ISSN 2220-315x (online)

World Journal of *Experimental Medicine*

Quarterly Volume 15 Number 1 March 20, 2025

Published by Baishideng Publishing Group Inc

World Journal of Experimental Medicine

Contents

Quarterly Volume 15 Number 1 March 20, 2025

EDITORIAL

REVIEW

MINIREVIEWS

ORIGINAL ARTICLE

Retrospective Cohort Study

Observational Study

Prospective Study

Basic Study

LETTER TO THE EDITOR

World Journal of Experimental Medicine

Quarterly Volume 15 Number 1 March 20, 2025

Contents

ABOUT COVER

Peer Reviewer of *World Journal of Experimental Medicine*, Wu Duan, MD, PhD, Assistant Professor, Attending Doctor, Department of Endocrinology, Qilu Hospital of Shandong University, Jinan 250012, Shandong Province, China. duanwu@qiluhospital.com

AIMS AND SCOPE

The primary aim of the *World Journal of Experimental Medicine* (*WJEM*, *World J Exp Med*) is to provide scholars and readers from various fields of experimental medicine with a platform to publish high-quality basic and clinical research articles and communicate their research findings online.

WJEM mainly publishes articles reporting research results and findings obtained in the field of experimental medicine and covering a wide range of topics including clinical laboratory medicine (applied and basic research in hematology, body fluid examination, cytomorphology, genetic diagnosis of hematological disorders, thrombosis and hemostasis, and blood typing and transfusion), biochemical examination (applied and basic research in laboratory automation and information system, biochemical methodology, and biochemical diagnostics), *etc*.

INDEXING/ABSTRACTING

The *WJEM* is now abstracted and indexed in PubMed, PubMed Central, Scopus, Reference Citation Analysis, China Science and Technology Journal Database, and Superstar Journals Database. The *WJEM*'s CiteScore for 2023 is 1.7 and Scopus CiteScore rank 2023: Internal medicine is 109/167.

RESPONSIBLE EDITORS FOR THIS ISSUE

NAME OF JOURNAL
World Journal of Experimental Medicine

ISSN
ISSN 2220-315x (online)

LAUNCH DATE
December 20, 2011

FREQUENCY
Quarterly

PUBLICATION DATE
March 20, 2025

PUBLISHING PARTNER
Department of Clinical Laboratory, The Affiliated Suzhou Hospital of Nanjing Medical University, Suzhou Municipal Hospital

INSTRUCTIONS TO AUTHORS
https://www.wjgnet.com/bpg/gerinfo/204

GUIDELINES FOR ETHICS DOCUMENTS
https://www.wjgnet.com/bpg/GerInfo/287

GUIDELINES FOR NON-NATIVE SPEAKERS OF ENGLISH
https://www.wjgnet.com/bpg/gerinfo/240

PUBLICATION ETHICS
https://www.wjgnet.com/bpg/GerInfo/288

PUBLICATION MISCONDUCT
https://www.wjgnet.com/bpg/gerinfo/208

POLICY OF CO-AUTHORS
https://www.wjgnet.com/bpg/GerInfo/310

ARTICLE PROCESSING CHARGE
https://www.wjgnet.com/bpg/gerinfo/242

STEPS FOR SUBMITTING MANUSCRIPTS
https://www.wjgnet.com/bpg/GerInfo/239

ONLINE SUBMISSION
https://www.f6publishing.com

PUBLISHING PARTNER's OFFICIAL WEBSITE
http://www.smh.cc/home2020/page/index/index.html

World Journal of Experimental Medicine

Submit a Manuscript: https://www.f6publishing.com

World J Exp Med 2025 March 20; 15(1): 94022

DOI: 10.5493/wjem.v15.i1.94022

ISSN 2220-315x (online)

ORIGINAL ARTICLE

Basic Study

SARS-CoV-2 proteins show great binding affinity to resin composite monomers and polymerized chains

Pedro Henrique Sette-de-Souza, Moan Jéfter Fernandes Costa, Boniek Castillo Dutra Borges

Specialty type: Medicine, research and experimental

Provenance and peer review: Invited article; Externally peer reviewed.

Peer-review model: Single blind

Peer-review report's classification

Scientific Quality: Grade B
Novelty: Grade B
Creativity or Innovation: Grade B
Scientific Significance: Grade B

P-Reviewer: Arumugam EAP

Received: March 10, 2024
Revised: October 3, 2024
Accepted: October 30, 2024
Published online: March 20, 2025
Processing time: 291 Days and 0.9 Hours

Pedro Henrique Sette-de-Souza, Moan Jéfter Fernandes Costa, Faculdade de Odontologia, Universidade de Pernambuco-campus Arcoverde, Arcoverde 56503-146, Pernambuco, Brazil

Pedro Henrique Sette-de-Souza, Programa de Pós-Graduação em Saúde e Desenvolvimento Socioambiental, Universidade de Pernambuco-campus Garanhuns, Garanhuns 55294-902, Pernambuco, Brazil

Moan Jéfter Fernandes Costa, Programa de Pós-Graduação em Biologia Celular e Molecular Aplicada, Universidade de Pernambuco-campus Santo Amaro, Recife 50100-130, Pernambuco, Brazil

