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DAFTAR PUSTAKA

Abidia, R. F., El-Hejazi, A. A., Azam, A., Al-Qhatani, S., Al-Mugbel, K., AlSulami, M., & Khan, A. S. (2023). In vitro comparison of natural tooth-whitening remedies and professional tooth-whitening systems. *The Saudi Dental Journal*, *35*(2), 165–171. https://doi.org/10.1016/j.sdentj.2023.01.007

Adasme, M. F., Linnemann, K. L., Bolz, S. N., Kaiser, F., Salentin, S., Haupt, V. J., & Schroeder, M. (2021). PLIP 2021: expanding the scope of the protein–ligand interaction profiler to DNA and RNA. *Nucleic Acids Research*, *49*(W1), W530–W534. https://doi.org/10.1093/nar/gkab294

Agarwal, R., Vasani, N., Mense, U. S., Prasad, N., Shetty, A., Natarajan, S., Dutta, A., & Thomas, M. S. (2024). Effects of online marketplace-sourced over-the-counter tooth whitening products on the colour, microhardness, and surface topography of enamel: an in vitro study. *BDJ Open*, *10*(1), 67. https://doi.org/10.1038/s41405-024-00253-0

Agu, P. C., Afiukwa, C. A., Orji, O. U., Ezeh, E. M., Ofoke, I. H., Ogbu, C. O., Ugwuja, E. I., & Aja, P. M. (2023). Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management. *Scientific Reports*, *13*(1), 13398. https://doi.org/10.1038/s41598-023-40160-2

Aida Ariella. (2019). Kadar Proline-Rich Protein Sebagai Indikator Early Childhood Caries = Salivary Proline-Rich Protein Levels as a Detection for Early Childhood Caries. *Fakultas kedokteran gigi universitas indonesia*.

Akter, R., Asgor Moral, M. A., Md, K., & A. K. M., B. (2025). Biomimetic Effect of Saliva on Human Tooth Enamel: A Scanning Electron Microscopic Study. *International Journal of Dentistry*, *2025*(1). https://doi.org/10.1155/ijod/1664620

Alkahtani, R., Stone, S., German, M., & Waterhouse, P. (2020). A review on dental whitening. *Journal of Dentistry*, *100*, 103423. https://doi.org/10.1016/j.jdent.2020.103423

AlShehri, A., AlRefeai, M. H., AlZamil, F., AlOtaibi, N., & AlKinani, Y. (2022). Effect of Over-The-Counter Tooth-Whitening Products on Enamel Surface Roughness and Microhardness. *Applied Sciences*, *12*(14), 6930. https://doi.org/10.3390/app12146930

Anil, A., Ibraheem, W. I., Meshni, A. A., Preethanath, R., & Anil, S. (2022). *Demineralization and Remineralization Dynamics and Dental Caries*. www.intechopen.com

UNIVERSITAS GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Antonio Nanci. (2024). *Ten's Cate Oral Histology* (10 ed.). Elsevier.

Antunes, E. V. G., Basting, R. T., do Amaral, F. L. B., França, F. M. G., Turssi, C. P., Kantovitz, K. R., Bronze-Uhle, E. S., Filho, P. N. L., & Basting, R. T. (2023). Titanium dioxide nanotubes in a hydrogen peroxide-based bleaching agent: physicochemical properties and effectiveness of dental bleaching under the influence of a poliwave led light activation. *Clinical Oral Investigations*, *27*(4), 1745–1755. https://doi.org/10.1007/s00784-022-04802-5

Araujo, T. T., Dionizio, A., Carvalho, T. de S., Debortolli, A. L. B., Vertuan, M., de Souza, B. M., Camara, J. V. F., Henrique-Silva, F., Chiaratti, M., Santos, A., Alves, L., Ferro, M., Magalhães, A. C., & Buzalaf, M. A. R. (2024). Acquired pellicle and biofilm engineering with CaneCPI-5: Insights from proteomic and microbiomics analysis. *Archives of Oral Biology*, *166*, 106025. https://doi.org/10.1016/j.archoralbio.2024.106025

Arifin, S. N., & Pratiwi, D. (2017). Studi in Silico senyawa flavonoid dari ekstrak kacang panjang (Vigna sinensiL) sebagai penumbuh rambut dengan reseptor androgen. *Jurnal Farmagazine*, *4*, 31–37.

Asmawati, A., & Rieuwpassa, I. E. (2018). Comparison of enamel hardness after dental bleaching agent application strawberry gel and carbamide peroxide 10%. *Journal of Dentomaxillofacial Science*, *3*(1), 17. https://doi.org/10.15562/jdmfs.v3i1.626

Avila, V., Proctor, G., Velandia-Romero, M., Castellanos, J. E., Beltrán, E. O., Lynham, S., & Martignon, S. (2024). Proteome of the 2-h in vivo Formed Acquired Enamel Pellicle of Adolescents with Erosive Tooth Wear, Caries, or Sound. *Caries Research*, 1–12. https://doi.org/10.1159/000541026

Aziz, H. A. (2020). Studi In Silico Aktivitas Penghambatan Senyawa Turunan Kuersetin Terhadap Protease HIV-1. *Universitas Nasional*.

