Documents

Tze Lin, K.[a] , Mahat, N.A.[a b c] , Azman, A.R.[a b] , Wahab, R.A.[a b] , Oyewusi, H.A.[a b] , Abdul Hamid, A.A.[d e]

Interaction of the nanobio-based reagent with sodium fluorescein and lipids via bioinformatics for forensic fingerprint visualisations

(2023) *Journal of Biomolecular Structure and Dynamics*, .

DOI: 10.1080/07391102.2023.2186709

[a] Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, Johor, Skudai, Malaysia
[b] Enzyme Technology and Green Synthesis Research Group, Faculty of Science, Universiti Teknologi Malaysia, Johor, Skudai, Malaysia
[c] Centre for Sustainable Nanomaterials, Ibnu Sina Institute for Scientific and Industrial Research, Universiti Teknologi Malaysia, Johor, Skudai, Malaysia
[d] Department of Biotechnology, Kuliyyah of Science, International Islamic University Malaysia, Kuantan, Bandar Indera Mahkota, Malaysia
[e] Research Unit for Bioinformatics and Computational Biology (RUBIC), Kulliyyah of Science, International Islamic University Malaysia, Pahang, Kuantan, Malaysia

Abstract
Being commonly found at crime scenes, fingerprints are crucial for human identification, attributable to their uniqueness, persistence and systematic classification of ridge patterns. In addition to latent fingerprints being invisible to the naked eye, the escalating trends of disposing forensic evidence bearing such prints in watery bodies would further complicate criminal investigations. Taking into account the toxicity of small particle reagent (SPR) commonly used in visualising latent fingerprints on wet and non-porous objects, a greener alternative using the nanobio-based reagent (NBR) has been suggested. However, NBR only applies to white and/or relatively light-coloured objects. Thus, conjugation of sodium fluorescein dye with NBR (f-NBR) may be beneficial for increasing the contrast of fingerprint on multi-colored objects. Hence, this study was aimed at investigating the possibility of such conjugation (i.e., f-NBR) as well as proposing suitable interactions between the f-NBR and lipid constituents of fingerprints (tetra-, hexa- and octadecanoic acids) via molecular docking and molecular dynamics simulations. The binding energies between CRL with its ligands were observed at −8.1, −5.0, −4.9 and −3.6 kcal/mole for sodium fluorescein, tetra-, hexa- and octadecanoic acids, respectively. Besides, the formations of hydrogen bonds observed in all complexes (ranged between 2.6 and 3.4 Å), further supported by the stabilized root mean square deviation (RMSDs) plots in MD simulations. In short, the conjugation of f-NBR was computationally feasible, and thereby merits further investigations in the laboratory. Communicated by Ramaswamy H. Sarma.

Author Keywords
Candida rugosa lipase; Latent fingerprints; nanobio-based reagent; sodium fluorescein; structural bioinformatics

References

- Abdul Wahab, R., Puspanadan, J.K., Mahat, N.A., Azman, A.R., Ismail, D.
  Potassium triiodide enhanced multi-walled carbon nanotubes supported lipase for expediting a greener forensic visualization of wetted fingerprints
  (2021) *Chemical Papers*, 75 (4), pp. 1401-1412.
- Acharya, V., Arutselvan, R., Pati, K., Rout, A.K., Dehury, B., Chauhan, V.B.S., Nedunchezhiyan, M.
  Structural insights into the RNA interaction with Yam bean Mosaic virus (coat protein) from Pachyrhizus erosus using bioinformatics approach
  (2022) *PLoS One*, 17 (7).
- Alsolmy, E., Abdelwahab, W.M., Martinez, V., Henary, M., Patonay, G.
  Investigation of benzophenoxazine derivatives for the detection of latent

fingerprints on porous surfaces
(2020) *Journal of Photochemistry and Photobiology A: Chemistry*, 392, p. 112416.

