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We have used PDinsight.py, a python program developed for this manuscript, for the generation of:

table 1, numerical columns (e.g., fig7\_pars.txt)

table 2; Appendix 5 table 1 (tab1\_pars.txt)

figure 7 (fig7\_pars.txt, fig7d\_pars.txt)

figure 8b (fig8b\_pars.txt)

Parameter files indicated in brackets. These are available as Source code 1. Documentation on the use of PDinsight.py is included as an appendix to the manuscript with additional information at the head of the example parameter file. More extensive documentation is included with PDinsight on github: https://github.com/eedeinum/PDinsight . PDinsight also has a citable DOI through Zenodo: 10.5281/zenodo.3536704.

For cross validation, figure 6 was recreated using PDinsight (fig6\_pars.txt) (note that with the default model, Rn = Rdt + 2 alpha\_bar = 8 nm + 2 alpha\_bar).