Boniek Castillo Dutra Borges, Department of Odontologia, Universidade Federal do Rio Grande do Norte, Natal 59056-000, Rio Grande do Norte, Brazil

Boniek Castillo Dutra Borges, Programa de Pós-Graduação em Ciências Odontológicas, Universidade Federal do Rio Grande do Norte, Natal 59056-000, Rio Grande do Norte, Brazil

Corresponding author: Pedro Henrique Sette-de-Souza, DDS, MSc, PhD, Full Professor, Faculdade de Odontologia, Universidade de Pernambuco-campus Arcoverde, Rua Cícero Monteiro de Melo, s/n-São Cristóvão, Arcoverde/PE, Arcoverde 56503-146, Pernambuco, Brazil. pedro.souza@upe.br

Abstract

BACKGROUND

Due to saliva and salivary glands are reservoir to severe acute respiratory syndrome-coronavirus 2 (SARS-CoV-2), aerosols and saliva droplets are primary sources of cross-infection and are responsible for the high human–human transmission of SARS-CoV-2. However, there is no evidence about how SARS-CoV-2 interacts with oral structures, particularly resin composites.

AIM

To evaluate the interaction of SARS-CoV-2 proteins with monomers present in resin composites using in silico analysis.

METHODS

Four SARS-CoV-2 proteins [*i.e.* main protease, 3C-like protease, papain-like protease (PLpro), and glycoprotein spike] were selected along with salivary amylase as the positive control, and their binding affinity with bisphenol-A glycol

dimethacrylate, bisphenol-A ethoxylated dimethacrylate, triethylene glycol dimethacrylate, and urethane dimethacrylate was evaluated. Molecular docking was performed using AutoDock Vina and visualised in Chimera UCSF 1.14. The best ligand–protein model was identified based on the binding energy (ΔG–kcal/moL).

RESULTS

Values for the binding energies ranged from -3.6 kcal/moL to -7.3 kcal/moL. The 3-monomer chain had the lowest binding energy (*i.e*. highest affinity) to PLpro and the glycoprotein spike. Non-polymerised monomers and polymerised chains interacted with SARS-CoV-2 proteins *via* hydrogen bonds and hydrophobic interactions. Those findings suggest an interaction between SARS-CoV-2 proteins and resin composites.

CONCLUSION

SARS-CoV-2 proteins show affinity to non-polymerised and polymerised resin composite chains.

Key Words: Composite resins; COVID-19; SARS-CoV-2; Dental restorations; Molecular docking simulation; Dentistry

Core Tip: The severe acute respiratory syndrome-coronavirus 2 (SARS-CoV-2) may interact with monomers of resin composites; triethylene glycol dimethacrylate has the smallest affinity with SARS-CoV-2 among monomers; bisphenol-A glycol dimethacrylate and bisphenol-A ethoxylated dimethacrylate show a remarkable affinity mainly with papain-like protease.

Citation: Sette-de-Souza PH, Fernandes Costa MJ, Dutra Borges BC. SARS-CoV-2 proteins show great binding affinity to resin composite monomers and polymerized chains. *World J Exp Med* 2025; 15(1): 94022
URL: https://www.wjgnet.com/2220-315x/full/v15/i1/94022.htm
DOI: https://dx.doi.org/10.5493/wjem.v15.i1.94022

INTRODUCTION

Saliva and salivary glands are a significant reservoir for severe acute respiratory syndrome-coronavirus 2 (SARS-CoV-2) [1]. Aerosols and saliva droplets are primary sources of cross-infection and are responsible for the high human–human transmission of SARS-CoV-2[2,3]. Once saliva wets oral tissues, tooth structures, and dental restoratives present in the oral cavity, SARS-CoV-2 can bind to them, thereby increasing the permanence of microorganisms in the mouth.

Among dental restoratives, resin composites are widely used to restore decayed teeth[4] due to their aesthetic properties and capacity to preserve healthy tooth tissues. Such materials contain organic monomers such as bisphenol A glycol dimethacrylate [bisphenol-A glycol dimethacrylate (Bis-GMA)], bisphenol A ethoxylated dimethacrylate [bisphenol-A ethoxylated dimethacrylate (Bis-EMA)], triethylene glycol dimethacrylate (TEGDMA), and urethane dimethacrylate (UDMA), along with inorganic filler particles[5]. Those monomers present chemical components such as hydroxyl, oxygen, and nitrogen that affect intermolecular interactions with substrates[6,7]. It has been demonstrated that, aside from taking shelter on dental biofilms, SARS-CoV-2 can interact with oral tissues and tooth structures[8,9]. However, it remains unclear whether SARS-CoV-2 proteins interact with resin composites.

Knowing the sites within the mouth that can harbour SARS-CoV-2 is essential for understanding its spread once saliva is not the only oral harbour for viruses[9]. However, the mechanism by which SARS-CoV-2 colonises dental biofilm remains unclear. At the same time, the acquired pellicle (AP) may form on any exposed surface, including dental materials, through the selective adsorption of proteins[10]. Thus, SARS-CoV-2 proteins may interact with dental materials and collaborate in the formation of AP.

