



Drug in Action According to Nano Force of Interaction

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ABSTRACT

One of the strong forces of attraction coming from the carbon role is discussed here as the main force of interaction in the protein association during relief work. One can consider several examples of drug interaction with the protein of interest. Here it is taken as microbial controlling beta-lactamase binding oxacillin one for study and to detail out the force of involvement and associated principles. Our results clearly explain the role of carbon in the interaction between the drug of action and associated protein. One can take this principle coming out of carbon value for further study on drug development or protein inhibition value. We conclude here that the carbon value is the best treatment of all sort of interaction associated with drug-protein interaction and all other forces are merely there for the association and not at all important for study in drug development further on.

Keywords: Nanone, ICOD, Drug action, Drug-protein interaction, Carbon value, Fundamental force, Carbon profile

INTRODUCTION

Several potential drugs prohibit pain of our body in the nervous system. Understanding the action of these potential drugs is yet to be realized at the atomic scale. One of the dominant force of the existence of cohesiveness comes from such drugs is the focus of this work in nature [1-9]. However, dealing with such cohesiveness is very difficult to adjust the parameter to be in the code of contact and all. At this juncture, it is believed that nano-force coming from a carbon point of view is crucial for any new development at the drug to be in action and all. Accordingly, the sequence of protein where and all binding is to be characterized for suitability and necessary change in the global and local structure of intervening atoms. Nevertheless, the action of the drug to the binding site evolved from the internal one coming from the carbon of protein side, not in drug one. Drug one side in internal one to get adjusted and maintain code of contact with carbon force coming with a value of 0.3144. Otherwise, call it as intervening change that and all hoped to be in the vicinity to act accordingly. Hope this phenomenon is met with adequate flexibility and alteration at the atomic level of change of amino acids and drug one. Altering any of these two might be interesting in finding a better or more sensitive solution of action at the site interest, otherwise going to be insolvable in the internal one to get auctioned. Needless to say that the molecule of interest must meet the necessary changes that and all in the internal one very near to the point of action. Overall one should look upon the internal one along with the local one to be satisfied. Overall one may be invaluable in the code of contact is considered. One should ignore this way of binding in the vicinity where only the local structure and all is important in getting effective binding. Over and above it may be better to find the operation at all level that and all feasible for eloping molecule that binds to the system of disease character and only the incoming need to be fulfilling these action of the drug and adjust to the adequate carbon profile that is coming from cohesiveness and alternative force of nanone all along mutually. Adjacent to the active site all other amino acids are adequately arranged to provide all necessary alteration that and all meeting the requirement of nanone to exist which eventually adjust during binding and alters its orientation accordingly. Very many points of interest meet this phenomenon of binding but only one of them meets this phenomenon effectively adjusting every other to accommodate everywhere in the system that adjusts to meet out the effective point of the profile of carbon

value coming from adjustable elements. Otherwise going to be inefficient binding that may not affect the protein and all in the binding of ineffective drug one. Eventually, lead to salvation less action coming from inefficient drug one. Over and above it may be placed in such a way that it is complementing each other ineffective binding and all. The cohesiveness of the nanone one coming here is elevated to a higher level. A much faster code of contact may be provided to accommodate drugs in the vicinity which holds this phenomenon of drug action which is taken up here as a point of the study.

Though one can go on synthesizing different potential drugs for such action, fundamentally one has to realize that carbon role in inflammation and also in anti-inflammatory powerful force comes from cohesive nanopores are important for the foundation of such actionable drugs that cause relief during a difficult time of action in force [10-13]. One has to study a detailed explanation on how, where it acts for such interaction. The drug used for microbial control is taken here to detail out the protein-drug interactions.

METHODS

Protein and its complex structures were retrieved from the PDB website. This includes the native form of lactamase (5xp6) and the complex formed (4eyb). The files are having atomic coordinates of 42 to 270 and 30 to 270 in native form and complex structure respectively. Rest are missing residues as in crystal structure found by X-ray crystallography. Though it is good enough for comparison, alteration may be there with all other elements. The program was evolved to find out carbon atoms of interest from carbon value calculation that arranges to provide details of the domain of atoms involved and also the non-coding regions. Otherwise, call it the arrangement of carbon domain calculation for internal one of all atoms that can provide input on alteration for mutational study and also for effective binding of the drug to protein.