Banerjee, P., Kemmler, E., Dunkel, M., & Preissner, R. (2024). ProTox 3.0: a webserver for the prediction of toxicity of chemicals. *Nucleic Acids Research*, *52*(W1), W513–W520. https://doi.org/10.1093/nar/gkae303

Blasse, C., Saalfeld, S., Etournay, R., Sagner, A., Eaton, S., & Myers, E. W. (2017). PreMosa: Extracting 2D surfaces from 3D microscopy mosaics. *Bioinformatics*, *33*(16), 1–7. https://doi.org/10.1093/bioinformatics/xxxxxx

Burnett, C. L., Bergfeld, W. F., Belsito, D. V., Hill, R. A., Klaassen, C. D., Liebler, D. C., Marks, J. G., Shank, R. C., Slaga, T. J., Snyder, P. W., & Heldreth, B. (2022). Amended Safety Assessment of Malic Acid and Sodium Malate as Used in Cosmetics. *International Journal of Toxicology*, *41*(3_suppl), 69–76. https://doi.org/10.1177/10915818221117535

UNIVERSITAS GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Butera, A., Maiorani, C., Rederiene, G., Checchi, S., & Nardi, G. M. (2024). Evaluation of the Effectiveness of Different Types of Professional Tooth Whitening: A Systematic Review. *Bioengineering*, *11*(12), 1178. https://doi.org/10.3390/bioengineering11121178

Carpio-Salvatierra, B., da Silva, K. L., Favoreto, M. W., González, C., Ordóñez, M. C. R. B., Loguercio, A. D., & Farago, P. V. (2024). Effect of an experimental desensitizer with a hydroxyapatite-capsaicin composite applied before in-office dental bleaching on hydrogen peroxide diffusion, color and surface changes. *Clinical Oral Investigations*, *28*(12). https://doi.org/10.1007/s00784-024-06041-2

Chawhuaveang, D. D., Yu, O. Y., Yin, I. X., Lam, W. Y. H., Mei, M. L., & Chu, C. H. (2021a). Acquired salivary pellicle and oral diseases: A literature review. Dalam *Journal of Dental Sciences* (Vol. 16, Nomor 1, hlm. 523–529). Association for Dental Sciences of the Republic of China. https://doi.org/10.1016/j.jds.2020.10.007

Chen, C., Huang, X., Zhu, W., Ding, C., Huang, P., & Li, R. (2021a). TRPA1 triggers hyperalgesia and inflammation after tooth bleaching. *Scientific Reports*, *11*(1). https://doi.org/10.1038/s41598-021-97040-w

Costa, M. J. F., Sette-De-souza, P. H., & Borges, B. C. D. (2023). In silico affinity between analgesic/anti-inflammatory drugs and the transient receptor potential A1 to predict potential pharmacological managing approaches for bleaching sensitivity. *Anais da Academia Brasileira de Ciencias*, *95*. https://doi.org/10.1590/0001-3765202320230555

de Boa, P. W. M., de Sousa Santos, K., da Silva Souza, A. M., da Silva-Júnior, A. A., & Borges, B. C. D. (2025). Impact of nanostructured additives in tooth bleaching agents on enhancing color change and reducing side effects: a scoping review. *Clinical oral investigations*, *29*(1), 70. https://doi.org/10.1007/s00784-025-06148-0

De Borja, J. R., & Cabrera, H. S. (2024). In Silico Drug Screening for Hepatitis C Virus Using QSAR-ML and Molecular Docking with Rho-Associated Protein Kinase 1 (ROCK1) Inhibitors. *Computation*, *12*(9), 175. https://doi.org/10.3390/computation12090175

de Oliveira, T. A., Medaglia, L. R., Maia, E. H. B., Assis, L. C., de Carvalho, P. B., da Silva, A. M., & Taranto, A. G. (2022). Evaluation of Docking Machine Learning and Molecular Dynamics Methodologies for DNA-Ligand Systems. *Pharmaceuticals*, *15*(2), 132. https://doi.org/10.3390/ph15020132

Deng, Q., Wong, H. M., & Peng, S. (2024). Alterations in salivary profile in individuals with dental caries and/or obesity: A systematic review and meta-analysis. *Journal of Dentistry*, *151*, 105451. https://doi.org/10.1016/j.jdent.2024.105451

UNIVERSITAS
GADJAH MADA
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Diedrich, K., Krause, B., Berg, O., & Rarey, M. (2023a). PoseEdit: enhanced ligand binding mode communication by interactive 2D diagrams. *Journal of Computer-Aided Molecular Design*, *37*(10), 491–503. https://doi.org/10.1007/s10822-023-00522-4

Eberhardt, J., Santos-Martins, D., Tillack, A. F., & Forli, S. (2021). AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. *Journal of Chemical Information and Modeling*, *61*(8), 3891–3898. https://doi.org/10.1021/acs.jcim.1c00203

Enax, J., Fandrich, P., Schulze zur Wiesche, E., & Epple, M. (2024). The Remineralization of Enamel from Saliva: A Chemical Perspective. Dalam *Dentistry Journal* (Vol. 12, Nomor 11). Multidisciplinary Digital Publishing Institute (MDPI). https://doi.org/10.3390/dj12110339

Enax, J., Ganss, B., Amaechi, B. T., Schulze zur Wiesche, E., & Meyer, F. (2023). The composition of the dental pellicle: an updated literature review. *Frontiers in Oral Health*, *4*. https://doi.org/10.3389/froh.2023.1260442

