



ChemTech

International Journal of ChemTech Research

CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.10 No.13, pp 60-65, 2017

Identification of Bioactive Lead Compound against Central Hypothyroidism – An *Insilico* Approach

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Abstract : Computational approaches are intended to provide system level insight into complex biological processes that underlie serious diseases. In this work, an attempt has been made to utilize *in-silico* docking procedures to study a clinically important and common disease – Central hypothyroidism(CH). Currently, there is a significant burden of thyroid disease around the world; the most crucial part is people are unaware of the condition and mostly women are 5-8 times more likely than men to have thyroid problem. Although several treatment procedures are available *i.e.*, Synthetic and Ayurveda methods; most of these drugs create various side effects and thus forcing the patients to continue the medication throughout their life. Taking this gaps into consideration, this study has focused on several bioactive components from plant that has the ability to treat CH. Through virtual screening and docking procedure, β -glucan, a group of β -D-glucose polysaccharides present in oats (*Avena sativa*) was identified as lead compound. Additionally, it was confirmed from various literature survey that they pose anti-oxidant properties and thus have a unique ability to be used as nutraceutical in treating the symptoms of CH.

Keywords : Ayurveda, Central hypothyroidism, Molecular docking, Nutraceuticals.

Ram Kothandan *et al* /International Journal of ChemTech Research, 2017,10(13): 60-65.
