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EDITED BY

Dimitrios Koutsouras,
University of Bath, United Kingdom

REVIEWED BY

Angsuman Sarkar,
Kalyani Government Engineering College
(KGEC), India

*CORRESPONDENCE

Rupam Goswami,
✉ rupam21@tezu.ernet.in

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Beyond ideal models: non-idealities in TCAD simulations of dielectric-modulated FETs for label-free biosensing

Rupam Goswami^{1*}, Vivek Menon U ², Suman Kumar Mitra³,
Deepjyoti Deb⁴, Prachuryya Subash Das¹, Hirakjyoti Choudhury⁵
and Raja Vipul Gautam¹

¹Technology in Semiconductors and Devices Laboratory, Department of ECE, School of Engineering, Tezpur University, Tezpur, Assam, India, ²Department of Engineering “Enzo Ferrari”, University of Modena and Reggio Emilia, Modena, Italy, ³Quest-Global, Bengaluru, Karnataka, India, ⁴Department of ECE, SRM Institute of Science and Technology-Vadapalani Campus, Chennai, Tamil Nadu, India, ⁵Department of Electronics, North Lakhimpur University, Lakhimpur, Assam, India

Dielectric modulation in field-effect transistors (FETs) for label-free biosensing have been extensively explored to date, mostly due to the availability of semiconductor device technology computer-aided design (TCAD) tools. Of these works, many reports have revolved around TCAD simulations and focused on ideal or slightly deviated-from-ideal conditions, rather than on the inclusion of non-idealities to create actual biosensing test scenarios. This perspective presents a status of label-free dielectric-modulated biosensing in FETs. It highlights the five most important but rarely used or missing non-idealities in semiconductor TCAD tools, viz., multispecies representation, biomolecular kinematics, cavity profile, hybridization, and transient response. To better align TCAD frameworks with experimental studies, this article recommends adopting method-specific TCAD-integrated modeling (MSTIM) approaches.

KEYWORDS

TCAD, dielectric-modulated biosensor, steric hindrance, kinematics, selectivity, sensitivity, cavity profile, hybridization

1 Introduction

Dielectric modulation in field-effect transistors (FETs) for biosensing purposes has garnered widespread interest since the demonstration of the phenomenon (Im et al., 2007). While the fabrication of the biosensor using a conventional CMOS fabrication process flow was significant in the timeline, it was the simulation framework that inspired research work on dielectric-modulated (DM) biosensing using FETs.

Technology computer-aided design (TCAD) tools for semiconductor devices have revolutionized the electronics design and technology sector on many fronts while reducing financial and design costs (SDU Manual, 2022; Sarkar, 2018). Major functional advantages of TCAD tools include (a) design and simulation of two-dimensional and three-dimensional device architectures; (b) flexibility and options of using several physics-based models to describe device principles; (c) parametric visualization of electrical

parameters; (d) definition of new material properties for simulation; (e) device-to-circuit and mixed mode analyses.

The ability of the TCAD tools to conveniently design and simulate FETs has shaped the way research has progressed in the area of DM label-free biosensing using FETs. The design of cavities in the gate dielectric of FETs for dielectric-modulated biosensing has led to the emergence of different configurations of DM biosensors across devices of multiple architectures and principles of operation, which include metal oxide semiconductor (MOS) FETs (Das et al., 2025; Yojo et al., 2021), tunnel FETs (Vadizadeh et al., 2025; Elshafie et al., 2025; Kondavitee et al., 2025; Hussian et al., 2024), fin-shaped FETs (Gandhi and Kondekar, 2025), nanotube FETs (Hadded et al., 2024; Ho et al., 2024), and junctionless FETs (Singh et al., 2024; Son et al., 2025). While the number of studies of FET architectures for biosensing is exceptional, there has been slow progress in the design of simulation environments with near-practical test scenarios.