Alternatively one can go on calculating the internal one obtainable from sequence information that may not complete in the sense that the internal one differs from carbon-rich regions. The overall pattern of carbon-rich and carbon domain regions may be obtained from this sequence information additionally to internal one of the 3D structures obtained from X-ray crystallography. An alternative to the complex formed, one can get information on where are all the internal one and carbon-rich portion that might have changed during complex formation. Fantastic about this is that an internal one called carbon domain may be obtainable from simple sequence information that can be extrapolated to protein 3D structure of all-atom involved. Arranged in the protein information in the sequence for three-dimensional structures to be adopted. It can be called arrangement of the atomic profile of the carbon domain and an active portion along with the sequence information. When in need one can calculate these portion identified from Carbon distribution (CARd) analysis of sequence information which are shown here additional to CARd3D or bond from C α -C bond of back bond atoms [14,15].

One of the important facts is that cohesive force coming from carbon alone is responsible for complex formed and released during drug binding and release which are analyzed and discussed here as part of the drug-protein topic of macromolecular association in biological systems that control disease and alter biological phenomena of binding [16].

Oxacillin and New Delhi Metallo-Beta-Lactamase-1 are the two arranged molecules for the case study here. Otherwise, a lot of other well-known structures found in PDB can be analyzed for a clear picture of protein-drug interaction. Arranged are only the demos of the nuclear picture of carbon value and bond length variation at atomic-level understanding for complex formation. Nuclear means that atomic coordinates are the main picture of all calculations involved and neglecting atom's particle of the native structure that can be better over the nuclear one.

Part of the calculations, arranged are the group evaluation for a broader sense of amino acid involved. Accordingly, amino acids that can possess atomic details can be put together 75 atoms or so are taken into account for a clear picture of the variation of bond length character with internal one and non-COD parameters. Additionally, other factors involved in active regions are to be taken here at an average of 5 amino acids. Otherwise group average of 5 amino acids is essential for comparison with internal one obtainable from 16Å. Here are shown only the CA-C bond and compared.

One of the factors of internal one calculation is that the sequence information retrieved from the amino acid sequence is being done using our homemade PERL coded CARd program which runs on any platform of the research program. Otherwise one might want to use this program to identify sequential burial of information for the fact of carbon

domain value which is happening here at the last of the result section. The parameters are standardized and no other information may be required in calculating the internal results. The only sequence is good enough for calculation. Retrieval may of interest for internal calculation. Otherwise call it the adhesive of additional force in protein internal for binding of drug focused in treatment of diseases including fever, vomiting, and/or nervousness.

RESULTS AND DISCUSSION

Socio-demographic Characteristics

The picture of beta-lactamase bound to the drug (yellow-colored sulfur seen in) is given here (Figure 1) to show that cohesive forces are involved in binding of the drug to protein which is not part of the other modeling work coming from electrostatic and van der Waals forces of attraction. As can be seen here the active stretches are away from drug bound portion. Cohesive force is the major driving force of all this attraction and binding. Additional to drug binding other portions are affected for further molecular interaction during drug action which is evident from the internal one drawing obtained for 16Å and shown in Figure 2.



Figure 1 Picture showing protein-drug complex; yellow and associated colored atoms are seen as drug component and the other side the colored protein atoms are the portion that got altered upon binding; cohesiveness is explained rather than binding itself considered.

