Materials Design Analysis Reporting (MDAR) Checklist for Authors

The MDAR framework establishes a minimum set of requirements in transparent reporting applicable to studies in the life sciences (see Statement of Task: doi:10.31222/osf.io/9sm4x.). The MDAR checklist is a tool for authors, editors and others seeking to adopt the MDAR framework for transparent reporting in manuscripts and other outputs. Please refer to the MDAR Elaboration Document for additional context for the MDAR framework.

Materials

Antibodies	**Yes (indicate where**	**n/a**
For commercial reagents, provide supplier name, catalogue number and RRID, if available.		N/A, because we did not have the commercial reagents.

Cell materials	**Yes (indicate where**	**n/a**
Cell lines: Provide species information, strain. Provide accession number in repository **OR** supplier name, catalog number, clone number, **OR** RRID		N/A, because we did not have the cell materials.
Primary cultures: Provide species, strain, sex of origin, genetic modification status.		N/A, because we did not have the cell materials.

Experimental animals	**Yes (indicate where**	**n/a**
Laboratory animals: Provide species, strain, sex, age, genetic modification status. Provide accession number in repository **OR** supplier name, catalog number, clone number, **OR** RRID		N/A, because we did not have the experimental animals.
Animal observed in or captured from the field: Provide species, sex and age where possible		N/A, because we did not have the experimental animals.
Model organisms: Provide Accession number in repository (where relevant) **OR** RRID		N/A, because we did not have the experimental animals.

Plants and microbes	**Yes (indicate where**	**n/a**
Plants: provide species and strain, unique accession number if available, and source (including location for collected wild specimens)		N/A, because we did not have the plants and microbes.
Microbes: provide species and strain, unique accession number if available, and source		N/A, because we did not have the plants and microbes.

Human research participants	**Yes (indicate where**	**n/a**
Identify authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		N/A, because we did not have the human research participants.
Provide statement confirming informed consent obtained from study participants.		N/A, because we did not have the human research participants.
Report on age and sex for all study participants.		N/A, because we did not have the human research participants.

Design

Study protocol	**Yes (indicate where**	**n/a**
For clinical trials, provide the trial registration number **OR** cite DOI in manuscript.		N/A, because we did not have the clinical trials in our study.

Laboratory protocol	**Yes (indicate where**	**n/a**
Provide DOI or other citation details if detailed step-by-step protocols are available.		N/A, because we did not have detailed step-by-step protocols.

Experimental study design (statistics details)	Yes (indicate where	n/a
State whether and how the following have been done**, or** if they were not carried out.		
Sample size determination		N/A, because we did not have experimental study.
Randomisation		N/A, because we did not have experimental study.
Blinding		N/A, because we did not have experimental study.
Inclusion/exclusion criteria		N/A, because we did not have experimental study.

Sample definition and in-laboratory replication	Yes (indicate where	n/a
State number of times the experiment was replicated in laboratory		N/A, because we did not have Sample definition and in-laboratory replication.
Define whether data describe technical or biological replicates		N/A, because we did not have Sample definition and in-laboratory replication.

Ethics	Yes (indicate where	n/a
Studies involving human participants: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		N/A, because we did not have the studies involving human participants.
Studies involving experimental animals: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		N/A, because we did not have Studies involving experimental animals.
Studies involving specimen and field samples: State if relevant permits obtained, provide details of authority approving study; if none were required, explain why.		N/A, because we did not have Studies involving specimen and field samples.

Dual Use Research of Concern (DURC)	Yes (indicate where	n/a
If study is subject to dual use research of concern, state the authority granting approval and reference number for the regulatory approval		N/A, because the study is not subject to dual use research of concern.

Analysis

Attrition	Yes (indicate where	n/a
State if sample or data point from the analysis is excluded, and whether the criteria for exclusion were determined and specified in advance.	Yes, we used *P-value* <0.05 to exclude the date point from the analysis (page 9 line 1; page 12 line 7; page 13 line 6) and we used OB $\geqslant$ 30% , DL $>$ 0.18 to screen the compounds and targets. (page 7 line 11) And the target screening AUC $\geqslant$ 0.7, and the result score $\geqslant$ 0.5 (page 7 line 19)	

Statistics	Yes (indicate where	n/a
Describe statistical tests used and justify choice of tests.	Yes, we used the Metascape database with statistical tests. (page 8 line 20)	

Data Availability	Yes (indicate where	n/a
State whether newly created datasets are available, including protocols for access or restriction on access.		N/A, because we did not create new databases.
If data are publicly available, provide accession number in repository or DOI or URL.		N/A, because we did not create new databases.
If publicly available data are reused, provide accession number in repository or DOI or URL, where possible.		N/A, because we did not create new databases.

Code Availability	Yes (indicate where	n/a
For all newly generated code and software essential for replicating the main findings of the study:		N/A, because we did not generate new code and software.
State whether the code or software is available.		N/A, because we did not generate new code and software.
If code is publicly available, provide accession number in repository, or DOI or URL.		N/A, because we did not generate new code and software.

Reporting

Adherence to community standards	Yes (indicate where provided: section/paragraph)	n/a
MDAR framework recommends adoption of discipline-specific guidelines, established and endorsed through community initiatives. Journals have their own policy about requiring specific guidelines and recommendations to complement MDAR.	Yes, the authors have followed Materials Design Analysis Reporting (MDAR), relevant guidelines, and relevant checklists. (page 23, line 1)	
State if relevant guidelines (eg., ICMJE, MIBBI, ARRIVE) have been followed, and whether a checklist (eg., CONSORT, PRISMA, ARRIVE) is provided with the manuscript.	ICMJE guidelines were followed, as the journal follows ICMJE recommendations for publication.	

Article information: http://dx.doi.org/10.21037/apm-20-1759