

## राष्ट्रीय रासायनिक प्रयोगशाला

(वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद) डॉ. होमी भाभा रोड, पुणे - 411 008. भारत

## NATIONAL CHEMICAL LABORATORY

(Council of Scientific & Industrial Research) Dr. Homi Bhabha Road, Pune - 411008, India



## Gangadhar J. Sanjayan

Chief Scientist & AcSIR Professor of Chemistry Division of Organic Chemistry, Pune - 411 008, India Phone (O): 0091-20-25902082, E-mail: gj.sanjayan@ncl.res.in

Research Group: https://gjsanjayan.wixsite.com/csir-ncl

Sun Pharma Science Foundation. 8C, 8th Floor, Hansalaya Building, 15-Barakhamba Road, Connaught Place, New Delhi - 110001, INDIA

27th August 2024

Subject: Citation (brief summary) on the research work of the applicant by nominator

## Award Committee Chair:

I am writing to provide a citation and summary of the research work submitted for Sun Pharma Science Foundation Research Scholar Award in the field of Pharmaceutical Sciences by Nilu Gone in the development of a novel class of SARS-CoV-2 Main Protease (Mpro) inhibitor which has been published recently - Nilu Gone et al: "Discovery of SARS-CoV-2 Inhibitors Featuring Novel Histidine α-Nitrile Motif" Chem. Biodiversity., 2023, e202300957 (DOI: https://doi.org/10.1002/cbdv.202300957). Patent application filed: Nilu V. Gone, Kiran Bokar, G. J. Sanjayan, "SARS-COV-2 inhibitors and method of preparation thereof". Patent application number: 0051NF2024/IN, 2021. Nilu Gone's research work primarily aimed in discovery of a novel class of inhibitors against the SARS-CoV-2, bearing histidine α-nitrile motif embedded on a simple dipeptide framework. Her research work is having twofold advantage: firstly, the designing and short synthesis of histidine α-nitrile dipeptides as simplest peptidomimetics inhibitors; secondly, it successfully identifies these histidine  $\alpha$ -nitrile dipeptides as SARS-CoV-2 main protease (M<sup>pro</sup>) inhibitor agents. The antiviral assay and computational analysis revealed that the potent histidine  $\alpha$ -nitrile dipeptides 6i displayed strong SARS-CoV-2 viral reduction (EC<sub>50</sub> = 0.48 μM) and M<sup>pro</sup>-inhibitors binding energies in the range of -34.2 Kcal/mol, respectively. Overall, her research work led to the development of histidine  $\alpha$ -nitrile dipeptides as a novel class of SARS-CoV-2 inhibitors that would raise the hope as a potent drug candidate to fight the dreaded SARS-CoV-2 and its variants. The practical utility of histidine  $\alpha$ -nitrile dipeptides could have a positive effect in future pandemics, reducing the risks to both lives and the economy.

With best regards and season's greetings,

Gangadhar J. Sanjayan

+91 20 25902639 (Business Development)

URL: www.ncl-india.org