Homology modeling and docking studies to explore the novel drug for monocyte differentiation antigen CD14

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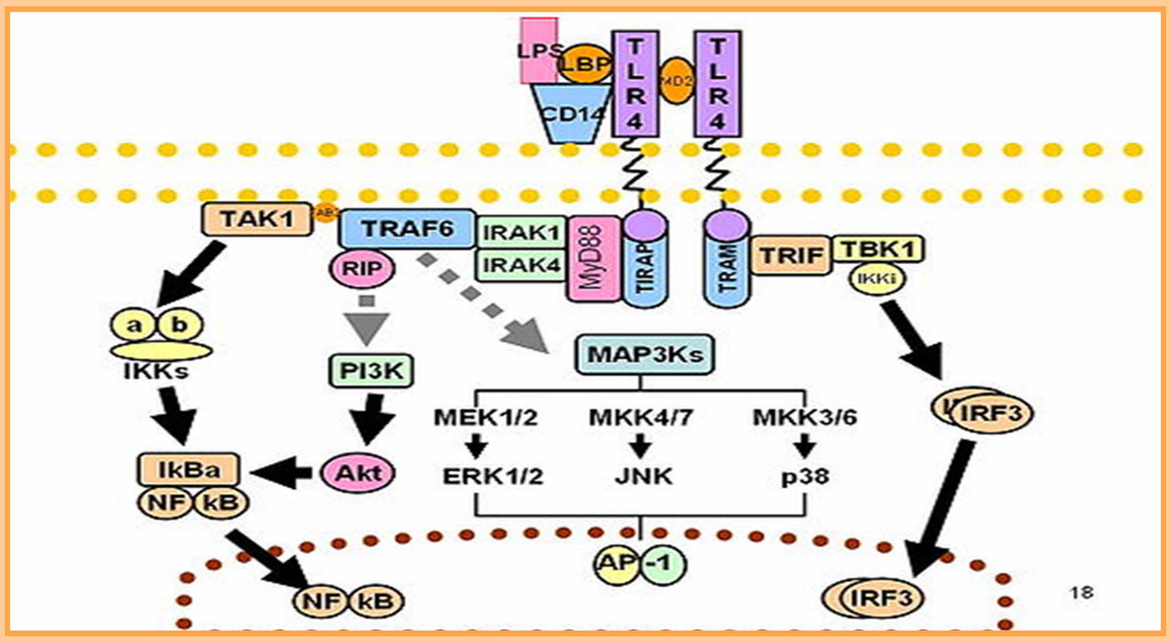
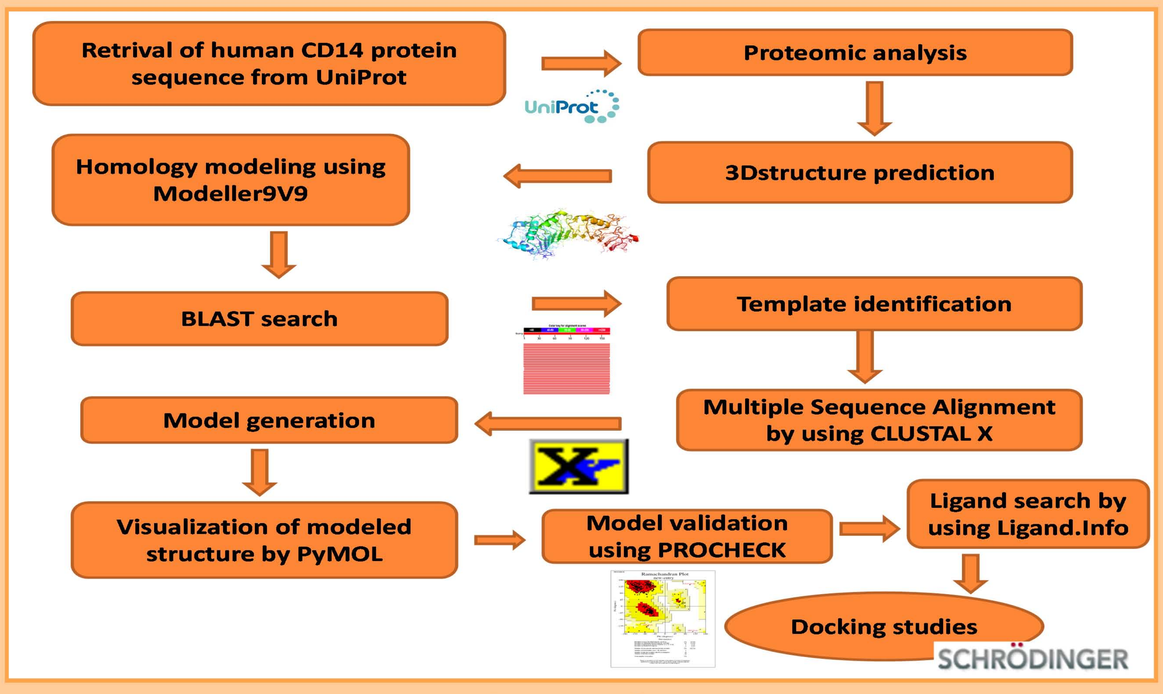
Key points