The major challenge in most TCAD tools is the absence of full-scale biomolecular kinematics and electrochemical models. This roadblock in the evolution of the TCAD environment includes the non-idealities encountered in real-world DM biosensing applications. Another concern is that while few articles have attempted to explore this area and presented interesting solutions, the same does not apply to benchmarking the simulation environments for such works. This has not only affected the way in which TCAD simulations are carried out for DM biosensors but also has led to methods that have become repeatable and mostly predictable.

The primary objective of this article is to assess the current state of the art in FET-based DM biosensors and present the gaps in TCAD frameworks that can be explored to propel the research in this area with better test scenarios and methods. To avoid ambiguity, it is to be noted that any one of the terminologies—*label-free biosensors*, *dielectric-modulated (DM) biosensors*, *FET-based DM biosensors*, or *FET-based biosensors*—refers to cavity-embedded FET-based label-free dielectric-modulated biosensors.

2 Current status, gaps, and challenges

2.1 Architecture

In the context of label-free biosensing, dielectric modulation refers to the principle by which altering the material properties (dielectric constant, κ , or charge, Q_T) of the gate dielectric in a FET leads to alteration of the device's electrical parameters, such as, but not limited to, drain current (I_D), threshold voltage (V_{TH}), and subthreshold swing (SS).

As mentioned in Section 1, the currently proposed TCAD analyses of DM biosensors originate from the work of Im et al. (2007). The fabricated DM FET-based biosensor reported by the authors had a partially etched chromium cavity (leading to an air gap) beneath the gold electrodes. To demonstrate dielectric modulation in a biotin–streptavidin system, the reported FET was fabricated with a cavity length of 200 nm in experiments (400 nm using a TCAD tool) and a cavity height of 15 nm (Im et al., 2007). Using a dielectric constant of 2.1 in the cavity, TCAD simulations showed a shift in the threshold voltage of the device; a similar trend was observed for the experimental measurement. The

report further proved that the biotin–streptavidin binding can be reversibly broken, showing that after it is broken, V_{TH} recovered to the value corresponding to the state before the biotin–streptavidin binding occurred.

Based on the work mentioned in the preceding paragraph, it is a fundamental design principle in current TCAD frameworks that while creating any FET-based DM biosensor in a TCAD tool, the gate dielectric region beneath the gate material is divided into at least two dielectric materials. One material that represents the actual gate dielectric partially fills the region, provides support to the gate material in principle, and has a fixed dielectric constant. The other dielectric material is used to represent the etched cavity—its dielectric constant (κ) is set to 1 to represent an empty or air-filled cavity and set to a specific value to represent the biomolecules when occupied. The change in the cavity dielectric constant and charge affects the surface potential in a conventional MOS system, and therefore, a change in its electrical parameters can be observed.

While several works have focused on specific biomolecules such as breast cancer markers (Prasanthi et al., 2025), uricase, APTES, bacteriophage, keratin (Mohanty et al., 2021), and SARS-CoV-2 (Yadav et al., 2021), others have demonstrated the performance of DM FET biosensors using values of dielectric constants and charge (Raut et al., 2025; Goswami and Bhowmick, 2019). Sensitivity in such biosensors is measured according to the relative change in an electrical parameter like drain current and threshold voltage with reference to an air-filled cavity, mathematically described by the following form: $Sensitivity = |P(\kappa_a) - P(\kappa_{air})/P(\kappa_{air})|$, where $P(\kappa_a)$ is the value of the electrical parameter when the cavity is filled with the bioanalytes, and $P(\kappa_{air})$ is the value of the electrical parameter when the cavity is empty (filled with air) (Mohanty et al., 2021; Goswami and Bhowmick, 2019).

2.2 Considerations and deviations in TCAD simulations

This section highlights the methods through which key conditions are currently considered in TCAD simulations and their deviations from practical scenarios, if any. These methods and conditions are discussed in a tabular format (Table 1) to fill the gaps and missing cases in TCAD frameworks that may be reliably used to create test scenarios that are close to actual scenarios.

