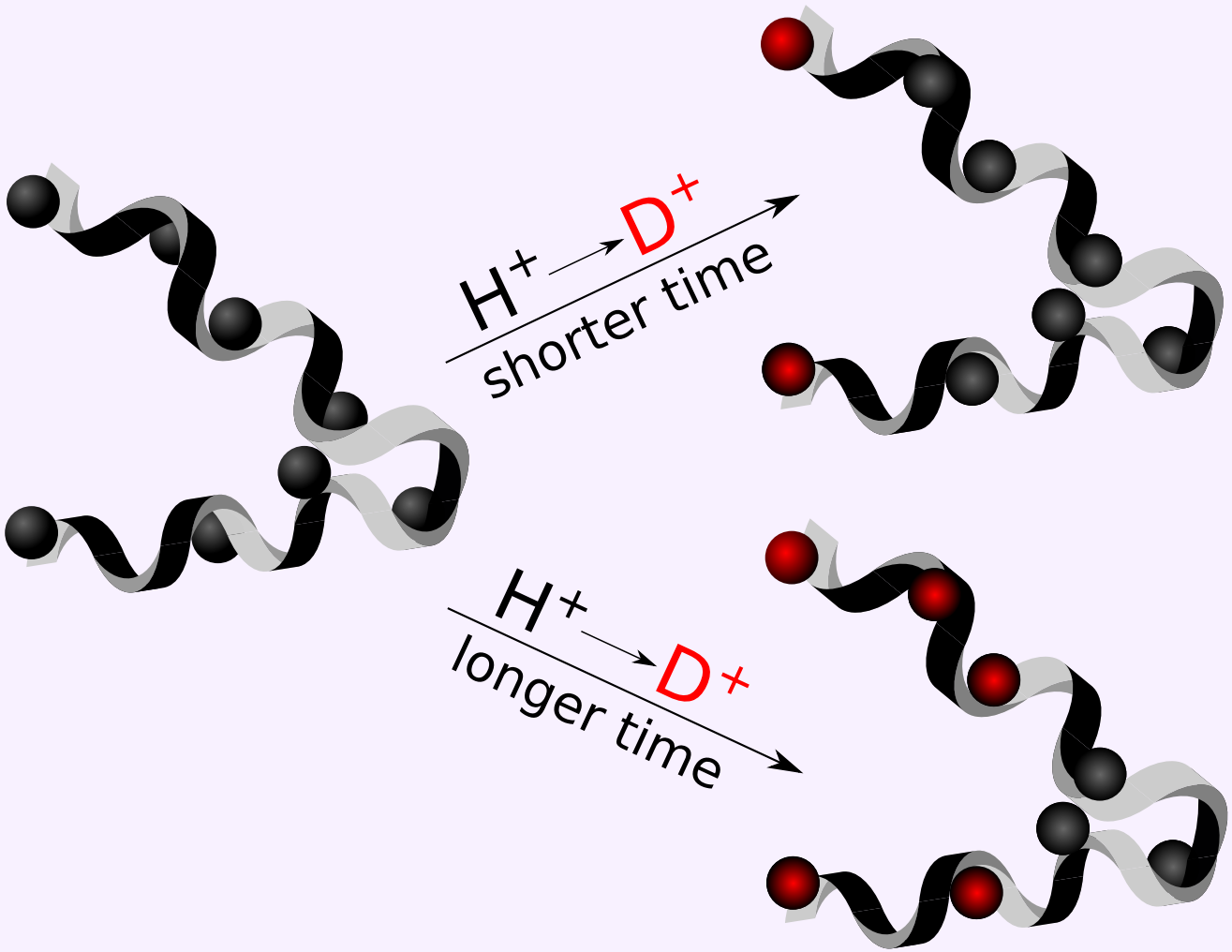
HaDeX: an R package and web-server for analysis of data from HDX-MS experiments

