Data Article

The data on molecular docking of cinnamic acid amide on dengue viral target NS2B/NS3

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\textbf{A R T I C L E  I N F O}

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\textbf{A B S T R A C T}

A natural occurring class compound, cinnamic acid is composed of a benzene ring, an alkene double bond and an acrylic acid functional group. Due to the feasibility of its structure modifications with a variety of compounds, cinnamic acids have been actively explored to improve their biological efficacy. Cinnamic acid derivatives have been reported to exhibit an antimicrobial property. Despite the beneficial properties of cinnamic acid derivatives, the antiviral activity of the amide derivatives especially against the dengue virus is poorly defined. Herein, the cinnamic amide derivatives were evaluated for their potential as an anti-dengue virus through the \textit{in-silico} analysis of the derivatives. This data aimed to analyze the interactions of the derivatives against the non-structural protein of viral target, dengue virus type 2 (DENV-2) NS2B/N3. The evaluation was based on binding affinity, interaction type (bond type and distance) and interaction with amino acids. Three derivatives (CAA15, CAA16 and CAA17) with the best docking score were reported. Enhanced understanding of the interaction acquired from this analysis provide a useful information on for the

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Specifications Table

| Subject | Chemistry |
|---------|-----------|
| Specific subject area | Molecular docking |
| Type of data | Table |
| | Image |
| | Figure |
| How data were acquired | Molecular docking (AutoDock 4.2), ChemDraw Professional 16.0, OpenBabel GUI, Discovery Studio 2020 Client. |
| Data format | Raw |
| | Analyzed |
| Parameters for data collection | Docking score and interaction of the ligand with amino acid residues in the binding pocket |
| Description of data collection | The structure of cinnamic amide derivatives was constructed and energy minimized using ChemDraw software. The minimized structures were docked on selected anti-viral targets using AutoDock software. |
| Data source location | Institution: Universiti Malaysia Terengganu |
| | City/Town/Region: Kuala Nerus, Kuala Terengganu |
| | Country: Terengganu |
| Data accessibility | Tables and Figures of the docking are accessible in the article. Molecular docking files for Figure 2–4 are available at https://data.mendeley.com/datasets/838gm89sr2/1.
| | doi: 10.17632/838gm89sr2.1 |

Value of the Data

- The data provide on the interaction between cinnamic amide derivatives with the viral target NS2B/NS3 protease (NS2B/NS3pro) protein.
- The in-silico analysis of the antiviral properties of cinnamic amide derivatives may indicate the direction for future research in the field of anti-dengue therapy.
- The screening data help minimized research time considerably by enable the researchers to rapidly identify promising compounds and its interaction with the viral target.
- The data are useful for research scholars with insufficient software and hardware requirements which not affordable by them.
- The data can facilitate on the direction of the functional design of cinnamic amide derivatives specifically to target dengue virus infection.

1. Data Description

The predominant circulating dengue virus (DENV) serotype is dengue virus type 2 (DENV-2). Although many research have been conducted in finding an effective antiviral against it, there is still no specific treatment currently available [1]. Nonetheless, there is emerging interest in development of an effective inhibitor against the NS2b/NS3 serine protease which responsible for seven different polyprotein cleavages in the virus life cycle [2]. Cinnamic acid (Fig. 1) occur in all green plant and is known for their various biological activities [3,4]. The provided docking data
of 30 cinnamic amide derivatives against DENV-2 may be useful to develop new drug candidates for the treatment of DENV infections. In this article, Table 1 provides the details of the viral target (as retrieved from Wichapong et al [5].), Table 2 provides the structure of cinnamic amide derivatives, while the free binding energy, interaction type and bond length of the docking are shown in Table 3. The 3D interaction of the top 3 best-docked compounds with the target are shown in Figs. 2–4. The selection was made based on the lowest free binding energy with the highest number of Hydrogen bonding.
Table 2
List of cinnamic acids and cinnamic amide derivatives.

| No. | Ligand | Structure |
|-----|--------|-----------|
| 1.  | CAA01  | ![Structure 1](image1) |
| 2.  | CAA02  | ![Structure 2](image2) |
| 3.  | CAA03  | ![Structure 3](image3) |
| 4.  | CAA04  | ![Structure 4](image4) |
| 5.  | CAA05  | ![Structure 5](image5) |
| 6.  | CAA06  | ![Structure 6](image6) |
| 7.  | CAA07  | ![Structure 7](image7) |

