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Radiative transfer and inversion codes for characterizing planetary atmospheres: an overview

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The study of planetary atmospheres is crucial for understanding the origin, evolution, and processes that shape celestial bodies like planets, moons and comets. The interpretation of planetary spectra requires a detailed understanding of radiative transfer (RT) and its application through computational codes. With the advancement of observations, atmospheric modelling, and inference techniques, diverse RT and retrieval codes in planetary science have been proliferated. However, the selection of the most suitable code for a given problem can be challenging. To address this issue, we present a comprehensive mini-overview of the different RT and retrieval codes currently developed or available in the field of planetary atmospheres. This study serves as a valuable resource for the planetary science community by providing a clear and accessible list of codes, and offers a useful reference for researchers and practitioners in their selection and application of RT and retrieval codes for planetary atmospheric studies.

KEYWORDS

atmospheres, radiative transfer, planets and satellites, retrieval, exoplanets

1 Introduction

Planetary science, including the study of exoplanets, is currently a very active and fascinating multi-disciplinary field covering astronomy, astrophysics, geophysics, astrobiology, among other fields. By studying planets, we can answer fundamental questions about their origin, formation, evolution, potential for life, and physico-chemical processes. The spectrum of a planet contains valuable information about its atmospheric chemical composition and physical processes. Deriving atmospheric properties like the vertical thermal structure, chemical composition and dynamics is essential to understand the origin, evolution, and how the atmospheres are influenced by physical and chemical mechanisms. Numerous physico-chemical problems in planetary atmospheres require a detailed understanding of radiative transfer (RT) of photons in different environments. Detailed solutions of the RT equation demand high computational capabilities. The technical implementation of these solutions in codes is a rapidly developing area, and numerous RT approaches have been attempted in recent years. Several groups then attacked the problem from a variety of perspectives by using completely different, independent and dedicated numerical algorithms. Some atmospheric RT codes have been developed with a particular aim or for the interpretation of a particular planet. Later on, in some cases, their functionalities have been extended beyond their original purposes but still limited to the study of a specific type of planets. In recent years, breakthroughs in atmospheric retrieval have been made possible through a combination of advancements in instrumentation, computational resources, sophisticated atmospheric modelling, and powerful statistical inference techniques.

There are varying levels of complexity in atmospheric models and the physico-chemical processes considered in RT and inversion codes, motivated by atmospheric observations. As a result, a significant number of RT and inversion codes have been developed and widely used in different atmospheric contexts, depending on whether the planet being studied is Earth, another planet or body in the Solar System, or an exoplanet. Spectra of Solar System planets can be spatially distributed and have a high signal-to-noise ratio, and can be supplemented with *in situ* measurements or *a priori* knowledge. However, exoplanetary spectroscopy currently lacks this observational capability, and retrievals must navigate a much larger parameter space for exoplanetary atmospheres than that for Solar System planets.

The selection of a particular code may depend on various factors, such as the physical problem to face, the estimation technique, computation time, flexibility, user-friendliness, among others. The selection of the most appropriate code suited for a specific problem may result in more accurate and reliable results, highlighting the importance of having a comprehensive list of available codes. This mini-review provides a comprehensive overview of the current RT and inversion codes used in the planetary and exoplanetary communities, as seen from the perspective of a user. These codes are crucial in predicting and interpreting spectra of planetary atmospheres, both in hydrostatic equilibrium and in expanding comas. The quality and extent of these codes are critical for the effective use of space and ground-based telescopes facilities. Madhusudhan (2018) has already provided a review of exoplanetary atmospheric retrieval, some existing retrieval codes, and a description of their differences, Barstow and Heng (2020) provides a discussion of open problems in retrieval analysis, and more recently, MacDonald and Batalha (2023) provides a catalogue of the atmospheric retrieval codes for exoplanets published to date. In this mini-review, we expand and update the codes list, including a large new generation of RT and atmospheric retrieval codes for Solar System and exoplanets.

