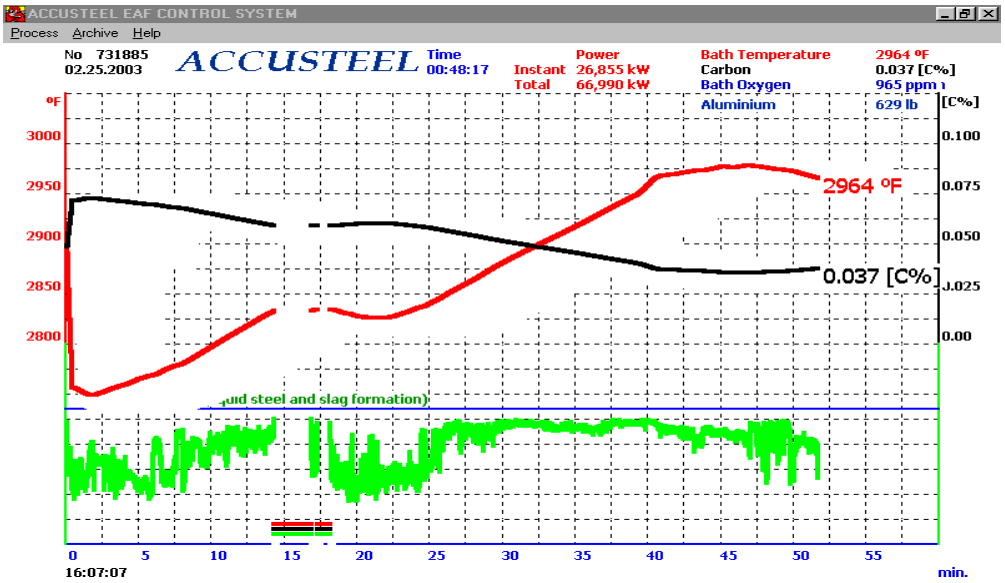


*Fig. 5:* Heat diagram № 731885 from 02.25.2003

This is heat diagram of one the first heats in the start of Accusteel system test on DC EAF furnace. We can see that from 27-th minute of the process the melt bath was formed and the period of melt refining was started in the closed arc mode. The period of melt refining is characterized by the maximum consumption of the energy supplied to the melt. From 40-th minute within 12 minutes the process is made with an open electric arc because intensive tapping of the slag phase. This process control mode causes poor absorption of energy entering the melt.

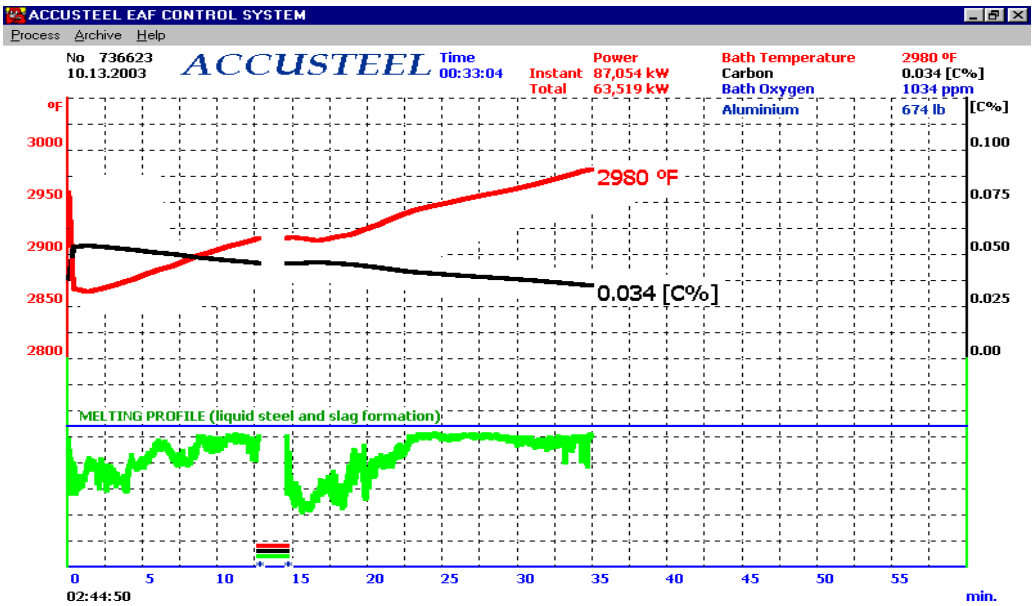


*Fig. 6:* Heat diagram № 736623 from 10.13.2003

Fig.6 shows that after 9 months of the Accusteel system's work the smelting process was optimized. The melting cycle has been reduced from 72 minutes to 48 minutes with a saving of 6 megawatts of electrical energy and also amount of the oxygen blast to melt.

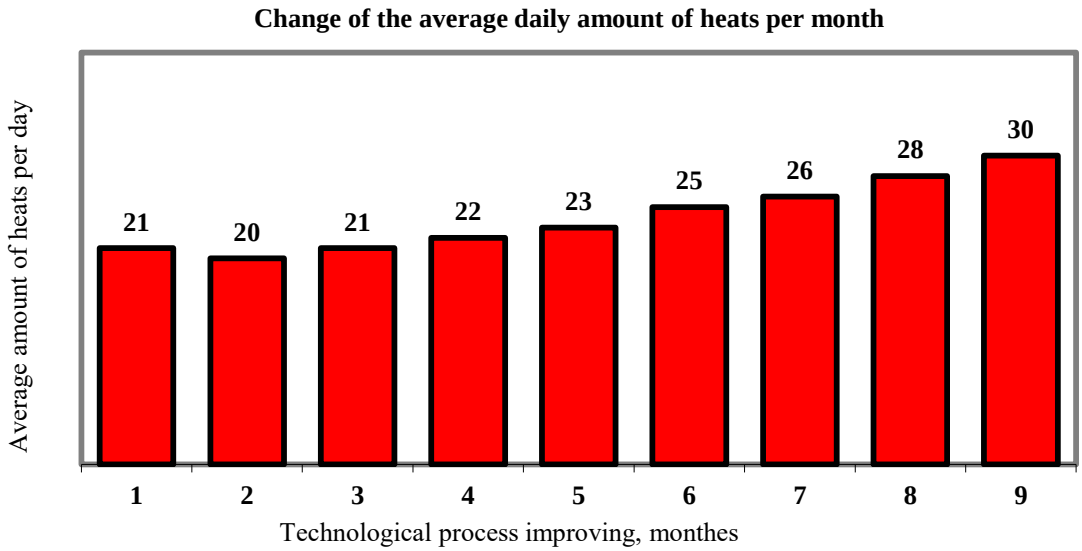


*Fig. 7:* Diagram of the average-daily performance per month on EAF furnace of 150t as a result of the technological process optimization using the Accusteel system's information

Fig. 7 shows that using information of the Accusteel system for nine months production was increased from an average of 21-22 to 30 heats per day for DC EAF with a charge 150 tons.

Lets consider the possibility of using the Accusteel system on the BOF where the "drop-bomb" thermocouples computer temperature control system is used. The tests were made using the Accusteel system on the 80t charge blast oxygen furnace (BOF), company Mannesmann, Brazil. It is known that the BOF process is controlled visually by a torch on the neck of the furnace using the experience of the BOF operator. Temperature control during the melting is made for 3-4 minutes or 15-20% oxygen blow before the end of the process without stopping the process by the thermocouple computer system by immersion in the melt "drop-bomb" thermocouple. The chemistry of the melt is determined by the local method by taking a sample of the melt for express analysis after stopping the process.

The results of statistical data analyses of temperature by "drop-bomb" thermocouple and chemistry of the melt are presented in table 3.