- Azman, A.R., Mahat, N.A., Abdul Wahab, R., Abdul Razak, F.I., Hamzah, H.H.
Novel safranin-tinted Candida rugosa lipase nanoconjugates reagent for visualizing latent fingerprints on stainless steel knives immersed in a natural outdoor pond
(2018) *International Journal of Molecular Sciences*, 19 (6), p. 1576.

- Azman, A.R., Mahat, N.A., Abdul Wahab, R., Ahmad, W.A., Mohamed Huri, M.A., Abdul Hamid, A.A., Adamu, A., Mat Saat, G.A.
Characterisation and computational analysis of a novel lipase nanobio-based reagent for visualising latent fingerprints on water-immersed glass slides
(2020) *Process Biochemistry*, 96, pp. 102-112.

- Azman, A.R., Zulkifli, N., Mahat, N.A., Ahmad, W.A., Hamzah, H.H., Wahab, R.A.
Visualisation of latent fingerprints on non-porous object immersed in stagnant tap water using safranin-tinted Candida rugosa lipase reagent
(2019) *Malay Journal of Fundamental and Applied Sciences*, 15 (6), pp. 781-783.

- Bahaman, A.H., Wahab, R.A., Abdul Hamid, A.A., Abd Halim, K.B., Kaya, Y.
Molecular docking and molecular dynamics simulations studies on β-glucosidase and xylanase Trichoderma asperellum to predict degradation order of cellulosic components in oil palm leaves for nanocellulose preparation
(2021) *Journal of Biomolecular Structure & Dynamics*, 39 (7), pp. 2628-2641.

- Bayramoglu, G., Celikbicak, O., Kilic, M., Yakup Arica, M.
Immobilization of Candida rugosa lipase on magnetic chitosan beads and application in flavor esters synthesis
(2022) *Food Chemistry*, 366, p. 130699.

- Becker, R.F., Nordby, S.H., Jon, J.
(2013) *Underwater forensic investigation*,
CRC Press

- Berg, J.M., Tymoczko, J.L., Stryer, L.
(2002) *Biochemistry*,
WH Freeman

- Cavalcanti, E.D., Aguieiras, É.C., da Silva, P.R., Duarte, J.G., Cipolatti, E.P., Fernandez-Lafuente, R., da Silva, J.A.C., Freire, D.M.
Improved production of biolubricants from soybean oil and different polyols via esterification reaction catalyzed by immobilized lipase from Candida rugosa
(2018) *Fuel*, 215, pp. 705-713.

- Chakraborty, H.J., Rout, A.K., Behera, B.K., Parhi, J., Parida, P.K., Das, B.K.
Insights into the aquaporin 4 of zebrafish (Danio rerio) through evolutionary analysis, molecular modeling and structural dynamics
(2018) *Gene Reports*, 11, pp. 101-109.

- Delgado-García, M., Rodríguez, J.A., Mateos-Díaz, J.C., Aguilar, C.N., Rodríguez-Herrera, R., Camacho-Ruíz, R.M.
Halophilic archaeal lipases and esterases: Activity, stability, and food applications
(2018) *Enzymes in Food Technology: Improvements and Innovations*, pp. 243-262.
Kuddus M., (ed), Springer Nature Singapore, &,. (Ed

- Eldridge, S.
  Every contact leaves a trace
  (2017) *Investigating trace evidence*, pp. 9-18.
  In, (). Retrieved from

- Girod, A., Weyermann, C.
  Lipid composition of fingermark residue and donor classification using GC/MS
  (2014) *Forensic Science International*, 238, pp. 68-82.

- Goguet, M., Narwani, T.J., Petermann, R., Jallu, V., de Brevern, A.G.
  In silico analysis of Glanzmann variants of Calf-1 domain of α IIb β 3 integrin revealed dynamic allosteric effect
  (2017) *Scientific Reports*, 7 (1), pp. 1-13.

- Gray, T., Matthews, B.
  Intrahelical hydrogen bonding of serine, threonine and cysteine residues within α-helices and its relevance to membrane-bound proteins
  (1984) *Journal of Molecular Biology*, 175 (1), pp. 75-81.