Given the above, in silico analyses play a remarkable role in investigations involving cellular and molecular processes [11,12]. The molecular docking method, which entails searching for probable interactions between microorganisms' proteins and substrates, has been used worldwide as the first step to understanding probable interactions with SARS-CoV-2[13]. That computational approach is an essential tool due to the urgent need to better understand SARS-CoV-2's effects on human health.

Against that background, in our study we evaluated the possible interaction of SARS-CoV-2 proteins with monomers and polymers present in resin composite in silico. The null hypothesis tested was that an interaction between the SARS-CoV-2 proteins and the monomers and other proteins would not occur.

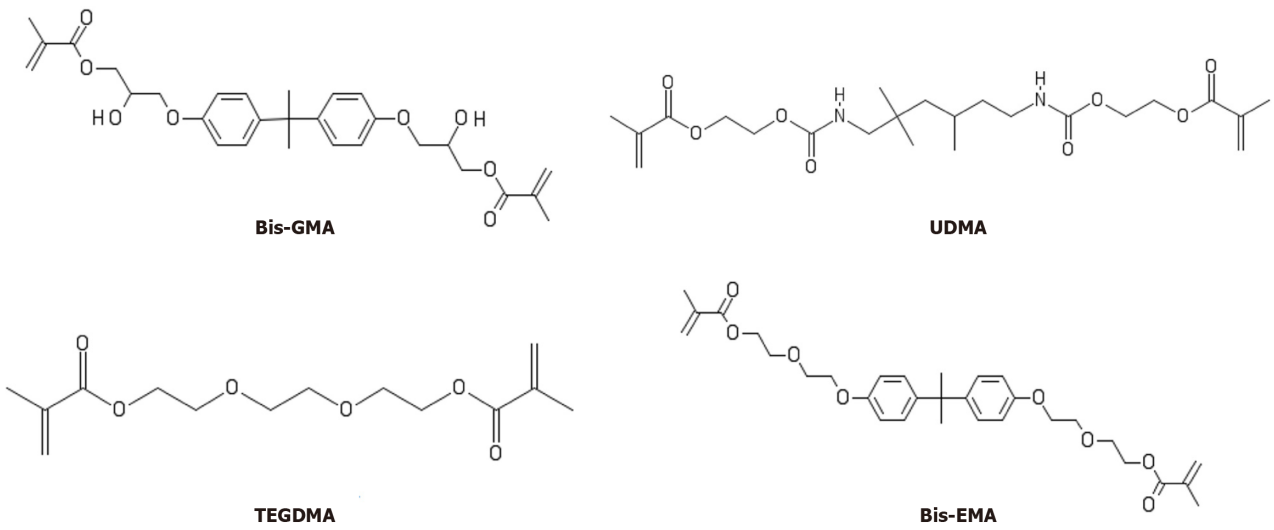

Figure 1 Chemical structure of the tested monomers: Bisphenol-A glycol dimethacrylate, bisphenol-A ethoxylated dimethacrylate, triethylene glycol dimethacrylate, and urethane dimethacrylate. Bis-EMA: Bisphenol-A ethoxylated dimethacrylate; Bis-GMA: Bisphenol-A glycol dimethacrylate; UDMA: Urethane dimethacrylate; TEGDMA: Triethylene glycol dimethacrylate.

MATERIALS AND METHODS

Protein selection and structure preparation

SARS-CoV-2 has some proteins involved in biological processes related to coronaviruses[14]. Thus, to simulate a whole new coronavirus, four different SARS-CoV-2 protein groups-the main protease (Mpro) (PDB: 6LU7), 3C-like protease (3CLpro) (PDB: 6M2N), papain-like protease (PLpro) (PDB: 6W9C), and glycoprotein spike (PDB: 6VYB)-were selected in light of previous studies[15–17]. For a positive control, we used salivary amylase (PDB: 3BLP) because it is involved in AP formation on multiple surfaces[10].

The crystal structures of SARS-CoV-2 proteins were obtained from the GenBank National Center for Biotechnology Information (RRID: SCR_002760). The AutoDock (RRID: SCR_012746) was used to delete duplicated chains, heteroatoms, and water molecules, as well as add polar hydrogens atoms and the charge of all atoms in the protein structure. Gasteiger charges were computed, and the structure was saved as a PDBQT file for the docking studies.

Ligand selection and structure preparation

The monomers Bis-GMA ($C_{29}H_{36}O_8$, PubChem CID: 15284), TEGDMA ($C_{14}H_{22}O_6$, PubChem CID: 7979), UDMA ($C_{23}H_{38}N_2O_8$, PubChem CID: 170472), and Bis-EMA ($C_{31}H_{40}O_8$, PubChem CID: 92523) were used in this study. Their chemical structures appear in Figure 1.

After retrieving SMILE codes from the National Center for Biotechnology Information's chemical structure library (RRID: SCR_004284), we constructed multiple chains through monomer combination using PubChem Draw (RRID: SCR_021249). We also linked the individual chains to simulate the natural polymerised resin composite. Next, we simulated various polymerised chains linking the monomer methacrylate regions during polymerisation, after which we transformed the new SMILE code in a PDB file in Chimera UCSF 1.14 (RRID: SCR_004097).

