

Serbian Biochemical Society
Eighth Conference
with international participation

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“Coordination in Biochemistry and Life”

Foreword

Dear Colleagues

Welcome to the 8th Conference of the Serbian Biochemical Society, entitled "*Coordination in Biochemistry and Life*".

The title of this year's Conference refers to an important place of coordination chemistry in biochemistry and biomedicine, but also to a need to coordinate the efforts towards new knowledge with fellow scientists from other fields in order to reach more. The collaboration within FEBS3+ (Croatia, Hungary, Slovenia, and Serbia) Meeting Programme continues with the invited lecture of our dear colleague Tantos Ágnes from Research Center for Natural Sciences, Budapest, Hungary. For the first time we have 'Diaspora Lecture' that will be delivered by Miloš Filipović, a top 'product' of Serbian biochemistry who is now affiliated at the Université de Bordeaux. We have more than forty PhD students from Serbia, Hungary, and Belarus with poster presentations, and for the first time the Conference is held outside the capital. It believe that we are getting better each year, and that we are prepared for future challenges.

I would like to express my gratitude to the members of the Scientific Board who suggested lecturers, to all respected colleagues who accepted the invitation, and to our dear hosts from the University of Novi Sad.

Editor of the Proceedings
Ivan Spasojević

Computational analysis of non-covalent interactions in phycocyanin subunit interfaces

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Phycocyanins (C-phycocyanin and allophycocyanin) are stable water-soluble trimers ($\alpha\beta$)₃ or hexamers ($\alpha\beta$)₆, containing dark-blue covalently attached phycocyanobilin chromophore with variety of pharmacological properties. Molecular forces (non-covalent interactions) responsible for the observed differences in thermal and chemical stability of different phycocyanin complexes are not completely understood¹.

In this study, we used the manually curated non-redundant dataset of 118 interfaces from 20 X-ray phycocyanin structures (PDB ID codes: 1all, 1b33, 1kn1, 2vjt, 3dbj, 4f0u, 4po5, 4rmp, 1pcp, 1gh0, 1f99, 1jbo, 1phn, 2bv8, 2vml, 3o18, 411e, 4lm6, 4lms, 4yjj) to gain additional insight to this phenomenon using a robust inter-atomic non-covalent interaction analyzing tool PPCheck (<http://caps.ncbs.res.in/ppcheck>). For our dataset, the mean interface area was 1088 Å² and there were on average 59 residues per interface. Most of the individual interface parameters are clustered at the middle of the range which we call “standard-size” interfaces. Our observations indicate that there is relatively high composition (51%) of hydrophobic residues at the phycocyanin interfaces; most frequent amino acids in interfaces are Ala (11.4%), Leu (10.0%), Arg (9.5%) and Thr (8.3%).

The analysis shows that about 42% of the total hydrogen bonds in the interfaces under consideration are involved in the formation of multiple hydrogen bonds; 52.8% of total number of hydrogen bonds is formed by water (as donor or acceptor; Figure 1); the hydrogen bonds across the interfaces are predominantly the O–N type; the largest numbers are side chain–side chain hydrogen bonds (55.9%) between the phycocyanin interfaces; most of hydrogen bonds possess distances in the region 2.8–4.2 Å, indicating their moderate and weak strength. The mean number of hydrophobic interactions per interface is 13.6 (max 30); the hydrophobic side chains make larger number of these interactions than side chains of charged and the hydrophilic amino acid. On average, there are about 3 salt bridges per interface in phycocyanin interfaces (max 7); less than one-tenth of the salt bridges in our database are networked, to form several triads, and the remaining are isolated ones. Most salt bridges (~80%) contain at least one hydrogen bond between the atoms in their side-chain charged groups; there is no preferred combination of donors and acceptors.

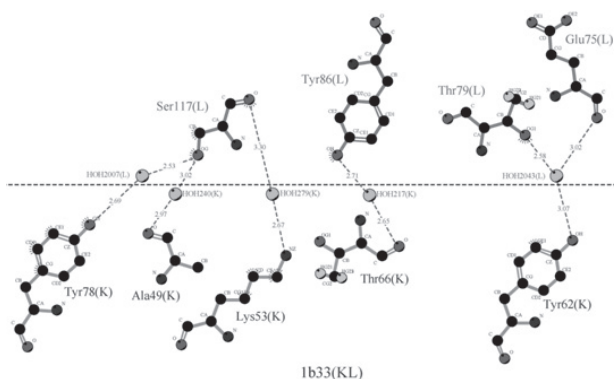


Figure 1. View of the water-bridged hydrogen bonds (KL interface) of Allophycocyanin from *Mastigocladus laminosus* (PDB 1b33). The flattened diagram places atoms and bonds on the 2D page to minimize the overlap of atoms and the crossing of bonds in the final diagram. Hydrogen bonds are indicated by dashed green lines (with the distance between donor and acceptor printed in the middle) between the atoms involved. The Figure was prepared using program LigPlot+ v.2.1.

The stability of a non-covalent complex is usually related to the complexation energy, which is proportional to the strength of the interactions involved. Analysis shows that hydrogen bond energies contribute to about 88% to the total energy. Van der Waals and electrostatic energy contributes to 9.3% and 1.9% on average in these complexes, respectively. Thus, hydrogen bonds contribute maximally towards the stability of protein–protein complexes. Results show the total binding energy is more for large phycocyanin interfaces. The normalized energy per residue was less than -16 kJ mol^{-1} , while most of them have energy in the range from -6 to -14 kJ mol^{-1} . The non-covalent interacting residues in phycocyanin protein interfaces were found to be highly conserved (ConSurf server: <http://consurf.tau.ac.il/2016/>); salt bridge forming residues have average conservation scores 7.3; for those involved in hydrogen bonds is 7.0; the amino acid residues forming hydrophobic interactions and water-bridged hydrogen bonds both have average conservation scores of 5.9 (on scale 1–9). Obtained results might contribute to the understanding of structural stability of this class of evolutionary essential proteins with increased practical application and future designs of novel protein–bioactive compound interactions.

Acknowledgements

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References

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