Dominik Cysewski

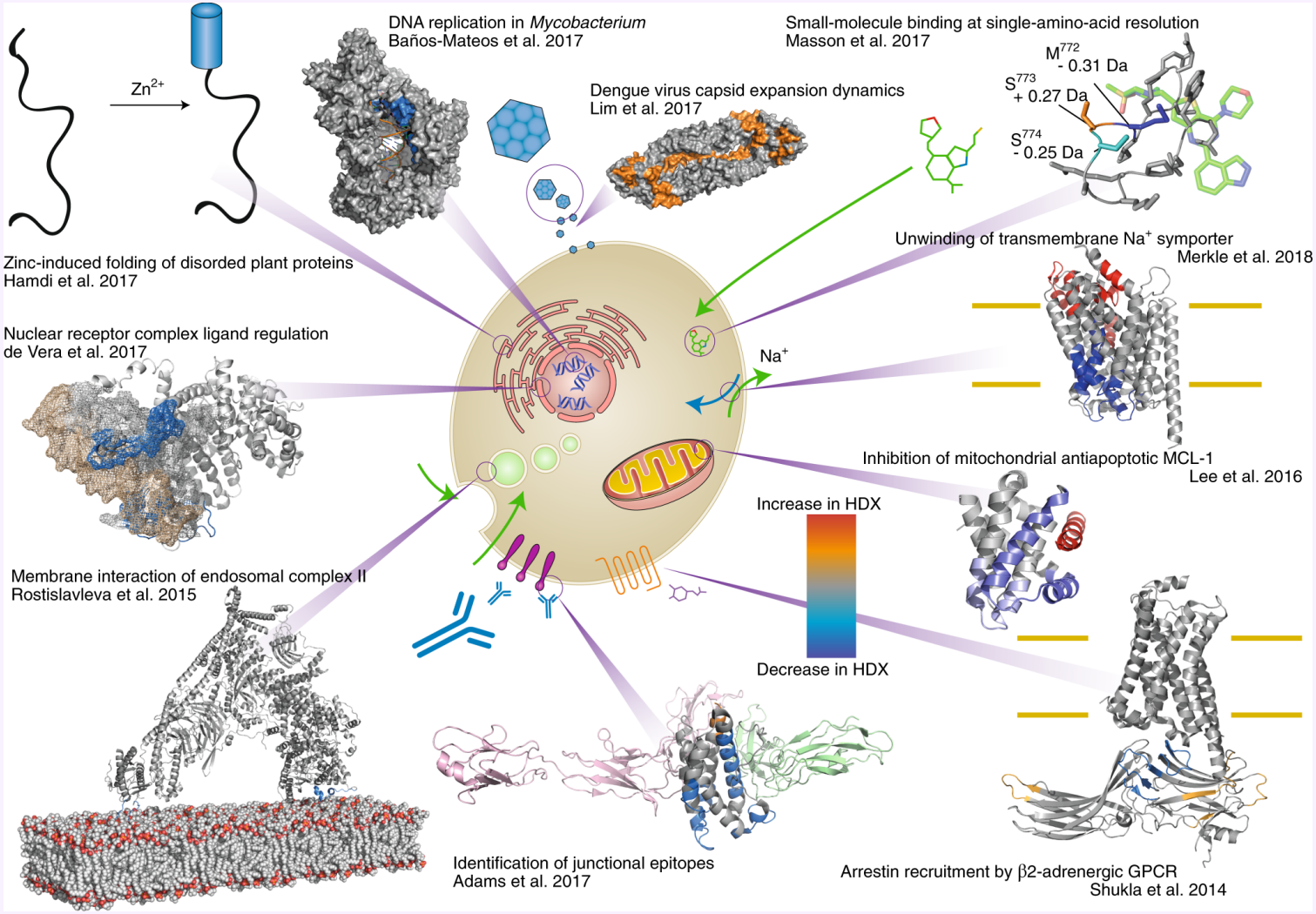
Institute of Biochemistry and Biophysics
Polish Academy of Sciences