The rotatable bonds of the ligands were defined using AutoDock, and the structures were saved as PDBQT files for use in the docking studies.

Docking procedure

The Autogrid algorithm created the three-dimensional grids to generate the grid parameter files (RRID: SCR_015982). Each grid map was set to the centre of chain A, docking parameters were set according to the protein (Table 1), and all analyses were performed with a/an exhaustiveness value of 8.

Molecular docking was performed using AutoDock Vina (RRID: SCR_011958), and the best ligand–protein model was identified based on the binding energy (ΔG–kcal/moL)[18].

Docking visualisation

The results obtained through the docking procedure were visualised in Chimera UCSF 1.14 (RRID: SCR_004097). The two-dimensional interactions of the complex protein–ligand structure, including hydrogen bonds and bond lengths, were analysed in LigPlot+ (RRID: SCR_018249) for all interactions[19]. The step-by-step methodological approach that we followed is depicted in Figure 2.

Table 1 Binding energy (ΔG–kcal/mol) and standard deviation of the interaction between the severe acute respiratory syndrome-coronavirus 2 proteins and resin composite

Chain	Binding energy (ΔG–kcal/mol)				
	6LU7[1]	6M2N[1]	6W9C[1]	6VYB[1]	3BLP+
3-monomer-chain	-4.95 ± 0.53	-5.28 ± 0.65	-5.46 ± 0.83	-5.15 ± 0.49	-5.63 ± 0.48
2-monomer-chain	-4.71 ± 0.72	-4.93 ± 0.71	-4.78 ± 0.83	-4.85 ± 0.56	-5.17 ± 1.30
Monomers	-5.05 ± 0.66	-5.28 ± 0.47	-5.25 ± 1.10	-5.03 ± 0.53	-5.05 ± 0.76
Hydroxyapatite	-4.2	-4.6	-5.1	-4.9	-4.8
PO_4	-3.3	-3.2	-3.6	-3.6	-3.7

[1]Severe acute respiratory syndrome-coronavirus 2.
6LU7: Main protease; 6M2N: 3C-like protease; 6W9C: Papain-like protease; 6VYB: Glycoprotein spike; 3BLP: Salivary amylase.

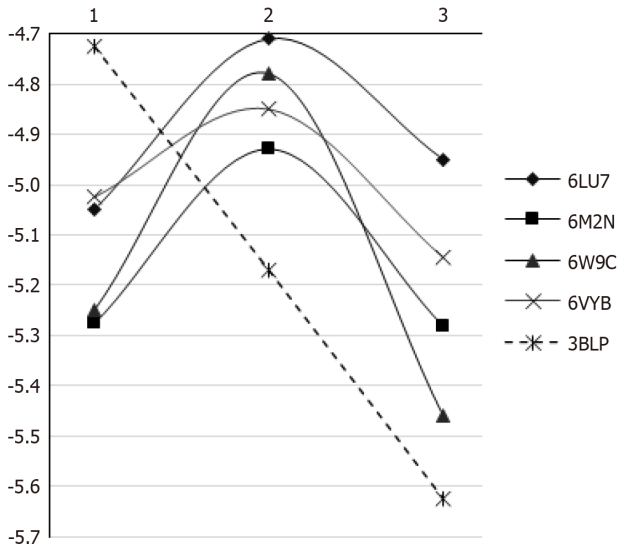

Figure 2 Binding energy between severe acute respiratory syndrome-coronavirus 2 proteins and resin composite chains. 1: Monomer; 2: Two-monomer chain; 3: Three-monomer chain.

RESULTS

Binding energy evaluation

Binding energies ranging from -3.1 kcal/moL to -8.0 kcal/moL were found. The 3-monomer chain had the lowest binding energy (*i.e.* highest affinity) to PLpro, the glycoprotein spike, and salivary amylase (Table 1). For all tested proteins, the 2-monomer chain demonstrated the highest binding energy.

Interaction analyses

To observe the specific interactions between monomers and proteins, we used LigPlot+. The central oxygen and nitrogen atoms from monomers were involved in hydrogen bonds with amino acid residues, and some alkene groups of monomers presented hydrophobic interactions with the residues. Those interactions were also observed in the polymerised chains.

Non-polymerised monomers and polymerised chains interacted with SARS-CoV-2 proteins *via* hydrogen bonds and hydrophobic interactions (Figure 3). Beyond that, any SARS-CoV-2 protein may have interacted with many non-polymerised and polymerised chains simultaneously (Figure 4).

DISCUSSION

The null hypothesis tested in our study-that an interaction between the SARS-CoV-2 proteins and the monomers and polymers would not occur-was rejected because the binding affinity between all monomers and polymers and all proteins (*i.e.* Mpro, 3CLpro, PLpro, and the glycoprotein spike) was observed.