3 Method-specific TCAD-integrated modeling (MSTIM): perspectives for better models

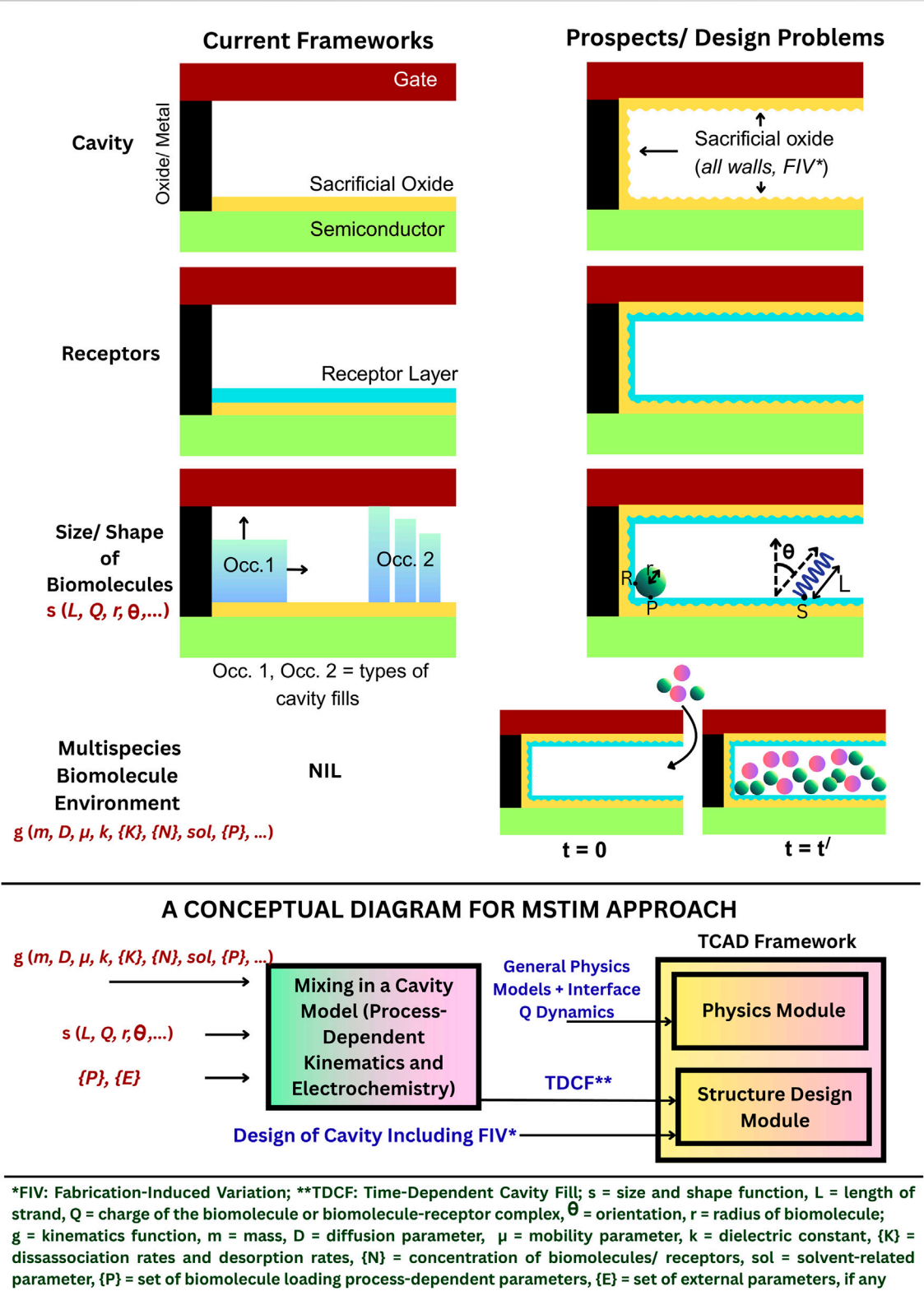
It is evident from Section 2 that advances in the domain of DM biosensors using TCAD tools have occurred from the standpoint of architectures and types of devices and placement of the cavity. The primary purpose of TCAD tools is to create predictive frameworks for real-world scenarios so that time, effort, and cost are minimized and optimization is done before fabricating a device. Progress in the areas of design of experiment-mimicking models and measurement methods using TCAD tools is expected to complement the work in experimental biosensing.