Eric, J., Ciobanu, O., Abdallah, M. N., Nelea, V. D., Gupta, N., Abotaleb, A., & Tamimi, F. (2025). The effect of Hydrogen Peroxide treatments on dental enamel porosity and protein structure and its long-term implications on tooth hardness and optical properties. *Journal of Dentistry*, *156*. https://doi.org/10.1016/j.jdent.2025.105714

Farooq, I., & Bugshan, A. (2021). The role of salivary contents and modern technologies in the remineralization of dental enamel: a narrative review. *F1000Research*, *9*, 171. https://doi.org/10.12688/f1000research.22499.3

Ferrari, C. R., HANNIG, M., & BUZALAF, M. A. R. (2025). Acquired pellicle engineering: a fascinating approach to prevent demineralization. *Journal of Applied Oral Science*, *33*. https://doi.org/10.1590/1678-7757-2024-0359

Frameski, I., Muga, R., Rahmawati, D. L., & Rachmawati, F. (2022). White Pomegranate Extract Gel's Efficacy as A Teeth-Whitening Agent. *International Journal Of Health Science*, *2*(2), 1–5. https://ejurnal.politeknikpratama.ac.id/index.php

Fuhrmann, J., Rurainski, A., Lenhof, H., & Neumann, D. (2010). A new Lamarckian genetic algorithm for flexible ligand-receptor docking. *Journal of Computational Chemistry*, *31*(9), 1911–1918. https://doi.org/10.1002/jcc.21478

Fung, K.-M., Lai, S.-J., Lin, T.-L., & Tseng, T.-S. (2022). Antigen-Antibody Complex-Guided Exploration of the Hotspots Conferring the Immune-Escaping Ability of the SARS-CoV-2 RBD. *Frontiers in molecular biosciences*, *9*, 797132. https://doi.org/10.3389/fmolb.2022.797132

UNIVERSITAS
GADJAH MADA
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Gasmi Benahmed, A., Gasmi, A., Menzel, A., Hrynovets, I., Chirumbolo, S., Shanaida, M., Lysiuk, R., Shanaida, Y., Dadar, M., & Bjørklund, G. (2022). A review on natural teeth whitening. *Journal of Oral Biosciences*, *64*(1), 49–58. https://doi.org/10.1016/j.job.2021.12.002

Gkavela, G., Kakouris, V., Pappa, E., & Rahiotis, C. (2024). Effect of Bleaching Agents on Healthy Enamel, White Spots, and Carious Lesions: A Systematic Review and Meta-Analysis. *Dentistry Journal*, *12*(5), 140. https://doi.org/10.3390/dj12050140

Goettems, M. L., Fernandez, M. dos S., Donassollo, T. A., Henn Donassollo, S., & Demarco, F. F. (2021). Impact of tooth bleaching on oral health-related quality of life in adults: A triple-blind randomised clinical trial. *Journal of Dentistry*, *105*. https://doi.org/10.1016/j.jdent.2020.103564

Gopikrishna, V. (2021). *GROSSMAN'S ENDODONTIC PRACTICE 14TH EDITION* (Fourteenth edition). Wolters Kluwer (India) .

Hand, A. R., & Frank, M. E. (2014). *Fundamentals of Oral Histology and Physiology*. John Wiley & Sons, Inc.

Hany, M., Abdelghany, A., Abdurhman, K., Alqarni, A., Jaber, S. B., Hesham, H., & Elsherif, E. (t.t.). *Cronicon Salivary Statherin-An Overview*.

Harren, T., Gutermuth, T., Grebner, C., Hessler, G., & Rarey, M. (2024). Modern <scp>machine-learning</scp> for binding affinity estimation of <scp>protein–ligand</scp> complexes: Progress, opportunities, and challenges. *WIREs Computational Molecular Science*, *14*(3). https://doi.org/10.1002/wcms.1716

Hata, H., Phuoc Tran, D., Marzouk Sobeh, M., & Kitao, A. (2021). Binding free energy of protein/ligand complexes calculated using dissociation Parallel Cascade Selection Molecular Dynamics and Markov state model. *Biophysics and Physicobiology*, *18*(0), bppb-v18.037. https://doi.org/10.2142/biophysico.bppb-v18.037

Hughes, J. A., West, N. X., Parker, D. M., Van Den Braak, M. H., & Addy, M. (t.t.). *Effects of pH and concentration of citric, malic and lactic acids on enamel, in vitro*. www.elsevier.com/locate/jdent

IIZUKA, J., KUNIMATSU, Y., MIKUNI-TAKAGAKI, Y., & MUKAI, Y. (2022). Evaluation of the mineral-promoting effects of in-office bleaching on experimental subsurface enamel lesions. *Dental Materials Journal*, *41*(4), 2021–2229. https://doi.org/10.4012/dmj.2021-229

Iizuka, J., MUKAI, Y., TANIGUCHI, M., MIKUNI-TAKAGAKI, Y., TEN CATE, J. M., & TERANAKA, T. (2014). Chemical alteration by tooth bleaching of human salivary proteins that infiltrated subsurface enamel lesions —Experimental study

UNIVERSITAS
GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

with bovine lesion model systems—. *Dental Materials Journal*, *33*(5), 663–668. https://doi.org/10.4012/dmj.2014-046

Irmaleny, I., Prisinda, D., & Susilo, M. (2023). Differences of Enamel Microhardness Post External Bleaching After Application with Casein Phosphopeptide Amorphous Phosphate (CPP-ACP) and 5% Sodium Fluoride (NAF). *The Open Dentistry Journal*, *17*(1). https://doi.org/10.2174/18742106-v17-e230216-2022-103