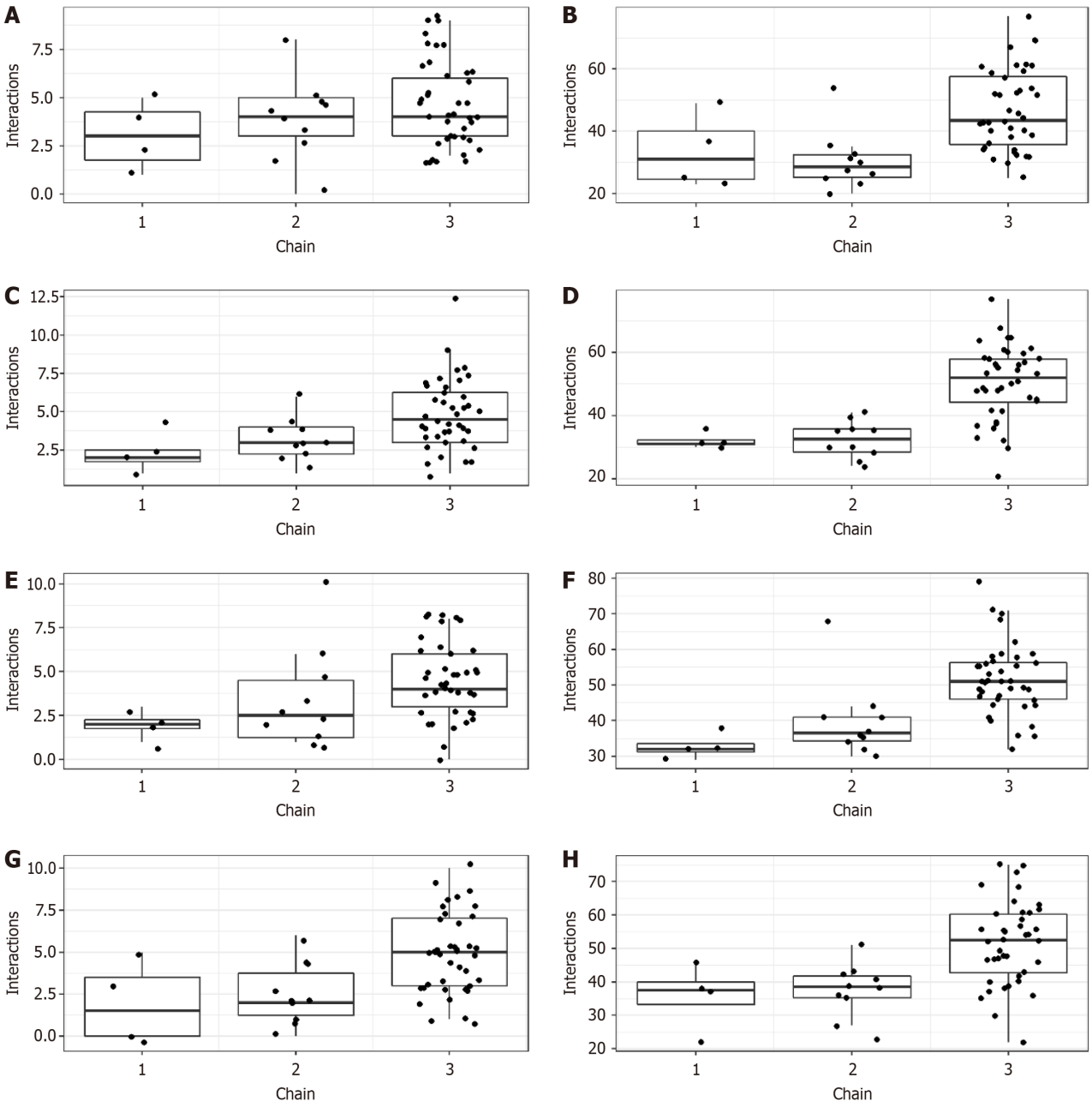

Figure 3 Interactions between severe acute respiratory syndrome-coronavirus 2 proteins and resin composite. A: Hydrogen bond between 6LU7 and resin composite; B: Hydrophobic interactions between 6LU7 and resin composite; C: Hydrogen bond between 6M2N and resin composite; D: Hydrophobic interactions between 6M2N and resin composite; E: Hydrogen bond between 6VYB and resin composite; F: Hydrophobic interactions between 6VYB and resin composite; G: Hydrogen bond between 6W9C and resin composite; H: Hydrophobic interactions between 6W9C and resin composite.

Among other results, Bis-GMA and Bis-EMA showed remarkable binding energy with all tested proteins, with ΔG values equal to or less than -5.0 kcal/moL. Such affinity relates to the number of interactions presented (*i.e.* hydrogen bonds and hydrophobic interactions) such that hydrogen bonds are more potent than hydrophobic interactions[20]. A higher number of oxygen atoms and a central, highly hydrophobic group present in Bis-GMA and Bis-EMA formed hydrogen bonds with hydroxyl radicals of polar amino acid residues and hydrophobic interactions with nonpolar amino acid residues. The fact that Mpro showed the highest binding energy to UDMA can be due to many interactions, primarily hydrogen bonds. A highly hydrophobic central area of Bis-EMA promoted many hydrophobic interactions with residues of PLpro, which was responsible for promoting the highest binding energy. Meanwhile, the highest binding energy (*i.e.* lowest affinity) obtained between TEGDMA and all proteins tested related to its having the smallest area of the monomers, which decreased the number of interactions with amino acid residues.