*Table 3:* Statistics of technological parameters of BOF heats

| | T1°C | Ta1°C | T2°C | Ta2°C | %C1 | %Ca1 | %C2 | %Ca2 | %P1 | %Pa1 | %P2 | %Pa2 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Count | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| Average | 1617 | 1616 | 1560 | 1618 | 0.038 | 0.042 | 0.19 | 0.041 | 0.01 | 0.01 | 0.012 | 0.013 |
| StDev | ±27 | ±16 | ±24 | ±17 | ±0.0111 | ±0.004 | ±0.21 | ±0.004 | ±0.0037 | ±0.0035 | ±0.0035 | ±0.0036 |

Where: T1°C is the temperature determined by the "drop-bomb" thermocouple, the second temperature for performing statistical and correlation analysis is the temperature T2°C determined by the thermocouple in the ladle. For statistical and correlation analysis of the chemistry of the melt were used data of the carbon percentage %C in the furnace %C1 and in the ladle %C2 and for the phosphorus percentage in the furnace %P1 and in the ladle %P2. Data of temperature and chemistry determined by the Accusteel system: Ta1°C - temperature, chemical element concentrations %Ca1 and %Pa1 taken in time of measurements made by the "drop-bomb" and in the end of heat (100% blast) temperature Ta2°C, carbon and phosphorus percentage %Ca2 and %Pa2.

The table 3 shows that the average temperatures T1°C and Ta1°C corresponded. The difference in StDev - standard deviations, errors in determining the temperature and chemical composition of the melt, can be explained by the local definition of data for the thermocouple, heterogeneity of the melt where there are intense heat exchange processes accompanied by convective currents due to the temperature gradient presence. For the Accusteel system data the mass-average temperature of the gas in the furnace cavity characterizes the thermophysical properties of the melt. For evaluation of the reliability of the information received the correlation analysis of data determined by computer systems was performed.

The correlation analysis results of the temperature and chemistry of the melt are presented in table 4.

*Table 4:* Correlation analysis of technological parameters

| Function | T1(T2) | Ta1(Ta2) | C1(C2) | Ca1(Ca2) | P1(P2) | Pa1(Pa2) |
|---|---|---|---|---|---|---|
| Coefficient | 0.03 | 0.97 | -0.022 | 0.97 | 0.6 | 0.97 |

The results of the correlation analysis in Table 4 confirm the low reliability of the information obtained for the temperatures determined by the "drop-bomb" thermocouple system and the chemistry of the melt. Indicates low reliability of the information received. The correlation of the temperature and chemistry data of 0.97 indicates the reliability of the data determined by the Accusteel system.

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# Efficient and Facile One-Pot Synthesis of Novel Benzimidazoles using Rice Husk

By Suman, Rajvir Singh, Susheel Gulati & Suprita
*Chaudhary Charan Singh Haryana Agricultural University*

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*Keywords: rice husk, green catalyst, benzimidazole, metal-free, atom economy.*

*GJSFR-B Classification: FOR Code: 030299*


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## I. Introduction

In recent years, the progress of science and technology gradually shifted more towards environmentally benign, sustainable, and green resources. In this series, much attention has been focused on the utilization of plant biomass as biocatalyst. Amongst the various biomasses, with abundant and renewable energy sources, rice husk is not only a potential source of energy but also a value-added by-product[1].In the last days, there were many reasons associated with rice husk for not being effectively like (i) lack of awareness of its potential by farmers and industry persons, (ii) socio-economic problems, (iii) penetration of technology, (iv)lack of environmental concern and many others. The only solution to these problems associated with the utilization of this solid waste needs to be detected both in quality and quantity aspects. Benzimidazole and its derivatives have reported the number of biological importance like they can be used as anticonvulsant, antibacterial, antifungal, antitumor, anthelmintic, ant amoebic, analgesic, and antiulcer [2-3]. Recent results indicate that the benzimidazole structure can bind in the DNA minor groove and can act as a ligand to transition metals. So, it must be necessary to develop a mild and easy procedure for the synthesis of these bioactive chemicals. Generally, benzimidazoles were prepared by CAN [4], microwave-assisted[5], lead peroxide [6].Despite of these methods, polycondensation of o-phenylenediamine with aryl aldehydes is more efficient and facile. Recently, some of the green protocol for the synthesis of benzimidazole derivatives has been carried out, such as the use of pectin in water [7]. In continuation of these series, we want to explain the applicability of RHA.$CaCl_2$ as a newly reported green catalyst which is reusable many times without loss of activity and performs the reaction under mild conditions with high yields.

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## II. Experimental Details

The contents of rice husk are hemicellulose 24.3%, cellulose 34.4%, lignin19.2%, ash 18.85%and the other substances are3.25% [8]. Cellulose and lignin did not show the bonding properties because these are mostly inert but the monomeric components of hemicelluloses such as methyl glucuronic acid (monosaccharides), which become polar due to the electrometric effect of carboxylic acidic part. The active acidic monosaccharide can be extracted by removing lignin and cellulose from rice husk with an alkaline metal treatment [9]. All reagents and solvents were used in analytical grade and used without purification. Melting points were determined in open capillaries on a Ganson electric melting point apparatus and are uncorrected. Infrared spectra (4000-350 $cm^{-1}$) of the synthesized compounds were recorded in KBr pellets on Perkin Elmer FT-IR-R2X spectrophotometer, and frequency was expressed in $cm^{-1}$. The $^1$HNMR spectrum was recorded in $CDCl_3$ or DMSO-$d_6$ using tetra methyl silanean internal reference on "Brucker Ac 400 F"(400 MHz) nuclear magnetic resonance spectrometer. The chemical shift values were quoted in delta (ppm).

### a) *General procedure of the synthesis of biocatalyst*

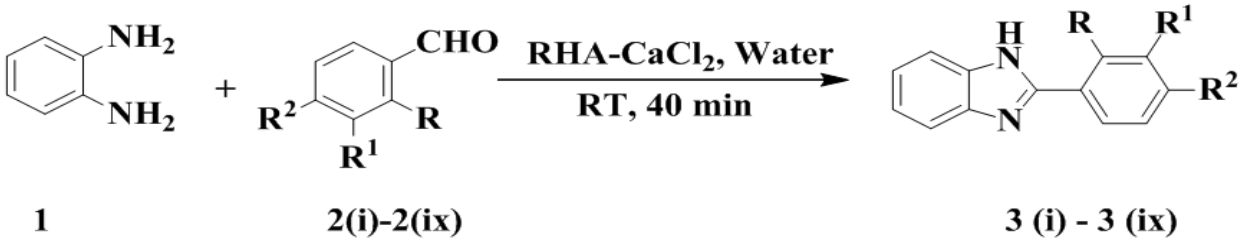
The catalyst was prepared by sorption of anaqueous solution of $CaCl_2.2H_2O$ (7.35 gm, 0.05 mmol) in per mL distilled water on rice husk (0.25 gm). The mixture was heated at 100 °C for 4 hours to give RHA.$CaCl_2$ [9].

### b) *General procedure of the synthesis of benzimidazole*

O-phenylenediamine(20 mmol) was added to a mixture of RHA.$CaCl_2$ (20 mg), substituted aldehydes (20 mmol),and 10 mL distilled water .Thus the resulting mixture was stirred at room temperature for 40 min. The progress of reaction was monitored by thin-layer

chromatography (Ethyl acetate: n-hexane 2:8). After completion of the reaction, the mixture was workup by the addition of ice-coldwater. The yellow solid products was separated by simple filtration and recrystallized from ethanol. If the product was gummy, it was extracted with ethyl acetate, and the organic phase was washed with water and dried over sodium sulfate. The reaction was found to complete within 40 min to give 2-(1*H*-benzimidazole-2yl) phenol 3(i) a product in quantitative yield (Table 3, entry 1). Various derivatives of benzimidazole and their yield formed was shown in Table 2 under (Scheme-1). Also, the specialty of the catalyst in comparison of other is shown in Table 3.

