

Dear Reviewer,

we want to thank you for your time and effort in reviewing our paper. Here's a detailed response.

RC1

In this paper, the authors develop a bioavailable Sr isoscape for South America using a machine learning approach. The model is trained on a compilation of published Sr data across the continent, complemented by new plant samples from two regions in Brazil. This work represents a valuable contribution, as spatially explicit Sr isoscapes remain scarce at the local and continental scales in South America, and such models have strong potential for applications in archaeology, ecology, and provenance studies.

Overall, the manuscript is well written and easy to follow. The introduction provides the necessary background and clearly frames the objectives. The methods are clearly described and rely on a robust and widely used modelling framework. The results are presented in a clear and detailed manner.

I only have a comment regarding the discussion. I was wondering whether there are published Sr datasets from southern Brazil (Santa Catarina or Rio Grande do Sul) that could be used for a qualitative comparison with the isoscape predictions. I am not suggesting a formal validation with statistical tests, but rather a brief and simple consistency check. It would help the reader assess how well the model performs in real-world contexts.

A: We thank the reviewer for the suggestion. We have incorporated all documents, to the best of our knowledge, pertaining to the areas of investigation into the construction of the model proposed here.

I only have a few minor comments:

- L248: Can you provide the description of the predictors that you included in the model? (e.g. as a table in SI). This would allow the reader to understand the variables without having to consult previous publications. It would also make it unnecessary to redefine abbreviations in the results section.

A: we added a Table in the main text, reporting the used predictors and their respective reference:

Variables	Description	Resolution	Type	Source
r.m1	Median bedrock model	1 km	Discrete	Bataille et al. 2018
r.srsrq1	1st quartile bedrock model	1 km	Discrete	Bataille et al. 2018
r.srsrq3	3rd Quartile bedrock model	1 km	Discrete	Bataille et al. 2018
r.age	Terrane age attribute	1 km	Discrete	Mooney et al. 1998
r.dust	Multi-models average (g.m-2.yr-1)	1°x1°	Continuous	Mahowald et al., 2006

r.map	Mean annual precipitation (mm.yr-1)	30-arc sec	Continuous	Hijmans et al., 2005
r.salt.t	CCSM.3 simulation	1.4°×1.4°	Continuous	Mahowald et al. 2006
r.pet	Global Potential Evapo-Transpiration	30-arc sec	Continuous	Zomer et al. 2008
r.ai	Global Aridity Index	30-arc sec	Continuous	Zomer et al. 2008
r.elevation	SRTM (m)	90 m	Continuous	Jarvis et al., 2008
r.ph	Soil pH in H2O solution (x10)	250 m	Continuous	Hengl et al., 2017
r.clay	Clay (weight %)	250 m	Continuous	Hengl et al., 2017
r.bulk	Bulk density (kg m-3)	250 m	Continuous	Hengl et al., 2017
r.GUM	Global unconsolidated sediment map	1 km	Continuous	Börker et al., 2018
r.ssaw	Multi-models average sea salt wet deposition (kg.ha-1.yr-1)	1° x 1°	Continuous	Vet et al., 2014
r.ssa	Multi-models average Sea salt wet+dry deposition (kg.ha-1.yr-1)	1° x 1°	Continuous	Vet et al., 2014
r.cec	Cation Exchange Capacity	250 m	Continuous	Hengl et al., 2017
r.bouguer	WGM2012_Bouguer	2 min	Continuous	Balmino et al., 2012
r.mat	Mean annual temperature (°C)	30-arc sec	Continuous	Hijmans et al., 2005
r.maxage_geol	GLiM age attribute (Myrs)	1 km	Discrete	Hartmann and Moosdorf, 2012
r.minage_geol	GLiM age attribute (Myrs)	1 km	Discrete	Hartmann and Moosdorf, 2012
r.meanage_geol	GLiM age attribute (Myrs)	1 km	Discrete	Hartmann and Moosdorf, 2012
r.nfert	Global Nitrogen Fertilization	30-arc	Continuous	Potter et al., 2010
r.volc	Atmospheric deposition of volcanic material (kg.m-2.s-1)	0.5°	Continuous	Brahney et al. 2015

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- L254: parameter “mtry” not “mtyr”

A: We amended accordingly.

- L295: What do you mean by “anomalous values”? Higher than expected? And how did you handled these data? Removed as you did for the extreme Sr values of water or kept in the model?

