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Existence of Carbon Domain Alters Bond Orders in Protein

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Abstract- Program has been developed to interpret the rule of law of carbon in effective learning or designing probe molecule for disease control. In biological functions the probe need not be in active site at all where it is necessary to satify only the carbon deficiency everywhere in the protein. One of the alternative force coming from this carbon is brought here for verification and alteration. According to this frame work carbon domain dictates everything from folding to function. Interestingly the bond length varies accordingly which are critically analysed for validation here. Results are in agreement with that of role of carbon in explaining phenomena of binding. According to the rule of law, oneness of bond lenth is preferred overall.
Keywords – internal COD, bond order variation, carbon rule of law, carbon domain, protein

I. INTRODUCTION

Internal carbon optimised domain (COD) is one of the promising phenomena of carbon rule of law increasingly evident that carbon rule of law governs protein structure and activity [1-4]. Seems to be important that internal COD can identify the cohessiveness of rule of law based on carbon value. Interestingly internal COD becoming one of the predominant force of all attraction present in biological system say here protein which is dominant over the other forces coming from non bonded interaction like van der Waals and electrostatic forces of interaction. Hopefully India can be front runner over the issue of internal COD population everywhere in the universe whole heartedly. Every now and then internal COD promises interesting results over the issue of binding studies leading to drug discovery and all. Overall internal COD dominate over the electrostatic and Lennard-Jones potential for non bonded interaction. Interestingly internal COD include both bonded and nonbonded interaction in the calculation where in internal COD influence the bond of all present in vicinity of internal COD value where as in nonCOD regions it is not so. These are measurable quantity coming from X-Ray or NMR structure which are taken up here. That is to say that internal COD dominancy is measured interms of bondlength over the nonCOD regions which are non obedient for rule of law where incoming molecule can be partly satisfy them adequately altering entire gamet of protein struture for the same. Adequacy needs to be the thumb rule here for all involved in internal COD dominant force of interaction where in adequate rule of law is followed for self satisfaction. Needless to say that qdequacy principle of carbon rule of law drives entire gamet of protein to obey oneness uniformly everywhere in the structure, where the bonded atoms are altered its position for self sufficient carbon rule of law where in the reduced or altered and or increased bonds tells all of its happening which are measured here as quantity for internal COD determination where as in nonCOD regions these are not followed which again reflects in the bonded atoms that was captured for non obedient atoms of interaction where oneness of principled atoms absent. Interestingly non obedient atoms follow up interactive molecule for self sufficency, needlessly altering the position of atoms that are following rule of law which are captured here as COD. Nevertheless internal COD dominate rule of law which are captured as measurable quntity in terms of bond order of individual atoms involved in the local arrangement over the entire structure of protein that alter accordingly. Needless to say that arrangements are carried out in such a way that COD can be the ruler here which is captured as measurable quantity the bondlength of all involved.

Measured bondlengths dictate here the internal COD involvement at local structure predominant over entire gamet of accepted bond of all forces coming from rule of law entirely adjusting to the local needs, predominantly over the arrangement at 16Å where in local needs to be under control within the framework where self satisfaction need of the hour. One cannot expect the uniform principle of rule of law that are non obedient to the COD where in flexibility seems to be the dominant character of aminoacids that involved in local bonded in nature of interaction. Welcoming these non obedient chanracter of aminoacids that fascinate the external forces of attraction for binding that alter the local acenario for self sufficiency rule of law where as in nonCOD region becoming self sufficient that follow principled COD of law arising out of carbon alone not even nonbonded interaction such as van der Waals and electrostatic forces.

Having defined atomic detail [5], particularly carbon role in pattern finding [6,7], stability of protein [8], disorders [9,10], diseases [11] and mutational responsibility [12-14], it is time for reconciliation of all related problems of

biological nature. Studies on protein evolution [15] can be revaluated to address the carbon role in macromolecular system of biological nature.

II. MATERIALS AND METHODS

2.1 Data –

The reference here is the protein SOD in standalone condition available in PDB as 1rk7 and also the cofactors attached condition as in 1ba9. Both are NMR structure available for calculations including here as metal ion binding in its chanracteristic functinal role. The cofactors are Cu and Zn ions which are attached to the SOD structure including binding site neither of them are not in functional site where it supposed to be.