*Chemical reaction*




*Scheme-1*

## III. Result and Discussion

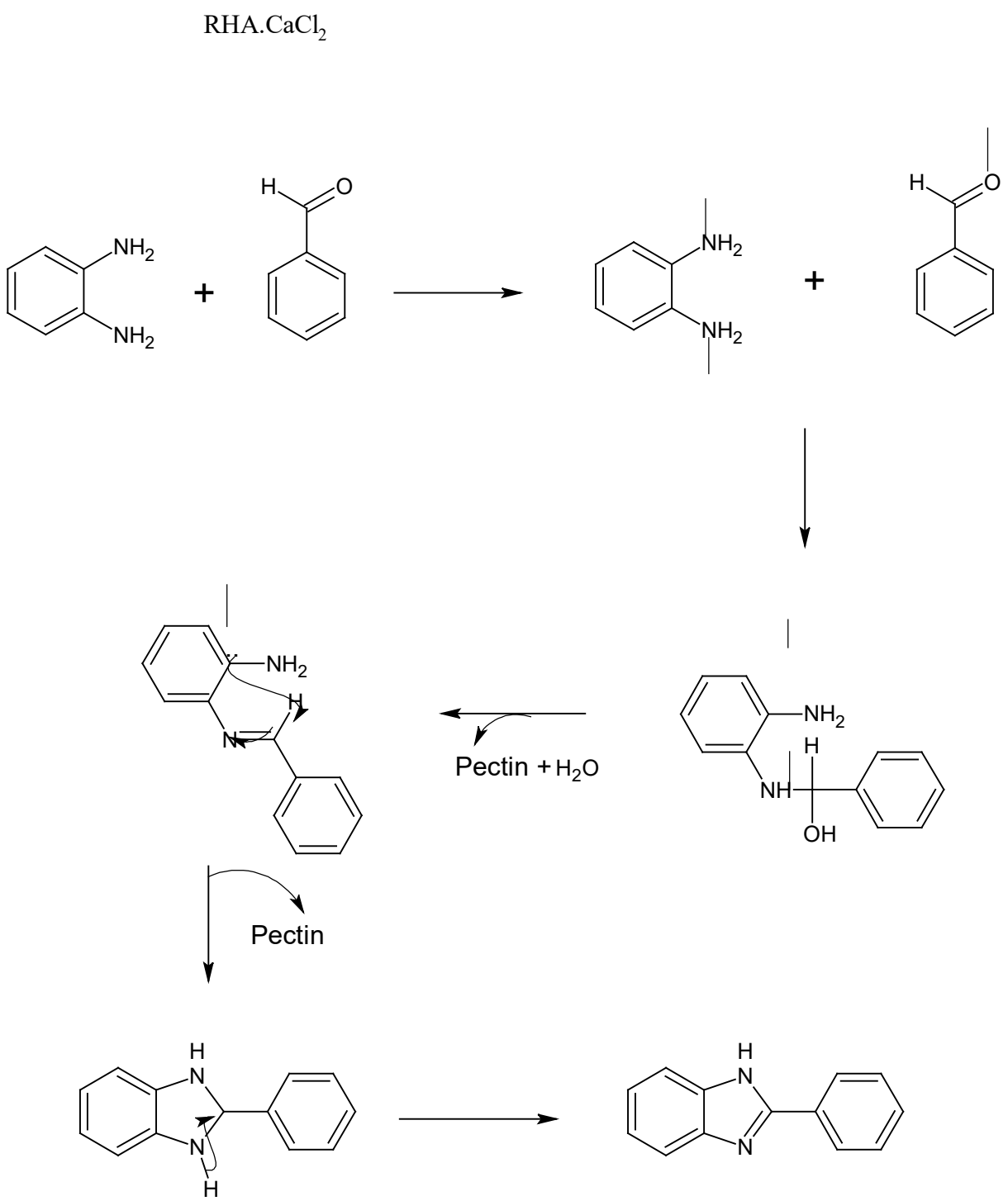
The model reaction between salicylaldehyde 2(i) (2.44g; 20mmoles) and o-phenylene diamine(1) (3.74g; 20mmoles) in the presence of RHA.$CaCl_2$ was taken in the flask and stirred for 40 min on the magnetic stirrer. The solid that separated and worked up with cold water and recrystallized from ethanol to furnish 3(i) as the product in quantitative yield (Table 3, Entry 1).Inspired by this result, the concentration of catalyst was optimized through the above reaction by using different amounts of catalyst i.e.0.12, 0.25, 0.50, 0.75, 1.00 gm (Table 1, Entry 1-5) of RHA.$CaCl_2$ in the water at room temperature for 40 min to give the desired products 3(i). The reaction procedure was performed in the absence of catalyst at the same condition; a low yield is obtained, which shows the value of the prescribed agitator. Fig.1a shows SEM images of untreated rice husk; this figure represents an irregular shape of fibers and rough surface; but a smooth and regular form was showed after treatment with hydrated calcium chloride ($CaCl_2.2H_2O$). At low magnification, RHA.$CaCl_2$(Fig 1b, c) shows a regular surface, but the shape of fiber particles does not appear accurately. But at high magnification RHA.$CaCl_2$(Fig. 1d)seems to be composed of regular-shapedp articles with a uniform distribution of $CaCl_2$ on the surface. Due to this, calcium treatment improves the fiber surface and bond uniqueness by removing hemicelluloses and producing regular surface. This topography offers better fiber-matrix interface bond and an increase in mechanical properties. Treatment by alkali and alkaline reduces the lignin and hemicellulose content in natural fibers, increases the surface area, allowing the dissemination of water molecules to the inner layers, and breaks the bonds between lignin-carbohydrate and hemicellulose [17].

*a) Catalyst recycles*

Reusability is one attractive advantage of green catalysts. A recycling experiment was conducted using the above-mentioned model reaction (Scheme 1). The syntheses were performed three times and the effect of recycling catalysts on yields of 3(i), as shown in Table 2. In every cycle, the catalyst was almost quantitatively recovered, and after second and third-time use of catalyst, the decreasing yield is not much more significant.

*b) Plausible Mechanism for Synthesis of Benzimidazole in the presence of RHA. $CaCl_2$*

The possible mechanism for the synthesis of benzimidazole (Scheme 1) depicted below. The reaction proposed that the aryl aldehyde was first activated by green catalyst by nucleophilic attack on carbonyl group, then o-phenylene diamine attacks the activated carbonyl group of the compound, which leads to the formation of the intermediate and intermolecular cyclization proceeds to form the desired product.




c) *Spectral data of some selected compounds*

i. *2-(1H-benzimidazol-2yl)phenol:* pale yellow solid. mp: 293–296°C; $^1$H NMR (400 Hz, $CDCl_3$): $\delta$ 3.62 (brd, 1H, OH); 7.30-8.91(m, 8H, Ar-H); 10.38 (s, 1H, NH); IR (KBr) cm$^{-1}$3366 (OH), 3165 (N-H), 3035(C=CH), 1618 (C=C, aromatic)

ii. *2-(2-chlorophenyl)-1H-benzimidazole:* pale yellow solid. mp: 225–226°C; $^1$H NMR (400 Hz, $CDCl_3$):$\delta$6.97-8.24 (m, 8H, Ar-H), 11.01 (s, 1H, NH);IR (KBr) cm$^{-1}$:3261 (N-H), 3030(C=CH), 1596 (C=C, aromatic), 754 (C-Cl)

iii. *2-(3-nitrophenyl)-1H-benzimidazole:* pale yellow solid. mp: 164-186°C; $^1$H NMR (400 Hz, $CDCl_3$): $\delta$ 6.12-8.28 (m, 8H, Ar-H), 10.33 (s, 1H, NH); IR (KBr) cm$^{-1}$: 3326 (N-H), 2968 (C=CH), 1590 (C=C, aromatic), 1318 ($NO_2$)

*d) Comparison of the results of the present methods for the synthesis of benzimidazoles with the reported methods*

Table 4 indicates the comparison of the activity of different catalysts by considering the yield of the reaction. We observed that the RHA.$CaCl_2$ gives catalytic activity in terms of product yield, solvent, and response time of reaction compared to other catalysts in the literature such as CAN, p-TsOH, Metal-Nitrate, Ammonium Chloride, Ring-Closing. RHA.$CaCl_2$is a readily available and inexpensive biocatalyst, which makes this method green and mild. Also the above catalyst is a renewable catalyst that follows one of the green chemistry principles regarding the maximum yield of renewable resources.