(continued on next page)
Table 2 (continued)

| No. | Ligand | Structure |
|-----|--------|-----------|
| 8.  | CAA08  | ![Structure image](image_url1) |
| 9.  | CAA09  | ![Structure image](image_url2) |
| 10. | CAA10  | ![Structure image](image_url3) |
| 11. | CAA11  | ![Structure image](image_url4) |
| 12. | CAA12  | ![Structure image](image_url5) |
| 13. | CAA13  | ![Structure image](image_url6) |
| 14. | CAA14  | ![Structure image](image_url7) |

(continued on next page)
| No.  | Ligand | Structure |
|-----|--------|-----------|
| 15. | CAA15  | ![Structure of CAA15](image1) |
| 16. | CAA16  | ![Structure of CAA16](image2) |
| 17. | CAA17  | ![Structure of CAA17](image3) |
| 18. | CAA18  | ![Structure of CAA18](image4) |
| 19. | CAA19  | ![Structure of CAA19](image5) |
| 20. | CAA20  | ![Structure of CAA20](image6) |

(continued on next page)
Table 2 (continued)

| No. | Ligand | Structure |
|-----|--------|-----------|
| 21. | CAA21  | ![Structure 21](image) |
| 22. | CAA22  | ![Structure 22](image) |
| 23. | CAA23  | ![Structure 23](image) |
| 24. | CAA24  | ![Structure 24](image) |
| 25. | CAA25  | ![Structure 25](image) |
| 26. | CAA26  | ![Structure 26](image) |

(continued on next page)
Table 2 (continued)

| No. | Ligand | Structure |
|-----|--------|-----------|
| 27. | CAA27  | ![CAA27](image1) |
| 28. | CAA28  | ![CAA28](image2) |
| 29. | CAA29  | ![CAA29](image3) |
| 30. | CAA30  | ![CAA30](image4) |

Fig. 3. The 3D interaction of compound CAA16 (FEB: −7.03) against viral target NS2B/NS3pro.
### Table 3
Cinnamic amide derivatives and their interactions.

| Sr. No. | Ligand    | Free Binding energy, FEB (kcal/mol) | Interaction | Type of interaction | Bond distance (Å) |
|---------|-----------|------------------------------------|-------------|--------------------|------------------|
| 1.      | CAA01     | −6.66                              | ILE B:36    | π-Alkyl            | 4.94             |
|         |           |                                    | VAL B:52    | π-Alkyl            | 5.24             |
|         |           |                                    | ASP B:129   | Carbon H-Bond      | 3.01             |
|         |           |                                    | PHE B:130   | H-Bond             | 2.71             |
|         |           |                                    | PRO B:132   | H-Bond             | 2.18             |
|         |           |                                    | TYR B:161   | π-π Stacked        | 5.62             |
|         |           |                                    |             | π-Sigma            | 3.66             |
| 2.      | CAA02     | −6.56                              | ILE B:36    | π-Alkyl            | 5.28             |
|         |           |                                    | VAL B:52    | π-Alkyl            | 2.89             |
|         |           |                                    | HIS B:51    | H-Bond             | 2.08             |
|         |           |                                    | SER B:135   | H-Bond             | 1.90             |
|         |           |                                    | TYR B:150   | π-Alkyl            | 4.82             |
| 3.      | CAA03     | −6.60                              | ILE B:36    | Alkyl              | 3.94             |
|         |           |                                    | VAL B:52    | π-Alkyl            | 5.27             |
|         |           |                                    | PRO B:132   | H-Bond             | 1.98             |
| 4.      | CAA04     | −6.45                              | ILE B:36    | Alkyl              | 3.83             |
|         |           |                                    | VAL B:52    | π-Alkyl            | 5.39             |
|         |           |                                    | PRO B:132   | H-Bond             | 2.00             |
| 5.      | CAA05     | −6.85                              | ARG B:54    | 3 H-Bonds          | 1.75, 2.37, 2.63 |
|         |           |                                    | PRO B:132   | H-Bond             | 2.51             |
|         |           |                                    | TYR B:150   | π-Alkyl            | 5.22             |
|         |           |                                    | TYR B:161   | π-Alkyl            | 5.17             |
| 6.      | CAA06     | −6.01                              | HIS B:51    | Carbon H-Bond      | 3.26             |
|         |           |                                    | ASP B:75    | Pi-Anion           | 3.28             |
|         |           |                                    | SER A:83    | Carbon H-Bond      | 3.07             |
|         |           |                                    | MET A:84    | H-Bond             | 1.95             |
|         |           |                                    | ASN B:152   | 2 H-Bonds          | 1.78, 2.00       |
|         |           |                                    | GLY B:153   | Pi-Donor H-Bond    | 3.07             |
| 7.      | CAA07     | −6.66                              | TRP B:50    | π-Alkyl            | 5.07             |
|         |           |                                    | VAL B:72    | Alkyl              | 4.77             |
|         |           |                                    | ILE A:86    | Alkyl              | 4.06             |
|         |           |                                    | GLY B:153   | H-Bond             | 2.05             |
|         |           |                                    | VAL B:154   | π-Sigma            | 3.72             |
|         |           |                                    |               | Alkyl              | 4.16             |
|         |           |                                    | VAL B:155   | H-Bond             | 1.91             |
|         |           |                                    |             | π-Alkyl            | 5.07             |
|         |           |                                    |             | Alkyl              | 5.07             |
| 8.      | CAA08     | −6.81                              | ILE B:36    | π-Alkyl            | 5.29             |
|         |           |                                    |               | Alkyl              | 3.61             |
|         |           |                                    |               | Pi-Lone pair       | 2.95             |
|         |           |                                    | HIS B:51    | H-Bond             | 2.04             |
|         |           |                                    | VAL B:52    | π-Alkyl            | 5.25             |
|         |           |                                    | SER B:135   | H-Bond             | 1.86             |
|         |           |                                    | TYR B:150   | π-Alkyl            | 4.81             |