2.2 Cohessiveness –

Otherwise satisfying the deficiency observed in fuctional site which is called cohessive force of interaction then and there called intervening force of COD. Verifying this forces of interaction would probably yield net force for bioinformatics calculations where all problems will be sorted out without hinges where are all unknown elements is noticed in the functional site within the ranges of 16 Å. Neither the metal ions in these range of interaction. Hopefully cohessive can explain this very well than that of other forces like van der Waals or electrostatic forces would yield in the vicinity of probe binding. Wherever binding of metal ion take place, only selected of them are involved in the vicinity whereas in cohesive line form the extended nonlinear form of interaction studied here whereas every now and then it needs to be important in biomolecular study of disease solving human life saving technology development for the furturistic application in the form of research taking place whereas it is important to note that every now and then there ought to be verification these COD in every biomolecular simulation that are useful for human life saving technique in biology is concerened.

2.3 CARd3D calculation –

The cohessiveness of interactive forces can be observed from our inbuilt home made PERL program available for simple performance based on our intervening validation neither in the market nor for nonacademic calculation, only through arrangement based on personal interaction for certain verification of all atom interaction in the binding of incoming molecule for futuristic application. Calculations involve reading of atomic coordinates into array, arrange them into smaller spherical dia where the intervening forces can be influential adequately (16 Å here), verify the carbon percentage to meet out the required threshold of 0.3144, when in threshold line calculate the atoms that are contigues aminoacid wise, arrange them according to their merit of involment in COD of all atom concerned, when aminoacids sometime atoms involved in these COD are considered to be involved in cohessiveness rather than that of nonCOD aminoacids that are not in line with internal COD value, obsolutely zero value. Neither COD nor nonCOD aminoacids follow the principle of 0.3144 carbon value where the aminoacids are hydrophilic type for longer than 5 aminoacids.

XY plot is obtained to observe the cohessiveness all along the protein sequence at every aminoacid position where in negative value never obtained, either zero or magnitude of interger numbers without fraction for net force calculation, where in magnitude indicate the involment of particular aminoacid in COD of cohessiveness where as others are not invlved in the cohessive force inviting other forces from external molecules for binding leading to productivity of biochemical reactions where in incoming molecules interact to replace or attach functional units in the proteins for fuction as probe binder.

2.4 Bondlength Calculation –

Understandably the probe binding will have to be alter the protein structure necessarily in the fuctional role of binding where in incoming probe can withstand effectively for further course of action where as the van der Waals and electrostatic forces of interaction not adequate to tamper this obviously as external probe can be satifying them adequately needlessly in the active form of interaction. What next then, the only alternative to this phenomena of binding would evolve only from cohessiveness of carbon role in the biomolecular structure that alter chemical bond everywhere in the structure of protein during interaction which is captured here as measurable quatity from pdb structure of individual atoms that are arranged according the principle of cohessive interaction of forces of attraction available from the principle of 31.44% carbon rule of law. Negative sense that the atoms are not involved in the forces of alternative force arising from carbon rule of law. Either zero or non negative indicate the COD and nonCOD portions which is basis for bond alteration during intercourse. Alternative to the existing forces of interaction say van der Waals and electrostatics, cohessiveness coming from carbon role alters bond lengths considerably which are measurable quantity for cohessive force adequately in the absence all other forces of alteration. Adequate to explain the phenomena of binding atleast here.

Arranged the atoms of pdb coordinates in the array of elements for probability prediction of adequate to evolve nonCOD and or COD of domain that are adjusted bond elements arranged according to principle of rule of law. To say something the carbon-carbon single bonds are condensed at COD regions whereas in nonCOD it's not so. Needless to say that the bonds are tend to become one in all sense of alteration that the double bond tend to be single bond including aromatic π electrons tend to be delocalised which are evidence for carbon role in adequacy principle of law of rule. During the delocalisation the single bond character alter the atomic structure of individual elements in the due course that alter internal COD value adequately evidently this phenomena of internal COD can perform oneness of carbon rule of law for effective rule that govern all attractive force for incoming probe to bind where it adequately supply enough material to fulfil all deficiency of internal COD in the structure where as nonCOD fulfil all adequacy problem and that may arise another portion to be active for another binding where the incoming needs to see only the second problem to be fulfilled where it ignore previous rule of law that were there earlier, negative to this may be leads to the collabse of the whole structure where nothing can be interactive at alternate probably where in nil reaction take place especially in binding of alternative sources of interaction that are carbon rule of law.