HDX-MS



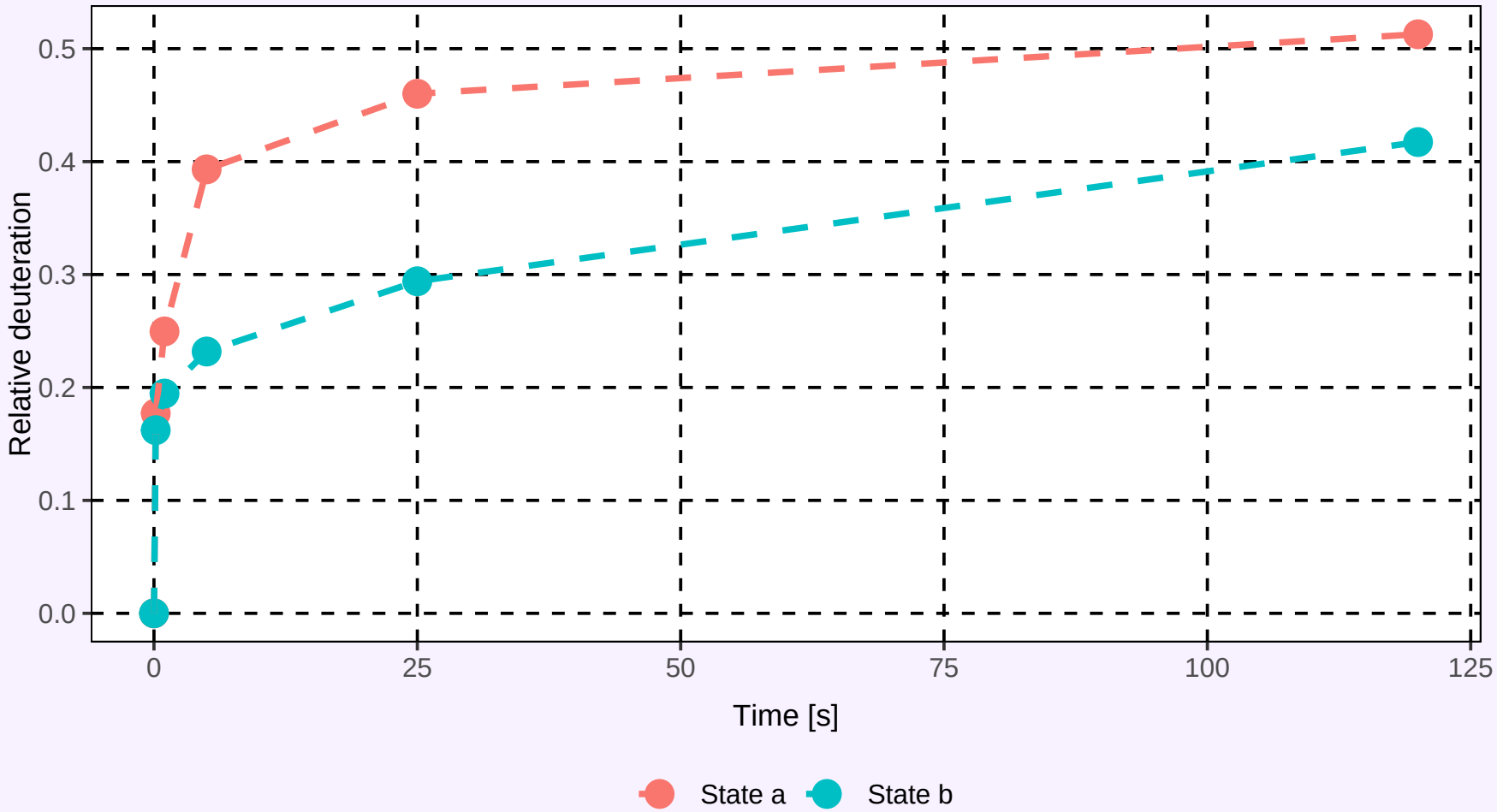
The longer incubation time, the more protected hydrogens are being replaced by deuters.