We evaluated binding energy values and interactions between SARS-CoV-2 proteins and non-polymerised methacrylate monomers and polymerised chains of resin composites. The growth of polymeric chains occurs when monomers are linearly connected by converting double C = C bonds into C–C bonds from different terminal methacrylate groups [21]. Monomers, especially Bis-GMA, may also be cross-linked *via* hydrogen bonds between hydroxyl groups and nitrogen or oxygen[22]. Thus, because hydrogen bonds and hydrophobic interactions between each non-polymerised

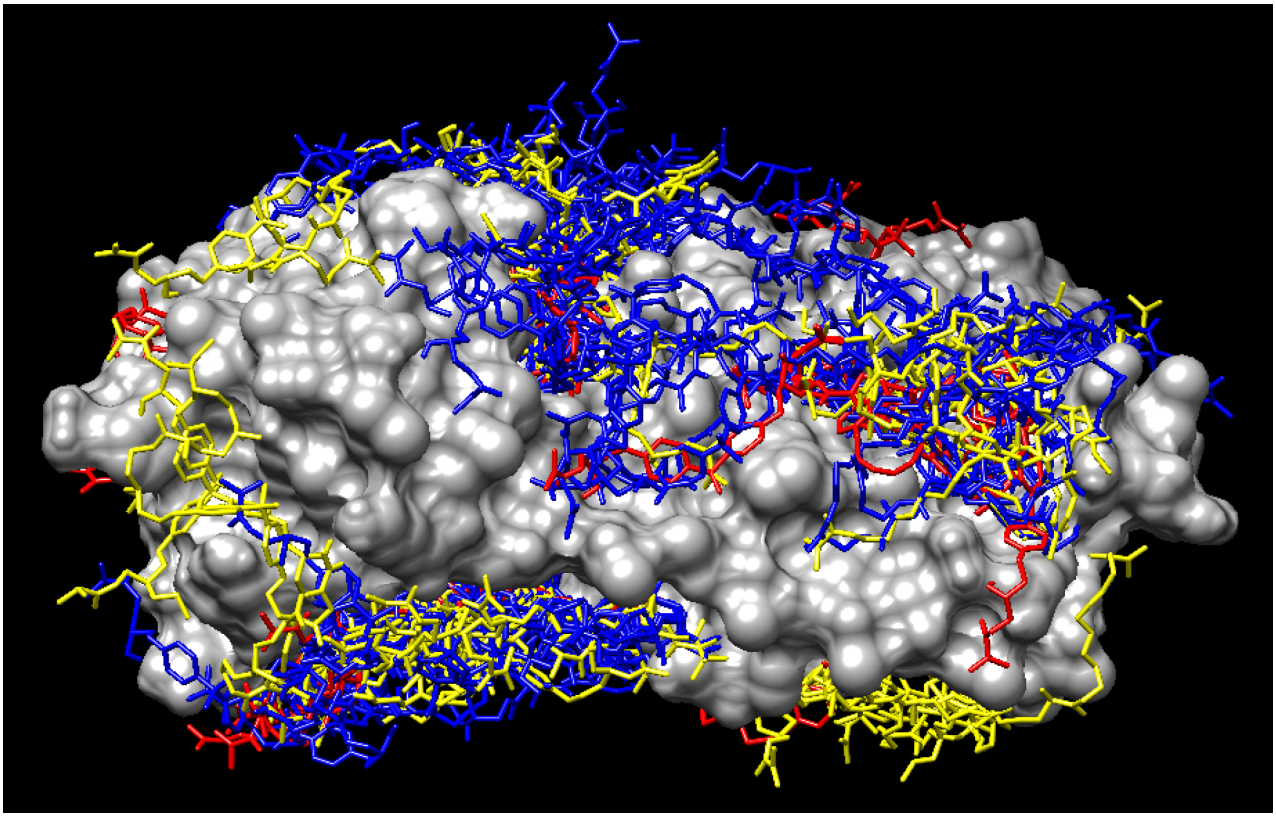

Figure 4 Graphical interaction between unpolymerised chain (red), 2-monomer chain (yellow), 3-monomer polymerised chain (blue), and the severe acute respiratory syndrome-coronavirus 2 protein.

monomer and SARS-CoV-2 proteins did not involve terminal methacrylate groups or hydroxyl groups in Bis-GMA, it was probable that similar binding between SARS-CoV-2 proteins and a polymerised chain would occur. Our results validate that assumption.

In a tooth preparation restored with resin composite, polymer chains of polymerised monomers and filler particles are likely present[21]. In general, resin composite restorations are polished in clinical conditions in order to achieve adequate smoothness and aesthetic properties and expose filler particles[23]. Thus, further investigations should evaluate the binding affinity of SARS-CoV-2 proteins to different filler particles. If a high binding affinity between them were found, then an increase the number of microorganisms might increase in resin composite restorations, and all implications highlighted by our results might increase. At the same time, another study[10] has shown that salivary amylase interacts with resin composites and collaborates in AP formation in filled resin composites. Thus, given our results, we believe that SARS-CoV-2 may also collaborate in AP formation.