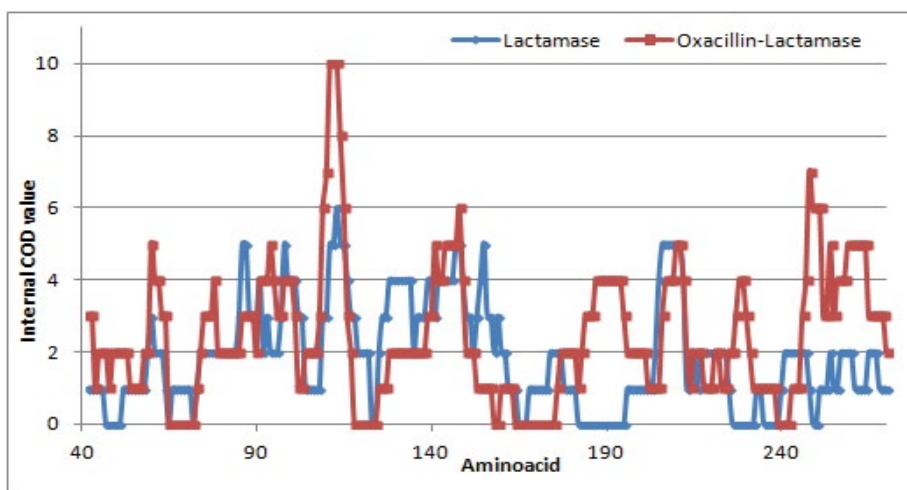


Figure 2 Internal one obtained from CARD3D program for Lactamase (blue) and drug complex of lactamase (dark brown); arrangements are to follow non-COD are having internal one values zero; non zero portions are one with cohesive force involved forming internal one; break in internal one of zero indicates that complex formation is favored otherwise not all involved in the formation of the complex during mixing of drug with protein which is shown here as a demo of internal one versus active suspects

Figure 3 represents the image diagram showing active spot and internal one portions obtained from CARd3D for 16Å. Red color indicates the active region along the sequence and associated stretch in yellow color, otherwise altogether active regions accordingly in protein 3D structure. And also seen are blue color centered dark blue are domain regions additionally involved in the stable domain of all atoms. A program called ImageOne from PERL instruction is developed to generate this image for clear visualization of active and domain portion along the sequence otherwise called optimization of arranged amino acids according to the internal one and deletion for optimization during the mutational study of amino acid binding at the active region for effective control over.

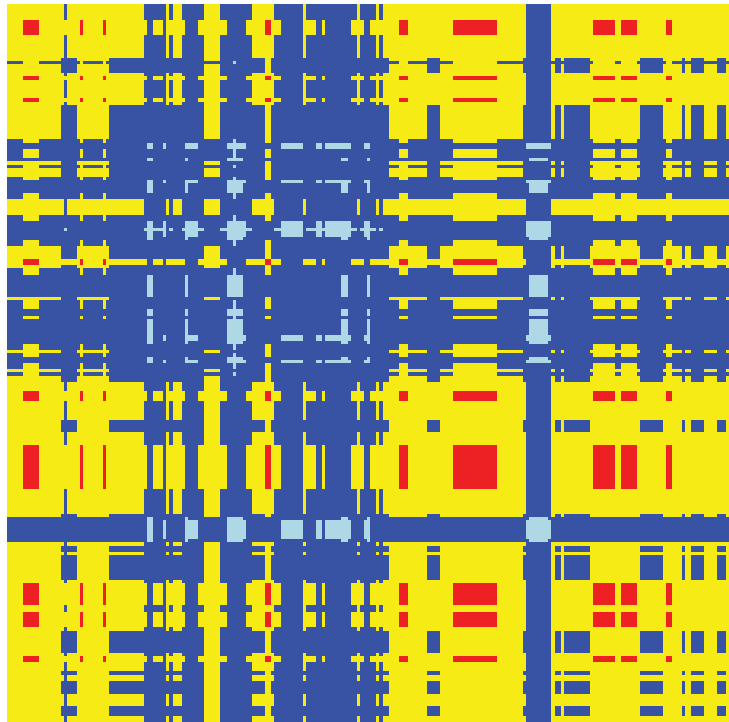


Figure 3 Based on the internal one value the identified active regions are in red; blue validate internal one regions obeying carbon value for uniform distribution; dark blue and yellow are corresponding lower degree of internal one and non-internal one stretches