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| Sr. No. | Ligand | Free Binding energy, FEB (kcal/mol) | Interaction | Type of interaction | Bond distance (Å) |
|---------|--------|-----------------------------------|-------------|--------------------|------------------|
| 9.      | CAA09  | $-6.75$                           | ILE B:36    | $\pi$-Alkyl        | 5.45             |
|         |        |                                   |             | Alkyl              | 3.85             |
|         |        |                                   | HIS B:51    | H-Bond             | 1.98             |
|         |        |                                   | VAL B:52    | $\pi$-Alkyl        | 5.31             |
|         |        |                                   | PRO B:132   | H-Bond             | 1.85             |
|         |        |                                   | TYR B:150   | $\pi$-Alkyl        | 5.27             |
|         |        |                                   | TYR B:161   | $\pi$-Sigma        | 3.74             |
|         |        |                                   |             | $\pi$-$\pi$ Stacked| 4.53             |
| 10.     | CAA10  | $-6.61$                           | ILE B:36    | $\Pi$-Alkyl        | 5.24             |
|         |        |                                   |             | Alkyl              | 3.55             |
|         |        |                                   | PRO B:132   | H-Bond             | 1.83             |
|         |        |                                   | TYR B:161   | $\pi$-Alkyl        | 5.09             |
|         |        |                                   |             | $\pi$-Alkyl        | 3.61             |
| 11.     | CAA11  | $-6.72$                           | HIS B:51    | H-Bond             | 2.11             |
|         |        |                                   |             | $\pi$-Cation       | 4.83             |
|         |        |                                   |             | $\pi$-$\pi$ T-shaped| 5.20             |
|         |        |                                   | ARG B:54    | 3 H-Bonds          | 1.85, 2.56, 2.60  |
|         |        |                                   | PRO B:132   | $\pi$-Alkyl        | 5.22             |
|         |        |                                   | SER B:135   | H-Bond             | 2.20             |
|         |        |                                   | TYR B:161   | $\pi$-$\pi$ T-shaped| 3.90             |
|         |        |                                   |             | $\pi$-Sigma        | 5.11             |
| 12.     | CAA12  | $-5.99$                           | ILE B:36    | $\pi$-Alkyl        | 5.23             |
|         |        |                                   |             | Alkyl              | 3.47             |
|         |        |                                   | VAL B:52    | $\pi$-Alkyl        | 5.24             |
|         |        |                                   | PRO B:132   | H-Bond             | 1.98             |
|         |        |                                   | GLY B:151   | H-Bond             | 1.98             |
| 13.     | CAA13  | $-6.66$                           | ILE B:36    | $\pi$-Alkyl        | 5.26             |
|         |        |                                   |             | Alkyl              | 4.46             |
|         |        |                                   |             | $\pi$-Lone pair    | 2.95             |
|         |        |                                   | HIS B:51    | H-Bond             | 2.18             |
|         |        |                                   | VAL B:52    | $\pi$-Alkyl        | 5.24             |
|         |        |                                   | ASP B:29    | H-Bond             | 2.76             |
|         |        |                                   | PHE B:130   | H-Bond             | 1.97             |
|         |        |                                   | PRO B:132   | H-Bond             | 1.81             |
|         |        |                                   | TYR B:161   | $\pi$-$\pi$ Stacked| 4.67             |
| 14.     | CAA14  | $-7.05$                           | HIS B:51    | $\pi$-Alkyl        | 3.87             |
|         |        |                                   | VAL B:52    | $\pi$-Alkyl        | 5.33             |
|         |        |                                   |             | Alkyl              | 3.58             |
|         |        |                                   | ASP B:29    | H-Bond             | 2.39             |
|         |        |                                   | PHE B:130   | H-Bond             | 2.07             |
|         |        |                                   | PRO B:132   | H-Bond             | 1.97             |
|         |        |                                   |             | Alkyl              | 4.62             |
|         |        |                                   | TYR B:161   | $\pi$-$\pi$ Stacked| 4.35             |
| 15.     | CAA15  | $-7.22$                           | ILE B:36    | Alkyl              | 4.15             |
|         |        |                                   | HIS B:51    | H-Bond             | 2.13             |
|         |        |                                   | VAL B:52    | $\pi$-Alkyl        | 5.42             |
|         |        |                                   | ASP B:29    | H-Bond             | 1.91             |
|         |        |                                   | PHE B:130   | H-Bond             | 2.43             |
|         |        |                                   | PRO B:132   | H-Bond             | 1.73             |
|         |        |                                   | TYR B:161   | $\pi$-$\pi$ Stacked| 4.15             |

