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Structure-functional annotation, GO, PPI, binding sites, and antigenicity identification of an uncharacterized protein of Acinetobacter baumannii: A computational study

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INTRODUCTION & AIM

- Acinetobacter baumannii, a drug-resistant bacteria that infects critically ill individuals, has several uncharacterized proteins that may be necessary for its survival and illness [1].
- This study used computational approaches to predict the physicochemical, functional, three-dimensional, active site, and antigenic features of an uncharacterized A. baumannii protein.
- This protein is acidic and hydrophilic, involved in aminoacyl-tRNA production, with a structure rich in α-helices and random coils, and non-antigenic. Additional experiments and therapy intervention are supported by these findings.

METHOD

The UniProtKB database provided the protein sequence, and the ProtParam service assessed its physical and chemical properties.

→ Functional annotation was employed through STRING (v. 12.0), NCBI CD search, ScanProsite, and Gene Ontology.

→ The SOPMA server determined secondary structural characteristics.

→ The protein's 3D structure was modeled using AlphaFold, Swiss-Model, and I-TASSER servers.

→ SAVES PROCHECK program and the Pro-SA web for structural assessment

→ The CASTp server predicts the active site.

RESULTS & DISCUSSION

Functional annotation & Gene ontology Analysis

- The functional annotation analyses the protein contained Asn-tRNA(Asn) or Gln-tRNA(Gln) amidotransferase subunit C.
- Most biology and molecular biology employ gene ontology [2].This protein regulates translation, glutaminyl-tRNAGln synthesis, and translational fidelity.

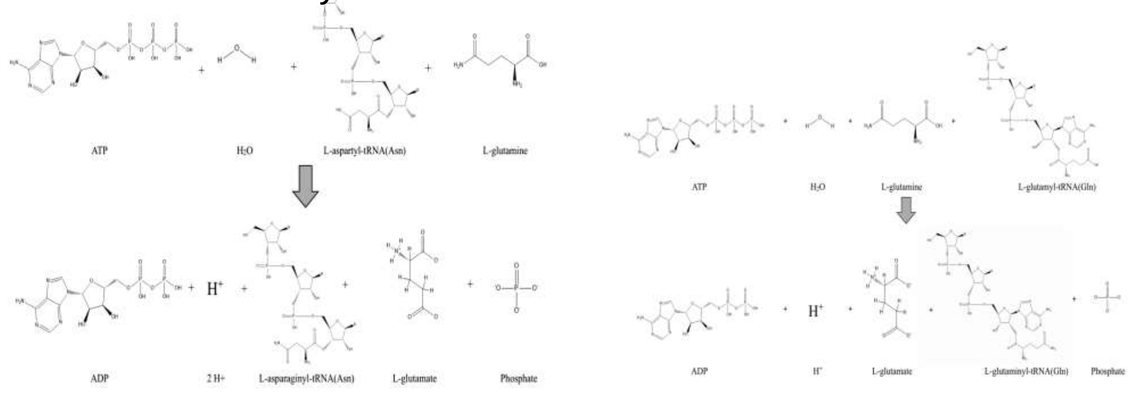
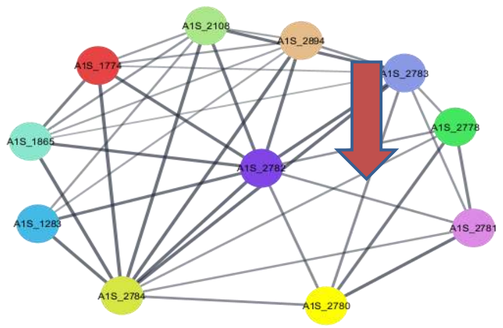


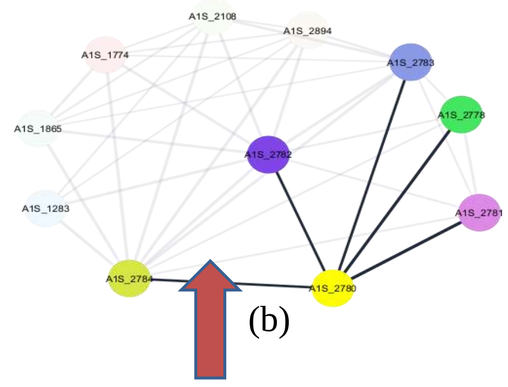
Fig.1. Asn- or Gln-tRNA amidotransferase subunit C assessed

❖ *PPI*

- Protein interaction - a complete overview of interacting components that interacted with ten other proteins



(a)

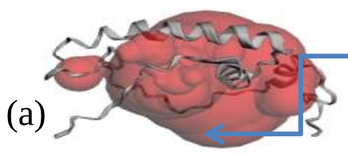


(b)

- The STRING Network Stats - nodes (11), edges (37), average node degree (6.73), and PPI enrichment p-value (2.36×10^{-10}).

