

EDITORIAL TRACE RESPONSES

Author: Please verify the changes made to the above addresses..... 1

YES THESE ADDRESSES ARE CORRECT

Author: A citation to Table 1 was added here because it is not cited in the paper. Is this location correct?..... 11

YES THIS IS THE CORRECT LOCATION

Author: Please supply the name and location of the publisher in ref 4.28

Name of publisher: European Chemicals Agency

Location: Helsinki, Finland

URL: <https://echa.europa.eu/information-on-chemicals/pre-registered-substances>

Author: Please verify the changes made to the above reference. 28

AGREE

Author: Please supply the volume number and page range, and name and location of the publisher in ref 27. 29

PLEASE CHANGE ref 27 to:

Martin MT, Judson RS, Reif DM, Kavlock RJ, Dix DJ. Profiling chemicals based on chronic toxicity results from the U.S. EPA ToxRef Database. *Environmental Health Perspectives*. 117: 392-9. PMID [19337514](https://pubmed.ncbi.nlm.nih.gov/19337514/) DOI: [10.1289/ehp.0800074](https://doi.org/10.1289/ehp.0800074)

Author: Please supply the name and location of the publisher in ref 33. 30

THIS REFERENCE IS FOR THE RDKit OPENSOURCE SOFTWARE PUBLISHED ON THE WEB AT <http://www.rdkit.org> by G. Landrum.

Author: Please verify the changes made to the above reference. 31
AGREE

Author: Please verify the changes made to the above reference. 31
AGREE

Author Corrections

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Corresponding Author Name:	Imran Shah

Please provide your text corrections in the table below and then send this document and any other necessary files by e-mail to acsproof@acs.org.

NOTE that the first three rows shown are simply examples to show how to fill out the table. They can be deleted if you prefer.

Line Number	Action	Current Text	New Text
Line 24	Change	classification, and regression trees	classification and regression trees
Line 355	Change	FF1	F1
Line 217	Change	bioactivity assays are	bioactivity assays is
Line 442	Change	Figure. 2	Figure 2
Global search replace	Change	posthoc	post hoc
Lines 612-613	Change	HepG2MicrotubuleCSK	HepG2 Microtubule CSK

The “machine learning workflow” on page D after line 365 line breaks, which should be removed. If it is not possible to remove the line breaks then they should be shown as follows:

Statement 1

Statement 2 with some formula

Statement 3 with some
formula and line-break

The indentation after the line break should be at the same level as the parent line +1 space