A: We thank the reviewer for this comment. With "anomalous values" we refer to data that deviate from the expected isotopic range for these unconsolidated Quaternary sediments. We expected the values to generally show a strontium isotopic range of approximately 0.708 to 0.715, while our datasets show unusually radiogenic $^{87}\text{Sr}/^{86}\text{Sr}$ ratios compared to the rest of the sedimentary units. These values represent statistical outliers (Tukey's fences) as reported in Figure 3. We considered these values as related to the heterogeneity of source deposits, such as fluvial/marine reworking processes and floodplain sources contributing to mixed sedimentary sources enriched by older local radiogenic lithologies. These samples come indeed from sediments near high isotopic Sr ratios in older formations of the Mantiqueira Province and Dom Feliciano Belt and that the higher values could be consistent with sediments derived from these formations. The data were kept in the models. Conversely, we removed from our dataset the extreme values (>0.900) from the Parguaza Batholith because they show remarkably high residuals in the RF models. .

We have clarified this point in the main manuscript and we report the text here:

'The presence of isotopic outliers in our plant dataset, with ratios higher than those expected for unconsolidated coastal deposits, can be explained by the heterogeneity of the Holocene and Pleistocene deposits (fluvial, marine, aeolian) on which the plants grew, and the characteristics of the parental lithologies. Since these values reflect geological variability, they were retained in the model. In contrast, the extremely radiogenic values for river waters (>0.900) were excluded.'

- L433-439: This is more out of curiosity and does not need to be included in the manuscript. Have you tested your model with the global dataset provided by Bataille et al. 2020 or more recent updates? Your reported R^2 is higher than studies using a global dataset to run their RF. I agree that when regional data coverage is good, a regional model is often preferable to a global one, but I would be interested to know how your model compares in that context.

A: This is a well-known issue in the field: whether to use global datasets when modeling local bioavailable Sr isotope variability. In our experience, incorporating data from highly diverse eco-geological settings often leads to worse predictions for the specific area of interest. While this is not universally true, it can be particularly problematic in geologically complex regions (e.g., Madagascar; Bataille et al., 2020). Additionally, the increased computational cost further discouraged us from using a global dataset to train the RF model. We do not claim that our approach is optimal in all cases, but we consider it a cautious and reasonable choice. The lower R^2 reported for the global isoscape by Bataille et al. is coherent when considering the much larger dataset used in their model. Such broad coverage likely reduces overall residuals at the global scale, even if local variability is likely

underrepresented. In contrast, our dataset is smaller and derived entirely from a geologically complex region, where higher local variability can lead to lower model fit.

RC2

This manuscript presents an important new bioavailable $^{87}\text{Sr}/^{86}\text{Sr}$ dataset from southern Brazil ($n = 233$ plant samples) and compiles a continental-scale dataset for South America to generate random forest-based Sr isoscapes. The new field data are clearly valuable, geographically well distributed, and analytically robust. In particular, the analytical methods and metadata for the newly generated samples are exceptionally well documented, which is unfortunately still rare in isoscape studies and deserves explicit recognition. The authors should be congratulated for this. However, while the new dataset itself is very strong, there are some issues related to data compilation, attribution, metadata completeness, and reproducibility that must be addressed before publication. Most of these issues concern adherence to FAIR data principles. In its current form, the manuscript does not yet meet the standards expected for a fully reproducible data paper in Earth System Science Data.

My concerns are outlined below.

1. Compilation transparency, provenance, and FAIR compliance

The manuscript relies heavily on a large compilation of previously published bioavailable Sr datasets (1588 datapoints from 883 sites), yet the compilation process itself is insufficiently described and documented.

Specifically it is unclear how the data were identified, selected, filtered, cleaned, harmonized, and quality-controlled. The manuscript or the zenodo link/metadata do not clearly explain many of the rationale for how non-local samples (e.g., humans, fauna) were assessed and excluded across all contributing studies. How many and why? This sort of sample selection needs clear/define criteria. How inconsistent metadata across studies were standardized. How duplicate sampling locations were handled beyond brief mention of “sites”? How were coordinates obtained when not explicitly reported in the original studies? How was analytical heterogeneity treated (i.e., some datasets use TIMS, others MC-ICPMS, others ICPMS) and these techniques have different precision, accuracy, and susceptibility to interferences? How was preparation protocol affected the data quality? For example soil digestion methods vary considerably across studies and do not represent the same bioavailable Sr pool.