## IV. Conclusion

In summary, we have developed an efficient catalytic system for the synthesis of substituted benzimidazoles by using rice husk. Under the improved method, it offers several benefits over the previous methods, which includes the elimination of toxic chemicals, cheap, and the main product was obtained in good to excellent yields. Furthermore, the rice husk catalytic system could be reuse up to three times without significant loss of activity. All synthesized compounds were obtained by precipitation without the need for column purification. This current improved method is capable of minimizing the use of hazardous chemicals and, at the same time, provides an alternative way of bio-waste management. We predict that the current procedure will provide a great utility in the synthesis of other heterocyclic compounds shortly.

## Acknowledgment

We are very thankful to Chaudhary Charan Singh HAU Hisar for providing necessary research facilities and also Sophisticated Analytical Instrumentation Facility, PU Chandigarh for NMR, IR, and SEM analysis.

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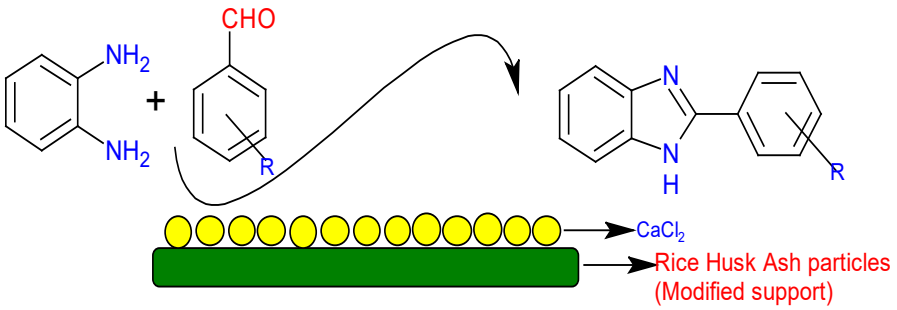
*Figures*

*Graphical Abstract:*



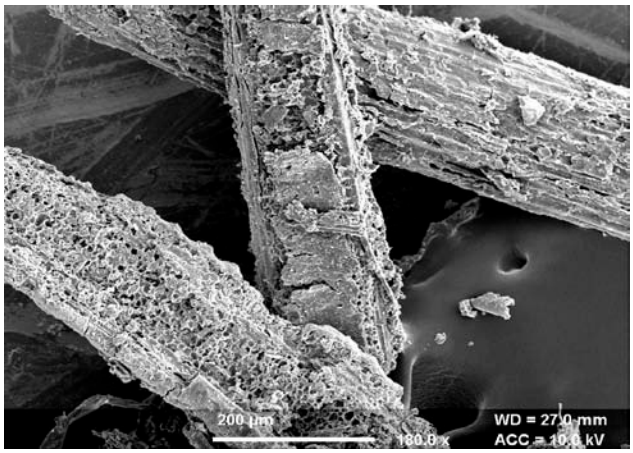
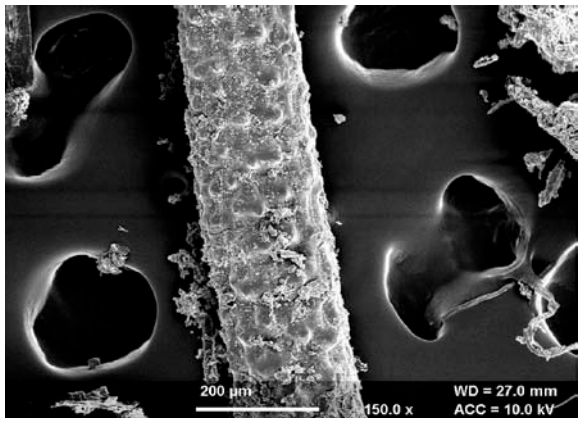




*Fig.:* 1a SEM Images of untreated Rice Husk



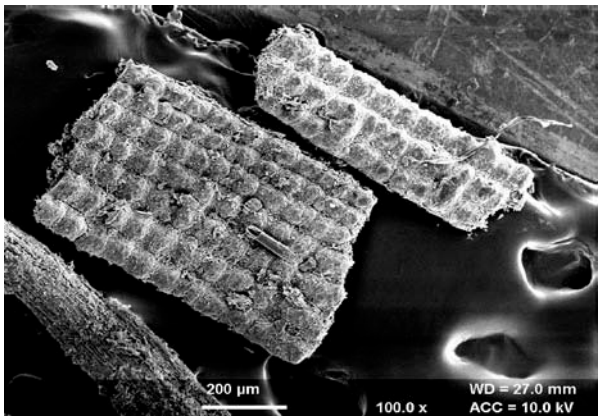




*Fig.:* 1b, c SEM of RH.$CaCl_2$ at low magnification

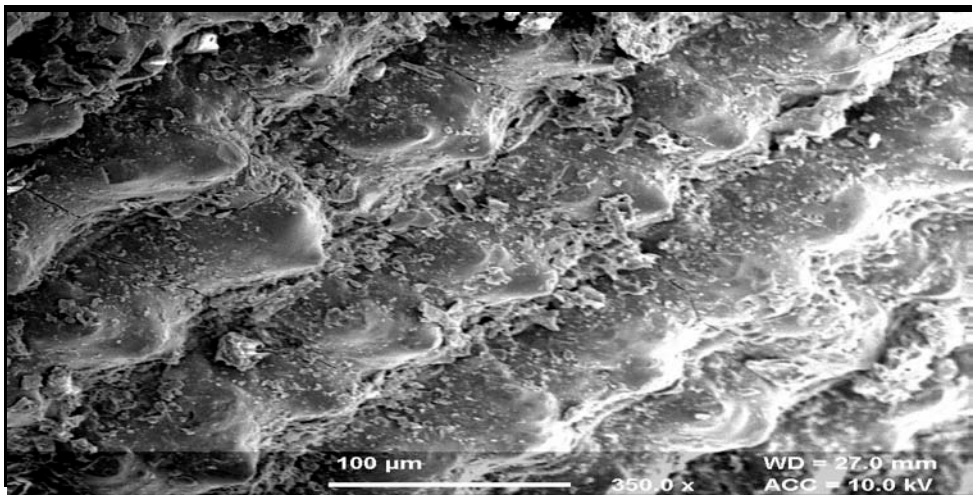



*Fig.:* 1d SEM of RHA.$CaCl_2$ at high magnification

*Tables*

*Table 1:* Screening of RHA.$CaCl_2$ for the synthesis of 3(i)

| Entry | Amount of Catalyst (gm) | Time (min) | Yield |
|---|---|---|---|
| 1. | 0.12 | 75 | 79 |
| 2 | 0.25 | 40 | 82 |
| 3 | 0.50 | 30 | 80 |
| 4 | 0.75 | 25 | 76 |
| 5 | 1.00 | 25 | 76 |

*Entry 2 is the best concentration for the prescribed catalyst*

*Table 2:* Reusability of catalyst

| Reuse Cycle | Fresh | First | Second | Third |
|---|---|---|---|---|
| Time (min) | 40 | 40 | 60 | 90 |
| Yield (%) | 82 | 82 | 78 | 76 |

*Table 3:* Synthesis of benzimidazoles in presence of RHA.$CaCl_2$

| Entry | R | $R^1$ | $R^2$ | Product | Yield | Phase | MPt. (°C) [Ref] |
|---|---|---|---|---|---|---|---|
| 1 | OH | H | H | 3(i) | 82 | Solid | 180-182 [10] |
| 2 | H | OH | H | 3(ii) | 92 | Solid | 282-284 [11] |
| 3 | Cl | H | H | 3(iii) | 88 | Solid | 225-226 [10] |
| 4 | $CH_3$ | $CH_3$ | H | 3(iv) | 86 | Gummy | --------- |
| 5 | H | OH | OH | 3(v) | 90 | Gummy | --------- |
| 6 | H | $NO_2$ | H | 3(vi) | 84 | Solid | 164-186 [10] |
| 7 | H | H | $OCH_3$ | 3(vii) | 90 | Solid | 223-225 [10] |
| 8 | H | H | OH | 3(viii) | 82 | Solid | 285-287 [11] |
| 9 | H | H | Cl | 3(ix) | 78 | Solid | 294-296 [10] |

*Table 4:* Comparison of the results with the reported methods

| S. No. | Catalyst | Solvent | Temperature (°C) | Time (min) | Yield (%) | Literature |
|---|---|---|---|---|---|---|
| 1 | CAN | PEG | 50 | 120 | 90 | [4] |
| 2 | *p*-TsOH | DMF | 80 | 10 | 82 | [12] |
| 3 | Metal-Nitrate | Methanol | RT | 30 | 80 | [13] |
| 4 | Ammonuim Chloride | Ethanol | 80-90 | 120 | 78 | [14] |
| 5 | Ring-Closing | Ethanol | 90 | 120 | 78 | [15] |
| 7 | RHA.$CaCl_2$ | Water | RT | 40 | 82 | Present work |

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The primary objective is to recognize the leaders in research and scientific fields of the current era with a global perspective and to create a channel between them and other researchers for better exposure and knowledge sharing. Members are most eminent scientists, engineers, and technologists from all across the world. Fellows are elected for life through a peer review process on the basis of excellence in the respective domain. There is no limit on the number of new nominations made in any year. Each year, the Open Association of Research Society elect up to 12 new Fellow Members.

