

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 provided: section/paragraph)	n/a
For commercial reagents, provide supplier name, catalogue number and RRID, if available.		x

Cell materials	Yes (indicate where provided: section/paragraph)	n/a
Cell lines: Provide species information, strain. Provide accession number in repository OR supplier name, catalog number, clone number, OR RRID		x
Primary cultures: Provide species, strain, sex of origin, genetic modification status.		x

Experimental animals	Yes (indicate where provided: section/paragraph)	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		x
Animal observed in or captured from the field: Provide species, sex and age where possible		x
Model organisms: Provide Accession number in repository (where relevant) OR RRID		x

Plants and microbes	Yes (indicate where provided: section/paragraph)	n/a
Plants: provide species and strain, unique accession number if available, and source (including location for collected wild specimens)		x
Microbes: provide species and strain, unique accession number if available, and source		x

Human research participants	Yes (indicate where provided: section/paragraph)	n/a
Identify authority granting ethics approval (IRB or equivalent committee(s)), provide reference number for approval.		x
Provide statement confirming informed consent obtained from study participants.		x
Report on age and sex for all study participants.		x

Design

Study protocol	Yes (indicate where provided: section/paragraph)	n/a
For clinical trials, provide the trial registration number OR cite DOI in manuscript.		x

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Laboratory protocol	Yes (indicate where provided: section/paragraph)	n/a
Provide DOI or other citation details if detailed step-by-step protocols are available.		x

Experimental study design (statistics details)	Yes (indicate where provided: section/paragraph)	n/a
State whether and how the following have been done, or if they were not carried out.	Page 4 The method has explained the data was from the open website.	
Sample size determination		x
Randomisation	Page 4 Method explained the results were based on the websites.	
Blinding		x
Inclusion/exclusion criteria	page 2 the abstract provide the statistics details.	

Sample definition and in-laboratory replication	Yes (indicate where provided: section/paragraph)	n/a
State number of times the experiment was replicated in laboratory		x
Define whether data describe technical or biological replicates		x

Ethics	Yes (indicate where provided: section/paragraph)	n/a
Studies involving human participants: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		x
Studies involving experimental animals: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		x
Studies involving specimen and field samples: State if relevant permits obtained, provide details of authority approving study; if none were required, explain why.		x

Dual Use Research of Concern (DURC)	Yes (indicate where provided: section/paragraph)	n/a
If study is subject to dual use research of concern, state the authority granting approval and reference number for the regulatory approval		x

Analysis

Attrition	Yes (indicate where provided: section/paragraph)	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.	Page 4 Main active compounds and targets of the TCM drugs. Page 4 We have explained the method and how to get the result.	

Statistics	Yes (indicate where provided: section/paragraph)	n/a
Describe statistical tests used and justify choice of tests.	Page 5 Molecular docking validation	

Data Availability	Yes (indicate where provided: section/paragraph)	n/a
State whether newly created datasets are available, including protocols for access or restriction on access.	Page 4 Collection of disease-related targets With Anxiety Disorders as the keyword, human genes were searched in databases including DisGeNET (https://www.disgenet.org/), Online Mendelian Inheritance in Man (OMIM) (http://www.omim.org), Drugbank (https://www.drugbank.ca), GeneCards (https://www.genecards.org/), and Comparative	

	Toxicogenomics Database (CTD) (http://ctdbase.org/)	
If data are publicly available, provide accession number in repository or DOI or URL.	Page 4 All the websites are available to access	
If publicly available data are reused, provide accession number in repository or DOI or URL, where possible.	Page 4 Main active compounds and targets of the TCM drugs The SMILES codes of all active compounds were confirmed through PubChem (http://pubchem.ncbi.nih.gov).	

Code Availability	Yes (indicate where provided: section/paragraph)	n/a
For all newly generated code and software essential for replicating the main findings of the study:	Page 4 Main active compounds and targets of the TCM drugs The SMILES codes of all active compounds were confirmed through PubChem (http://pubchem.ncbi.nih.gov).	
State whether the code or software is available.	Page2 <i>abstract</i> and page 4 <i>method has explained the code and website</i>	
If code is publicly available, provide accession number in repository, or DOI or URL.	Page 4 Main active compounds and targets of the TCM drugs The SMILES codes of all active compounds were confirmed through PubChem (http://pubchem.ncbi.nih.gov).	

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.		
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	

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