Virtual screening of bioactive anti-SARS-CoV natural products and identification of 3β,12-diacetoxyabieta-6,8,11,13-tetraene as a potential inhibitor of SARS-CoV-2 virus and its infection related pathways by MD simulation and network pharmacology

A.K.M. Moyeenul Huq\textsuperscript{a,b,*}, Miah Roney\textsuperscript{a,c,*}, Syahrul Imran\textsuperscript{d,e}, Shafi Ullah Khan\textsuperscript{f}, Md. Nazim Uddin\textsuperscript{g}, Thet Thet Hta\textsuperscript{h}, Atif Amin Baig\textsuperscript{i}, Mohiuddin Ahmed Bhuiyan\textsuperscript{j}, Zainal Amiruddin Zakaria\textsuperscript{a}, Mohd Fadhlizil Fasihi\textsuperscript{a,c} and Saiful Nizam Tajuddin\textsuperscript{a,c,*}

\textsuperscript{a}Bio Aromatic Research Centre, Universiti Malaysia Pahang, Kuantan, Pahang, Malaysia; \textsuperscript{b}School of Medicine, Department of Pharmacy, University of Asia Pacific, Dhaka, Bangladesh; \textsuperscript{c}Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang, Kuantan, Pahang, Malaysia; \textsuperscript{d}Atta-ur-Rahman Institute for Natural Product Discovery (AuRIns), Universiti Teknologi MARA Cawangan Selangor Kampus Puncak Alam, Puncak Alam, Selangor, Malaysia; \textsuperscript{e}Faculty of Applied Science, Universiti Teknologi MARA (UiTM), Shah Alam, Selangor, Malaysia; \textsuperscript{f}Product & Process Innovation Department, Qarshi Brands (Pvt) Ltd, Haripur, KP, Pakistan; \textsuperscript{g}Institute of Food Science and Technology, Bangladesh Council of Scientific and Industrial Research, Dhaka, Bangladesh; \textsuperscript{h}School of Pharmacy, Monash University Malaysia, Subang Jaya, Selangor, Malaysia; \textsuperscript{i}Faculty of Medicine, Universiti Sultan Zainal Abidin, Kuala Terengganu, Terengganu, Malaysia; \textsuperscript{j}Department of Biomedical Sciences, Faculty of Medicine and Health Sciences, Universiti Malaysia Sabah, Jalan UMS, Kota Kinabalu, Sabah, Malaysia

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1. Introduction

Coronaviruses (CoVs) are the most frequent source of mild to acute respiratory illnesses. In 2003 and 2012, two especially virulent CoVs, the severe acute respiratory syndrome coronavirus (SARS-CoV) and the Middle East respiratory syndrome coronavirus (MERS-CoV), both transferred through animals to people, sparked global pandemics with significant mortality rates (Cavasotto & Di Filippo, 2021). In December 2019, the public health officials of China first reported to the World Health Organization (WHO) about an unknown virus from Wuhan which caused illness similar to pneumonia (Khan & Fahad, 2020). They quickly identified the virus as a member of the coronavirus (CoV) category, which was fast propagating outside from Wuhan to other places or countries and was named novel coronavirus disease 2019 (COVID-19) (Hasan et al., 2021) with flue like symptoms including fever, cough, pneumonia, nausea and tiredness. WHO declared a worldwide emergency on 30\textsuperscript{th} January 2020 and a pandemic on 11\textsuperscript{th} March 2020 for the coronavirus illness (COVID-19) (Hua & Shaw, 2020). As of August 07, 2021, the global number of coronavirus cases had reached 202.59 million, with 4.29 million deaths (https://www.worldometers.info/coronavirus/). COVID-19 is regarded as a serious public health threat worldwide. During the last 1.5 years, different variants of this virus have evolved with greater transmissibility and associated disease severely (https://www.who.int/en/activities/tracking-SARS-CoV-2-variants/). With the evolution of vaccines for SARS-CoV-2 and continuous vaccination through world, a significant decline in new transmission and death brought hope...