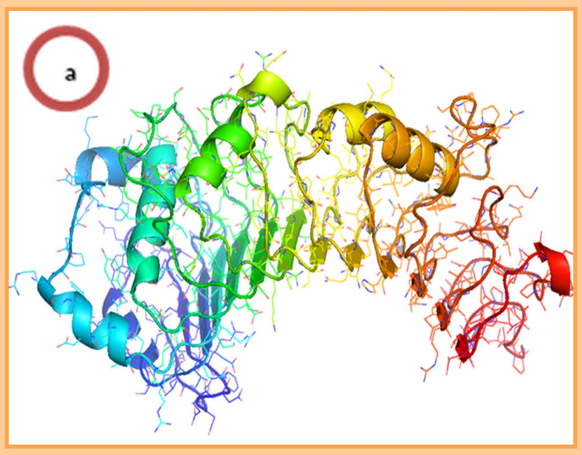
- **Monocyte differentiation antigen CD14 belongs to leucine rich family.**
- **CD14 and toll-like receptor4 (TLR4) plays a major role in inflammatory response and elevated levels cause ischemic heart diseases, neuropathic pain and LPS (endotoxin) induced septic shock.**

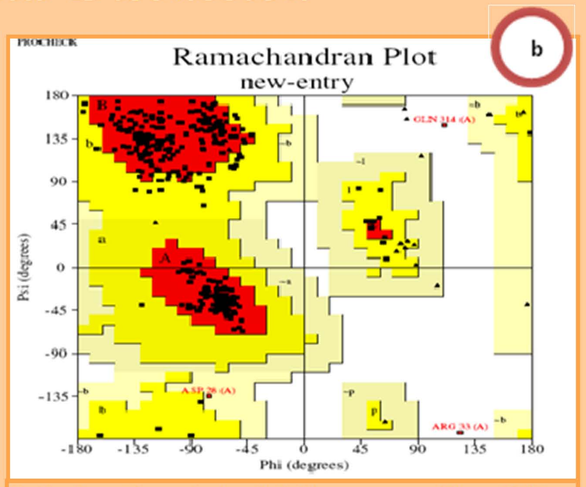


Materials and Methods

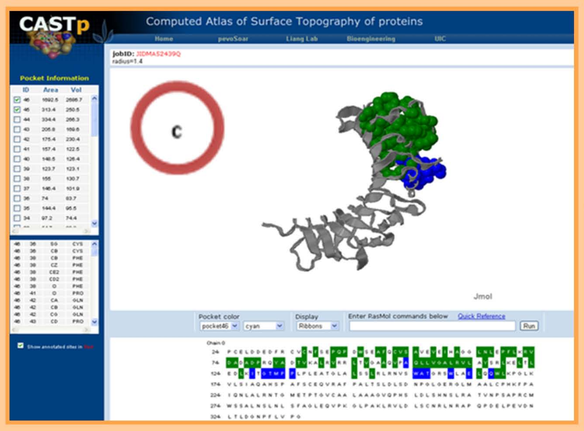


Results and Discussion

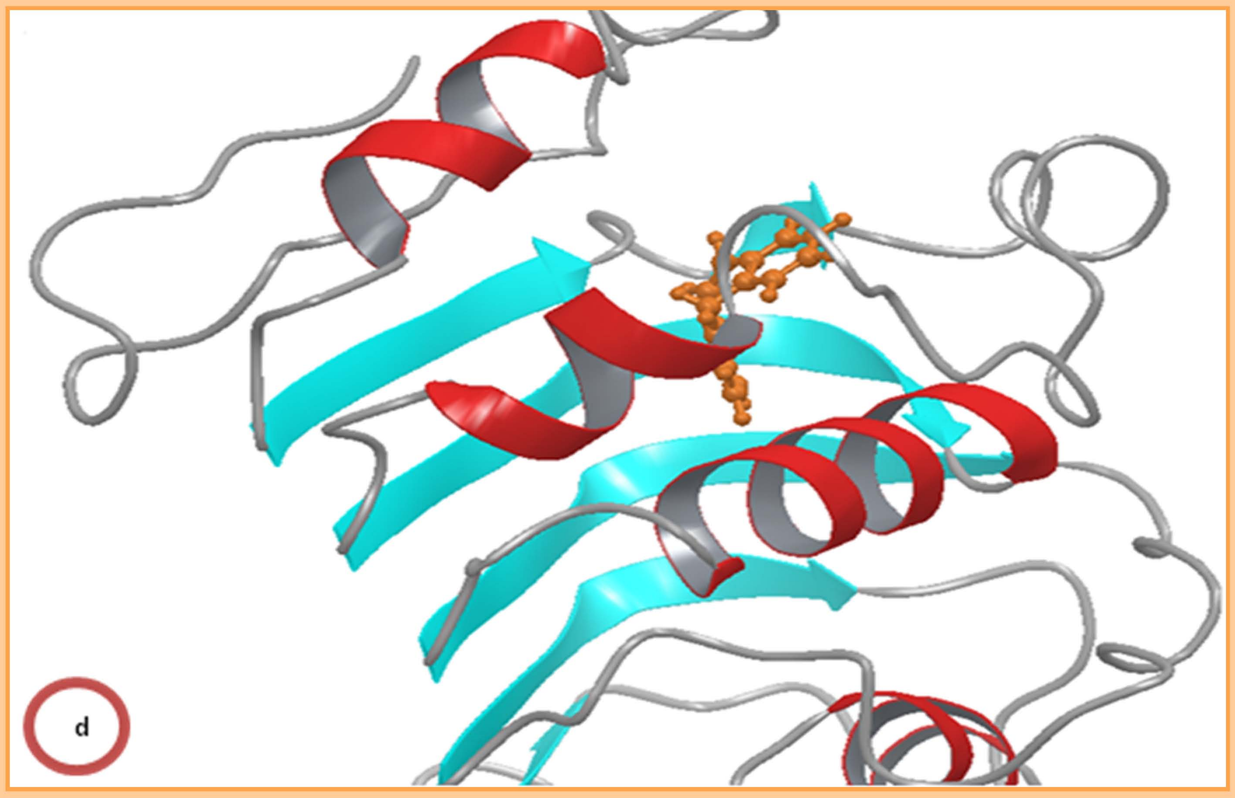


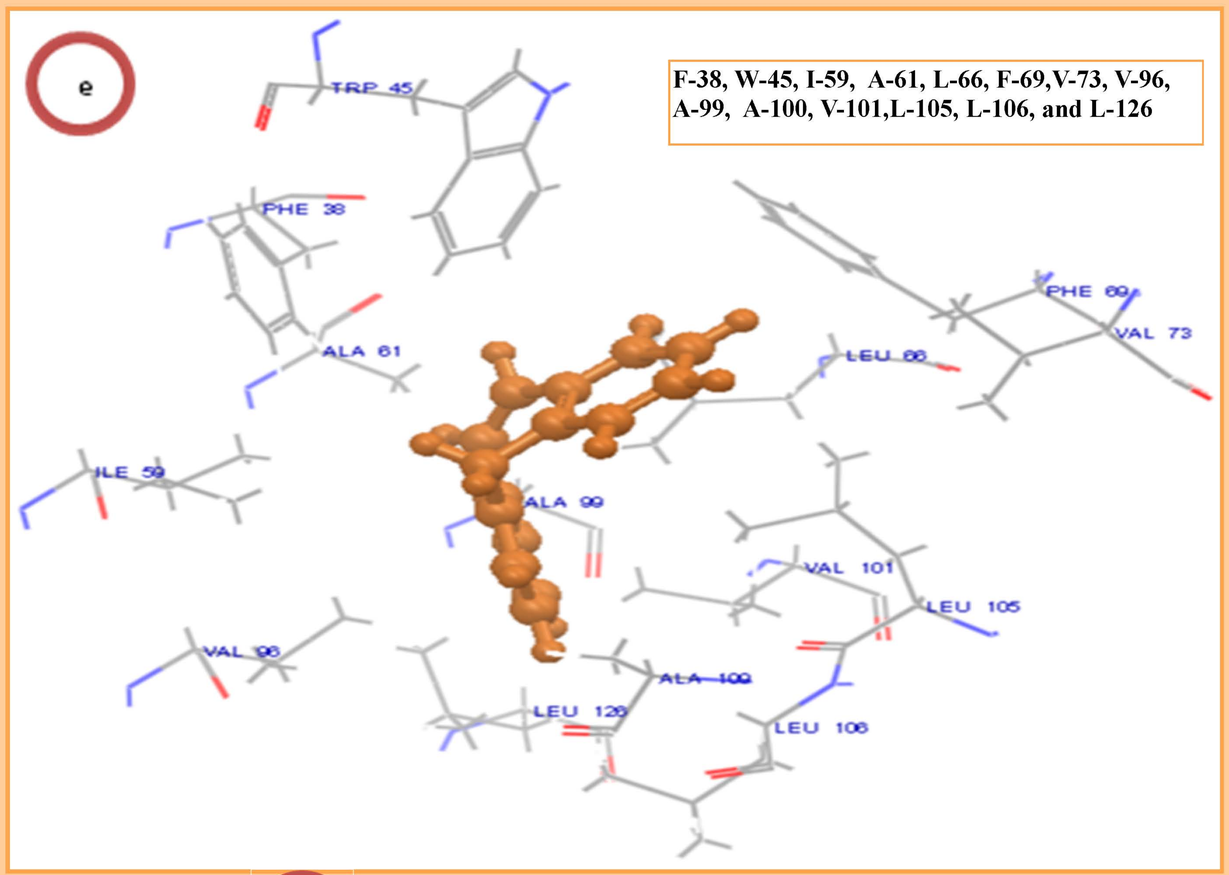


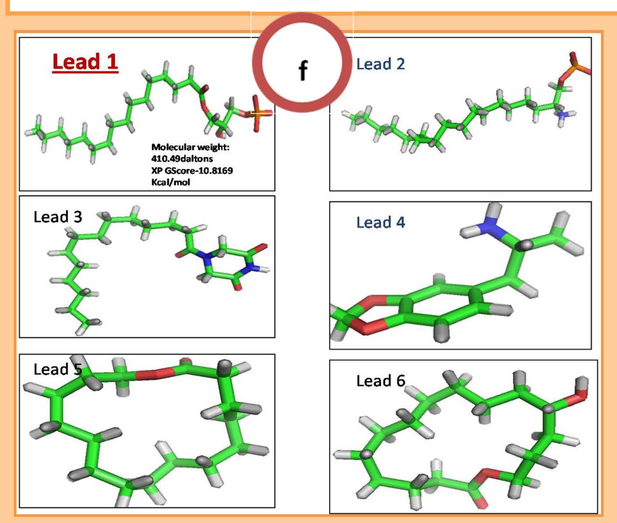
Residues in most favoured regions [A, B, L]	274	85.9%
Residues in additional allowed regions [a, b, l, p]	42	13.2%
Residues in generously allowed regions [~a, ~b, ~l, ~p]	1	0.3%
Residues in disallowed regions	2	0.6%
Number of non-glycine and non-proline residues	319	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	24	
Number of proline residues	30	
Total number of residues	375	



Lig Prep	2947
Post Lig Prep	1992
Qik Prop	1665
GLIDE HTVS	162
SP Docking	22
XP Docking	17







a)Visualisation of modeled structure.
b) PROCHECK analysis.
c) Prediction of binding site residues using CASTp.
d) Docking complex of CD14 with lead1.
e) Residues involved in van der Waal interactions.
f) Proposed leads.

CONCLUSION

- **The reliable modeled structure for human CD14 protein was predicted using modller9v9. Six leads were proposed with good pharmacological properties.**
- **The lead '1' is having a least docking score of -10.8169 Kcal/mol was suggested as the potent inhibitor for blocking the human CD14 functional activity in turn control ischemic heart diseases.**

AKNOWLEDGEMENTS

My deep sense of gratitude to Dr. B.Vengamma, Director, SVIMS University, Tirupati and DBT, Ministry of Science and Technology, Govt. of India and for providing all the necessary facilities to carryout project.