# Benefit

## To the institution

### Get letter of appreciation

Global Journals sends a letter of appreciation of author to the Dean or CEO of the University or Company of which author is a part, signed by editor in chief or chief author.

## Exclusive Network

### Get access to a closed network

A FSFRC member gets access to a closed network of Tier 1 researchers and scientists with direct communication channel through our website. Fellows can reach out to other members or researchers directly. They should also be open to reaching out by other.

Career | Credibility | Exclusive | Reputation


## Certificate

### Receive a print ed copy of a certificate

Fellows receive a printed copy of a certificate signed by our Chief Author that may be used for academic purposes and a personal recommendation letter to the dean of member's university.

Career | Credibility | Exclusive | Reputation


## Designation

### Get honored title of membership

Fellows can use the honored title of membership. The “FSFRC” is an honored title which is accorded to a person’s name viz. Dr. John E. Hall, Ph.D., FSFRC or William Walldroff, M.S., FSFRC.

Career | Credibility | Exclusive | Reputation

## Recognition on the Platform

### Better visibility and citation

All the Fellow members of FSFRC get a badge of "Leading Member of Global Journals" on the Research Community that distinguishes them from others. Additionally, the profile is also partially maintained by our team for better visibility and citation. All fellows get a dedicated page on the website with their biography.

Career | Credibility | Reputation

## Future Work

### Get discounts on the future publications

Fellows receive discounts on future publications with Global Journals up to 60%. Through our recommendation programs, members also receive discounts on publications made with OARS affiliated organizations.

Career | Financial

## GJ Internal Account

### Unlimited forward of Emails

Fellows get secure and fast GJ work emails with unlimited forward of emails that they may use them as their primary email. For example,
john [AT] globaljournals [DOT] org.

Career | Credibility | Reputation

## Premium Tools

### Access to all the premium tools

To take future researches to the zenith, fellows and associates receive access to all the premium tools that Global Journals have to offer along with the partnership with some of the best marketing leading tools out there.

Financial

## Conferences & Events

### Organize seminar/conference

Fellows are authorized to organize symposium/seminar/conference on behalf of Global Journal Incorporation (USA). They can also participate in the same organized by another institution as representative of Global Journal. In both the cases, it is mandatory for him to discuss with us and obtain our consent. Additionally, they get free research conferences (and others) alerts.

Career | Credibility | Financial

## Early Invitations

### Early invitations to all the symposiums, seminars, conferences

All fellows receive the early invitations to all the symposiums, seminars, conferences and webinars hosted by Global Journals in their subject.

Exclusive


## Publishing Articles & Books

### Earn 60% of sales proceeds

Fellows can publish articles (limited) without any fees. Also, they can earn up to 60% of sales proceeds from the sale of reference/review books/literature/ publishing of research paper. The FSFRC member can decide its price and we can help in making the right decision.

Exclusive | Financial

## Reviewers

### Get a remuneration of 15% of author fees

Fellow members are eligible to join as a paid peer reviewer at Global Journals Incorporation (USA) and can get a remuneration of 15% of author fees, taken from the author of a respective paper.

Financial

## Access to Editorial Board

### Become a member of the Editorial Board

Fellows may join as a member of the Editorial Board of Global Journals Incorporation (USA) after successful completion of three years as Fellow and as Peer Reviewer. Additionally, Fellows get a chance to nominate other members for Editorial Board.

Career | Credibility | Exclusive | Reputation

## And Much More

### Get access to scientific museums and observatories across the globe

All members get access to 5 selected scientific museums and observatories across the globe. All researches published with Global Journals will be kept under deep archival facilities across regions for future protections and disaster recovery. They get 10 GB free secure cloud access for storing research files.

## ASSOCIATE OF SCIENCE FRONTIER RESEARCH COUNCIL

ASSOCIATE OF SCIENCE FRONTIER RESEARCH COUNCIL is the membership of Global Journals awarded to individuals that the Open Association of Research Society judges to have made a 'substantial contribution to the improvement of computer science, technology, and electronics engineering.

The primary objective is to recognize the leaders in research and scientific fields of the current era with a global perspective and to create a channel between them and other researchers for better exposure and knowledge sharing. Members are most eminent scientists, engineers, and technologists from all across the world. Associate membership can later be promoted to Fellow Membership. Associates are elected for life through a peer review process on the basis of excellence in the respective domain. There is no limit on the number of new nominations made in any year. Each year, the Open Association of Research Society elect up to 12 new Associate Members.

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Career | Credibility | Exclusive | Reputation


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Career | Credibility | Financial

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Exclusive


## Publishing Articles & Books

### Earn 30-40% of sales proceeds

Associates can publish articles (limited) without any fees. Also, they can earn up to 30-40% of sales proceeds from the sale of reference/review books/literature/publishing of research paper.

Exclusive | Financial

## Reviewers

### Get a remuneration of 15% of author fees

Associate members are eligible to join as a paid peer reviewer at Global Journals Incorporation (USA) and can get a remuneration of 15% of author fees, taken from the author of a respective paper.

Financial

## And Much More

### Get access to scientific museums and observatories across the globe

All members get access to 2 selected scientific museums and observatories across the globe. All researches published with Global Journals will be kept under deep archival facilities across regions for future protections and disaster recovery. They get 5 GB free secure cloud access for storing research files.

| Associate | Fellow | Research Group | Basic |
|---|---|---|---|
| $4800<br>**lifetime designation** | $6800<br>**lifetime designation** | $12500.00<br>**organizational** | APC<br>**per article** |
| **Certificate,** LoR and Momento<br>**2** discounted publishing/year<br>**Gradation** of Research<br>**10** research contacts/day<br>**1 GB** Cloud Storage<br>**GJ** Community Access | **Certificate,** LoR and Momento<br>**Unlimited** discounted publishing/year<br>**Gradation** of Research<br>**Unlimited** research contacts/day<br>**5 GB** Cloud Storage<br>**Online Presense** Assistance<br>**GJ** Community Access | **Certificates,** LoRs and Momentos<br>**Unlimited** free publishing/year<br>**Gradation** of Research<br>**Unlimited** research contacts/day<br>**Unlimited** Cloud Storage<br>**Online Presense** Assistance<br>**GJ** Community Access | **GJ** Community Access |

# Preferred Author Guidelines

**We accept the manuscript submissions in any standard (generic) format.**

We typeset manuscripts using advanced typesetting tools like Adobe In Design, CorelDraw, TeXnicCenter, and TeXStudio. We usually recommend authors submit their research using any standard format they are comfortable with, and let Global Journals do the rest.

Alternatively, you can download our basic template from https://globaljournals.org/Template.zip

Authors should submit their complete paper/article, including text illustrations, graphics, conclusions, artwork, and tables. Authors who are not able to submit manuscript using the form above can email the manuscript department at submit@globaljournals.org or get in touch with chiefeditor@globaljournals.org if they wish to send the abstract before submission.

