

Life Sciences Reporting Summary

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Please do not complete any field with "not applicable" or n/a. Refer to the help text for what text to use if an item is not relevant to your study. For [final submission](#): please carefully check your responses for accuracy; you will not be able to make changes later.

► Experimental design

1. Sample size

Describe how sample size was determined.

As our study presents a new method for analyzing mass spectrometry data, rather than an attempt to illustrate a statistically significant biological phenomenon, no sample size considerations were relevant.

2. Data exclusions

Describe any data exclusions.

We excluded data that would be considered "noise" in mass spectrometry data, i.e. signals of very low intensity relative to the main signal of interest. This was based on pre-established quantitative criteria.

3. Replication

Describe the measures taken to verify the reproducibility of the experimental findings.

All mass spectrometry experiments were performed at least in duplicate (most often in triplicate), with high reproducibility in almost all cases.

4. Randomization

Describe how samples/organisms/participants were allocated into experimental groups.

One of our experiments did involve assignments of synthetic peptides to groups, which were randomly chosen by co-author Samuel Myers.

5. Blinding

Describe whether the investigators were blinded to group allocation during data collection and/or analysis.

For the synthetic peptide experiment, group assignment was chosen randomly by co-authors S.M. while analysis was performed by R.P., who had no knowledge of the members of each group.

Note: all in vivo studies must report how sample size was determined and whether blinding and randomization were used.

6. Statistical parameters

For all figures and tables that use statistical methods, confirm that the following items are present in relevant figure legends (or in the Methods section if additional space is needed).

n/a Confirmed

- The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement (animals, litters, cultures, etc.)
- A description of how samples were collected, noting whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
- A statement indicating how many times each experiment was replicated
- The statistical test(s) used and whether they are one- or two-sided
Only common tests should be described solely by name; describe more complex techniques in the Methods section.
- A description of any assumptions or corrections, such as an adjustment for multiple comparisons
- Test values indicating whether an effect is present
Provide confidence intervals or give results of significance tests (e.g. P values) as exact values whenever appropriate and with effect sizes noted.
- A clear description of statistics including central tendency (e.g. median, mean) and variation (e.g. standard deviation, interquartile range)
- Clearly defined error bars in all relevant figure captions (with explicit mention of central tendency and variation)

See the web collection on [statistics for biologists](#) for further resources and guidance.

► Software

Policy information about [availability of computer code](#)

7. Software

Describe the software used to analyze the data in this study.

The purpose of our study was to present a new software tool. As stated in the manuscript, our custom code is available on GitHub at github.com/rpeckner-broad/Specter.

For manuscripts utilizing custom algorithms or software that are central to the paper but not yet described in the published literature, software must be made available to editors and reviewers upon request. We strongly encourage code deposition in a community repository (e.g. GitHub). *Nature Methods* [guidance for providing algorithms and software for publication](#) provides further information on this topic.

► Materials and reagents

Policy information about [availability of materials](#)

8. Materials availability

Indicate whether there are restrictions on availability of unique materials or if these materials are only available for distribution by a third party.

No unique materials were used.

9. Antibodies

Describe the antibodies used and how they were validated for use in the system under study (i.e. assay and species).

No antibodies were used.

10. Eukaryotic cell lines

a. State the source of each eukaryotic cell line used.

PC3 cell lines were obtained from ATCC (catalog number CRL-1435).

b. Describe the method of cell line authentication used.

DNA fingerprinting was applied using the following SNPs: Chromosome SNP ID Position
 5 rs10037858 156766708
 1 rs532905 189620278
 1 rs2229857 154573967 20 rs6104310 44354538 18 rs9304229 38247872 6 rs2273827 160211339 5 rs2036902 49696932
 1 rs6679393 31770944
 5 rs2369754 99156362
 1 rs1052053 156202173 2 rs6726639 112753097 11 rs2512276 124115370 17 rs6565604 79589242 7 rs6972020 68182022
 8 rs13269287 124453662 1 rs10888734 52266242 7 rs6966770 115895718 7 rs2639 6066461
 2 rs10186291 112748514 2 rs7598922 39082344
 4 rs2709828 152355268 2 rs1131171 232326417 4 rs7664169 99037859 17 rs1437808 4175846
 3 rs11917105 183371250 12 rs10876820 55978465 5 rs2910006 140590766 24 AMG_3b 6737949
 14 rs8015958 67086676 13 rs3105047 55937194 3 rs5009801 101058775 6 rs9277471 33053682 18 rs3744877 77894844 9 rs1549314 127910307 6 rs9369842 48994615 5 rs390299 153363334 2 rs1734422 10932207 22 rs9466 38273749
 19 rs4517902 29851078 13 rs6563098 79887237 9 rs965897 77175017

c. Report whether the cell lines were tested for mycoplasma contamination.

The cell lines were tested for mycoplasma contamination.

d. If any of the cell lines used are listed in the database of commonly misidentified cell lines maintained by [ICLAC](#), provide a scientific rationale for their use.

None of the cell lines we used are listed in the ICLAC database.

► Animals and human research participants

Policy information about [studies involving animals](#); when reporting animal research, follow the [ARRIVE guidelines](#)

11. Description of research animals

Provide all relevant details on animals and/or animal-derived materials used in the study.

No animals were used.

Policy information about [studies involving human research participants](#)

12. Description of human research participants

Describe the covariate-relevant population characteristics of the human research participants.

The study did not involve human research participants.