Jaha, H. S., Alhejoury, H. A., Fayad, A. A., Alnafisah, A. M., Bahshan, I. A., Assiri, S. I., & Alsubhi, A. S. (2021). Knowledge, Practices, and Perceptions about Tooth Whitening among Female Population in Saudi Arabia – A Cross-Sectional Study. *Journal of Pharmacy and Bioallied Sciences*, *13*(Suppl 1), S817–S820. https://doi.org/10.4103/jpbs.JPBS_769_20

Kalliath, C., Mukunda, A., Pynadath, M., Venugopal, V., & Prethweeraj, J. (2018a). Comparison between the effect of commercially available chemical teeth whitening paste and teeth whitening paste containing ingredients of herbal origin on human enamel. *AYU (An international quarterly journal of research in Ayurveda)*, *39*(2), 113. https://doi.org/10.4103/ayu.ayu_82_18

Khelef, A. E., Hadni, H., Gouzi, H., & Grama, B. S. (2024). Artemisia campestris L. as a promising source of potential antiviral drugs for SARS-CoV-2: Docking and dynamic simulation studies. *Scientific African*, *26*, e02445. https://doi.org/10.1016/j.sciaf.2024.e02445

Kim, S., Chen, J., Cheng, T., Gindulyte, A., He, J., He, S., Li, Q., Shoemaker, B. A., Thiessen, P. A., Yu, B., Zaslavsky, L., Zhang, J., & Bolton, E. E. (2021). PubChem in 2021: new data content and improved web interfaces. *Nucleic Acids Research*, *49*(D1), D1388–D1395. https://doi.org/10.1093/nar/gkaa971

Komatsu, T., Kobayashi, K., Morimoto, Y., Helmerhorst, E., Oppenheim, F., & Chang-il Lee, M. (2020). Direct evaluation of the antioxidant properties of salivary proline-rich proteins. *Journal of Clinical Biochemistry and Nutrition*, *67*(2), 131–136. https://doi.org/10.3164/jcbn.19-75

Kuban-Jankowska, A., Tuszynski, J. A., Winter, P., Gorska, M., Knap, N., & Wozniak, M. (2012). Activation of Hydrogen Peroxide to Peroxytetradecanoic Acid Is Responsible for Potent Inhibition of Protein Tyrosine Phosphatase CD45. *PLoS ONE*, *7*(12), e52495. https://doi.org/10.1371/journal.pone.0052495

Kury, M., Hiers, R. D., Zhao, Y. D., Picolo, M. Z. D., Hsieh, J., Khajotia, S. S., Esteban Florez, F. L., & Cavalli, V. (2022a). Novel Experimental In-Office Bleaching Gels Containing Co-Doped Titanium Dioxide Nanoparticles. *Nanomaterials*, *12*(17). https://doi.org/10.3390/nano12172995

UNIVERSITAS
GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Lee, J., Hao Nguyen, C., & Mamitsuka, H. (2025). Beyond rigid docking: deep learning approaches for fully flexible protein–ligand interactions. *Briefings in Bioinformatics*, *26*(5). https://doi.org/10.1093/bib/bbaf454

Li, J., Song, P., Wang, H., Lian, W., Li, J., Wang, Z., Zhang, Y., Cai, Q., Yang, H., & Cheng, M. (2025). Selectivity mechanism of inhibition towards Phosphodiesterase 1B and phosphodiesterase 10A in silico investigation. *Computational Biology and Chemistry*, *115*, 108322. https://doi.org/10.1016/j.compbiolchem.2024.108322

Li, K., Chen, S., Wang, J., Xiao, X., Song, Z., & Liu, S. (2024). Tooth whitening: current status and prospects. Dalam *Odontology* (Vol. 112, Nomor 3, hlm. 700–710). Springer. https://doi.org/10.1007/s10266-024-00914-4

Li, Q., Xu, B. T., Li, R., Yu, H., & Wang, Y. N. (2010). Quantitative evaluation of colour regression and mineral content change of bleached teeth. *Journal of Dentistry*, *38*(3), 253–260. https://doi.org/10.1016/j.jdent.2009.11.005

Liu, Y., Yang, X., Gan, J., Chen, S., Xiao, Z. X., & Cao, Y. (2022). CB-Dock2: improved protein-ligand blind docking by integrating cavity detection, docking and homologous template fitting. *Nucleic Acids Research*, *50*(W1), W159–W164. https://doi.org/10.1093/nar/gkac394

Lucio, F. N. M., Gomes, A. O. C. V., Bandeira, P. N., Ferreira, M. K. A., Ribeiro, W. H. F., Romão, I. C., Roberto, C. H. A., Marinho, M. M., Teixeira, A. M. R., Marinho, E. S., de Gomes, A. F. C., de Menezes, J. E. S. A., & dos Santos, H. S. (2025). Synthesis, characterization, anxiolytic and anticonvulsant activity, DFT, molecular docking, DMPK studies of chalcone derived from maleic anhydride. *Journal of Molecular Structure*, *1322*. https://doi.org/10.1016/j.molstruc.2024.140466