2 RT and inversion codes

One commonly used way to interpret the measured spectra is calculating a synthetic spectrum for comparison with that measured by solving the radiative transfer (forward model) -i.e., computation of the outgoing radiation from the planetary surface for a given set of free parameters-, and inferring parameters like temperature and chemical abundance profiles. This last step is called inversion or retrieval and consists in comparing the measured and best modelled/synthetic spectra adjusting the atmospheric parameters in such a way as to minimise any discrepancy. A number of radiative transfer codes or forward models and inversion algorithms are already constructed, and generally available and used by the planetary and exoplanetary characterisation communities. A comprehensive list of RT and retrieval codes in the literature is shown in **Table 1**, indicating where to find them (if available) and the estimation technique employed (**Section 3**).

Retrieval codes can use either parametric models or self-consistent equilibrium models to estimate the composition and pressure-temperature (P-T) profiles from spectral data. Parametric models do not make any assumptions about thermochemical and radiative-convective equilibrium, using instead parametric forms for the P-T profile and composition. Self-consistent models compute profiles based on assumptions of the atmosphere's physical and chemical properties and processes, with varying levels of complexity from 1-D atmospheres to full 3-D general circulation models. We do not cover 3-D general circulation codes specifically in this paper, they are complex and couple many processes together in a three-dimensional time-marching calculation. For a discussion of the principles of atmospheric retrievals of exoplanets see Gandhi and Madhusudhan (2017). When calculating a synthetic atmospheric spectrum, lines are read from atomic and molecular databases -databases differ in completeness and accuracies-, and opacities are calculated via diverse approaches (Rengel, 2022).

Some RT models used for Solar System planets and exoplanets have their roots in Earth codes. There are several RT codes used in the Earth atmospheric community but they are just listed here: 4A/OP [Scott (1974); Scott and Chedin (1981)], 6S [Lee et al. (2020)], AccuRT[1] [Stamnes et al. (2018)]; ARMS Weng et al. (2020), BIRRA[2] [Gimeno García et al. (2011)], BTRAM[3] [Chapman et al. (2004)], DISORT [Stamnes et al. (1988)], Eradiate[4] [Govaerts et al. (2022)], FASCODE [Smith et al. (1978); Clough et al. (1981)], FUTBOLIN [Martin-Torres and Mlynczak (2005)], GARLIC [Schreier et al. (2014)], GENLN2 [Edwards (1992)], IMAP-DOAS [Frankenberg et al. (2005)], IMLM Gloudemans et al. (2005), KCARTA[5,6] [DeSouza-Machado et al. (2020)], LBLRTM[7,8] [Clough et al. (2005)], LEEDR [Fiorino et al. (2014)], LinePak[9] [Gordley et al. (1994)], libRadtran[10] [Mayer and Kylling (2005)], MODTRAN[11] [Berk et al. (1998)], MPI[12] [Gropp et al. (1998)], PUMAS[13] [Villanueva et al. (2015); Villanueva et al. (2022)], RFM[14] [Dudhia (2017)], RTMOM [Govaerts (2006)], RTTOV[15]

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[1] http://www.geminor.com/accurt.html.

[2] https://www.dlr.de/eoc/en/desktopdefault.aspx/tabid-5447/9970_read-20673/.

[3] https://blueskyspectroscopy.com/?page_id=21.

[4] https://www.eradiate.eu/site/.

[5] http://asl.umbc.edu/pub/packages/kcarta.html.

[6] https://github.com/sergio66/kcarta_gen.

[7] http://rtweb.aer.com/lblrtm.html.

[8] https://github.com/AER-RC/LBLRTM.

[9] https://spectralcalc.com/info/about.

[10] http://www.libradtran.org/doku.php.

[11] http://modtran.spectral.com.

[12] https://mitpress.mit.edu/9780262571234/mpi-the-complete-reference/.

[13] https://psg.gsfc.nasa.gov/.

[14] http://eodg.atm.ox.ac.uk/RFM/.

[15] https://nwp-saf.eumetsat.int/site/software/rttov/.

TABLE 1 Some radiative transfer and inversion codes used in the (exo) planetary community. Symbols: OE algorithm (†), nested sampling (‡), MCMC method (▲), Grid search (•), and ML approaches (⧫).