TABLE 1 TCAD strategies for DM FET-based biosensors, their current status, and deviations from practical scenarios.

Condition	Considerations/assumptions in TCAD frameworks	Deviation(s) from practical scenarios
Kinematics/transport of biomolecules and fill factor, cavity profile	<p>TCAD strategies are based on the assignment of a dielectric material region to represent the cavity, which points to the assumption that the hybridization has already occurred. The dielectric constant and the charge of the region or interface define the type of biomolecule. The general consideration is that the fill factor, which defines the percentage of the volume of the cavity when filled with biomolecules, is taken to be 100% for maximum performance (Raut et al., 2025; Mohanty et al., 2021; Goswami and Bhowmick, 2019).</p> <p>In cases of partial hybridization when fill factors are lower than 100%, a one-dimensional scenario is generally considered in TCAD simulations (Raut et al., 2025; Mohanty et al., 2021; Goswami and Bhowmick, 2019). Only a few works have reported the impact of the orientation of DNA strands on the performance of biosensors (Kalra et al., 2016).</p> <p>Additionally, the cavity profile is assumed ideally damage-free with no edge roughness due to etching.</p>	<p>The kinematics and transport of the biomolecules inside the cavity in a single-species or multispecies environment are not considered.</p> <p>In practice, fill factors are not 100%. The accurate fill factor in practical conditions depends on the physical state of the etched cavity (size and roughness), size and orientation of the biomolecules, and non-uniform partial hybridization in three dimensions.</p> <p>The nanocavity profile plays an important role in the biosensing process. During the etching process, the walls of the cavity may undergo undesirable damage, which can be extracted from a TEM (micrograph) profile of a fabricated cavity. The design of such a realistic cavity profile is expected to lead to an accurate representation of DM biosensing.</p>
Steric hindrance and partial hybridization	<p>Steric hindrance is a case of partial hybridization in which biomolecules inside the cavity prevent the entry of further biomolecules.</p> <p>By taking different profiles of the biomolecule-represented dielectric region in TCAD tools (<i>widely used are monotonically increasing, monotonically decreasing, concave, and convex</i>), the steric hindrance scenario is tested for a single type of biomolecule (Kumar and Chauhan, 2023; Bhattacharyya et al., 2020; Bhattacharyya et al., 2022; Goswami and Bhowmick, 2019).</p>	<p>Steric hindrance is usually relevant when larger molecules block the path for smaller molecules, which generally indicates a scenario in which more than one type of molecule is present. Generally, only one type of molecule is considered in the TCAD simulations.</p> <p>In another scenario, the blockade can be due to the same type of biomolecules, a problem that the current literature addresses appropriately with limited TCAD models.</p>
Selectivity and specificity (multispecies environment)	<p>Selectivity of a biomolecule refers to the distinct biorecognition of a specific target biomolecule by the biosensor despite the presence of other biomolecules or analytes. Specificity refers to the ability of a probe to bind with the specific target biomolecules (Morales and Halpern, 2018).</p> <p>Current TCAD strategies do not possess a model for executing a probe-target binding electrochemistry. To represent hybridization (binding) in a TCAD scenario, one designates a filled region with the assignment of dielectric constant and charge at the interface (Goswami and Bhowmick, 2019).</p> <p>Existing as a measurable metric, selectivity is presented as a relative difference of an electrical parameter, usually drain current, between a target biomolecule and non-target biomolecules:</p> <p>Selectivity = $\frac{I_{DS}(\kappa_a) - I_{DS}(\kappa_{ref})}{I_{DS}(\kappa_{ref})}$, where $I_{DS}(\kappa_a)$ is the drain current of the measured analyte, and $I_{DS}(\kappa_{ref})$ is the drain current of the reference biomolecule. It does not, however, represent a multispecies environment (Elshafie et al., 2025).</p>	<p>There are two cases in experimental scenarios, one in which the responses of the biosensor to the target biomolecules and non-target biomolecules are measured one at a time, and two, in which a multispecies environment is considered simultaneously.</p> <p>In TCAD analyses, there is a partial provision for the former case in which the dielectric constant and the charge of the biomolecules are used to define selectivity in terms of an electrical parameter.</p> <p>However, there is no simulation test scenario proposed to date for the latter, considering the size, orientation, transport, and kinematics of the biomolecules.</p>
Transient analysis	<p>A few works have reported transient simulations on TCAD for DM biosensors (Choudhary et al., 2025; Dwivedi et al., 2021). The extraction of settling time has been incorporated in TCAD simulations (Dwivedi et al., 2021); however, a mechanism to measure the recovery time of the biosensor is yet to be implemented</p>	<p>In practical scenarios, transient measurements with instants of exposure and removal of target and non-target biomolecules one after another are used to determine the response and recovery times of the biosensor, along with the amplitude of the sensing parameter. This effect has been partially achieved in TCAD simulations, as mentioned in the adjacent column.</p>