Luo, J., Wang, Y., Wang, K., Jiang, W., Li, X., & Zhang, L. (2020). Comparative proteomic analysis on acquired enamel pellicle at two time points in caries-susceptible and caries-free subjects. *Journal of Dentistry*, *94*, 103301. https://doi.org/10.1016/j.jdent.2020.103301

Mailart, M., Sakassegawa, P., Torres, C., Palo, R., & Borges, A. (2020). Assessment of Peroxide in Saliva During and After At-home Bleaching With 10% Carbamide and Hydrogen Peroxide Gels: A Clinical Crossover Trial. *Operative Dentistry*, *45*(4), 368–376. https://doi.org/10.2341/19-127-C

Makeneni, S., Thieker, D. F., & Woods, R. J. (2018). Applying Pose Clustering and MD Simulations To Eliminate False Positives in Molecular Docking. *Journal of chemical information and modeling*, *58*(3), 605–614. https://doi.org/10.1021/acs.jcim.7b00588

Mandal, M., & Mandal, S. (2024a). MM/GB(PB)SA integrated with molecular docking and ADMET approach to inhibit the fat-mass-and-obesity-associated protein using

UNIVERSITAS
GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

bioactive compounds derived from food plants used in traditional Chinese medicine. *Pharmacological Research - Modern Chinese Medicine*, *11*, 100435. https://doi.org/10.1016/j.prmcm.2024.100435

Maran, B. M., Matos, T. de P., de Castro, A. dos S., Vochikovski, L., Amadori, A. L., Loguercio, A. D., Reis, A., & Berger, S. B. (2020). In-office bleaching with low/medium vs. high concentrate hydrogen peroxide: A systematic review and meta-analysis. Dalam *Journal of Dentistry* (Vol. 103). Elsevier Ltd. https://doi.org/10.1016/j.jdent.2020.103499

Marin, L. M., Xiao, Y., Cury, J. A., & Siqueira, W. L. (2022). Modulation of Streptococcus mutans Adherence to Hydroxyapatite by Engineered Salivary Peptides. *Microorganisms*, *10*(2), 223. https://doi.org/10.3390/microorganisms10020223

Marques, C., Sotiles, A. R., Farias, F. O., Oliveira, G., Mitterer-Daltoé, M. L., & Masson, M. L. (2020). Full physicochemical characterization of malic acid: Emphasis in the potential as food ingredient and application in pectin gels. *Arabian Journal of Chemistry*, *13*(12), 9118–9129. https://doi.org/10.1016/j.arabjc.2020.10.036

Martis, E. A. F., & Téletchéa, S. (2025a). Ten quick tips to perform meaningful and reproducible molecular docking calculations. *PLoS computational biology*, *21*(5), e1013030. https://doi.org/10.1371/journal.pcbi.1013030

Matthews, C. J., Andrews, E. S. V., & Patrick, W. M. (2021). Enzyme-based amperometric biosensors for malic acid – A review. *Analytica Chimica Acta*, *1156*, 338218. https://doi.org/10.1016/j.aca.2021.338218

Melo, M., Fioresta, R., Sanz, J. L., Pecci-Lloret, M. P., & Llena, C. (2022). Effect of highly concentrated bleaching gels on enamel microhardness and superficial morphology, and the recovery action of four remineralizing agents. *BMC Oral Health*, *22*(1), 645. https://doi.org/10.1186/s12903-022-02693-2

Mena-Serrano, A., Sanchez, S., Granda-Albuja, M. G., Favoreto, M. W., Carneiro, T. de S., Cordeiro, D. C. F., Loguercio, A. D., & Reis, A. (2024). Hydrogen Peroxide in the Pulp Chamber and Color Change in Maxillary Anterior Teeth After In-Office Bleaching. *Brazilian Dental Journal*, *35*. https://doi.org/10.1590/0103-6440202405793

Mohamad Saberi, F. N., Sukumaran, P., Ung, N. M., & Liew, Y. M. (2022). Assessment of demineralized tooth lesions using optical coherence tomography and other state-of-the-art technologies: a review. Dalam *BioMedical Engineering Online* (Vol. 21, Nomor 1). BioMed Central Ltd. https://doi.org/10.1186/s12938-022-01055-x

Mohammadipour, H. S., Shokrollahi, P., Gholami, S., Bagheri, H., Namdar, F., & Sekandari, S. (2024). Do Different Tooth Bleaching-Remineralizing Regimens

UNIVERSITAS GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Affect the Bleaching Effectiveness and Enamel Microhardness In Vitro? *International journal of dentistry*, *2024*, 6893472. https://doi.org/10.1155/2024/6893472

Montaner, M., Sanz, J. L., Llena, C., Melo, M., Puig-Herreros, C., & Ghilotti, J. (2024). Cytotoxicity of Bleaching Products: A Systematic Review. *Applied Sciences*, *14*(9), 3680. https://doi.org/10.3390/app14093680

Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S., & Olson, A. J. (2009). AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. *Journal of Computational Chemistry*, *30*(16), 2785–2791. https://doi.org/10.1002/jcc.21256

Muchtaridi, & Y. M. (2018). *Teori dan Prakter Penambatan Molekul (Molecular Docking)*. Unpad Press.