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Table 3 (continued)

| Sr. No. | Ligand | Free Binding energy, FEB (kcal/mol) | Interaction | Type of interaction | Bond distance (Å) |
|---------|--------|-------------------------------------|-------------|---------------------|------------------|
| 16.     | CAA16  | −7.03                               | ILE B:36    | Alkyl               | 4.14             |
|         |        |                                     | HIS B:51    | H-Bond              | 2.17             |
|         |        |                                     | VAL B:52    | π-Alkyl             | 5.37             |
|         |        |                                     | ASP B:29    | H-Bond              | 1.93             |
|         |        |                                     | PHE B:130   | H-Bond              | 2.56             |
|         |        |                                     | PRO B:132   | H-Bond              | 1.69             |
|         |        |                                     | TYR B:161   | π-π Stacked         | 4.16             |
| 17.     | CAA17  | −7.07                               | VAL B:52    | π-Alkyl             | 5.47             |
|         |        |                                     | ARG B:54    | 2 H-Bonds           | 2.02, 2.68       |
|         |        |                                     | ASP B:29    | H-Bond              | 2.73             |
|         |        |                                     | PHE B:130   | H-Bond              | 1.97             |
|         |        |                                     | PRO B:132   | H-Bond              | 2.20             |
|         |        |                                     | TYR B:161   | π-π Stacked         | 4.62             |
| 18.     | CAA18  | −6.23                               | GLN B:35    | H-Bond              | 2.34             |
|         |        |                                     | ILE B:36    | π-Lone pair         | 2.88             |
|         |        |                                     |             | π-Alkyl             | 5.20             |
|         |        |                                     | VAL B:52    | π-Alkyl             | 5.23             |
|         |        |                                     | ASP B:29    | H-Bond              | 2.99             |
|         |        |                                     | PHE B:130   | H-Bond              | 1.96             |
|         |        |                                     | PRO B:132   | H-Bond              | 1.81             |
|         |        |                                     | TYR B:161   | π-π Stacked         | 5.13             |
| 19.     | CAA19  | −7.74                               | TRP B:50    | π-Alkyl             | 5.04             |
|         |        |                                     | VAL B:72    | Alkyl               | 4.83             |
|         |        |                                     | ILE A:86    | Alkyl               | 4.03             |
|         |        |                                     | GLY B:153   | H-Bond              | 2.05             |
|         |        |                                     | VAL B:154   | π-Sigma             | 3.69             |
|         |        |                                     |             | Alkyl               | 4.09             |
|         |        |                                     | VAL B:155   | H-Bond              | 1.90             |
|         |        |                                     |             | π-Alkyl             | 5.07             |
|         |        |                                     |             | Alkyl               | 5.12             |
| 20.     | CAA20  | −7.18                               | TRP B:50    | π-Alkyl             | 5.08             |
|         |        |                                     | VAL B:72    | Alkyl               | 4.91             |
|         |        |                                     | GLY B:153   | H-Bond              | 2.09             |
|         |        |                                     | VAL B:154   | π-Alkyl             | 5.40             |
|         |        |                                     | VAL B:155   | π-Alkyl             | 4.83             |
|         |        |                                     |             | Alkyl               | 5.03             |
|         |        |                                     | TYR B:161   | π-Alkyl             | 5.00             |
| 21.     | CAA21  | −7.36                               | TRP B:50    | π-Alkyl             | 4.97             |
|         |        |                                     | HIS B:51    | π-π Stacked         | 4.44             |
|         |        |                                     | VAL B:72    | Alkyl               | 4.97             |
|         |        |                                     | ASP B:75    | π-Cation            | 3.85             |
|         |        |                                     | PHE B:130   | Halogen             | 3.10             |
|         |        |                                     | GLY B:153   | H-Bond              | 2.12             |
|         |        |                                     | TYR B:161   | π-Alkyl             | 3.98             |
|         |        |                                     |             | π-π Stacked         | 4.10             |
| 22.     | CAA22  | −7.14                               | TRP B:50    | π-Alkyl             | 5.10             |
|         |        |                                     | HIS B:51    | π-π Stacked         | 4.36             |
|         |        |                                     | VAL B:72    | Alkyl               | 5.07             |
|         |        |                                     | ASP B:75    | π-Anion             | 3.97             |
|         |        |                                     | GLY B:153   | H-Bond              | 2.12             |