Current considerations in TCAD simulations (Refer to Table 1) are yet to include several practical conditions. Some innovation prospects in TCAD frameworks are method-inclusive with sufficient considerations for non-idealities, such as the impact of the method of loading on steric hindrance (including size of biomolecules, and cavity profiles), partial hybridization (including real experimental profiles), and response and recovery times (reference to transient analyses). Therefore, a method-specific TCAD-integrated modeling (MSTIM) approach is proposed with emphasis on a holistic TCAD framework. Here, the terminology *method* is inclusive of all variables (related to functionalization, kinematics,

transport, cavity profile, shape, properties of biomolecules, device design, and measurement) that may decide the process of biosensing. Figure 1 shows the basis for an MSTIM approach, highlighting the importance of the design of the cavity with possibilities of including cavity designs based on actual post-etching profiles. Similarly, the representation of receptor layers may vary from a single layer to multi-wall layers, depending on the method of receptor functionalization. The inclusion of the size and shape of biomolecules in TCAD structural designs is another possibility. For cavities that are only 10–15 nm in height, the length or diameter and orientation of the molecules (bioanalytes and receptors), along with that of any self-



environment, which remains underrepresented in current TCAD frameworks.

One of the important scenarios in a multispecies environment is the *mixing-in-a-box* problem (e.g., rapid mixing process or diffusion-limited process) (Chanda et al., 2023). The process by which the biomolecules move and interact inside a cavity when inserted is important in small cavities. Such analyses using the Langmuir kinematics and diffusion-limited process have been reported for ion-sensing field-effect transistors (ISFETs) (Chanda et al., 2023; Wadhwa et al., 2024); however, similar kinematics and transport mechanisms have not been used in the case of DM FET biosensors.

Existing works on FET-based DM biosensors using TCAD tools generally refer to the dry or near-dry sensing of biomolecules (referring to a state in which a dry cavity is occupied with either vacuum or biomolecules or both, during measurement) instead of wet sensing as in ISFETs (Hu et al., 2023). However, the so-called *dry sensing* in FET-based DM biosensors depends on several wet steps (Im et al., 2007), which, if considered, can make the TCAD frameworks robust and more realistic. Interestingly, during the functionalization of the cavity in such biosensors, the receptors and bioanalytes are transported to the cavity using appropriate buffer solutions. The cavity is dried with ultra-pure nitrogen after every step of functionalization, or at the end (Im et al., 2007). This indicates that models for Langmuir kinematics and diffusion-limited processes in ISFETs can be applied to DM FET-based biosensors to determine the filling of the cavity (time-dependent cavity fill: TDCF). On the other hand, apart from kinematics and transport, measurement models can account for buffer residues due to incomplete or faulty nitrogen drying, an aspect that has not yet been discussed in reported works.