Muhammad, S. (2022). Experimental studies on the pH levels that affect demineralization and remineralization of human tooth enamel. *Erbil Dental Journal*, *5*(1), 57–66. https://doi.org/10.15218/edj.202.8

Münchow, E. A., Távora, W. S., de Oliveira, H. T., & Machado, L. S. (2025). White diet is not necessary during dental bleaching treatment: A systematic review and network meta-analysis of clinical studies. *Journal of Dentistry*, *153*, 105459. https://doi.org/10.1016/j.jdent.2024.105459

Mutahar, M., O'Toole, S., Carpenter, G., Bartlett, D., Andiappan, M., & Moazzez, R. (2017). Reduced statherin in acquired enamel pellicle on eroded teeth compared to healthy teeth in the same subjects: An in-vivo study. *PLoS ONE*, *12*(8). https://doi.org/10.1371/journal.pone.0183660

Ortiz, C. L. D., Completo, G. C., Nacario, R. C., & Nellas, R. B. (2019). Potential Inhibitors of Galactofuranosyltransferase 2 (GlfT2): Molecular Docking, 3D-QSAR, and In Silico ADMETox Studies. *Scientific Reports*, *9*(1), 17096. https://doi.org/10.1038/s41598-019-52764-8

Owda, R., & Sancakli, H. S. (2021). Effects of Different Bleaching Agents on the Surface Topography and the Microhardness of Artificial Carious Lesions. *European Journal of Dentistry*, *15*(4), 687–693. https://doi.org/10.1055/s-0041-1728237

Pappa, E., Vougas, K., Zoidakis, J., Papaioannou, W., Rahiotis, C., & Vastardis, H. (2021b). Downregulation of Salivary Proteins, Protective against Dental Caries, in Type 1 Diabetes. *Proteomes*, *9*(3), 33. https://doi.org/10.3390/proteomes9030033

Pateel, D. G. S., Gunjal, S., & Dutta, S. (2022). Association of salivary statherin, calcium, and proline-rich proteins: A potential predictive marker of dental caries.

UNIVERSITAS GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Contemporary Clinical Dentistry, *13*(1), 84–89. https://doi.org/10.4103/ccd.ccd_859_20

Pettersen, E. F., Goddard, T. D., Huang, C. C., Couch, G. S., Greenblatt, D. M., Meng, E. C., & Ferrin, T. E. (2004). UCSF Chimera—A visualization system for exploratory research and analysis. *Journal of Computational Chemistry*, *25*(13), 1605–1612. https://doi.org/10.1002/jcc.20084

Piknjac, A., Soldo, M., Illeš, D., & Zlataric, D. K. (2021). Patients' assessments of tooth sensitivity increase one day following different whitening treatments. *Acta Stomatologica Croatica*, *55*(3), 280–290. https://doi.org/10.15644/asc55/3/5

Pini, N. I. P., Theobaldo, J. D., Lima, D. A. N. L., & Aguiar, F. H. B. (2019). Consumption of different energy beverages and oral health. Dalam *Sports and Energy Drinks: Volume 10: The Science of Beverages* (hlm. 441–481). Elsevier. https://doi.org/10.1016/B978-0-12-815851-7.00013-9

PS, S., Karumaran, C. S., R S, A., Manuel, C. E., V, J. C., & Stalin, R. (2024). An In Vitro Study on the Effects of Hydrogen Peroxide-Based Bleaching Agents on Enamel: Field Emission Scanning Electron Microscopy (FESEM) With Energy Dispersive Spectroscopy (EDS) Evaluation. *Cureus*. https://doi.org/10.7759/cureus.58318

Rahman, F., Tabrez, S., Ali, R., Alqahtani, A. S., Ahmed, M. Z., & Rub, A. (2021). Molecular docking analysis of rutin reveals possible inhibition of SARS-CoV-2 vital proteins. *Journal of Traditional and Complementary Medicine*, *11*(2), 173–179. https://doi.org/10.1016/j.jtcme.2021.01.006

Ramírez, D., & Caballero, J. (2018). Is It Reliable to Take the Molecular Docking Top Scoring Position as the Best Solution without Considering Available Structural Data? *Molecules (Basel, Switzerland)*, *23*(5). https://doi.org/10.3390/molecules23051038

Rathore, A., Alam, A., Riaz, M., Arshad, A., Javed, M., Fayyaz, F., & Chaudhry, S. (2021). Quantitative analysis of Protective Role of salivary protein on demineralization of enamel. *Pakistan Journal of Medical and Health Sciences*, *15*(8), 2457–2459. https://doi.org/10.53350/pjmhs211582457

Reis, F. N., Francese, M. M., Silva, N. D. G. da, Pelá, V. T., Câmara, J. V. F., Trevizol, J. S., Pieretti, J. C., Seabra, A. B., Pessan, J. P., Honório, H. M., Crusca, E., Marchetto, R., & Buzalaf, M. A. R. (2023). Gels containing statherin-derived peptide protect against enamel and dentin erosive tooth wear in vitro. *Journal of the Mechanical Behavior of Biomedical Materials*, *137*, 105549. https://doi.org/10.1016/j.jmbbm.2022.105549

UNIVERSITAS GADJAH MADA
ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Reynaldi, M. A., Faradilla, A., Nurbaeti, S. N., Ih, H., & Fajriaty, I. (2023). JOURNAL PHARMACY OF TANJUNGPURA MOLECULAR DOCKING SENYAWA PADA KOMPOSISI CINCALOK TERHADAP RESEPTOR PLASMODIUM FALCIPARUM DIHYDROOROTATE DEHYDROGENASE MOLECULAR DOCKING COMPOUNDS IN CINCALOK COMPOSITION AGAINST THE PLASMODIUM FALCIPARUM DIHYDROOROTATE DEHYDROGENASE RECEPTOR. Dalam *JPOP* (Vol. 1). https://jurnal.untan.ac.id/index.php/JPOP

Romero, M. J. R. H., Nakashima, S., Nikaido, T., Sadr, A., & Tagami, J. (2016). In vitro dentine remineralization with a potential salivary phosphoprotein homologue. *Archives of Oral Biology*, *68*, 35–42. https://doi.org/10.1016/j.archoralbio.2016.03.014

Rotstein, I., & Ingle, J. I. (2019). *Ingle's ENDODONTICS 7*. PMPH USA, Ltd.