Code name	Link	References
Alfnoor ‡	—	Changeat et al. (2020)
APOLLO ▲	https://github.com/alexrhowe/APOLLO	Howe et al. (2017) and Howe et al. (2022)
ARCiS ‡	http://www.exoclouds.com	Min et al. (2020)
ARTS †	https://radiativetransfer.org/	Buehler et al. (2018)
ASIMUT †	—	Vandaele et al. (2006b) and Vandaele et al. (2006a)
ATMO ▲ ‡ •	https://www.erc-atmo.eu/?page_id=322	Tremblin et al. (2015), Wakeford et al. (2017), and Evans et al. (2017)
AURA ‡	—	e.g., Pinhas et al. (2018)
Aura-3D ‡	—	Nixon and Madhusudhan (2022)
Aurora ‡	—	Welbanks and Madhusudhan (2021)
BART ▲	https://github.com/exosports/BART	Blecic (2016)
Benneke & Seager ‡	—	Benneke and Seager (2013)
Brewster ‡▲	—	Burningham et al. (2017)
Carrión-González et al. ▲	—	Carrión-González et al. (2020)
Cerberus ▲	—	Swain et al. (2014)
CCF-sequence ⧫	—	Fisher et al. (2020)
CHIMERA †▲‡	https://github.com/mrline/CHIMERA	Line et al. (2013)
DISORT	http://www.rtatmocn.com/	Stamnes et al. (2000)
Dynesty ‡	https://dynesty.readthedocs.io/en/stable/	Speagle (2020)
Ehrenreich et al.	—	Ehrenreich et al. (2006)
exoCNN ⧫	https://gitlab.astro.rug.nl/ardevol/exocnn	Martínez et al. (2022)
ExoGAN ⧫	https://osf.io/6dxps/	Zingales and Waldmann (2018)
ExoJAX ▲	https://github.com/HajimeKawahara/exojax	Kawahara et al. (2022)
ExoReL ℛ‡	—	Damiano and Hu (2020)
exoretrievals ‡	—	Espinoza et al. (2018)
Exo-REM	https://gitlab.obspm.fr/Exoplanet-Atmospheres-LESIA/exorem	Baudino et al. (2015) and Baudino et al. (2017)
Fortney et al. •	—	Fortney et al. (2005) and Fortney et al. (2010)
gCMCRT	https://github.com/ELeeAstro/gCMCRT	Lee et al. (2022)
Gibson et al.▲	—	Gibson et al. (2020)
HARP	https://github.com/luminoctum/athena-harp	Li et al. (2018)
HELA ⧫	https://github.com/exoclime/HELA	Marquez-Neila et al. (2018)
HELIOS-R ‡	https://github.com/exoclime/HELIOS	Lavie et al. (2017) and Oreshenko et al. (2017)
Helios-r2 ‡	https://github.com/exoclime/Helios-r2	Kitzmann et al. (2020)
Home made (MPS) †	—	Jarchow (1998)
HRCCS ‡	https://www.dropbox.com/sh/0cxfolfmrs8ip37/AABZYoHr8nuRlHJG84dArX4ea?dl=0	Brogi and Line (2019)
HyDRA ‡	—	Gandhi and Madhusudhan (2017)
HyDRo ‡	—	Piette et al. (2021)
INARA ⧫	https://gitlab.com/frontierdevelopmentlab/astrobiology/inara	Soboczenski et al. (2018)
Johnson & Marley ⧫	https://github.com/WreckItTim/MLP-Estimating-Exoplanet-Parameters	Johnsen et al. (2020)

(Continued on the following page)

TABLE 1 (*Continued*) Some radiative transfer and inversion codes used in the (exo) planetary community. Symbols: OE algorithm (†), nested sampling (‡), MCMC method (▴), Grid search (•), and ML approaches (⧫).

