

Antiviral Action against SARS-CoV-2 of a Synthetic Peptide Based on a Novel Defensin Present in the Transcriptome of the Fire Salamander (*Salamandra salamandra*)

Ana Luisa A. N. Barros ^{1,2}, Vladimir C. Silva ³, Atvaldo F. Ribeiro-Junior ¹, Miguel G. Cardoso ^{1,4}, Samuel R. Costa ⁵, Carolina B. Moraes ⁶, Cecília G. Barbosa ⁷, Alex P. Coleone ⁸, Rafael P. Simões ⁹, Wanessa F. Cabral ¹, Raul M. Falcão ¹⁰, Andreanne G. Vasconcelos ^{1,11}, Jefferson A. Rocha ¹², Daniel D. R. Arcanjo ¹³, Augusto Batagin-Neto ^{8,14}, Tatiana Karla S. Borges ¹, João Gonçalves ⁴, Guilherme D. Brand ⁵, Lucio H. G. Freitas-Junior ⁷, Peter Eaton ^{15,16}, Mariela Marani ¹⁷, Massuo J. Kato ¹⁸, Alexandra Plácido ¹⁵ and José Roberto S. A. Leite ^{1,*}

¹ Núcleo de Pesquisa em Morfologia e Imunologia Aplicada, NuPMIA, Faculdade de Medicina, Universidade de Brasília, UnB, Brasília 70910-900, DF, Brazil

² Programa de Pós-graduação em Medicina Tropical, PGMT, Faculdade de Medicina, Universidade de Brasília, UnB, Brasília 70910-900, DF, Brazil

³ Laboratório de Vigilância Genômica e Biologia Molecular-Fundação Oswaldo Cruz Piauí, Teresina, PI 64001-350, Brazil

⁴ imed.Ulisboa-Research Institute for Medicines, Faculty of Pharmacy, University of Lisbon, 1649-003 Lisbon, Portugal

⁵ Instituto de Química, IQ, Universidade de Brasília, UnB, Brasília 70910-900, DF, Brazil

⁶ Department of Pharmaceutical Sciences, Federal University of São Paulo, Diadema 09913-030, SP, Brazil

⁷ Department of Microbiology, Institute of Biomedical Sciences, University of São Paulo, São Paulo 05508-000, SP, Brazil

⁸ Programa de Pós-graduação em Ciência e Tecnologia de Materiais (POSMAT), School of Sciences, São Paulo State University (UNESP), Bauru 17033-360, SP, Brazil

⁹ School of Agriculture, Department of Bioprocess and Biotechnology, São Paulo State University (UNESP), Botucatu 18618-689, SP, Brazil

¹⁰ Bioinformatics Postgraduate Program, Metr pole Digital Institute, Federal University of Rio Grande do Norte, Natal 59078-900, RN, Brazil

¹¹ People&Science Pesquisa Desenvolvimento e Inova  o LTDA, Centro de Desenvolvimento Tecnol gico (CDT), Universidade de Bras lia, UnB, Bras lia 70910-900, DF, Brazil

¹² Campus S o Bernardo, Universidade Federal do Maranh o, UFMA, S o Bernardo 65550-000, MA, Brazil

¹³ Department of Biophysics and Physiology, Federal University of Pia  , Teresina 64049-550, PI, Brazil

¹⁴ Institute of Sciences and Engineering, S o Paulo State University (UNESP), Itapeva 18409-010, SP, Brazil

¹⁵ Laborat rio Associado para a Qu mica Verde/Rede de Qu mica e Tecnologia (LAQV/REQUIMTE), Departamento de Qu mica e Bioqu mica, Faculdade de Ci ncias, Universidade do Porto, 4169-007 Porto, Portugal

¹⁶ School of Chemistry, The Bridge, University of Lincoln, Lincoln LN6 7EL, UK

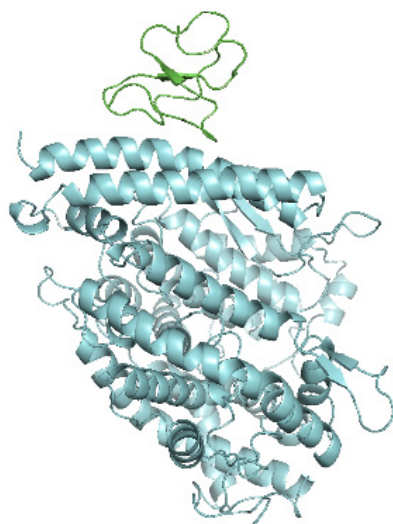
¹⁷ IPEEC-CONICET, Consejo Nacional de Investigaciones Cient ficas y T cnicas, Puerto Madryn 9120, Argentina