In our computational study of a new microorganism, evidence to compare and corroborate our findings was inadequate. In response, *in vitro* and *in vivo* analyses need to be performed to validate our findings. Further research should also be conducted to clarify the mechanisms of interaction observed in our study. Despite those limitations, the chief strength of our work lies in its being the first to provide data about a possible interaction between resin composites and SARS-CoV-2. Besides that, due to concerns about the degradation of the resin–dentin interface[24], further studies could be performed to determine whether the virus will adhere to resin and collaborate in the resin–dentin degradation in dental adhesive systems.

CONCLUSION

SARS-CoV-2 proteins (*i.e.* Mpro, 3CLpro, PLpro, and the glycoprotein spike) showed an affinity to non-polymerised and polymerised resin composite chains.

FOOTNOTES

Author contributions: Sette-de-Souza PH, Fernandes Costa MJ and Dutra Borges BC designed, performed the experiments, acquired, analyzed, and interpreted the data; all of the authors wrote the manuscript and approved the final version of the article.

Supported by The Coordenação de Aperfeiçoamento de Pessoal de Nível Superior-Brasil (CAPES), No. 001.

Conflict-of-interest statement: All authors declare no conflict of interest in publishing the manuscript.

Data sharing statement: Request to the corresponding author.

Country of origin: Brazil

ORCID number: Pedro Henrique Sette-de-Souza 0000-0001-9119-8435; Moan Jéfter Fernandes Costa 0000-0002-7250-5863; Boniek Castillo Dutra Borges 0000-0003-4313-5776.