Sadashivappa Pateel, D. G., Gunjal, S., & Dutta, S. (2022). Association of Salivary Statherin, Calcium, and Proline-Rich Proteins. *Contemporary Clinical Dentistry*, *13*(1), 84–89. https://doi.org/10.4103/ccd.ccd_859_20

Satish Chandra, Shaleen Chandra, & Girish Chandra. (2007). *Textbook of Operative Dentistry*. JAYPEE BROTHERS MEDICAL PUBLISHERS (P) LTD New Delhi.

Shah, S. (t.t.). *Statherin-Role in Biomimetic Early Caries Management*.

Shahzadi, Z., Yousaf, Z., Anjum, I., Bilal, M., Yasin, H., Aftab, A., Booker, A., Ullah, R., & Bari, A. (2024). Network pharmacology and molecular docking: combined computational approaches to explore the antihypertensive potential of Fabaceae species. *Bioresources and Bioprocessing*, *11*(1), 53. https://doi.org/10.1186/s40643-024-00764-6

Shayegan, A., Vozza, I., Bossù, M., & Malikzade, N. (2024). Impact of Exposure to Commonly Used Carbamide Peroxide on Dental Pulp Stem Cells. *Applied Sciences*, *14*(11), 4412. https://doi.org/10.3390/app14114412

Shraberg, J., Rick, S. W., Rannulu, N., & Cole, R. B. (2015). A study of procyanidin binding to Histatin 5 using Electrospray Ionization Tandem Mass Spectrometry (ESI-MS/MS) and molecular simulations. *Physical Chemistry Chemical Physics*, *17*(18), 12247–12258. https://doi.org/10.1039/C4CP05586A

Singh, S. V., Vidyapeeth, B., Mandlik, J., Sharma, P., Singh, S., Majumder, H., Kadam, M., & Dhawan, S. (t.t.). Evaluation of the effect of anticay application on enamel microhardness of teeth bleached with two different agents: an in-vitro study Section A-Research paper Evaluation of the effect of anticay application on enamel microhardness of teeth bleached with two different agents: an in-vitro study EVALUATION OF THE EFFECT OF ANTICAY APPLICATION ON ENAMEL MICROHARDNESS OF TEETH BLEACHED WITH TWO DIFFERENT

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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

AGENTS: AN IN-VITRO STUDY. *Eur. Chem. Bull*, *2023*(S2), 374–382. https://doi.org/10.31838/ecb/2023.12.s2.051

Soares, S., García-Estévez, I., Ferrer-Galego, R., Brás, N. F., Brandão, E., Silva, M., Teixeira, N., Fonseca, F., Sousa, S. F., Ferreira-da-Silva, F., Mateus, N., & de Freitas, V. (2018). Study of human salivary proline-rich proteins interaction with food tannins. *Food Chemistry*, *243*, 175–185. https://doi.org/10.1016/j.foodchem.2017.09.063

Sun, W., Ma, D., Bolscher, J. G. M., Nazmi, K., Veerman, E. C. I., Bikker, F. J., Sun, P., Lin, H., & Wu, G. (2020). Human Salivary Histatin-1 Promotes Osteogenic Cell Spreading on Both Bio-Inert Substrates and Titanium SLA Surfaces. *Frontiers in Bioengineering and Biotechnology*, *8*. https://doi.org/10.3389/fbioe.2020.584410

Sürmelioğlu, D., Gündoğar, H., Taysi, S., & Bağiş, Y. (2021). Effect of different bleaching techniques on DNA damage biomarkers in serum, saliva, and GCF. *Human & Experimental Toxicology*, *40*(8), 1332–1341. https://doi.org/10.1177/0960327121996030

Taira, E. A., Ferrari, C. R., Carvalho, G., Pelá, V. T., Ventura, T. M. O., Crusca, E., Marchetto, R., & Buzalaf, M. A. R. (2024). Statherin-Derived Peptide Protects against Intrinsic Erosive Enamel Wear in situ. *Caries Research*, 1–6. https://doi.org/10.1159/000541403

Tolosa, J., Barba, F. J., Pallarés, N., & Ferrer, E. (2020). Mycotoxin Identification and In Silico Toxicity Assessment Prediction in Atlantic Salmon. *Marine Drugs*, *18*(12), 629. https://doi.org/10.3390/md18120629

Tomer, A. K., Khandelwal, A., Mushtaq, H., Cecelia, L. L., Singh, S., Jain, S., & Kanika. (2021). BLEACHING WITH 37.5% HYDROGEN PEROXIDE-A CASE REPORT. *International Journal of Medical Science And Diagnosis Research*, *5*(6). https://doi.org/10.32553/ijmsdr.v5i6.823