One of the interesting phenomena of internal one obtainable from carbon value is to identify the active region of interest clear understanding of atoms to be edited and incorporated for protein to bind effectively which is happened here in Figure 2 as shown in the blue one with native internal one values and dark brown of complex formed during mixing of drug with the protein of interest. According to internal one evaluation the portions 182-194 and 226-231 are active sites in the native form of structure which are identified as a carbon-rich region in doublet score formation. According to the complex formation principle, these two sites are organized into internal one region in the complex formed. When in need internal one may be lost during complex formation, internal one stabilizes the complex and accordingly internal one activates other molecules to interact and proceed with a new course of reaction to be followed additionally under one roof of interaction. Accordingly in complex formation, the portions 65-72, 118-124, and 164-175 turn active sites. Seems to be 118-124 is a hydrophilic region and the other two 65-72 and 164-175 are carbon-rich regions.

Upon binding the internal domain remain unchanged at 52-64, 102-122, 124-164, 196-225, and 251-270. One of the interesting phenomena that take place during complexation is that the internal one is increasingly altered in some portion here at 109-118 that is seen as clear evidence for bond length change upon internal one formation due to cohesive force at 16Å. That is the bond length changed drastically at this site of interest of internal one. Never any doubt that there is the domain of carbon formation which is true. A direct measure of bond length variation clearly expresses these phenomena of a domain formed according to the nature of force involved in a cohesive one. Doubts may be there why not at dia of 15 which are not aligning, but it is the true story of carbon domain accordingly. According to the nature of law that the carbon domain favors a decrease of bond length but seen here are increased

bond length at 246-252 which demonstrates here that the active region at 239-242 interfering in arrangements active carbon to domain formation adjacent to carbon domain.

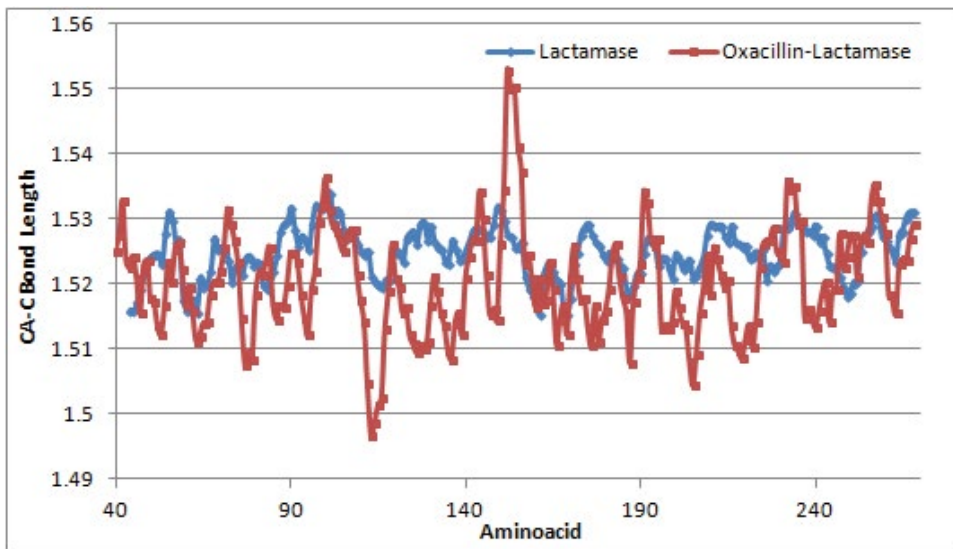


Figure 4 Internal one depicted from bond values of CA-C bond in lactamase (blue) and in drug bound one (red)

The alteration of non-carbon value to carbon one at active sites 182-194 and 226-231 is not seen with a drastic change in bond length as observed earlier in the domain to domain change but the adjustable neighbors got altered upon binding of the drug. That is to say, there is no change in CA-C bond length at the active site having a center around 187 and a significant reduction at neighboring internal one regions centered around 176 and 202 (Figure 4). Drug of action is felt at the internal one rather than binding energy. Bond values prove this phenomenon of catching the drug to the binding site. Drugs of all kinds may have this influence on internal one but an active one. Otherwise, call it site-specific binding of active drug in the vicinity of the internal one. Rather than the internal matter of binding, the effective binding may be designed accordingly. Nevertheless, the effectiveness is based on the neighboring internal matter. Otherwise, it is going to be an internal alteration that may not influence neighboring active regions. Based on carbon values improvements in binding can be worked out for effective drugs [17]. This seemingly shown here as another example for D16 involvement for bond length variation is that the rapid increase at 151-156 due to complex formed by oxacillin with lactamase creating another binding location for another molecule. The D16 expresses very well with bond length than the same with D15. So the D16 involvement clearly expressed and confirms the formation of an internal one based on cohesive force. That is bond length decreases with higher internal one formation.