I recommend the authors to explicitly document the compilation workflow, ideally with a dedicated subsection to follow existing best-practice compilation frameworks for isotope data as provided by IsoArch / IsoBank metadata fields. See for example recent compilations like ARDUOUS (e.g. ESSD 2026). These frameworks emphasize transparent provenance, versioning, and machine-readable metadata. Ideally, the compiled dataset should be restructure to conform to an IsoArch/IsoBank-style schema with metadata table describing source, material type, analytical method, coordinate source, uncertainty, and QC status for every entry.

A: We thank the reviewer for highlighting these points regarding transparency and compliance with FAIR principles. The dataset we produced in this study, available on Zenodo, contains useful information for reproducibility purposes, such as coordinates, geological unit, age, $^{87}\text{Sr}/^{86}\text{Sr}$ value, and related uncertainty. The literature dataset was compiled from existing databases and publications and includes all available information reported in those sources, such as sample names, coordinates, material type, and analytical uncertainties. Where such information was not provided in the original sources, we are unable to supply it, consistent with the approach taken in databases such as ARDUOS cited by the reviewer. We acknowledge the value and importance of the IsoArch metadata model; however, its structure may be less intuitive for some users, as it distributes information across multiple spreadsheets and introduces renamed sample identifiers. In contrast, our approach consolidates all relevant data into a single sheet (with full references provided separately), which we believe offers a more straightforward and user-friendly format for readers.

We acknowledge, however, that the documentation provided for compilation could be made more explicit. In the revised version of the manuscript, we have added a description of the criteria adopted for sample selection and exclusion, duplicate management, harmonization, and treatment of data heterogeneity.

Here we report the text added in section 3.4:

For the continental-scale compilation, we included both environmental samples (plants, lichens, soils, and water) and archaeological human and faunal samples identified as local in the original publications. Non-local individuals were excluded. Metadata relating to coordinates and material categories were harmonized, and duplicates were consolidated by site. Uncertainty values not reported in the original publications or datasets were excluded.

1. Missing citations and lack of credit to original data producers

Another important point is that the individual dataset used in the compilation are not cited in the main manuscript. While “Supplement Table S1” is mentioned, this is insufficient. The model presented here is built entirely on years of fieldwork, laboratory work, and interpretation by many research groups. Failing to properly cite each original dataset will discourage future data sharing and is technically not following FAIR principles. The same issue applies to predictor layers used in the random forest model. While the Dr. Bataille compiled, reprojected, and reorganized these layers and is cited, the primary creators of those datasets must also be properly cited and acknowledged. Many of us, including myself, have learned this “the hard way” during large compilations (e.g. ARDUOUS). I would encourage the authors to give credits to all scientists who made their work possible.

A: We thank the reviewer for his valuable comments.

We have revised the text taking his suggestions into account to ensure compliance with the FAIR principles.

Here we report the text added in section 3.4:

'All primary datasets used in the compilation, including the open-access IsoArch repository, Borges et al. (2021), Plomp (2021), Stantis et al. (2024) and Seferidou (2025), have been integrated with all additional sources and reported in Table S1. Overall data are from : Brass (1976), Palmer and Edmond (1989), Edmond et al. (1995; 1996), Hieronymus (1995), Henry et al. (1996), Gaillardet et al. (1997), Négrel and Lachassagne (2000), Grove et al. (2003), Knudson et al. (2004; 2013), Brunet et al. (2005), Pasquini et al. (2005), Knudson and Price (2007), Knudson (2008), Martins et al. (2008), Andrushko et al. (2009), Bastos (2009; 2014), Fiege et al. (2009), Hermenegildo (2009), Poszwa et al. (2009), Bastos et al. (2011; 2014; 2015; 2016; 2019; 2021), Laffoon et al. (2012), Lee et al. (2013), Machado (2013), Malaspinas et al. (2014), Pouilly et al. (2014), Santos et al. (2014), Oppitz (2015), Strauss et al. (2016), Barberena et al. (2017; 2019; 2020; 2021), Chala-Aldana et al. (2018), Duran et al. (2018), Slovak et al. (2018), Plomp et al. (2019), Moquet et al. (2020), Serna et al. (2020), Azevedo et al. (2021), Washburn et al. (2021), Fernandez et al. (2022), Quaggio et al.

(2022), Torres-Rouff et al. (2022), Avigliano et al. (2023), Seferidou et al. (2023), Silva et al. (2023), Kafino et al. (2024), Martinelli et al. (2025), Loponte et al. (2025), Scaggion et al. (2025a).'

