# <u>Materials Design Analysis Reporting (MDAR)</u> 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.

## For all that apply, please note where in the manuscript the required information is provided.

## Materials:

Newly created materials	indicate where provided: page no/section/legend)	n/a
The manuscript includes a dedicated "materials availability statement" providing transparent	pClneo-CD5-Δstalk-mouse PC1 CTF expression construct	
disclosure about availability of newly created materials including details on how materials can be	can be obtained by request from R. Maser.	
accessed and describing any restrictions on access.	(rmaser@kumc.edu)	
Antibodies	indicate where provided: page no/section/legend)	n/a
For commercial reagents, provide supplier name, catalogue number and RRID, if available.	TRAM2 rabbit monoclonal antibody [EPR2658]	
	Supplier: Abcam	
	Cat# ab109176	
	RRID:AB_10866211	
DNA and RNA sequences Short novel DNA or RNA including primers, probes: Sequences should be included or deposited in a public repository.	Primer sequences for cloning and mutagenesis are included as Table S5 in Supporting Information.	n/
Cell materials	indicate where provided: page no/section/legend	n/
Cell lines: Provide species information, strain.  Provide accession number in repository OR supplier name, catalog number, clone number, OR RRID.	HEK293T	11/
	Species: human	
	Supplier: ATCC	
	Cat #: CRL-3216	
<b>Primary cultures:</b> Provide species, strain, sex of origin, genetic modification status.		

Experimental animals	indicate where provided: page no/section/legend)	n/a
Laboratory animals or Model organisms: 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.		
Animal observed in or captured from the field: Provide species, sex, and age where possible.		

Plants and microbes	indicate where provided: page no/section/legend)	n/a
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<b>Plants:</b> provide species and strain, ecotype and cultivar where relevant, unique accession number if available, and source (including location for collected wild specimens).	
<b>Microbes:</b> provide species and strain, unique accession number if available, and source.	

Human research participants	indicate where provided: page no/section/legend) or state if these demographics were not collected	n/a
If collected and within the bounds of privacy		
constraints report on age, sex and gender or		
ethnicity for all study participants.		

#### Design:

Study protocol	indicate where provided: page no/section/legend)	n/a
If study protocol has been pre-registered, provide DOI. For clinical trials, provide the trial registration number <b>OR</b> cite DOI.		

Laboratory protocol	indicate where provided: page no/section/legend)	n/a
Provide DOI <b>OR</b> other citation details if detailed step-by-step protocols are available.		

Experimental study design (statistics details)		
For in vivo studies: State whether and how the	indicate where provided: page no/section/legend. If it	n/a
following have been done	could have been done, but was not, write not done	II/ a
Sample size determination		
Randomisation		
Blinding		
Inclusion/exclusion criteria		

Sample definition and in-laboratory replication	indicate where provided: page no/section/legend	n/a
State number of times the experiment was replicated in laboratory.	Numbers of experimental and technical replicates are provided in the legends for Figure 1 and Figure S2.	
Define whether data describe technical or biological replicates.		

Ethics	indicate where provided: page no/section/legend	n/a
<b>Studies involving human participants:</b> State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		
Studies involving experimental animals: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		
Studies involving specimen and field samples: State if relevant permits obtained, provide details of authority approving study; if none were required, explain why.		

Dual Use Research of Concern (DURC)	indicate where provided: page no/section/legend	n/a
If study is subject to dual use research of concern		
regulations, state the authority granting approval		
and reference number for the regulatory approval.		

### **Analysis:**

Attrition	indicate where provided: page no/section/legend	n/a
Describe whether exclusion criteria were		
preestablished. Report if sample or data points were		
omitted from analysis. If yes report if this was due to		
attrition or intentional exclusion and provide		
justification.		

Statistics	indicate where provided: page no/section/legend	n/a
Describe statistical tests used and justify choice of		
tests.	One-way ANOVA was used to compare means of	
	reporter activity between multiple conditions in Figures	
	1 and S2. Post hoc analysis used Tukey-Kramer Test.	

Data availability	indicate where provided: page no/section/legend	n/a
For newly created and reused datasets, the manuscript includes a data availability statement that provides details for access or notes restrictions on access.		
If newly created datasets are publicly available, provide accession number in repository <b>OR</b> DOI <b>OR</b> URL and licensing details where available.		
If reused data is publicly available provide accession number in repository <b>OR</b> DOI <b>OR</b> URL, <b>OR</b> citation.		

Code availability	indicate where provided: page no/section/legend	n/a
For all newly generated custom computer code/software/mathematical algorithm or re-used code essential for replicating the main findings of the study, the manuscript includes a data availability statement that provides details for access or notes restrictions.	Free energy profiles for p9, p17 and p21-bound ΔStalk  CTF as reported in Figures 2, 3 and 4 were generated  using the PyReweighting toolkit.  (https://www.med.unc.edu/pharm/miaolab/resources/P  yReweighting)  Pep-GaMD simulations were performed on p9, p17 and p21-bound ΔStalk CTF systems using the AMBER  simulation package (https://ambermd.org/)	
If newly generated code is publicly available, provide accession number in repository, <b>OR</b> DOI <b>OR</b> URL and licensing details where available. State any restrictions on code availability or accessibility.  If reused code is publicly available provide accession number in repository <b>OR</b> DOI <b>OR</b> URL, <b>OR</b> citation.		

#### Reporting

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.

Adherence to community standards	indicate where provided: page no/section/legend	n/a
State if relevant guidelines (e.g., ICMJE, MIBBI,		
ARRIVE) have been followed, and whether a checklist		
(e.g., CONSORT, PRISMA, ARRIVE) is provided with		
the manuscript.		