Torres-Rochera, B., Manjón, E., Escribano-Bailón, M. T., & García-Estévez, I. (2023). Role of Anthocyanins in the Interaction between Salivary Mucins and Wine Astringent Compounds. *Foods*, *12*(19), 3623. https://doi.org/10.3390/foods12193623

Usman, S., You, Y., & Waseem, A. (2025). Exploring the Healing Powers of Histatins: From Oral Health to Therapeutics. *International Journal of Molecular Sciences*, *26*(11), 5019. https://doi.org/10.3390/ijms26115019

Ventura, T. M. O., Buzalaf, M. A. R., Baumann, T., Pelá, V. T., Niemeyer, S. H., Crusca, E., Marchetto, R., Lussi, A., & Carvalho, T. S. (2023). New insights into the protective effect of statherin-derived peptide for different acquired enamel pellicle

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ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

formation times on the native human enamel surfaces. *Archives of Oral Biology*, *148*, 105643. https://doi.org/10.1016/j.archoralbio.2023.105643

Vittorio, S., Lunghini, F., Morerio, P., Gadioli, D., Orlandini, S., Silva, P., Jan Martinovic, Pedretti, A., Bonanni, D., Del Bue, A., Palermo, G., Vistoli, G., & Beccari, A. R. (2024). Addressing docking pose selection with structure-based deep learning: Recent advances, challenges and opportunities. *Computational and Structural Biotechnology Journal*, *23*, 2141–2151. https://doi.org/10.1016/j.csbj.2024.05.024

Wade, R. C., & Goodford, P. J. (1989). The role of hydrogen-bonds in drug binding. *Progress in clinical and biological research*, *289*, 433–444.

Wang, K., Zhou, X., Li, W., & Zhang, L. (2019). Human salivary proteins and their peptidomimetics: Values of function, early diagnosis, and therapeutic potential in combating dental caries. Dalam *Archives of Oral Biology* (Vol. 99, hlm. 31–42). Elsevier Ltd. https://doi.org/10.1016/j.archoralbio.2018.12.009

Wu, N., Zhang, R., Peng, X., Fang, L., Chen, K., & Jestilä, J. S. (2024). Elucidation of protein–ligand interactions by multiple trajectory analysis methods. *Physical Chemistry Chemical Physics*, *26*(8), 6903–6915. https://doi.org/10.1039/D3CP03492E

Wu, Y., & Yue, S. (2024). Network pharmacology unveils the active components and potential mechanism of traditional efficacy of Mugua. *Medicine (United States)*, *103*(51), e41028. https://doi.org/10.1097/MD.0000000000041028

Xiong, G., Wu, Z., Yi, J., Fu, L., Yang, Z., Hsieh, C., Yin, M., Zeng, X., Wu, C., Lu, A., Chen, X., Hou, T., & Cao, D. (2021). ADMETlab 2.0: An integrated online platform for accurate and comprehensive predictions of ADMET properties. *Nucleic Acids Research*, *49*(W1), W5–W14. https://doi.org/10.1093/nar/gkab255

Xu, M., Shen, C., Yang, J., Wang, Q., & Huang, N. (2022a). Systematic Investigation of Docking Failures in Large-Scale Structure-Based Virtual Screening. *ACS Omega*, *7*(43), 39417–39428. https://doi.org/10.1021/acsomega.2c05826

Yu, O. Y., Zhao, I. S., Mei, M. L., Lo, E. C. M., & Chu, C. H. (2017). A review of the common models used in mechanistic studies on demineralization-remineralization for cariology research. Dalam *Dentistry Journal* (Vol. 5, Nomor 2). MDPI AG. https://doi.org/10.3390/dj5020020

Zeczkowski, M., Tenuta, L. M. A., Ambrosano, G. M. B., Aguiar, F. H. B., & Lima, D. A. N. L. (2015). Effect of different storage conditions on the physical properties of bleached enamel: An in vitro vs. in situ study. *Journal of Dentistry*, *43*(9), 1154–1161. https://doi.org/10.1016/j.jdent.2015.06.004

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ANALISIS ENERGI PENGIKATAN ASAM MALAT SEBAGAI BAHAN BLEACHING TERHADAP PROTEIN SALIVA PADA DEMINERALISASI EMAIL (Kajian In Silico)
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Universitas Gadjah Mada, 2026 | Diunduh dari http://etd.repository.ugm.ac.id/

Zhang, L., Pan, J., & Zhang, J. (2022). Integrated two-phase free radical hydrogel: Safe, ultra-fast tooth whitening and antibacterial activity. *Journal of Materials Science and Technology*, *100*, 59–66. https://doi.org/10.1016/j.jmst.2021.05.029

Zhang, Y., Chen, Y., Chen, C., Zhu, Y., Liu, M., & Chen, J. (2024). The enhancement mechanisms of mucin and lactoferrin on α-amylase activity in saliva: Exploring the interactions using QCM-D and molecular docking. *International Journal of Biological Macromolecules*, *257*. https://doi.org/10.1016/j.ijbiomac.2023.128710

Zheng, L., Meng, J., Jiang, K., Lan, H., Wang, Z., Lin, M., Li, W., Guo, H., Wei, Y., & Mu, Y. (2022). Improving protein–ligand docking and screening accuracies by incorporating a scoring function correction term. *Briefings in Bioinformatics*, *23*(3). https://doi.org/10.1093/bib/bbac051