Applications

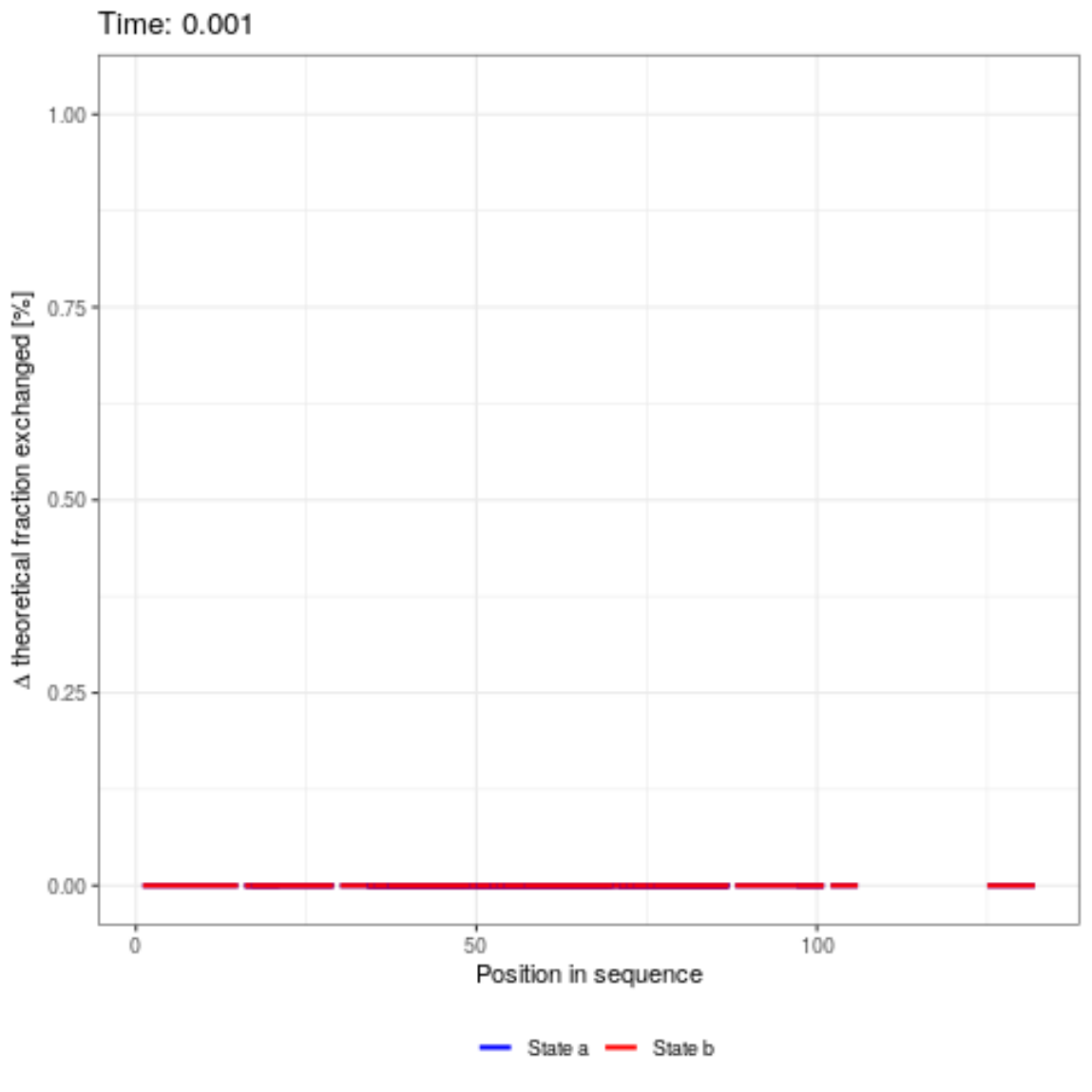


G. R. Masson et. al. (2019). Recommendations for performing, interpreting and reporting hydrogen deuterium exchange mass spectrometry (HDX-MS) experiments. Nature Methods, 16(7):595–602..

