Docking Interaction of Chromium(III) Phenylalanine with Protein Tyrosine Phosphatase

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Abstract

Chromium(III) complexes have been known to increase insulin absorption and decrease glucose levels in the blood, so Cr(III) complexes can be used as an anti-diabetic supplement especially for people with diabetes type 2. The experimentally Cr(III) complexes proven to decrease glucose level, but the role mechanism of Cr(III) complexes in the body until now there is no explain in detail. In this research, the interaction of Cr(III) phenylalanine [Cr(Phe)$_3$] with protein tyrosine phosphatase (PTP) was studied by molecular docking. The aim this study was to identify the active site of PTP that binding with those Cr(III) phenylalanine. This research performed by computational calculations Hartree-Fock with basis set 6-31G, the interaction with PTP used the Autodock Vina software. The results showed that [Cr(phe)$_3$] interact with 5 amino acids of PTP, i.e Leu(13), Arg(18), Ser(94), Asp(129) and Tyr(131) with the interaction energy of -6,6 Kcal/mol. The results showed that the interaction Cr(III) phenylalanine with PTP indicate hydrogen bonding with bond lenght from 1,8 Å to 2,9 Å

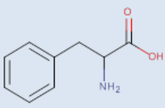
Method

- Structure prediction and energy calculation of Chromium(III) Phenylalanine were performed using HF method with 6-31G basis set
- The interaction with PTP used the Autodock Vina software
- The visualisation used Chemcraft 1.6 Software

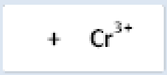
Results

Cr(Phe)$_3$ Complexes

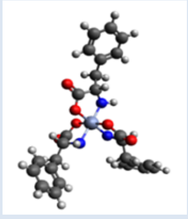
Phenylalanin



Chromium(III)



Cr(Phe)$_3$

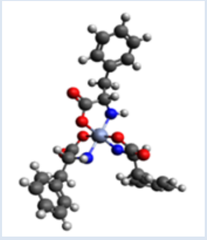


The Bond Lenght Calculation

No	Bond Type	Bond Lenght (Å)
1	Cr-O1	1,881
2	Cr-O2	1,915
3	Cr-O3	1,924
4	Cr-N1	2,052
5	Cr-N2	2,058
6	Cr-N3	2,023

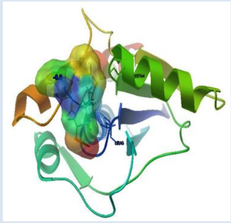
Docking Process

Cr(Phe)$_3$

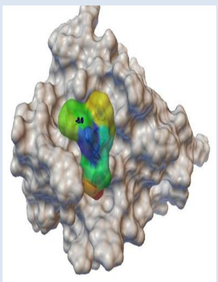


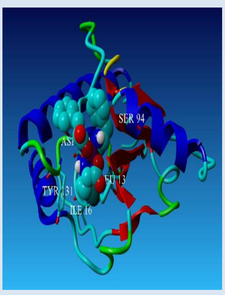
PTP

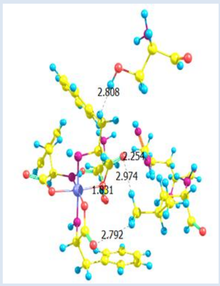
[Cr(Phe)$_3$-PTP]



The Interaction Cr(Phe)$_3$ - PTP







Summary

- The interaction between Cr(III) phenylalanine with PTP indicate Hydrogen Bonding interaction, and the distance 1,8 – 2,9 Å.
- The amino acids of PTP that interaction are Leu(13), Ile(16), Ser(47), Trp(49), Asn(50) and Tyr(131), the interaction energy is -6,6 kcal/mol

References

- Alonso H, Bliznyuk A.A, Gready E.J. (2006). Combining Docking and Molecular Dynamic Simulations in Drug Design. *Medicinal Research Reviews*. 26(5), 531-568
- Levina, A.,& Lay, P. A. (2008). Chemical Properties and Toxicity of Chromium(III) Nutritional Supplements. *Chemical Research Toxicology*, *21*, 563–571.

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