|         |        |                                     | TYR B:161   | π-Alkyl             | 4.21             |
|         |        |                                     |             | π-π Stacked         | 4.18             |
| Sr. No. | Ligand | Free Binding energy, FEB (kcal/mol) | Interaction | Type of interaction | Bond distance (Å) |
|---------|--------|-----------------------------------|-------------|-------------------|------------------|
| 23.     | CAA23  | −7.24                             | ILE B:36    | π-Alkyl           | 4.86             |
|         |        |                                   | ARG B:54    | H-Bond            | 2.28             |
|         |        |                                   | PRO B:132   | π-Alkyl           | 4.61             |
|         |        |                                   | SER B:135   | Carbon H-Bond     | 4.36             |
|         |        |                                   | TYR B:161   | π-Alkyl            | 4.48             |
|         |        |                                   |             | 2 π-Sigma         | 3.71, 3.90       |
| 24.     | CAA24  | −6.56                             | SER B:135   | 3 H-Bonds         | 1.99, 2.10, 3.01 |
|         |        |                                   | VAL B:155   | π-Alkyl           | 4.97             |
| 25.     | CAA25  | −6.70                             | GLN B:35    | Halogen           | 3.08             |
|         |        |                                   | ILE B:36    | π-Alkyl           | 4.95             |
|         |        |                                   |             | Alkyl             | 4.97             |
|         |        |                                   |             | π-Lone pair       | 2.80             |
|         |        |                                   | VAL B:52    | π-Alkyl           | 5.35             |
|         |        |                                   |             | Carbon H-Bond     | 2.97             |
|         |        |                                   | ASP B:29    | H-Bond            | 2.76             |
|         |        |                                   | PHE B:130   | H-Bond            | 2.12             |
|         |        |                                   | PRO B:132   | π-Alkyl           | 5.22             |
|         |        |                                   | TYR B:161   | π-Sigma           | 3.71             |
|         |        |                                   |             | π-π Stacked       | 5.58             |
| 26.     | CAA26  | −6.75                             | GLN B:35    | 2 Halogen         | 2.99, 3.68       |
|         |        |                                   | ILE B:36    | π-Alkyl           | 5.38             |
|         |        |                                   |             | Alkyl             | 5.26             |
|         |        |                                   |             | π-Lone pair       | 2.87             |
|         |        |                                   |             | Carbon H-Bond     | 4.14             |
|         |        |                                   |             | Halogen           | 3.37             |
|         |        |                                   | VAL B:52    | π-Alkyl           | 5.43             |
|         |        |                                   | HIS B:51    | H-Bond            | 2.19             |
|         |        |                                   | PRO B:132   | Alkyl             | 5.03             |
|         |        |                                   | SER B:135   | H-Bond            | 1.92             |
|         |        |                                   | TYR B:150   | π-Alkyl           | 4.75             |
| 27.     | CAA27  | −6.70                             | ILE B:36    | π-Alkyl           | 5.25             |
|         |        |                                   |             | Alkyl             | 3.95             |
|         |        |                                   | VAL B:52    | π-Alkyl           | 5.32             |
|         |        |                                   | ASP B:29    | 2 Halogens        | 2.78, 3.46       |
|         |        |                                   | PHE B:130   | Halogen           | 3.70             |
|         |        |                                   | PRO B:132   | H-Bond            | 1.97             |
|         |        |                                   | TYR B:161   | π-Alkyl           | 3.81             |
| 28.     | CAA28  | −6.52                             | ILE B:36    | π-Alkyl           | 5.26             |
|         |        |                                   |             | Alkyl             | 3.89             |
|         |        |                                   | VAL B:52    | π-Alkyl           | 5.35             |
|         |        |                                   | ASP B:29    | 2 Halogens        | 2.77, 3.65       |
|         |        |                                   | PHE B:130   | H-Bond            | 1.95             |
|         |        |                                   | PRO B:132   | π-Alkyl           | 3.70             |
| 29.     | CAA29  | −6.95                             | ARG B:54    | 2 H-Bonds         | 1.79, 2.19       |
|         |        |                                   | ASP B:29    | 2 Halogens        | 3.03, 3.60       |
|         |        |                                   | PHE B:130   | 2 Halogens        | 3.15, 3.46       |
|         |        |                                   | PRO B:132   | H-Bond            | 2.84             |
|         |        |                                   | TYR B:161   | π-Alkyl           | 5.31             |
|         |        |                                   |             | π-Lone pair       | 3.75             |
|         |        |                                   |             | π-π Stacked       | 5.48             |