## Before and during Submission

Authors must ensure the information provided during the submission of a paper is authentic. Please go through the following checklist before submitting:

1. Authors must go through the complete author guideline and understand and *agree to Global Journals' ethics and code of conduct,* along with author responsibilities.
2. Authors must accept the privacy policy, terms, and conditions of Global Journals.
3. Ensure corresponding author's email address and postal address are accurate and reachable.
4. Manuscript to be submitted must include keywords, an abstract, a paper title, co-author(s') names and details (email address, name, phone number, and institution), figures and illustrations in vector format including appropriate captions, tables, including titles and footnotes, a conclusion, results, acknowledgments and references.
5. Authors should submit paper in a ZIP archive if any supplementary files are required along with the paper.
6. Proper permissions must be acquired for the use of any copyrighted material.
7. Manuscript submitted *must not have been submitted or published elsewhere* and all authors must be aware of the submission.

**Declaration of Conflicts of Interest**

It is required for authors to declare all financial, institutional, and personal relationships with other individuals and organizations that could influence (bias) their research.

## Policy on Plagiarism

Plagiarism is not acceptable in Global Journals submissions at all.

Plagiarized content will not be considered for publication. We reserve the right to inform authors' institutions about plagiarism detected either before or after publication. If plagiarism is identified, we will follow COPE guidelines:

Authors are solely responsible for all the plagiarism that is found. The author must not fabricate, falsify or plagiarize existing research data. The following, if copied, will be considered plagiarism:

- Words (language)
- Ideas
- Findings
- Writings
- Diagrams
- Graphs
- Illustrations
- Lectures

- Printed material
- Graphic representations
- Computer programs
- Electronic material
- Any other original work

## Authorship Policies

Global Journals follows the definition of authorship set up by the Open Association of Research Society, USA. According to its guidelines, authorship criteria must be based on:

1. Substantial contributions to the conception and acquisition of data, analysis, and interpretation of findings.
2. Drafting the paper and revising it critically regarding important academic content.
3. Final approval of the version of the paper to be published.

**Changes in Authorship**

The corresponding author should mention the name and complete details of all co-authors during submission and in manuscript. We support addition, rearrangement, manipulation, and deletions in authors list till the early view publication of the journal. We expect that corresponding author will notify all co-authors of submission. We follow COPE guidelines for changes in authorship.

**Copyright**

During submission of the manuscript, the author is confirming an exclusive license agreement with Global Journals which gives Global Journals the authority to reproduce, reuse, and republish authors' research. We also believe in flexible copyright terms where copyright may remain with authors/employers/institutions as well. Contact your editor after acceptance to choose your copyright policy. You may follow this form for copyright transfers.

**Appealing Decisions**

Unless specified in the notification, the Editorial Board's decision on publication of the paper is final and cannot be appealed before making the major change in the manuscript.

**Acknowledgments**

Contributors to the research other than authors credited should be mentioned in Acknowledgments. The source of funding for the research can be included. Suppliers of resources may be mentioned along with their addresses.

**Declaration of funding sources**

Global Journals is in partnership with various universities, laboratories, and other institutions worldwide in the research domain. Authors are requested to disclose their source of funding during every stage of their research, such as making analysis, performing laboratory operations, computing data, and using institutional resources, from writing an article to its submission. This will also help authors to get reimbursements by requesting an open access publication letter from Global Journals and submitting to the respective funding source.

## Preparing your Manuscript

Authors can submit papers and articles in an acceptable file format: MS Word (doc, docx), LaTeX (.tex, .zip or .rar including all of your files), Adobe PDF (.pdf), rich text format (.rtf), simple text document (.txt), Open Document Text (.odt), and Apple Pages (.pages). Our professional layout editors will format the entire paper according to our official guidelines. This is one of the highlights of publishing with Global Journals—authors should not be concerned about the formatting of their paper. Global Journals accepts articles and manuscripts in every major language, be it Spanish, Chinese, Japanese, Portuguese, Russian, French, German, Dutch, Italian, Greek, or any other national language, but the title, subtitle, and abstract should be in English. This will facilitate indexing and the pre-peer review process.

The following is the official style and template developed for publication of a research paper. Authors are not required to follow this style during the submission of the paper. It is just for reference purposes.

***Manuscript Style Instruction (Optional)***

- Microsoft Word Document Setting Instructions.
- Font type of all text should be Swis721 Lt BT.
- Page size: 8.27" x 11'", left margin: 0.65, right margin: 0.65, bottom margin: 0.75.
- Paper title should be in one column of font size 24.
- Author name in font size of 11 in one column.
- Abstract: font size 9 with the word "Abstract" in bold italics.
- Main text: font size 10 with two justified columns.
- Two columns with equal column width of 3.38 and spacing of 0.2.
- First character must be three lines drop-capped.
- The paragraph before spacing of 1 pt and after of 0 pt.
- Line spacing of 1 pt.
- Large images must be in one column.
- The names of first main headings (Heading 1) must be in Roman font, capital letters, and font size of 10.
- The names of second main headings (Heading 2) must not include numbers and must be in italics with a font size of 10.

***Structure and Format of Manuscript***

The recommended size of an original research paper is under 15,000 words and review papers under 7,000 words. Research articles should be less than 10,000 words. Research papers are usually longer than review papers. Review papers are reports of significant research (typically less than 7,000 words, including tables, figures, and references)

A research paper must include:

a) A title which should be relevant to the theme of the paper.
b) A summary, known as an abstract (less than 150 words), containing the major results and conclusions.
c) Up to 10 keywords that precisely identify the paper's subject, purpose, and focus.
d) An introduction, giving fundamental background objectives.
e) Resources and techniques with sufficient complete experimental details (wherever possible by reference) to permit repetition, sources of information must be given, and numerical methods must be specified by reference.
f) Results which should be presented concisely by well-designed tables and figures.
g) Suitable statistical data should also be given.
h) All data must have been gathered with attention to numerical detail in the planning stage.

Design has been recognized to be essential to experiments for a considerable time, and the editor has decided that any paper that appears not to have adequate numerical treatments of the data will be returned unrefereed.

i) Discussion should cover implications and consequences and not just recapitulate the results; conclusions should also be summarized.
j) There should be brief acknowledgments.
k) There ought to be references in the conventional format. Global Journals recommends APA format.

Authors should carefully consider the preparation of papers to ensure that they communicate effectively. Papers are much more likely to be accepted if they are carefully designed and laid out, contain few or no errors, are summarizing, and follow instructions. They will also be published with much fewer delays than those that require much technical and editorial correction.

The Editorial Board reserves the right to make literary corrections and suggestions to improve brevity.

## Format Structure

***It is necessary that authors take care in submitting a manuscript that is written in simple language and adheres to published guidelines.***

All manuscripts submitted to Global Journals should include:

**Title**

The title page must carry an informative title that reflects the content, a running title (less than 45 characters together with spaces), names of the authors and co-authors, and the place(s) where the work was carried out.

**Author details**

The full postal address of any related author(s) must be specified.

**Abstract**

The abstract is the foundation of the research paper. It should be clear and concise and must contain the objective of the paper and inferences drawn. It is advised to not include big mathematical equations or complicated jargon.

Many researchers searching for information online will use search engines such as Google, Yahoo or others. By optimizing your paper for search engines, you will amplify the chance of someone finding it. In turn, this will make it more likely to be viewed and cited in further works. Global Journals has compiled these guidelines to facilitate you to maximize the web-friendliness of the most public part of your paper.

**Keywords**

A major lynchpin of research work for the writing of research papers is the keyword search, which one will employ to find both library and internet resources. Up to eleven keywords or very brief phrases have to be given to help data retrieval, mining, and indexing.

One must be persistent and creative in using keywords. An effective keyword search requires a strategy: planning of a list of possible keywords and phrases to try.

Choice of the main keywords is the first tool of writing a research paper. Research paper writing is an art. Keyword search should be as strategic as possible.

One should start brainstorming lists of potential keywords before even beginning searching. Think about the most important concepts related to research work. Ask, “What words would a source have to include to be truly valuable in a research paper?” Then consider synonyms for the important words.

It may take the discovery of only one important paper to steer in the right keyword direction because, in most databases, the keywords under which a research paper is abstracted are listed with the paper.

**Numerical Methods**

Numerical methods used should be transparent and, where appropriate, supported by references.

**Abbreviations**

Authors must list all the abbreviations used in the paper at the end of the paper or in a separate table before using them.