Code name	Link	References
KOPRA	https://www.imk-asf.kit.edu/english/312.php	Hoepfner et al. (1998), Stiller et al. (1998, 2000, 2002)
Lellouch et al. †	—	Lellouch et al. (2017)
Lupu et al. ▲‡	—	Lupu et al. (2016)
Madhusudhan & Seager •▲	—	Madhusudhan and Seager (2009)
Madhusudhan et al. ▲	—	Madhusudhan and Seager (2010) and Madhusudhan et al. (2011)
MARGE ⧫	github.com/exosports/marge	Himes et al. (2022)
Marley & McKay	—	Marley and McKay (1999)
MassSpec ▲	—	de Wit and Seager (2013)
MERC ‡	—	Seidel et al. (2020)
METIS ▲	—	Lacy and Burrows (2020)
MOLIERE †	—	Urban et al. (2004)
Moreno et al.	—	Moreno (1998) and Moreno et al. (2001)
NEMESIS †‡	https://users.ox.ac.uk/~atmp0035/nemesis.html	Irwin et al. (2008)
Nixon & Madhusudhan ⧫	—	Nixon and Madhusudhan (2020)
PETRA •▲	—	Lothringer and Barman (2020)
petitRADTRANS ‡▲	https://petitradtrans.readthedocs.io/en/latest/	Mollière et al. (2019)
PICASO	https://github.com/natashabatalha/picaso	Robbins-Blanch et al. (2022); Batalha et al. (2019)
plan-net ⧫	https://github.com/exoml/plan-net	Cobb et al. (2019)
PLATON ‡	https://github.com/ideasrule/platon	Zhang et al. (2020)
PLATON II ‡	https://github.com/ideasrule/platon	Zhang (2020)
PolyChord ‡	https://github.com/PolyChord/PolyChordLite	Handley et al. (2015a) and Handley et al. (2015b)
POSEIDON ‡	https://github.com/MartianColonist/POSEIDON	MacDonald and Madhusudhan (2017)
PSG †‡	https://github.com/nasapsg	Villanueva et al. (2018)
Pyrat-Bay ▲	https://pyratbay.readthedocs.io/en/latest/	Cubillos and Blecic (2021)
Pytmosph3R	https://pypi.org/project/pytmosph3r/	Caldas et al. (2019) and Falco et al. (2022)
p-winds▲	https://github.com/ladsantos/p-winds	Dos Santos et al. (2022)
REDFOX	—	Scheucher et al. (2020)
rfast▲	https://github.com/hablabx/rfast	Robinson and Salvador (2023)
SCARLET ‡▲	—	Benneke (2015)
smarter ‡	—	Lustig-Yaeger et al. (2022)
species ‡•▲	https://github.com/tomasstolker/species	Stolker et al. (2020)
Tau	https://cpc.cs.qub.ac.uk/summaries/AEPN_v1_0.html	Hollis et al. (2013)
TauREx 2.6 ‡▲	https://github.com/ucl-exoplanets/TauREx_public	Waldmann et al. (2015b) and Waldmann et al. (2015a)
TauREx 3.1 ‡	https://taurex3-public.readthedocs.io/en/latest/	Al-Refaie et al. (2021)
ThERESA ▲	—	Challener and Rauscher (2022)
tierra ▲	https://github.com/disruptiveplanets/tierra	Niraula et al. (2022)
TRIDENT	—	MacDonald and Lewis (2022)
Vasist et al. ⧫	—	Vasist et al. (2023)
VI-retrieval ⧫	—	Yip et al. (2022)

