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IN SILICO STUDIES OF (S)-2-AMINO-4-(3,5-DICHLOROPHENYL) BUTANOIC ACID AGAINST LAT1 AS A RADIOTHERANOSTIC AGENT OF CANCER

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Abstract

***Objective**: This study aims to obtain a good activity of radiotheranostic kit for cancer which is built by combining (S)-2-amino-4-(3,5-dichlorophenyl) butanoic acid (ADPB) with various bifunctional chelators.*

***Methods**: This study was conducted through in silico method that consists of molecular docking simulation using AutoDock 4 as well as ADMET prediction using vNN-ADMET and Pre-ADMET. Six bifunctional chelators (i.e. CTPA, DOTA, H2CB-TE2A, H2CB-DO2A, NOTA, and TETA) were conjugated with ADPB as a carrier molecule and further analyzed through molecular docking and ADMET prediction.*

***Results**: The results showed that the ADPB-NOTA has the best affinity with the Gibbs free energy (ΔG) of-7.68 kcal/mol with an inhibition constant of 2.36 μM and its ability to bind with the gating residue of LAT1 (ASN258) through hydrogen interactions. Besides that, the ADPB-NOTA compound has a good ADME profile and is predicted to be safe for human use.*

***Conclusion**: This study showed that ADPB-NOTA is the most prospective candidate to be used as a radiotheranostic agent.*

Author Keywords

Bifunctional chelators, Cancer, LAT1, In silico, Radiotheranostic

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