Fig.2. Interaction of the selected protein with other proteins

❖ Active site, 3D structure ,Secondary and tertiary structure analysis

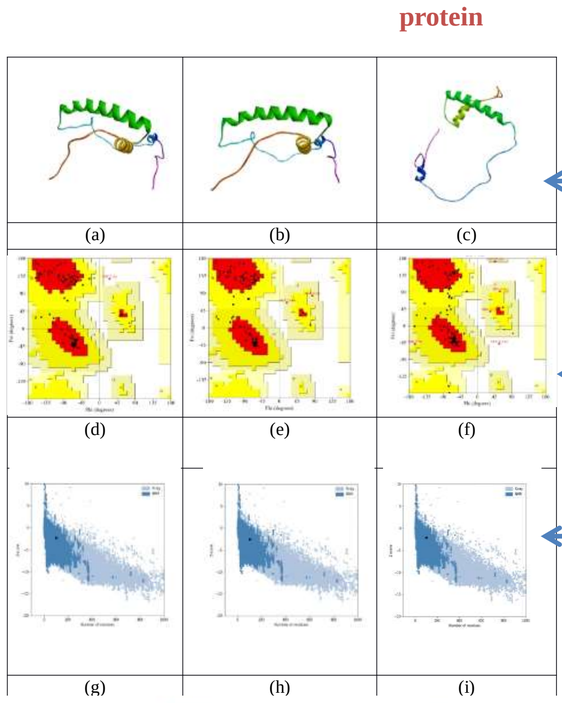


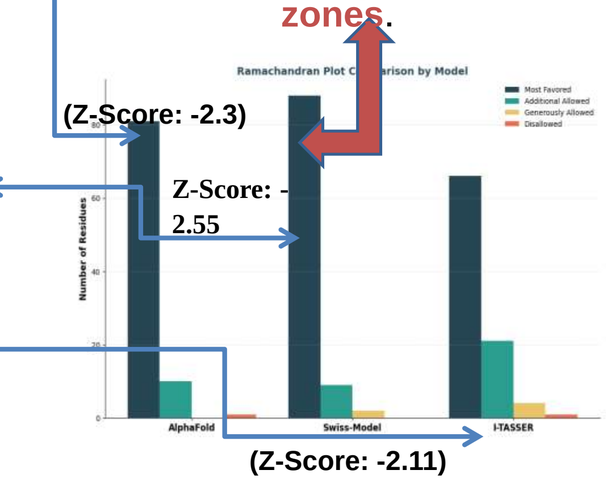
(a)

'red sphere' denotes the active pocket (surface area: 896.977 Å², volume: 4235.245 Å³) of the selected protein

The Swiss model the ideal balance in the most optimal locations with minimal residues in additional allowed and prohibited zones.

(b)



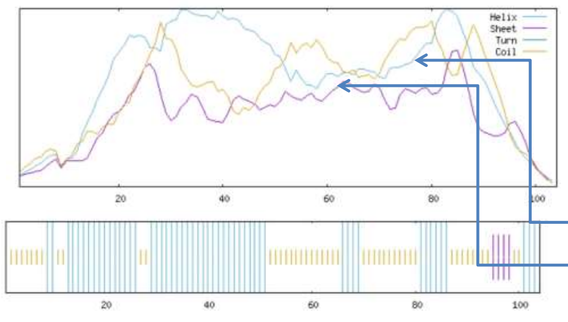


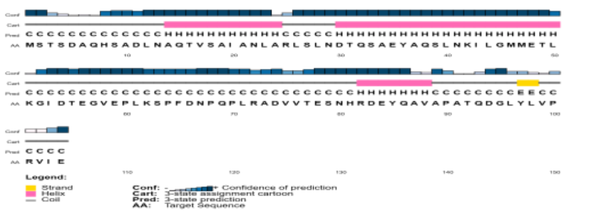
(Z-Score: -2.3)

Z-Score: -2.55

(Z-Score: -2.11)

(c)





alpha-helices (50%), fit into DNA grooves

46.15% random coils, structural dynamical flexibility.

Fig.3. Predict active site (a) and analysis of 3D structure (b), secondary and tertiary structure (c)

CONCLUSION

Uncharacterized Hydrophilic, acidic A. baumannii protein may produce tRNA. Non-antigenic, stable 3D structure, identified active site.
These results suggest a role in vital cellular functioning and warrant further study.

FUTURE WORK / REFERENCES

1. Rolain et al., 2013, Antimicrob. Agents Chemother. 57(1): 592–596
2. Gene Ontology Consortium, 2015, Nucleic Acids Res. 43(D1): D1049–D1056