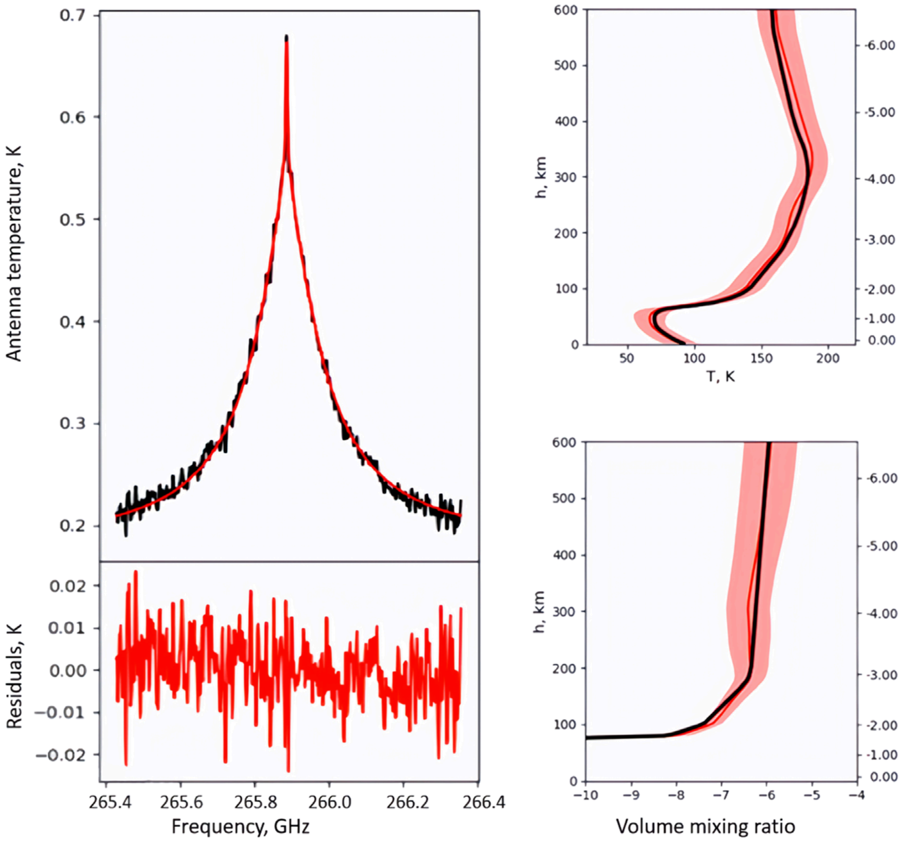

FIGURE 1
Example of forward model and retrieval applied to the case of HCN in Titan: Left: comparison between observed and best-fit simulated HCN (3-2) lines (black and red, respectively, upper panel), and the difference between the observed and fitted spectra (lower panel). Right: retrieved temperature and HCN distribution derived from the spectrum. The black and red lines, and the pink shadow show the initial and retrieved profiles, and the error bars, respectively. Figure based on Figure 1 in Rengel et al. (2022).

[Saunders et al. (1999); Matricardi (2007)], SARTA[16][17] [Strow et al. (2003)], SARTre [Mendrok (2006)], SASKTRAN[18] [Bourassa et al. (2008); Zawada et al. (2015)], SBDART[19] [Ricchiazzi et al. (2002)], SCIATRAN[20] [Rozanov et al. (2005); Rozanov et al. (2014)], SICOR[21] [Borsdorff et al. (2017); Borsdorff et al. (2018)], SKIRT[22] [Baes et al. (2003)], SMART-G[23] [Ramon et al. (2019)], TOMRAD [Dave (1964)], VDISORT [Lin et al. (2022)], VLIDORT/LIDORT[24] [Spurr and Christi (2019)], WFM-DOAS [Buchwitz et al. (2004); Buchwitz et al. (2005)] as well as models by Hartogh (1989), Tinetti et al. (2006a), Tinetti et al. (2006b) and Robinson et al. (2011).

3 Retrieval or parameter fitting or estimation techniques

The objective of an optimization algorithm is to extensively and efficiently sample a high-dimensional parameter space to find the best solution space given the data. The retrieval or parameter fitting or estimation techniques commonly used are Optimal Estimation (OE) algorithm (†), nested sampling (‡), Markov chain Monte Carlo (MCMC) method (▲), Grid search (●), and more recently, data-driven Machine Learning (ML) approaches (⧫). OE is popular in the Solar System community and assumes Gaussian statistics. It is fast and efficient and applicable to exoplanets under some specific conditions (e.g., Rengel et al., 2008; Hartogh et al., 2010; Lee et al., 2011; Line et al., 2012; Shulyak et al., 2019; Rengel et al., 2022; Villanueva et al., 2022). Grid search is simple and computationally cheap, but it can be inefficient (e.g., Madhusudhan & Seager, 2009). MCMC provides a better parameter exploration of the parameter space but with limitations in calculating the model evidence for model comparison and can be computationally expensive (e.g., Benneke and Seager, 2012; Madhusudhan et al., 2014; Waldmann et al., 2015b; Blecic, 2016; Cubillos, 2016; Evans et al., 2017; Wakeford et al., 2017; Lacy and Burrows, 2020). Nested sampling algorithm facilitates efficient

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[16] https://github.com/strow/sarta.

[17] https://github.com/clhepp/sarta.

[18] https://arg.usask.ca/docs/sasktran/.

[19] https://github.com/paulricchiazzi/SBDART.

[20] https://www.iup.uni-bremen.de/sciatran/.

[21] https://pypi.org/project/sicor/.

[22] https://skirt.ugent.be/root/_home.html.