Multi-state analysis

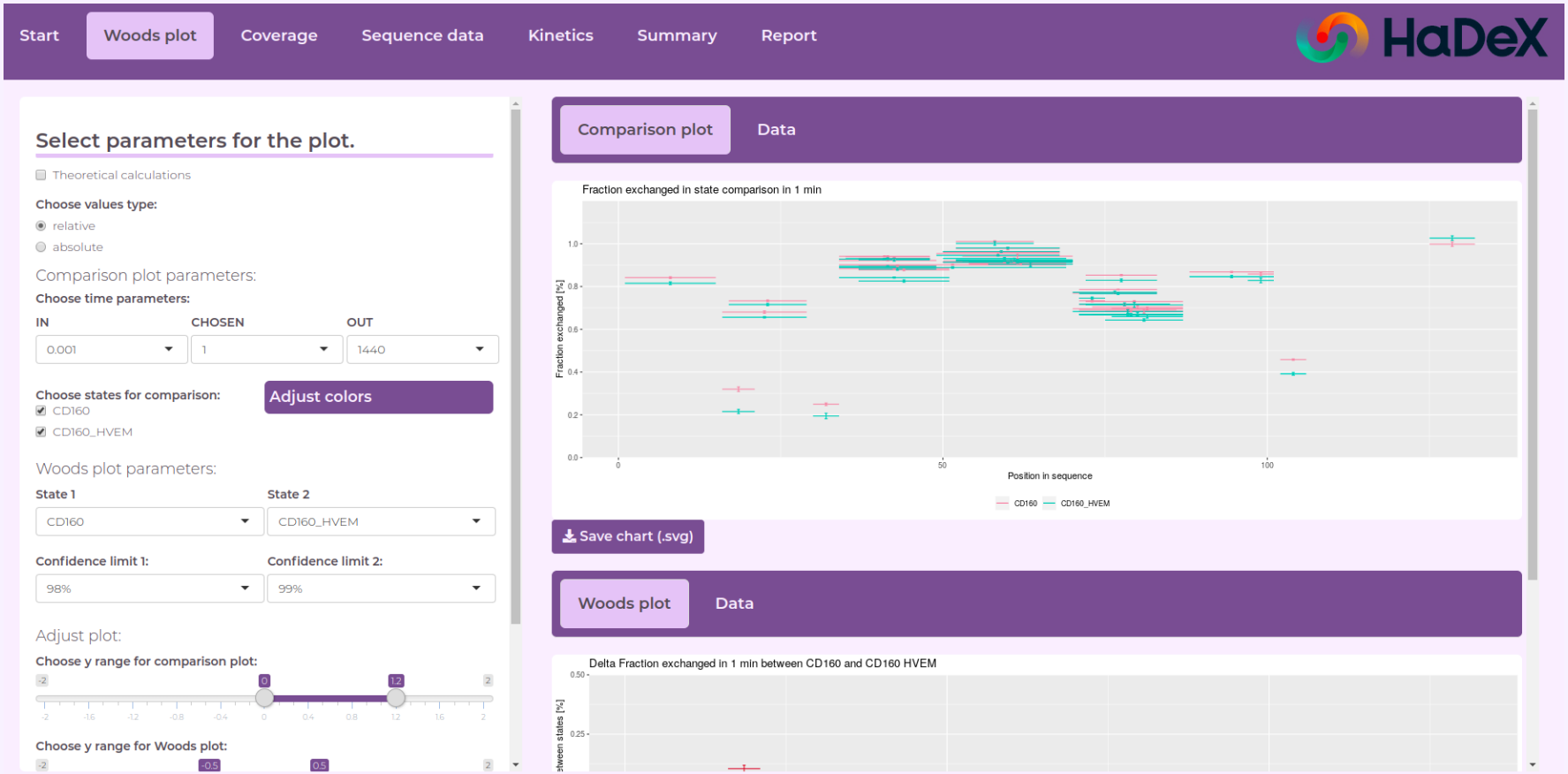


Peptides may come from proteins in differents states, i.e. bounded by different cofactors.



During the analysis of the HDX-MS data we have to consider both time of the incubation and position of a peptide in a sequence.

Relative deuteration



Deuteration kinetics

Start | Woods plot | Coverage | Sequence data | Kinetics | Summary | Report

HaDeX

Select parameters for the plot.