S-Editor: Luo ML
L-Editor: A
P-Editor: Zheng XM

REFERENCES

1 **Chen L**, Zhao J, Peng J, Li X, Deng X, Geng Z, Shen Z, Guo F, Zhang Q, Jin Y, Wang L, Wang S. Detection of SARS-CoV-2 in saliva and characterization of oral symptoms in COVID-19 patients. *Cell Prolif* 2020; **53**: e12923 [PMID: 33073910 DOI: 10.1111/cpr.12923]
2 **Adhikari SP**, Meng S, Wu YJ, Mao YP, Ye RX, Wang QZ, Sun C, Sylvia S, Rozelle S, Raat H, Zhou H. Epidemiology, causes, clinical manifestation and diagnosis, prevention and control of coronavirus disease (COVID-19) during the early outbreak period: a scoping review. *Infect Dis Poverty* 2020; **9**: 29 [PMID: 32183901 DOI: 10.1186/s40249-020-00646-x]
3 **Xu R**, Cui B, Duan X, Zhang P, Zhou X, Yuan Q. Saliva: potential diagnostic value and transmission of 2019-nCoV. *Int J Oral Sci* 2020; **12**: 11 [PMID: 32300101 DOI: 10.1038/s41368-020-0080-z]
4 **Cheng L**, Weir MD, Xu HH, Kraigsley AM, Lin NJ, Lin-Gibson S, Zhou X. Antibacterial and physical properties of calcium-phosphate and calcium-fluoride nanocomposites with chlorhexidine. *Dent Mater* 2012; **28**: 573-583 [PMID: 22317794 DOI: 10.1016/j.dental.2012.01.006]
5 **Alizadehgharib S**, Östberg AK, Dahlstrand Rudin A, Dahlgren U, Christenson K. The effects of the dental methacrylates TEGDMA, Bis-GMA, and UDMA on neutrophils in vitro. *Clin Exp Dent Res* 2020; **6**: 439-447 [PMID: 32543782 DOI: 10.1002/cre2.296]
6 **Müller C**, Lüders A, Hoth-Hannig W, Hannig M, Ziegler C. Initial bioadhesion on dental materials as a function of contact time, pH, surface wettability, and isoelectric point. *Langmuir* 2010; **26**: 4136-4141 [PMID: 19888741 DOI: 10.1021/la903299y]
7 **Nguyen S**, Adamczak M, Hiorth M, Smistad G, Kopperud HM. Interactions of liposomes with dental restorative materials. *Colloids Surf B Biointerfaces* 2015; **136**: 744-751 [PMID: 26519936 DOI: 10.1016/j.colsurfb.2015.10.024]
8 **Sabino-Silva R**, Jardim ACG, Siqueira WL. Coronavirus COVID-19 impacts to dentistry and potential salivary diagnosis. *Clin Oral Investig* 2020; **24**: 1619-1621 [PMID: 32078048 DOI: 10.1007/s00784-020-03248-x]
9 **Gomes SC**, Fachin S, da Fonseca JG, Angst PDM, Lamers ML, da Silva ISB, Nunes LN. Dental biofilm of symptomatic COVID-19 patients harbours SARS-CoV-2. *J Clin Periodontol* 2021; **48**: 880-885 [PMID: 33899251 DOI: 10.1111/jcpe.13471]
10 **Pelá VT**, Prakki A, Wang L, Ventura TMS, de Souza E Silva CM, Cassiano LPS, Brianezzi LFF, Leite AL, Buzalaf MAR. The influence of fillers and protease inhibitors in experimental resins in the protein profile of the acquired pellicle formed in situ on enamel-resin specimens. *Arch Oral Biol* 2019; **108**: 104527 [PMID: 31472277 DOI: 10.1016/j.archoralbio.2019.104527]
11 **Pappalardo F**, Russo G, Tshinanu FM, Viceconti M. In silico clinical trials: concepts and early adoptions. *Brief Bioinform* 2019; **20**: 1699-1708 [PMID: 29868882 DOI: 10.1093/bib/bby043]
12 **John JP**, Thirunavukkarasu P, Ishizuka K, Parekh P, Sawa A. An in-silico approach for discovery of microRNA-TF regulation of DISC1 interactome mediating neuronal migration. *NPJ Syst Biol Appl* 2019; **5**: 17 [PMID: 31098296 DOI: 10.1038/s41540-019-0094-3]
13 **Buonocore M**, Marino C, Grimaldi M, Santoro A, Firoznezhad M, Paciello O, Prisco F, D'Ursi AM. New putative animal reservoirs of SARS-CoV-2 in Italian fauna: A bioinformatic approach. *Heliyon* 2020; **6**: e05430 [PMID: 33173837 DOI: 10.1016/j.heliyon.2020.e05430]
14 **Tortorici MA**, Veesler D. Structural insights into coronavirus entry. *Adv Virus Res* 2019; **105**: 93-116 [PMID: 31522710 DOI: 10.1016/bs.aivir.2019.08.002]
15 **Ranjbar A**, Jamshidi M, Torabi S. Molecular modelling of the antiviral action of Resveratrol derivatives against the activity of two novel SARS CoV-2 and 2019-nCoV receptors. *Eur Rev Med Pharmacol Sci* 2020; **24**: 7834-7844 [PMID: 32744711 DOI: 10.26355/eurrev_202007_22288]
16 **Sette-DE-Souza PH**, Costa MJF, Amaral-Machado L, Araújo FADC, Almeida Filho AT, Lima LRA. Dental workers in front-line of COVID-19: an in silico evaluation targeting their prevention. *J Appl Oral Sci* 2021; **29**: e20200678 [PMID: 33787730 DOI: 10.1590/1678-7757-2020-0678]
17 **Hall DC Jr**, Ji HF. A search for medications to treat COVID-19 *via* in silico molecular docking models of the SARS-CoV-2 spike glycoprotein and 3CL protease. *Travel Med Infect Dis* 2020; **35**: 101646 [PMID: 32294562 DOI: 10.1016/j.tmaid.2020.101646]
18 **Trott O**, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *J Comput Chem* 2010; **31**: 455-461 [PMID: 19499576 DOI: 10.1002/jcc.21334]
19 **Abdel Bar FM**, Elsbaey M, Taha N, Elgaml A, Abdel-Fattah GM. Phytochemical, antimicrobial and antiquorum-sensing studies of pulicaria undulata L.: a revision on the structure of 1β,2α,3β,19α,23-pentahydroxy-urs-12-en-28-oic acid. *Nat Prod Res* 2020; **34**: 804-809 [PMID: 30422011 DOI: 10.1080/14786419.2018.1503658]
20 **Yadav R**, Imran M, Dhamija P, Chaurasia DK, Handu S. Virtual screening, ADMET prediction and dynamics simulation of potential compounds targeting the main protease of SARS-CoV-2. *J Biomol Struct Dyn* 2021; **39**: 6617-6632 [PMID: 32715956 DOI: 10.1080/07391102.2020.1796812]

21 **Pratap B**, Gupta RK, Bhardwaj B, Nag M. Resin based restorative dental materials: characteristics and future perspectives. *Jpn Dent Sci Rev* 2019; **55**: 126-138 [PMID: 31687052 DOI: 10.1016/j.jdsr.2019.09.004]

22 **Lemon MT**, Jones MS, Stansbury JW. Hydrogen bonding interactions in methacrylate monomers and polymers. *J Biomed Mater Res A* 2007; **83**: 734-746 [PMID: 17559132 DOI: 10.1002/jbm.a.31448]

23 **de Fátima Alves da Costa G**, Melo AMDS, de Assunção IV, Borges BCD. Impact of additional polishing method on physical, micromorphological, and microtopographical properties of conventional composites and bulk fill. *Microsc Res Tech* 2020; **83**: 211-222 [PMID: 31793704 DOI: 10.1002/jemt.23404]

24 **Amin F**, Fareed MA, Zafar MS, Khurshid Z, Palma PJ, Kumar N. Degradation and Stabilization of Resin-Dentine Interfaces in Polymeric Dental Adhesives: An Updated Review. *Coatings* 2022; **12**: 1094 [DOI: 10.3390/coatings12081094]

Published by **Baishideng Publishing Group Inc**
7041 Koll Center Parkway, Suite 160, Pleasanton, CA 94566, USA
Telephone: +1-925-3991568
E-mail: office@baishideng.com
Help Desk: https://www.f6publishing.com/helpdesk
https://www.wjgnet.com