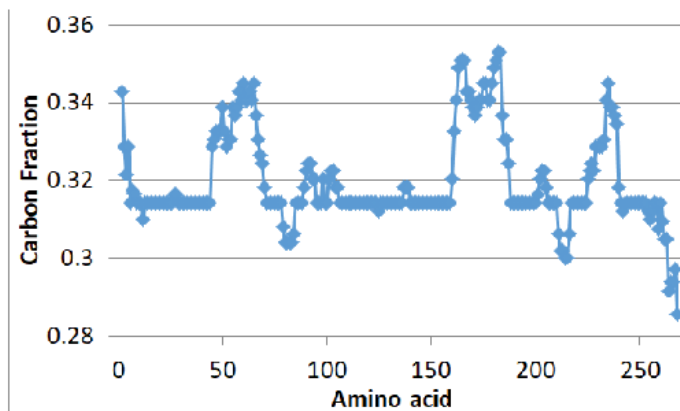


Figure 5 Protein sequence analysis for internal one; along the sequence are given the carbon fraction which indicates the internal one with carbon value of 0.3145 and other regions are carbon-rich and carbon-less regions; carbon-rich regions may act as active stretches where the incoming drug can bind and alter this into an internal one

One of the simplest things in the internal one calculation is the CARd score of internal one formation as shown in Figure 5. According to the nature of law that when portions of sequence retain a carbon fraction value of 0.3145 along the line then it maintains an internal one at the portion in 3D structure [18]. Whether there is a 3D structure available or not, the sequence gives an idea that domain and non-domain regions. The problem is the sequence remains the same but the internal one changes upon binding of the drug to protein. In the case of bond length calculation, the internal one may not be variable in sequence information but from the 3D structure. For understanding active versus nonactive regions in protein, one might want to use a 3D structure rather than a simple sequence. Overall it is fantastic with domain regions identification in native form but binding one requires 3D structure. Otherwise, call it a domain of native form for analysis of sequence information and retrieval of domain-related issues including internal domain calculation and carbon domain for stable regions, etc.

CONCLUSION

One of the interesting phenomena taking place in protein is the carbon domain which is measured in terms of carbon profile based on carbon value of 0.3145 which is assessed here as the ability to express binding free energy equivalent for binding of the protein to the drug which is demonstrated here. Otherwise, call it practical extraction of carbon domain for drug discovery and related issues. Carbon value with adequacy is the single most force of attraction in dealing with drug action in biomolecular systems. Otherwise one need not worry about other forces of interaction coming from van der Waals or electrostatic. Carbon alone is going to the interactive element in this action of the drug during pain relief. According to the nature of the interaction, it is the only force of attraction called nanonic force coming from carbon value fundamentally in the interacting molecules that are relieving painful action of the molecular system. Principally it is necessary to mention that carbon does play a role in deriving force from drug molecule which may of course be the principal driving force for binding and calculation leading to binding free energy like involvement might help design multiple drugs for the same target. Alternatively, arrangements can be made to increase the binding capability of the drug found already in complex with the protein of interest.