Theoretical calculations

Choose values type:

relative

absolute

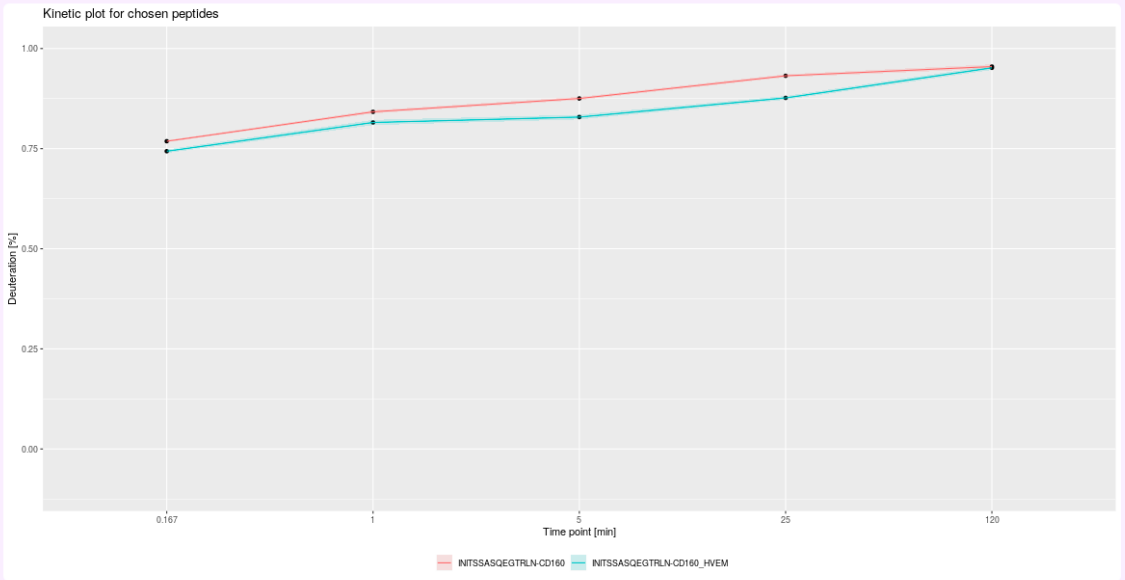
Choose time parameters:

IN	OUT
0.001	1440

Choose peptide:

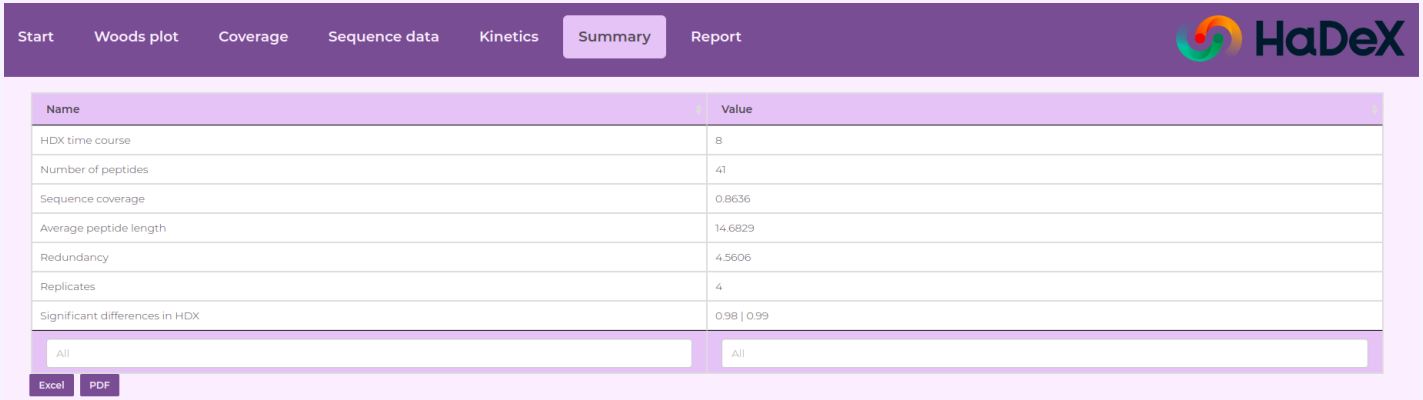
Sequence	State	Start	End
INITSSASQEGTRLN	CD160	1	15
INITSSASQEGTRLN	CD160_HVEM	1	15
LICTVW	CD160	16	21
LICTVW	CD160_HVEM	16	21
LICTVWHKKEEAEG	CD160	16	29
LICTVWHKKEEAEG	CD160_HVEM	16	29
ICTVWHKKEEAEG	CD160	17	29
ICTVWHKKEEAEG	CD160_HVEM	17	29
FVVFL	CD160	30	34
FVVFL	CD160_HVEM	30	34