Dielectric-modulated FET (DM FET) biosensors currently rely almost exclusively on aqueous-phase insertion of biomolecules into cavities. While effective, such wet-loading often suffers from uneven filling, nonspecific adsorption, and structural instability of biomolecules during processing. To move beyond these limitations, it is worth considering dry and near-dry loading methods that, although not yet implemented in DM-FETs, have shown promise in other biomolecule immobilization and pharmaceutical biomolecule or drug delivery technologies.

Aerosol or electrospray deposition may provide localized, reproducible loading by rapidly evaporating nebulized droplets, but shear forces and solvent compatibility with semiconductor surfaces are concerns (Mensink et al., 2017; Kavadiya and Biswas, 2018). Lyophilization-infiltration cycles offer a hybrid route to combine penetration with stability, although multiple drying steps may complicate device fabrication (Nadkarni et al., 2024; Kawasaki et al., 2019; Gaidhani et al., 2015). Vacuum-assisted dry loading could allow insertion of lyophilized biomolecules into cavities without exposing the dielectric to swelling or liquid-induced defects, although its efficiency in nanoscale pores remains unknown (Nadkarni et al., 2024; Mensink et al., 2017). Supercritical CO₂-assisted insertion is particularly attractive for its ability to deeply penetrate cavities and leave no solvent residues, but adapting high-pressure processes to semiconductor devices poses engineering challenges (do Nascimento Junior et al., 2021). Sublimation-based or electric-field-assisted sublimation deposition (Guo et al., 2015) has not yet been demonstrated in cavity-based FET biosensors, but

conceptually it could inspire solvent-free loading strategies, especially for smaller biomolecular species or for protective coatings that help stabilize larger biomolecules. The feasibility depends heavily on adapting the chemistry to preserve bioactivity during the sublimation process.

Although academic in principle, these methods highlight unexplored opportunities for DM FET biosensors. If adapted successfully, they could offer more uniform, residue-free, and stable biomolecule loading than conventional aqueous approaches. Systematic studies are needed to assess their feasibility. They represent a forward-looking direction for enhancing the robustness and reproducibility of label-free DM FET biosensing.

Although TCAD tools are devoid of method-specific models, externally designed time-dependent models can be used to determine the orientation and position of receptors and biomolecules inside the cavity so that their profile can be included in TCAD simulations.

4 Future directions

The domain of FET-based DM label-free biosensors is promising and has been explored to the best of the potential of the TCAD tools so far. With innovation in experiments growing with time, there is a need for progress in simulation frameworks for such biosensors. The current status of the DM biosensors reveals a one-directional progress, and therefore, the domain demands for innovation in TCAD strategies for DM biosensing. Method-specific models incorporating variables that describe the kinematics, nature of molecules, cavity design parameters, and other external parameters are expected to assist experimental studies. Holistic TCAD frameworks supported by such MSTIM approaches are expected to revolutionize the FET-based DM biosensing research. TCAD models could explore other bioanalyte loading methods that are widely used in other biomolecule immobilization strategies or in the pharmaceutical industries. While assessment is required to test alternative strategies, the process involved therein may open new avenues in modeling DM FET biosensors.

The advent of artificial intelligence (AI) and machine learning (ML) in the exploration of semiconductor devices is a boon to the industry. At a time when such state-of-the-art technologies are being applied to experiments in biosensing, TCAD frameworks must be built with better models and approaches so that the prediction of the performance of these biosensors is more efficient.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

RG: Conceptualization, Writing – review and editing, Investigation, Supervision, Writing – original draft. VMU: Writing – original draft, Resources, Investigation, Writing – review and editing. SM: Writing – original draft,

Supervision, Writing – review and editing. DD: Writing – review and editing, Investigation, Writing – original draft. PD: Investigation, Writing – review and editing, Writing – original draft. HC: Writing – original draft, Investigation, Writing – review and editing. RG: Writing – original draft, Writing – review and editing, Investigation.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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