**Formulas and equations**

Authors are advised to submit any mathematical equation using either MathJax, KaTeX, or LaTeX, or in a very high-quality image.

**Tables, Figures, and Figure Legends**

Tables: Tables should be cautiously designed, uncrowned, and include only essential data. Each must have an Arabic number, e.g., Table 4, a self-explanatory caption, and be on a separate sheet. Authors must submit tables in an editable format and not as images. References to these tables (if any) must be mentioned accurately.

**Figures**

Figures are supposed to be submitted as separate files. Always include a citation in the text for each figure using Arabic numbers, e.g., Fig. 4. Artwork must be submitted online in vector electronic form or by emailing it.

## Preparation of Eletronic Figures for Publication

Although low-quality images are sufficient for review purposes, print publication requires high-quality images to prevent the final product being blurred or fuzzy. Submit (possibly by e-mail) EPS (line art) or TIFF (halftone/ photographs) files only. MS PowerPoint and Word Graphics are unsuitable for printed pictures. Avoid using pixel-oriented software. Scans (TIFF only) should have a resolution of at least 350 dpi (halftone) or 700 to 1100 dpi (line drawings). Please give the data for figures in black and white or submit a Color Work Agreement form. EPS files must be saved with fonts embedded (and with a TIFF preview, if possible).

For scanned images, the scanning resolution at final image size ought to be as follows to ensure good reproduction: line art: >650 dpi; halftones (including gel photographs): >350 dpi; figures containing both halftone and line images: >650 dpi.

Color charges: Authors are advised to pay the full cost for the reproduction of their color artwork. Hence, please note that if there is color artwork in your manuscript when it is accepted for publication, we would require you to complete and return a Color Work Agreement form before your paper can be published. Also, you can email your editor to remove the color fee after acceptance of the paper.

## Tips for Writing a Good Quality Science Frontier Research Paper

Techniques for writing a good quality Science Frontier Research paper:

***1. Choosing the topic:*** In most cases, the topic is selected by the interests of the author, but it can also be suggested by the guides. You can have several topics, and then judge which you are most comfortable with. This may be done by asking several questions of yourself, like "Will I be able to carry out a search in this area? Will I find all necessary resources to accomplish the search? Will I be able to find all information in this field area?" If the answer to this type of question is "yes," then you ought to choose that topic. In most cases, you may have to conduct surveys and visit several places. Also, you might have to do a lot of work to find all the rises and falls of the various data on that subject. Sometimes, detailed information plays a vital role, instead of short information. Evaluators are human: The first thing to remember is that evaluators are also human beings. They are not only meant for rejecting a paper. They are here to evaluate your paper. So present your best aspect.

***2. Think like evaluators:*** If you are in confusion or getting demotivated because your paper may not be accepted by the evaluators, then think, and try to evaluate your paper like an evaluator. Try to understand what an evaluator wants in your research paper, and you will automatically have your answer. Make blueprints of paper: The outline is the plan or framework that will help you to arrange your thoughts. It will make your paper logical. But remember that all points of your outline must be related to the topic you have chosen.

***3. Ask your guides:*** If you are having any difficulty with your research, then do not hesitate to share your difficulty with your guide (if you have one). They will surely help you out and resolve your doubts. If you can't clarify what exactly you require for your work, then ask your supervisor to help you with an alternative. He or she might also provide you with a list of essential readings.

***4. Use of computer is recommended:*** As you are doing research in the field of science frontier then this point is quite obvious. Use right software: Always use good quality software packages. If you are not capable of judging good software, then you can lose the quality of your paper unknowingly. There are various programs available to help you which you can get through the internet.

***5. Use the internet for help:*** An excellent start for your paper is using Google. It is a wondrous search engine, where you can have your doubts resolved. You may also read some answers for the frequent question of how to write your research paper or find a model research paper. You can download books from the internet. If you have all the required books, place importance on reading, selecting, and analyzing the specified information. Then sketch out your research paper. Use big pictures: You may use encyclopedias like Wikipedia to get pictures with the best resolution. At Global Journals, you should strictly follow here.

***6. Bookmarks are useful:*** When you read any book or magazine, you generally use bookmarks, right? It is a good habit which helps to not lose your continuity. You should always use bookmarks while searching on the internet also, which will make your search easier.

***7. Revise what you wrote:*** When you write anything, always read it, summarize it, and then finalize it.

***8. Make every effort:*** Make every effort to mention what you are going to write in your paper. That means always have a good start. Try to mention everything in the introduction—what is the need for a particular research paper. Polish your work with good writing skills and always give an evaluator what he wants. Make backups: When you are going to do any important thing like making a research paper, you should always have backup copies of it either on your computer or on paper. This protects you from losing any portion of your important data.

***9. Produce good diagrams of your own:*** Always try to include good charts or diagrams in your paper to improve quality. Using several unnecessary diagrams will degrade the quality of your paper by creating a hodgepodge. So always try to include diagrams which were made by you to improve the readability of your paper. Use of direct quotes: When you do research relevant to literature, history, or current affairs, then use of quotes becomes essential, but if the study is relevant to science, use of quotes is not preferable.

***10. Use proper verb tense:*** Use proper verb tenses in your paper. Use past tense to present those events that have happened. Use present tense to indicate events that are going on. Use future tense to indicate events that will happen in the future. Use of wrong tenses will confuse the evaluator. Avoid sentences that are incomplete.

***11. Pick a good study spot:*** Always try to pick a spot for your research which is quiet. Not every spot is good for studying.

***12. Know what you know:*** Always try to know what you know by making objectives, otherwise you will be confused and unable to achieve your target.

***13. Use good grammar:*** Always use good grammar and words that will have a positive impact on the evaluator; use of good vocabulary does not mean using tough words which the evaluator has to find in a dictionary. Do not fragment sentences. Eliminate one-word sentences. Do not ever use a big word when a smaller one would suffice.

Verbs have to be in agreement with their subjects. In a research paper, do not start sentences with conjunctions or finish them with prepositions. When writing formally, it is advisable to never split an infinitive because someone will (wrongly) complain. Avoid clichés like a disease. Always shun irritating alliteration. Use language which is simple and straightforward. Put together a neat summary.

***14. Arrangement of information:*** Each section of the main body should start with an opening sentence, and there should be a changeover at the end of the section. Give only valid and powerful arguments for your topic. You may also maintain your arguments with records.

***15. Never start at the last minute:*** Always allow enough time for research work. Leaving everything to the last minute will degrade your paper and spoil your work.

***16. Multitasking in research is not good:*** Doing several things at the same time is a bad habit in the case of research activity. Research is an area where everything has a particular time slot. Divide your research work into parts, and do a particular part in a particular time slot.

***17. Never copy others' work:*** Never copy others' work and give it your name because if the evaluator has seen it anywhere, you will be in trouble. Take proper rest and food: No matter how many hours you spend on your research activity, if you are not taking care of your health, then all your efforts will have been in vain. For quality research, take proper rest and food.

***18. Go to seminars:*** Attend seminars if the topic is relevant to your research area. Utilize all your resources.

***19. Refresh your mind after intervals:*** Try to give your mind a rest by listening to soft music or sleeping in intervals. This will also improve your memory. Acquire colleagues: Always try to acquire colleagues. No matter how sharp you are, if you acquire colleagues, they can give you ideas which will be helpful to your research.

***20. Think technically:*** Always think technically. If anything happens, search for its reasons, benefits, and demerits. Think and then print: When you go to print your paper, check that tables are not split, headings are not detached from their descriptions, and page sequence is maintained.

***21. Adding unnecessary information:*** Do not add unnecessary information like "I have used MS Excel to draw graphs." Irrelevant and inappropriate material is superfluous. Foreign terminology and phrases are not apropos. One should never take a broad view. Analogy is like feathers on a snake. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Never oversimplify: When adding material to your research paper, never go for oversimplification; this will definitely irritate the evaluator. Be specific. Never use rhythmic redundancies. Contractions shouldn't be used in a research paper. Comparisons are as terrible as clichés. Give up ampersands, abbreviations, and so on. Remove commas that are not necessary. Parenthetical words should be between brackets or commas. Understatement is always the best way to put forward earth-shaking thoughts. Give a detailed literary review.