III. RESULTS AND DISCUSSION

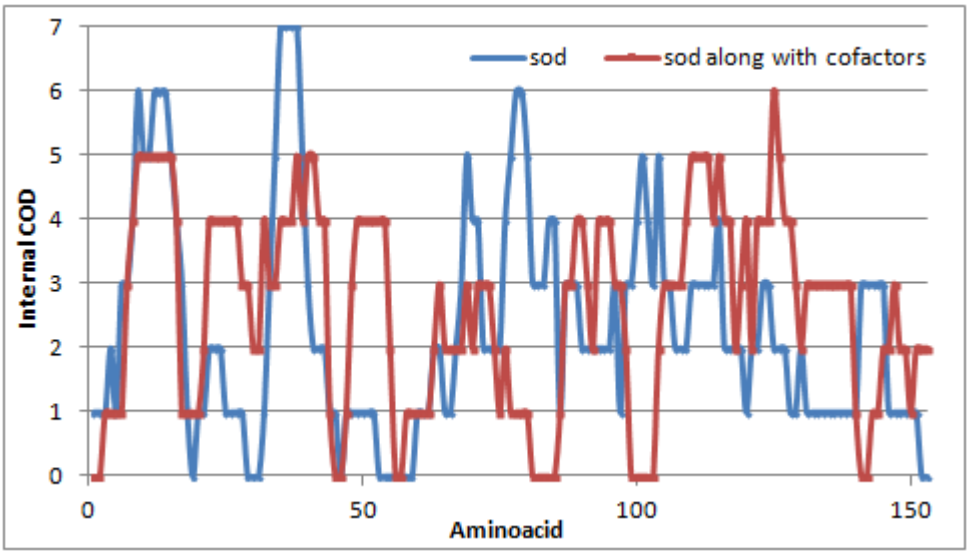

Figure 1 Plot of Internal COD against amino acid positions. Noteworthy to mention that the zero internal COD values are active regions which are responsible for binding. Higher internal COD values are dominant in stability wise which are reduced in bond length.

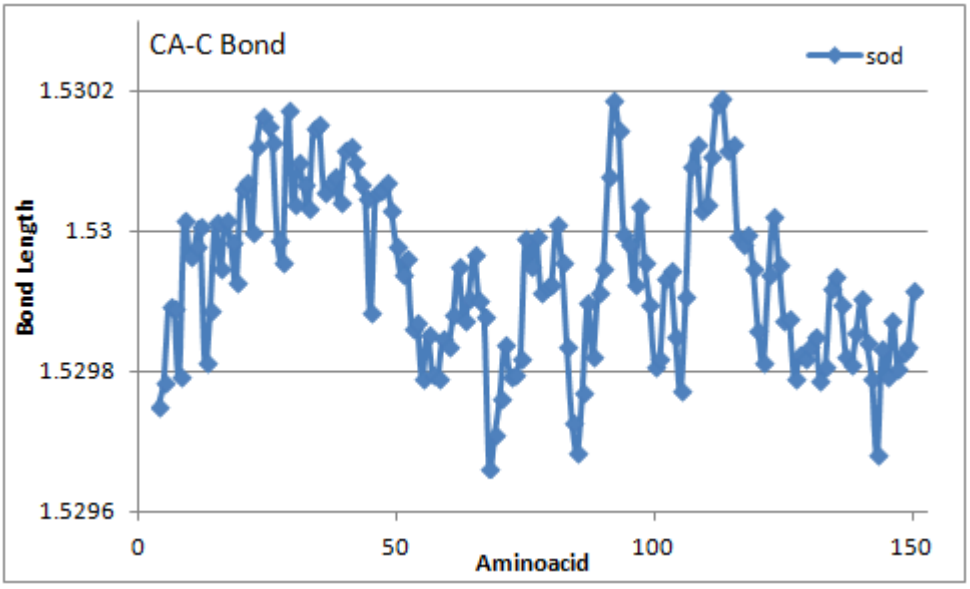

Figure 2 Plot showing bond length variations in unbound state of protein SOD. Wherever higher bond lengths observed, poor internal COD value which is non obedient internal wise. Magnitude of deviations is fractional and minimum. Also note that lower bond lengths are observed to be involved in internal COD.

