

Supporting Information

Thioguanine-based DENV-2 NS2B/NS3 protease inhibitors: Virtual screening, synthesis, biological evaluation and molecular modelling

Maywan Hariono^{1,2¶}, Sy Bing Choi^{1,9&}, Ros Fatimah Roslim^{1&}, Mohamed Sufian Nawi^{1,3&}, Mei Lan Tan⁴, Ezatul Ezleen Kamarulzaman¹, Nornisah Mohamed¹, Rohana Yusof⁵, Shatrath Othman⁶, Noorsaadah Abd Rahman⁶, Rozana Othman⁷, Habibah A. Wahab^{1,8*}

¹School of Pharmaceutical Sciences, Universiti Sains Malaysia, Minden, Pulau Pinang, Malaysia

²Faculty of Pharmacy, Sanata Dharma University, Maguwoharjo, Sleman, Yogyakarta, Indonesia

³Department of Pharmaceutical Chemistry, Kulliyah of Pharmacy, International Islamic University Malaysia, Kuantan, Pahang, Malaysia

⁴Advanced Medical and Dental Institute, Universiti Sains Malaysia, Bertam, Pulau Pinang, Malaysia

⁵Department of Molecular Medicine, Faculty of Medicine, Universiti Malaya, Kuala Lumpur, Malaysia

⁶Department of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur, Malaysia

⁷Department of Pharmacy, Faculty of Medicine, Universiti Malaya, Kuala Lumpur, Malaysia

⁸Malaysian Institute of Pharmaceuticals and Nutraceuticals, Ministry of Science, Technology and Innovation, Halaman Bukit Gambir, Bayan Lepas, Pulau Pinang, Malaysia

⁹School of Data Sciences, Perdana University, Blok B and d1, MAEPS Building, MARDI Complex, Jalan MAEPS Perdana, 43400 Serdang, Selangor

*Corresponding Author

E-mail: habibahw@usm.my ; bibwahab@gmail.com

&These authors contributed equally to this work

2 Fig