[23] https://www.hygeos.com/smartg.

[24] http://www.rtslidort.com/about_overview.html.

parameter space exploration and calculation of model evidence (e.g., Benneke and Seager, 2013; Waldmann et al., 2015a; Gandhi and Madhusudhan, 2017; Pinhas et al., 2018; Brogi and Line, 2019; Fisher and Heng, 2019; Mollière et al., 2019; Min et al., 2020; Seidel et al., 2020; Shulyak et al., 2020). ML algorithms can be computationally efficient, but they require large amounts of training data and can be sensitive to biases in the training set (e.g., Waldmann, 2016; Marquez-Neila et al., 2018; Soboczenski et al., 2018; Zingales and Waldmann, 2018; Cobb et al., 2019; Fisher et al., 2020; Hayes et al., 2020; Nixon and Madhusudhan, 2020). An example of an application of the forward model and retrieval technique is provided in **Figure 1**.

4 Verification and validation of RT and retrieval codes

The retrieval problem is a challenging one due to its ill-posed and ill-conditioned nature. This means that even a small change in measurements can result in a significant deviation in the estimated model, making the inverse solution computation extremely unstable (e.g., Ih and Kempton, 2021). Currently, each retrieval code has its unique method for computing opacities and input models, lacking community standards. Furthermore, models continue to become more complex and data quality improves, retrieval codes face increasingly complex and degenerate problems (e.g., Welbanks and Madhusudhan, 2019).

Verification and validation of planetary retrieval codes is an important aspect. Verification can be readily accomplished using synthetic measurements and code inter-comparison. Inter-model comparisons of forward and retrieval suites have already been underway, with notable studies by Clarmann et al., 2003; Baudino et al., 2017; Schreier et al., 2018; Barstow et al., 2020; Barstow et al., 2022). Validation is challenging due to the lack of reference "truth" data (e.g., *in situ* measurements). Thus, for an assessment of exoplanet atmospheric remote sensing, data dedicated to Solar System planets like Earth, Mars and Venus is an ideal test case. To our knowledge, this kind of data have been rarely used to demonstrate the capabilities of exoplanet atmospheric studies. Observing planetary transits in our own Solar System, for example, can serve as an invaluable benchmark and can provide crucial information for future exoplanet characterizations (e.g., Ehrenreich et al., 2011; Ehrenreich et al., 2012; Montañés-Rodríguez et al., 2015; López-Puertas et al., 2018; Schreier et al., 2018).

Results from inter-comparison show that small differences in the forward model setup can lead to noticeable differences in the retrieval outcome (Barstow et al., 2020). These efforts are crucial for improving the field and providing a clearer understanding of the sources of variability and their impact on the results. Such comparisons provide a roadmap for future advancements and refinements in modelling, enabling us to compare theoretical predictions with observations. They also offer an opportunity to identify any remaining problems, leading to the improvement of existing codes and the development of more reliable and consistent codes. The continued pursuit of inter-model comparisons will drive the field forward towards a better understanding of the retrieval problem. Furthermore, the inherent similarities in methods was investigated (Line et al., 2013), and there is now considerable work to understand and quantify the role of different modelling choices affecting accuracy and precision on constraints (Barstow et al., 2020).

5 Final remarks

Our current understanding of planetary atmospheres is limited by model completeness and robustness. Forward modelling and spectral retrieval is the leading technique for interpretation of spectra and is employed by various teams using a variety of forward models and parameter estimation algorithms. Numerous codes are available and continue been developed. The code employed which contain the complexity of models should be chosen with care depending on the specific questions whose answer is sought and on the nature of the data at hand (considering spectral coverage and region, resolution, precision, signal-to-noise ratio, etc.). The efficiency of these codes is a critical issue, but beyond the scope of this paper.

The study of RT in planetary atmospheres is a rapidly developing field, with numerous advances being made in both the understanding of the RT process and in the development of RT codes. With continued research and development including the improving of observational capabilities, it is likely that even more sophisticated RT codes and inversion algorithms will be developed in the future, enabling us to better understand the diversity of planetary systems beyond our own and the mechanisms shaping their atmospheres.

Author contributions

MR wrote the first draft of the manuscript. All authors contributed to the article and approved the submitted version.

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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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