All the articles and datasets are now cited also in the main text.

Yet, we would also like to stress that in the original version all source publications were referenced in the Supplementary information, as is common practice in our field (see e.g., Bataille et al., 2020 or e.g. Wang et al., 2024). We fully recognize the value of the ARDUOS dataset and its contribution to data standardization and accessibility. However, we note that it represents one of several possible approaches to data organization and dissemination, and alternative formats, such as the one adopted here, can also meet transparency and reproducibility requirements.

Finally, we stress that the primary aim of this study is to present newly-measured isotope data and their interpretation. Thus, this manuscript is not ultimately intended as a review paper *sensu stricto*, although we have made the compiled data fully available.

1. Treatment of outliers and model-performance comparisons

The discussion of outlier removal and model comparison needs some revision. While it is reasonable to remove extreme $^{87}\text{Sr}/^{86}\text{Sr}$ values it also fundamentally alters model performance metrics because RMSE and R^2 are strongly dependent on the value range and distribution. Models trained on datasets with fewer extreme values will always appear to perform better. As a result I don't think it is ideal to say that the plant+lichen model is "better" than the full dataset model in an absolute sense. I think differences in RMSE and R^2 primarily reflect training-set composition (see Fig. 2), not intrinsic model quality. The same comment is true when comparing with other published models (e.g. Dosseto et al. 2025; Bataille et al. 2020). Sampling strategy matters, but training-set distribution matters far more. For example, it would be easy to produce a bioavailable Sr model across Egypt that would achieve $\text{RMSE} < 0.001$ simply because carbonate geology dominates and is highly predictable and not very variable. Conversely, South America includes cratonic terrains with extremely high values along with young volcanic terrain with extremely low values, inflating RMSE but providing higher R^2 due to larger variance. So I would recommend the authors to mention some of those points when discussing model performance which in my view is almost entirely dependent on the selected training set distribution. Or the authors could provide a more stratified evaluation if they absolutely want to compare model to each other.

A: We think there is a misunderstanding. We agree that RMSE and R^2 are highly dependent on the isotopic distribution and variance of the training dataset and, therefore, cannot be interpreted as absolute indicators of model quality.

We intended to argue that the higher R^2 value observed in the plant+lichen model reflected the narrower isotopic range and more homogeneous composition of the dataset, rather than an intrinsically superior predictive performance.

This was in fact already reported in the original version of the manuscript at lines 338-341: 'The lower variance observed in these latter models likely reflects the smaller number and lower variability of samples compared to the 'All' dataset, which includes outliers with $^{87}\text{Sr}/^{86}\text{Sr}$ higher than 0.818 in water samples (Fig. 3).'

We have still revised the Discussion section to state more explicitly that the observed differences in RMSE and R^2 values, resulting from the comparison between our models, are relative and driven by the data selection.

Here we report the sentence added in Discussion:

'We reiterate that these differences in RMSE and R^2 more accurately reflect the isotopic range and internal heterogeneity of the training datasets, rather than intrinsic differences in model quality.'

Predictor choice and interpretability

I am surprised to see r.GUM included as a predictor, if you could justify its inclusion mechanistically?

A: The r.GUM variable represents the global distribution of unconsolidated sediments and was included among the covariates in the original framework of Bataille et al. (2020). From a mechanistic perspective, such sediments (largely present in South America) can influence local Sr isotope signatures through weathering, sediment-water interactions, and the eventual incorporation of allochthonous material. In our approach, rather than arbitrarily excluding predictors a priori, we kept the full set of original covariates and allowed the model to evaluate their relative importance after multicollinearity screening. As shown in Fig. 6, r.GUM shows the lowest predictive contribution among the selected variables, indicating that while it may retain some environmental variability, its influence on model performance is limited if not almost null.

1. Reproducibility and open science

I also recommend to fully follow FAIR principles to provide the entire modeling all scripts (data harmonization, predictor processing, modeling, validation, plotting) and the workflow should be archived on OSF or GitHub, with a permanent DOI. Ideally, provide a README explaining how the isoscapes can be regenerated from raw inputs.

A: We thank the reviewer for the suggestion. We have included our script in the Zenodo repository, although it is not intrinsically different from the Bataille et al. (2020) approach, and it was used from our group in other publications such as Scaggion et al. (2025), Armaroli et al. (2024), Gigante et al. (2023).