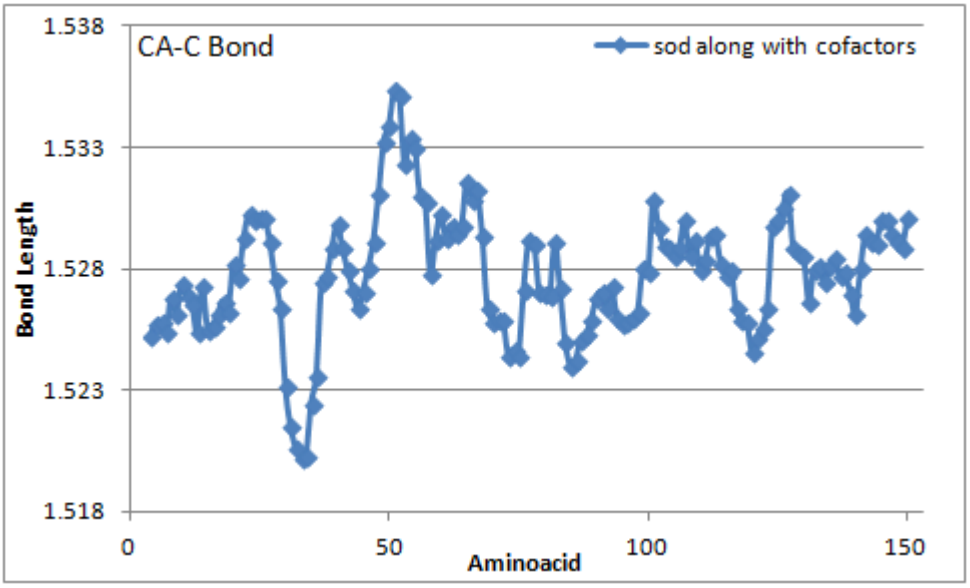

Figure 3 Same as plot 2 but for SOD in bound state of cofactors Cu and Zn. All observations are in line with internal COD value.

One of the most interesting stuff coming out of internal COD is that anyway conneted to the every single atom of others while performing internal COD evaluation but the fact is that internal COD obtained at dia 16 Å dominates the whole lot of stuff interveningly. Moreover the internal COD obtained via other dias may be there weaker than that one obtained at dia16. Most interestingly dia16 reflects all necessary components for binding, whereever necessary it can be computed for higher or lower dias using the same software. Infact it has been observed from 4Å to highest possible dias (dia that include all atoms) (5). From the point of observation, it has been decided to compute only for dia of 16 where are all binding is considered. Needless to say that dia 16 links almost all atoms that are contiguous atleast by 4 aminoacids. Many times it is working with necessary COD values where all amioacids involved in it. But the thing is that the nonCOD regions does not follow this minimum requirement of carbon value that becomes active region. Overall seems to be in COD except the active region. Binding of probe might be satisfying this site of interest where are all happy with internal COD. For example internal COD of SOD is shown here in plot 1 where the blue line indicates the internal COD for SOD without cofactors say copper and zinc. Careful observation that the nonCOD region from 20 to 33 is non obedient regions for rule of law where one would expect bond length be unaltered, interestingly high in bondlength plot obtained for the same SOD without metal ions.

Notably the bondlengths observed is high wherever the internal COD is minimum or zero value. Plot 2 where the length of particular bond is group averaged for 5 neighbouring amino acids indicates the bondlengths for those regions that are nonCOD which again relatively high indicate the involvement of COD in protein fold or binding. At the same plot one can observe that the internal COD intervening regions abide by rule of law are having lower bondlength which indicate that the internal COD reduces the bond lengths which is of CA-C bond. Otherwise it is different issue of change from one type of bond to another. For example the peptide bond reduces its character to become single bond, obviously reduces to lower bond order. Intervening forces can be involved in the reduction to oneness of all bonds everywhere in the structure.

At the same time the addition of cofactors should be involved in reducing deficiency of internal COD that automatically reduces the bondlengths considerably. Say here the regions that are lower in internal COD tend to be higher now which eventually reduces its bondlengths which is happening here in SOD amazingly. Obvious that internal COD does play an important role here in overall structure that are responsible for folding or binding. Plot 3 can be better exploited for internal COD obtained via SOD with metal ions bound as shown dark brown line in plot 1. Once again lower internal COD stretches become higher bondlength relatively. But interesting to note that the zero internal COD noticed for selected region, aminoacids 56-59 are increasingly high in bond length obtained

which is obvious reason why it should be. Overall interesting to tell that all because of internal COD which can be measurable quantity from bondlength factor. One thing is that the observed bondlength and overall COD might be interesting for accurate calculation where as here only the internal COD of dia 16 is compared to bondlength. Performance may be adjustable accordingly. Otherwise relative bondlengths and interal COD values are reflective each other at this dia of COD value. Mention that relative may be accurate here and obsolute may not be a criteria at all. Reflections are arranged accordingly in internal COD research work carried out here in this lab.

Scale of measure of protein robustness from bond length is possible where compactness, tightness, accessible surface area won't work here from bond of all atoms. It is clear from 7 group average of CA-C bonds of SOD and SODCuZn that internal COD at dia 16 plays an important role in determining bond order otherwise call it as nostalgia moment.

IV. CONCLUSION

To conclude the bond lenths seems to be a caliber for COD of biomolecular simulations where biomolecules tend to become oneness of bond length character which alter the aromatic double bonds into single bond character that assess for COD value. Evidences are reported here for internal COD calculation which promises very smart way of dealing with internal value. Evidence is also that single bonds tend to become lower value in the COD while is reverse in aromatic double bonds. Promisingly the COD can play an active role in the future for everlasting application of human diseases. Benefits are there to address the genetic disorders followed by growth and maitenence of human nature.

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