***22. Report concluded results:*** Use concluded results. From raw data, filter the results, and then conclude your studies based on measurements and observations taken. An appropriate number of decimal places should be used. Parenthetical remarks are prohibited here. Proofread carefully at the final stage. At the end, give an outline to your arguments. Spot perspectives of further study of the subject. Justify your conclusion at the bottom sufficiently, which will probably include examples.

***23. Upon conclusion:*** Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print for the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects of your research.

## Informal Guidelines of Research Paper Writing

***Key points to remember:***

- Submit all work in its final form.
- Write your paper in the form which is presented in the guidelines using the template.
- Please note the criteria peer reviewers will use for grading the final paper.

**Final points:**

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

*The introduction:* This will be compiled from reference matter and reflect the design processes or outline of basis that directed you to make a study. As you carry out the process of study, the method and process section will be constructed like that. The results segment will show related statistics in nearly sequential order and direct reviewers to similar intellectual paths throughout the data that you gathered to carry out your study.

**The discussion section:**

This will provide understanding of the data and projections as to the implications of the results. The use of good quality references throughout the paper will give the effort trustworthiness by representing an alertness to prior workings.

Writing a research paper is not an easy job, no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record-keeping are the only means to make straightforward progression.

**General style:**

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

**To make a paper clear:** Adhere to recommended page limits.

*Mistakes to avoid:*

- Insertion of a title at the foot of a page with subsequent text on the next page.
- Separating a table, chart, or figure—confine each to a single page.
- Submitting a manuscript with pages out of sequence.
- In every section of your document, use standard writing style, including articles ("a" and "the").
- Keep paying attention to the topic of the paper.
- Use paragraphs to split each significant point (excluding the abstract).
- Align the primary line of each section.
- Present your points in sound order.
- Use present tense to report well-accepted matters.
- Use past tense to describe specific results.
- Do not use familiar wording; don't address the reviewer directly. Don't use slang or superlatives.
- Avoid use of extra pictures—include only those figures essential to presenting results.

**Title page:**

Choose a revealing title. It should be short and include the name(s) and address(es) of all authors. It should not have acronyms or abbreviations or exceed two printed lines.

**Abstract:** This summary should be two hundred words or less. It should clearly and briefly explain the key findings reported in the manuscript and must have precise statistics. It should not have acronyms or abbreviations. It should be logical in itself. Do not cite references at this point.

An abstract is a brief, distinct paragraph summary of finished work or work in development. In a minute or less, a reviewer can be taught the foundation behind the study, common approaches to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study with the subsequent elements in any summary. Try to limit the initial two items to no more than one line each.

*Reason for writing the article—theory, overall issue, purpose.*

- Fundamental goal.
- To-the-point depiction of the research.
- Consequences, including definite statistics—if the consequences are quantitative in nature, account for this; results of any numerical analysis should be reported. Significant conclusions or questions that emerge from the research.

**Approach:**

- Single section and succinct.
- An outline of the job done is always written in past tense.
- Concentrate on shortening results—limit background information to a verdict or two.
- Exact spelling, clarity of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else.

**Introduction:**

The introduction should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable of comprehending and calculating the purpose of your study without having to refer to other works. The basis for the study should be offered. Give the most important references, but avoid making a comprehensive appraisal of the topic. Describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will give no attention to your results. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here.

*The following approach can create a valuable beginning:*

- Explain the value (significance) of the study.
- Defend the model—why did you employ this particular system or method? What is its compensation? Remark upon its appropriateness from an abstract point of view as well as pointing out sensible reasons for using it.
- Present a justification. State your particular theory(-ies) or aim(s), and describe the logic that led you to choose them.
- Briefly explain the study's tentative purpose and how it meets the declared objectives.

**Approach:**

Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done. Sort out your thoughts; manufacture one key point for every section. If you make the four points listed above, you will need at least four paragraphs. Present surrounding information only when it is necessary to support a situation. The reviewer does not desire to read everything you know about a topic. Shape the theory specifically—do not take a broad view.

As always, give awareness to spelling, simplicity, and correctness of sentences and phrases.

**Procedures (methods and materials):**

This part is supposed to be the easiest to carve if you have good skills. A soundly written procedures segment allows a capable scientist to replicate your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order, but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt to give the least amount of information that would permit another capable scientist to replicate your outcome, but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section.

When a technique is used that has been well-described in another section, mention the specific item describing the way, but draw the basic principle while stating the situation. The purpose is to show all particular resources and broad procedures so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step-by-step report of the whole thing you did, nor is a methods section a set of orders.

**Materials:**

*Materials may be reported in part of a section or else they may be recognized along with your measures.*

**Methods:**

- Report the method and not the particulars of each process that engaged the same methodology.
- Describe the method entirely.
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures.
- Simplify—detail how procedures were completed, not how they were performed on a particular day.
- If well-known procedures were used, account for the procedure by name, possibly with a reference, and that's all.

**Approach:**

It is embarrassing to use vigorous voice when documenting methods without using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result, when writing up the methods, most authors use third person passive voice.

Use standard style in this and every other part of the paper—avoid familiar lists, and use full sentences.

**What to keep away from:**

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings—save it for the argument.
- Leave out information that is immaterial to a third party.

**Results:**

The principle of a results segment is to present and demonstrate your conclusion. Create this part as entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.

**Content:**

- Sum up your conclusions in text and demonstrate them, if suitable, with figures and tables.
- In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation of an exacting study.
- Explain results of control experiments and give remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or manuscript.

**What to stay away from:**

- Do not discuss or infer your outcome, report surrounding information, or try to explain anything.
- Do not include raw data or intermediate calculations in a research manuscript.
- Do not present similar data more than once.
- A manuscript should complement any figures or tables, not duplicate information.
- Never confuse figures with tables—there is a difference.

**Approach:**

As always, use past tense when you submit your results, and put the whole thing in a reasonable order.

Put figures and tables, appropriately numbered, in order at the end of the report.

If you desire, you may place your figures and tables properly within the text of your results section.

**Figures and tables:**

If you put figures and tables at the end of some details, make certain that they are visibly distinguished from any attached appendix materials, such as raw facts. Whatever the position, each table must be titled, numbered one after the other, and include a heading. All figures and tables must be divided from the text.

**Discussion:**

The discussion is expected to be the trickiest segment to write. A lot of papers submitted to the journal are discarded based on problems with the discussion. There is no rule for how long an argument should be.

Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implications of the study. The purpose here is to offer an understanding of your results and support all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of results should be fully described.

Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact, you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved the prospect, and let it drop at that. Make a decision as to whether each premise is supported or discarded or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."

Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work.

- You may propose future guidelines, such as how an experiment might be personalized to accomplish a new idea.
- Give details of all of your remarks as much as possible, focusing on mechanisms.
- Make a decision as to whether the tentative design sufficiently addressed the theory and whether or not it was correctly restricted. Try to present substitute explanations if they are sensible alternatives.
- One piece of research will not counter an overall question, so maintain the large picture in mind. Where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

**Approach:**

When you refer to information, differentiate data generated by your own studies from other available information. Present work done by specific persons (including you) in past tense.

Describe generally acknowledged facts and main beliefs in present tense.

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| Topics | Grades | | |
|---|---|---|---|
| | **A-B** | **C-D** | **E-F** |
| ***Abstract*** | Clear and concise with appropriate content, Correct format. 200 words or below | Unclear summary and no specific data, Incorrect form<br><br>Above 200 words | No specific data with ambiguous information<br><br>Above 250 words |
| ***Introduction*** | Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited | Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter | Out of place depth and content, hazy format |
| ***Methods and Procedures*** | Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads | Difficult to comprehend with embarrassed text, too much explanation but completed | Incorrect and unorganized structure with hazy meaning |
| ***Result*** | Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake | Complete and embarrassed text, difficult to comprehend | Irregular format with wrong facts and figures |
| ***Discussion*** | Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited | Wordy, unclear conclusion, spurious | Conclusion is not cited, unorganized, difficult to comprehend |
| ***References*** | Complete and correct format, well organized | Beside the point, Incomplete | Wrong format and structuring |

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