¹⁸ Instituto de Qu mica (IQ), Universidade de S o Paulo (USP), S o Paulo 05508-900, SP, Brazil

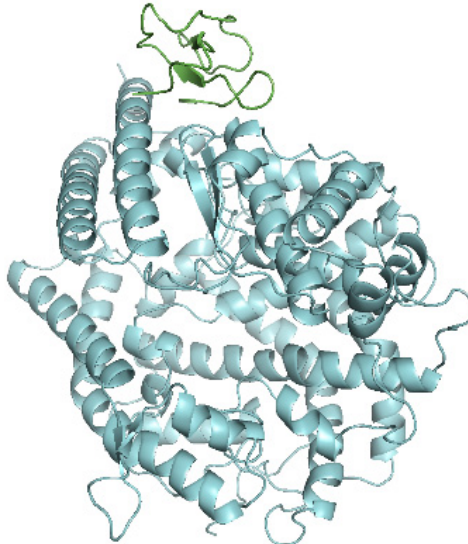
* Correspondence: jrsaleite@gmail.com

DOCKING SOLUTIONS

ACE2-PEP-S1



ACE2-PEP-S2



SPIKE-PEP-S1



SPIKE-PEP-S2

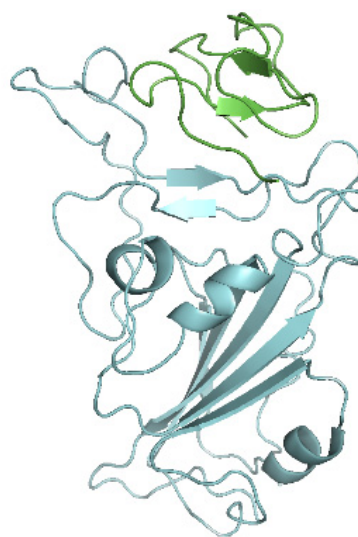


Figure S1. ACE2-PEP-S1, ACE2-PEP-S2, SPIKE-PEP-S1, and SPIKE-PEP-S2 molecular complexes obtained by docking analysis and used for MD simulations.

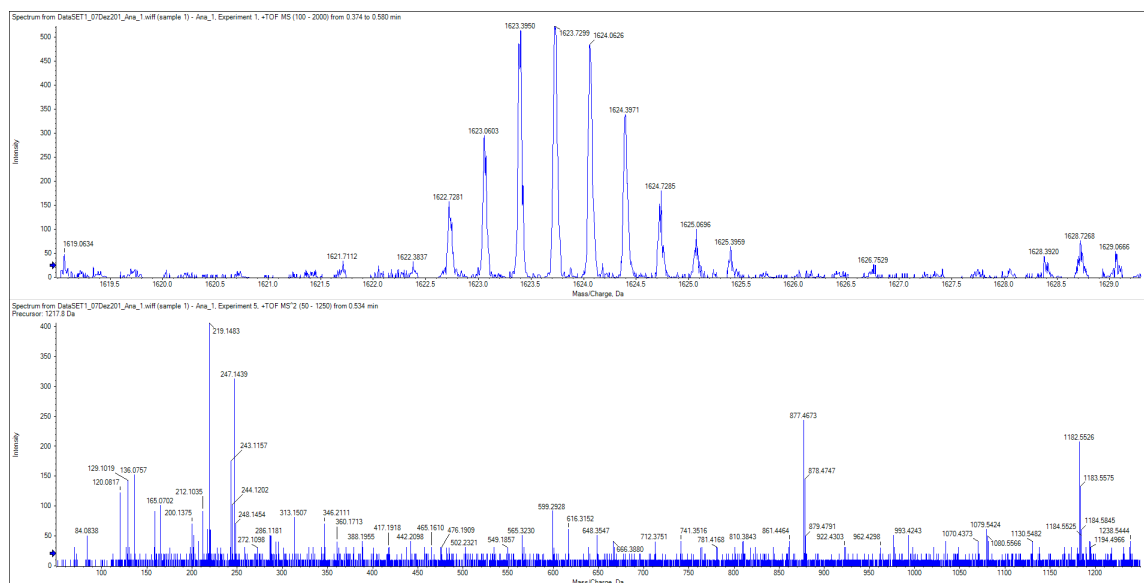


Figure S2. MS/MS Spectrum of the triply charged ion $[M+3H]^{3+}$ of SS-I.