- Harris, H.A., Lee, H.C.
  Fingerprints and other personal identification patterns
  (2019) *Introduction to forensic science and criminalistics*, pp. 117-142.
  2nd, CRC Press, &,. ed

- (2010) *IARC monographs on the evaluation of carcinogenic risks to humans*,
  International Agency for Research on Cancer

- Jityuti, B., Kuno, M., Liwporncharoenvong, T., Buranaprapuk, A.
  Selective protein photocleavage by fluorescein derivatives
  (2020) *Journal of Photochemistry and Photobiology. B, Biology*, 212, p. 112027.

- Joshi, T., Sharma, P., Joshi, T., Pundir, H., Mathpal, S., Chandra, S.
  Structure-based screening of novel lichen compounds against SARS Coronavirus main protease (Mpro) as potentials inhibitors of COVID-19
  (2021) *Molecular Diversity*, 25 (3), pp. 1665-1677.

- Liu, Y.-Y., Harbison, S.
  A review of bioinformatic methods for forensic DNA analyses
  (2018) *Forensic Science International. Genetics*, 33, pp. 117-128.

- Ma, M., Guan, P., Mukerabigwi, J.F., Yan, F., Chen, D., Sun, Y., Huang, X., Cao, Y.
  Nanodiamond conjugated fluorescein through ethylenediamine linker for cellular biomarking
  (2021) *Diamond and Related Materials*, 118, p. 108546.

- **Safety Data Sheet (C.I. 45350) 103887 Fluorescein sodium- indicator Reagent**
  (2021) *Darmstadt*,
  Merck,. In

- Morris, G.M., Huey, R., Lindstrom, W., Sanner, M.F., Belew, R.K., Goodsell, D.S., Olson, A.J.
  AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility
  (2009) *Journal of Computational Chemistry*, 30 (16), pp. 2785-2791.

- Motz, R.T., Tanksley, P., Liu, H., Mersha, T.B., Barnes, J.C.
Every contact leaves a trace: Contact with the criminal justice system, life outcomes, and the intersection with genetics
(2019) *Current Opinion in Psychology*, 27, pp. 82-87.

- O'Boyle, N.M., Banck, M., James, C.A., Morley, C., Vandermeersch, T., Hutchison, G.R.
Open Babel: An open chemical toolbox
(2011) *Journal of Cheminformatics*, 3 (1), p. 33.

- Oyewusi, H.A., Huyop, F., Wahab, R.A.
Molecular docking and molecular dynamics simulation of Bacillus thuringiensis dehalogenase against haloacids, haloacetates and chlorpyrifos
(2020) *Journal of Biomolecular Structure and Dynamics*, 40 (5), pp. 1979-1994.

- Ozyilmaz, E., Caglar, O., Sargin, I., Arslan, G.
Synergistic role of carbon quantum dots in the activity and stability of Candida rugosa lipase encapsulated within metal–organic frameworks (ZIF-8)
(2022) *Materials Today Communications*, 30, p. 103066.

- Ramharack, P., Soliman, M.E.S.
Bioinformatics-based tools in drug discovery: The cartography from single gene to integrative biological networks
(2018) *Drug Discovery Today*, 23 (9), pp. 1658-1665.

- Raschka, S., Wolf, A.J., Bemister-Buffington, J., Kuhn, L.A.
Protein–ligand interfaces are polarized: discovery of a strong trend for intermolecular hydrogen bonds to favor donors on the protein side with implications for predicting and designing ligand complexes
(2018) *Journal of Computer-Aided Molecular Design*, 32 (4), pp. 511-528.

- Rout, A.K., Acharya, V., Maharana, D., Dehury, B., Udgata, S.R., Jena, R., Behera, B., Behera, B.K.
Insights into structure and dynamics of extracellular domain of Toll-like receptor 5 in Cirrhinus mrigala (mrigala): A molecular dynamics simulation approach
(2021) *PLoS One*, 16 (1).

- Said, N.F.N., Abd. Rahman, N.S., Othman, P.J., Zakaria, Y., Nik Hassan, N.F.
Recovery of latent fingermarks on metal part of motorcycle submerged in different aquatic environments
(2021) *Sains Malaysiana*, 50 (8), pp. 2343-2354.