DECLARATIONS

Conflicts of Interest

The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

REFERENCES

- [1] Rajasekaran Ekambaram, R. Meenal, Prawin Angel Michael, and R. Indupriya. "Existence of nano level force in protein plays applications of maximum untold understanding of life form." *International Journal of Engineering and Advanced Technology (IJEAT)*, Vol. 9, No. 2, 2019, pp. 3722-26
- [2] Ekambaram, R., I. Rajasekaran, and M. Rajasekaran. "Domain formation in regions of protein probe interaction." *International Journal of Molecular Biology: Open Access*, Vol. 4, No. 5, 2019, pp. 167-69.
- [3] Rajasekaran, Indupriya, Meenal Rajasekaran, and Rajasekaran Ekambaram. "Existence of carbon domain alters bond orders in protein." *International Journal of Innovations in Engineering and Technology (IJIET)*, Vol. 13, No. 3, 2019, pp. 128-32.
- [4] Ekambaram, Rajasekaran, et al. "Nature of amino acid sequence instruct carbon value to be adopted in protein 3d structure." *2019 2nd International Conference on Intelligent Computing, Instrumentation and Control Technologies (ICICICT)*, Vol. 1, 2019, pp. 1354-59.
- [5] Rajasekaran, I., M. Rajasekaran, and K. Velusamy. "Drug protein interaction validates the internal cod formed due to cohesive force: Test of bond length variation in amino acids involved." *International Journal of Molecular Biology: Open Access*, Vol. 4, No. 3, 2019, pp. 113-17.
- [6] Ekambaram, R., and I. Rajasekaran. "Who power sickle cell disease: Carbon domain analysis tells all because of design in protein 3D arbitrary internal carbon domain (COD) arrangement." *International Journal of Molecular Biology: Open Access*, Vol. 4, No. 3, 2019, pp. 85-88.

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- [7] Ekambaram, Rajasekaran, et al. "Existence of cohesive force explains all phenomena that are in material which holds strong bond of all forces of attraction: A case study with carbon material." *AIP Conference Proceedings*, Vol. 2087, No. 1, 2019.
- [8] Ekambaram, Rajasekaran, Meenal Rajasekaran, and Indupriya Rajasekaran. "Paradigms in computer vision: Biology based carbon domain postulates nano electronic devices for generation next." *International Conference On Computational Vision and Bio Inspired Computing*, Springer, Cham, 2018.
- [9] Ekambaram, R. "Domains based in carbon dictate here the possible arrangement of all chemistry for biology." *International Journal of Molecular Biology: Open Access*, Vol. 3, No. 5, 2018, pp. 240-43.
- [10] Akila, K., N. Sneha, and E. Rajasekaran. "Study on carbon distribution at protein regions of disorder." *International Journal of Bioscience, Biochemistry and Bioinformatics*, Vol. 2, No. 2, 2012, pp. 68-70.
- [11] Mamboya, F. A., et al. "Carbon distribution analysis on mutations responsible for Li-Fraumeni syndrome." *GSTF International Journal on Bioinformatics and Biotechnology*, Vol. 1, No. 2, 2012, pp.1-9.
- [12] Rajasekaran, E., Sneha Nirmala John, and J. Jannet Vennila. "Carbon distribution in protein local structure direct superoxide dismutase to disease way." *Journal of Proteins and Proteomics*, Vol. 3, No. 2, 2013, pp. 99-104.
- [13] Rajasekaran, Ekambaram, Kannaiyan Akila, and Marimuthu Vijayasathy. "Allotment of carbon is responsible for disorders in proteins." *Bioinformation*, Vol. 6, No. 8, 2011, pp. 291-92.
- [14] Rajasekaran, Ekambaram. "CARd: Carbon Distribution analysis program for protein sequences." *Bioinformation*, Vol. 8, No. 11, 2012, pp. 508-12.
- [15] Ekambaram, Rajasekaran, et al. "CARd-3D: Carbon distribution in 3D structure program for globular proteins." *Bioinformation*, Vol. 10, No. 3, 2014, pp. 138-43.
- [16] Akila, K., P. Balamurugan, and E. Rajasekaran. "The nature of proteins in influenza." *Scientific Research: Open Access*, Vol. 4, No. 10, 2012, pp. 991-94.
- [17] Rajasekaran, E., and M. Palaniselvan. "High carbon content in drugs causes side effects." *Journal of Advanced Biotechnology*, Vol. 11, No. 5, 2011, pp. 11-12.
- [18] Rajasekaran, E., et al. "The nature of proteins." *2009 International Association of Computer Science and Information Technology-Spring Conference*. IEEE, 2009, pp.464-65.