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Table 3 (continued)

| Sr. No. | Ligand | Free Binding energy, FEB (kcal/mol) | Interaction | Type of interaction | Bond distance (Å) |
|---------|--------|----------------------------------|-------------|--------------------|------------------|
| 30.     | CAA30  | −5.89                            | HIS B:51    | H-Bond             | 2.90             |
|         |        |                                  | SER A:83    | 2 Halogens         | 3.52, 3.60       |
|         |        |                                  | MET A:84    | H-Bond             | 2.07             |
|         |        |                                  | SER B:135   | H-Bond             | 2.76             |
|         |        |                                  | ASN B:152   | Halogen            | 3.23             |
|         |        |                                  | GLY B:153   | Halogen            | 3.01             |
|         |        |                                  | VAL B:155   | Alkyl              | 5.36             |

Fig. 4. The 3D interaction of compound CAA17 (FEB: −7.07) against viral target NS2B/NS3pro.

2. Experimental Design, Materials and Methods

2.1. Selection and retrieval of targets structures

The virtual screening was carried out on the homology model of the dengue virus’s non-structural protein, NS2B/NS3pro developed by Wichapong et al [5]. The DENV-2 NS2B/NS3pro model was built based on the DENV-2 complex cofactor-protease using the crystal structure of NS2B/NS3pro West Nile Virus (WNV) as the template. The protein structure was prepared as a macromolecule prior to docking using AutoDock version 1.5.6 package (www.autodock.scrips.edu). Briefly, the protein preparation was done by removing the native ligand, tetrapeptide inhibitor (Bz-Nle-Lys-Ar-H) and water molecules, the addition of polar hydrogen and Kollmann charges.

2.2. Ligand preparation and molecular docking

The 3D structures of 30 cinnamic amide derivatives were constructed and energetically optimized using ChemDraw Professional 16.0. The minimised structures were saved in sdf format before being converted into pdb format using OpenBabel-3.1.1 software [6].
The validation of docking protocol was done by re-docking the inhibitor tetrapeptide (Bz-Nle-Lys-Ar-H) with the RMSD value not greater than 2.0 Å. The ligands were prepared by merging of non-polar hydrogen and assigned Gasteiger charged. The center of the grid box was employed around the protease active site at 23.038, 43.372, −0.316 in x, y, and z coordinate, respectively, with a box size of 60 × 60 × 60 dimensions and grid spacing 0.375 Å. The docking of ligands was run with the Lamarckian Genetics Algorithm (GA) search program applied to generate 100 runs. The binding modes of compounds were analyzed using Discovery Studio Client 2020 (www.accelrys.com).

The identification of hit compound was identified based on the conformations with the ones of lowest free binding energy and of the most populated cluster.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

CRediT Author Statement

Nadia Mohamed Yusoff: Data curation, Investigation, Methodology, Software, Writing – original draft; Asnuzilawati Asari: Conceptualization, Supervision; Siti Nor Khadijah Addis: Methodology, Validation, Writing – review & editing.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi: 10.1016/j.dib.2022.108036.

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