

## **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](https://doi.org/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**

<b>Antibodies</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
For commercial reagents, provide supplier name, catalogue number and RRID, if available.		The study did not involve the use of any antibodies.
<b>Cell materials</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
<b>Cell lines:</b> Provide species information, strain. Provide accession number in repository <b>OR</b> supplier name, catalog number, clone number, <b>OR</b> RRID		The study did not involve the use of any cell materials.
<b>Primary cultures:</b> Provide species, strain, sex of origin, genetic modification status.		The study did not involve the use of any primary cultures.
<b>Experimental animals</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
<b>Laboratory animals:</b> Provide species, strain, sex, age, genetic modification status. Provide accession number in repository <b>OR</b> supplier name, catalog number, clone number, <b>OR</b> RRID		The study did not involve the use of any laboratory animals.
<b>Animal observed in or captured from the field:</b> Provide species, sex and age where possible		The study did not involve the use of any animal observed in or captured from the field.
<b>Model organisms:</b> Provide Accession number in repository (where relevant) <b>OR</b> RRID		The study did not involve the use of any model organisms.
<b>Plants and microbes</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
<b>Plants:</b> provide species and strain, unique accession number if available, and source (including location for collected wild specimens)		The study did not involve the use of any plants.
<b>Microbes:</b> provide species and strain, unique accession number if available, and source		The study did not involve the use of any microbes.
<b>Human research participants</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
Identify authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.	The study was conducted under the approval of the Ethics Committee of Peking Union Medical College Hospital (ZS-1329). (See <b>Footnote, Ethical Statement</b> )	
Provide statement confirming informed consent obtained from study participants.	Written informed consent was obtained from each patient. (See <b>Footnote, Ethical Statement</b> )	
Report on age and sex for all study participants.	Clinical characteristics of cohorts, including age and sex, were reported in <b>Table 1</b>	

**Design**

<b>Study protocol</b>	<b>Yes</b>	<b>n/a</b>
For clinical trials, provide the trial registration number <b>OR</b> cite DOI in manuscript.		This is not a clinical trial.
<b>Laboratory protocol</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
Provide DOI or other citation details if detailed step-by-step protocols are available.	Detailed step-by-step protocols are available in the following publications: DOI: 10.1200/JCO.2010.29.6038 DOI: 10.1016/j.jtho.2017.06.017 (See in <b>Method, Database, sample collection, and NGS</b> )	
<b>Experimental study design (statistics details)</b>	<b>Yes</b>	<b>n/a</b>
State whether and how the following have been done, <b>or</b> if they were not carried out.		
Sample size determination		This is not a clinical trial.
Randomisation		This is not a clinical trial.
Blinding		This is not a clinical trial.
Inclusion/exclusion criteria	See in <b>Method, Database, sample collection, and NGS</b>	
<b>Sample definition and in-laboratory replication</b>	<b>Yes</b>	<b>n/a</b>
State number of times the experiment was replicated in laboratory		The study did not involve laboratory experiments.
Define whether data describe technical or biological replicates		The study did not involve technical/biological procedure that needs replication.
<b>Ethics</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
Studies involving human participants: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.	The study was conducted under the approval of the Ethics Committee of Peking Union Medical College Hospital (ZS-1329). (See <b>Footnote, Ethical Statement</b> )	
Studies involving experimental animals: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		The study did not involve the use of any 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.		The study did not involve the use of any specimen and field samples.
<b>Dual Use Research of Concern (DURC)</b>	<b>Yes</b>	<b>n/a</b>
If study is subject to dual use research of concern, state the authority granting approval and reference number for the regulatory approval		This study is not subjected to dual use research of concern

## Analysis

<b>Attrition</b>	<b>Yes (indicate where provided:</b>	<b>n/a</b>
State if sample or data point from the analysis is excluded, and whether the criteria for exclusion were determined and specified in advance.	Exclusion of data and its criteria are mentioned in <b>Methods, Database, sample collection, and NGS</b>	
<b>Statistics</b>	<b>Yes (indicate where provided:</b>	<b>n/a</b>
Describe statistical tests used and justify choice of tests.	Statistical tests are illustrated in <b>Methods, Statistical analysis</b>	
<b>Data Availability</b>	<b>Yes (indicate where provided:</b>	<b>n/a</b>
State whether newly created datasets are available, including protocols for access or restriction on access.		The newly created data are not shared out of privacy concerns.
If data are publicly available, provide accession number in repository or DOI or URL.		The newly created data are not shared out of privacy concerns.
If publicly available data are reused, provide accession number in repository or DOI or URL, where possible.	Code or software is available in the references mentioned in <b>Methods, Database, sample collection, and NGS</b>	
<b>Code Availability</b>	<b>Yes (indicate where provided:</b>	<b>n/a</b>
For all newly generated code and software essential for replicating the main findings of the study:		
State whether the code or software is available.	Code or software is available in the references mentioned in <b>Methods, Computational methods of simulation and energy analysis of lapatinib,</b>	
If code is publicly available, provide accession number in repository, or DOI or URL.	Code or software is available in the references mentioned in <b>Methods,</b>	

## Reporting

<b>Adherence to community standards</b>	<b>Yes (indicate where provided: section/paragraph)</b>	<b>n/a</b>
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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