ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA
DEMINERALISASI EMAIL (Kajian In Silico)
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ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN *BLEACHING* TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian *In Silico*)

INTISARI

Bahan *bleaching* ekstrakoronal seperti hidrogen peroksida efektif dalam *bleaching* gigi, namun memiliki efek samping demineralisasi email. Bahan *bleaching* asam malat diharapkan memiliki potensi efek samping minimal. Bahan *bleaching* menghidrolisis saliva sehingga email mengalami demineralisasi. Tujuan penelitian adalah untuk menganalisis energi pengikatan antara senyawa asam malat dan hidrogen peroksida terhadap protein saliva pada demineralisasi email melalui analisis *in silico*.

Senyawa ligan asam malat dan hidrogen peroksida dianalisis dengan *molecular docking* terhadap 3 reseptor protein saliva yaitu diantaranya proline rich protein haeIII subfamily1 (PRH1), statherin (STATH) dan histatin (HTN1) dengan menggunakan beberapa *tools* antara lain Chimera untuk pemodelan struktur molekul, CB-Dock2 untuk *blind docking* dan AutoDock untuk *docking* terarah. Valid jika protokol *docking* RMSD ≤ 2 Å. Setiap kompleks ligan–protein dilakukan 100 run, dengan output utama skor *docking* ΔG (kcal/mol) dan residu asam amino yang kontak dengan senyawa serta visualisasi 2D dan 3D dengan menggunakan Ligplot+.

Uji *Kruskal–Wallis* dan *Mann–Whitney* dengan data tidak berdistribusi normal dan varians tidak homogen (α=0,05). Hasil menunjukkan seluruh ligan berinteraksi melalui ikatan hidrogen atau elektrostatik pada permukaan protein dengan afinitas lemah (ΔG sekitar −1 hingga −4). Asam malat berikatan relatif lebih kuat pada statherin lalu histatin, terlemah pada proline rich protein haeIII subfamily1. Sedangkan hidrogen peroksida lebih kuat pada proline rich protein haeIII subfamily1, lalu histatin, dan terlemah pada statherin. Terdapat perbedaan bermakna antar keenam kelompok (H=565,69; p<0,001) dan seluruh perbandingan pasangan signifikan (p<0,001). Kesimpulannya terdapat interaksi molekuler antara kedua senyawa *bleaching* dengan 3 protein saliva proline rich protein haeIII subfamily1, histatin dan statherin.

Kata kunci : asam malat; hidrogen peroksida; demineralisasi email; molecular docking; saliva

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ANALYSIS OF MALIC ACID BINDING ENERGY AS A BLEACHING AGENT ON SALIVARY PROTEINS IN ENAMEL DEMINERALIZATION
(In Silico Study)

ABSTRACT

Extracoronal bleaching agents such as hydrogen peroxide have been proven effective in teeth bleaching, but they have the side effect of enamel demineralization. Malic acid bleaching agents are expected to have minimal side effects. Bleaching agents have been shown to hydrolyze saliva, causing enamel to undergo demineralization. The aim of this study was to analyze the binding energy between malic acid and hydrogen peroxide compounds and saliva proteins in enamel demineralization through in silico analysis.

Malic acid and hydrogen peroxide ligand compounds were analyzed by molecular docking against saliva protein receptors proline rich protein haeIII subfamily1 (PRH1), statherin (STATH), and histatin (HTN1) using several tools, including Chimera for molecular structure modeling, CB-Dock2 for blind docking, and AutoDock for directed docking. The docking protocol was considered valid if the RMSD was ≤ 2 Å. Each ligand-protein complex was run 100 times, with the main output being the docking score ΔG (kcal/mol) and amino acid residues in contact with the compound, as well as 2D and 3D visualizations using Ligplot+.

The Kruskal–Wallis and Mann–Whitney tests were used to the data were not normal and the variance was not homogeneous (α=0.05). The results showed that all ligands interacted through hydrogen/electrostatic bonds on the protein surface with weak affinity (ΔG around −1 to −4). Malic acid bound relatively stronger to statherin, then histatin, and weakest to proline rich protein haeIII subfamily1. Hydrogen peroxide binds more strongly to proline rich protein haeIII subfamily1, then histatin, and weakest to statherin. There were significant differences between the six groups ($H=565.69$; $p<0.001$) and all pairwise comparisons were significant ($p<0.001$). In conclusion, there is molecular interaction between the two bleaching compounds and the saliva proteins proline rich protein haeIII subfamily1, histatin, and statherin.

Keywords : malic acid; hydrogen peroxide; enamel demineralization; molecular docking; saliva