- Sampath, C., Belur, P.D., Iyyasami, R.
Enhancement of n-3 polyunsaturated fatty acid glycerides in Sardine oil by a bioimprinted cross-linked Candida rugosa lipase
(2018) *Enzyme and Microbial Technology*, 110, pp. 20-29.

- Schrödinger, L., DeLano, W.
(2020), Pymol. The PyMOL Molecular Graphics System, Version, 2

- (2020) *Safety Data Sheet SPR400UV small particle reagent- fluorescent*, Sirchie

- Su, L., Wu, R., Chen, X., Hou, W., Ruan, B.H.
FITC-labeled d-glucose analog is suitable as a probe for detecting insulin-dependent glucose uptake
(2018) *Bioorganic & Medicinal Chemistry Letters*, 28 (22), pp. 3560-3563.

- Subroto, E., Indiarto, R., Pangawikan, A., Huda, S., Yarlina, V.
  Characteristics, immobilization, and application of Candida rugosa lipase
  (2020) *Food Research*, 4 (5), pp. 1391-1401.

- Sufyan, M., Ali Ashfaq, U., Ahmad, S., Noor, F., Hamzah Saleem, M., Farhan Aslam, M., El-Serehy, H.A., Aslam, S.
  Identifying key genes and screening therapeutic agents associated with diabetes mellitus and HCV-related hepatocellular carcinoma by bioinformatics analysis
  (2021) *Saudi Journal of Biological Sciences*, 28 (10), pp. 5518-5525.

- Ting, C.W., Mahat, N.A., Azman, A.R., Muda, N.W., Anuar, N.
  Performance of the nanobio-based reagent for visualising wet fingerprints exposed to different levels of water salinity
  (2021) *Journal of Clinical and Health Sciences*, 6 (1Special), pp. 32-43.

- Tran, Q.-H., Nguyen, Q.-T., Vo, N.-Q.-H., Mai, T.T., Tran, T.-T.-N., Tran, T.-D., Le, M.-T., Thai, K.-M.
  Structure-based 3D-Pharmacophore modeling to discover novel interleukin 6 inhibitors: An in silico screening, molecular dynamics simulations and binding free energy calculations
  (2022) *PLoS One*, 17 (4).

- Trott, O., Olson, A.J.
  AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading
  (2010) *Journal of Computational Chemistry*, 31 (2), pp. 455-461.

- Tsang, M.-W., Leung, Y.-C., Wong, K.-Y.
  Rational design and construction of active-site labeled enzymes
  (2021) *Structural genomics*, pp. 13-22.
  Springer, &

- Win, K.N., Li, K., Chen, J., Viger, P.F., Li, K.
  Fingerprint classification and identification algorithms for criminal investigation: A survey
  (2020) *Future Generation Computer Systems*, 110, pp. 758-771.

- Yuan, C., Li, M., Wang, M., Cao, H., Lin, T.
  A critical review of fundamentals and applications of electrochemical development and imaging of latent fingerprints
  (2021) *Electrochimica Acta*, 390, p. 138798.

- Zhu, B., Ren, G., Tang, M., Chai, F., Qu, F., Wang, C., Su, Z.
  Fluorescent silicon nanoparticles for sensing Hg²⁺ and Ag⁺ as well visualization of latent fingerprints
  (2018) *Dyes and Pigments*, 149, pp. 686-695.

Correspondence Address
Mahat N.A.; Department of Chemistry, Johor, Malaysia; email: naji.arafat@utm.my
Azman A.R.; Department of Chemistry, Johor, Malaysia; email: aidarasyidah@utm.my

Publisher: Taylor and Francis Ltd.

ISSN: 07391102
CODEN: JBSDD
PubMed ID: 36880661
Language of Original Document: English

Abbreviated Source Title: J. Biomol. Struct. Dyn.
2-s2.0-85150455571
Document Type: Article
Publication Stage: Article in Press
Source: Scopus