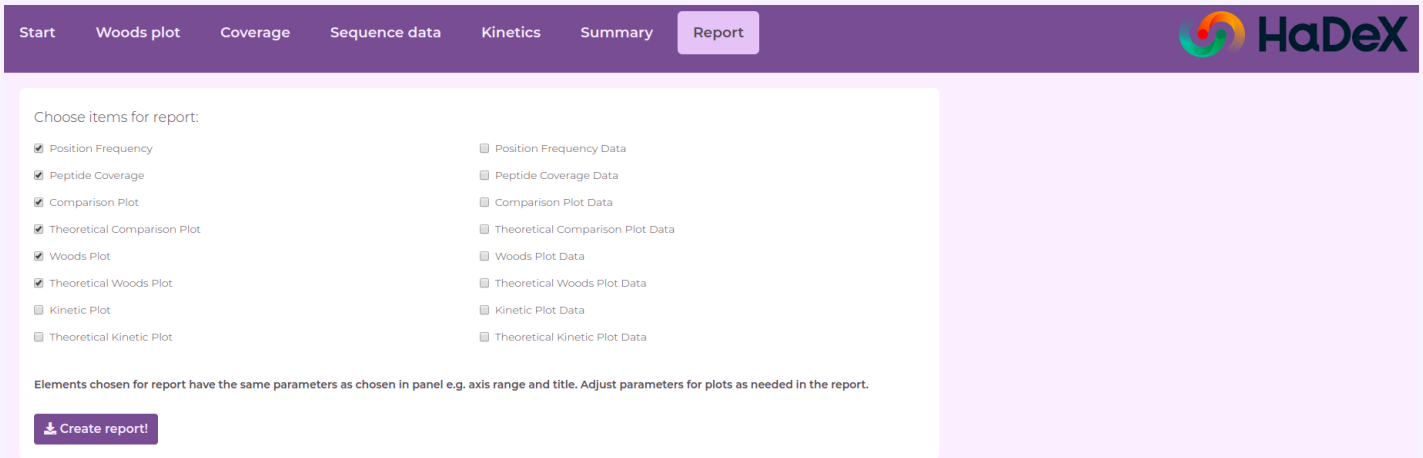
Kinetic plot | Data



Save chart (.svg)

Reporting


Start
Woods plot
Coverage
Sequence data
Kinetics
Summary
Report
HaDeX
Name
Value
HDX time course
8
Number of peptides
41
Sequence coverage
0.8636
Average peptide length
14.6829
Redundancy
4.5606
Replicates
4
Significant differences in HDX
0.98 | 0.99
All
All
Excel
PDF
Showing 1 to 7 of 7 entries
This table was adapted from the HDX Data Summary (Masson, G.R., Burke, J.E., Ahn, N.G., Anand, G.S., Borchers, C., Brier, S., Bou-Assaf, G.M., Engen, J.R., Englander, S.W., Faber, J., et al. (2019). Recommendations for performing, interpreting and reporting hydrogen deuterium exchange mass spectrometry (HDX-MS) experiments. Nat Methods 16, 595–602).


Start
Woods plot
Coverage
Sequence data
Kinetics
Summary
Report
HaDeX
Choose items for report:
Position Frequency
Peptide Coverage
Comparison Plot
Theoretical Comparison Plot
Woods Plot
Theoretical Woods Plot
Kinetic Plot
Theoretical Kinetic Plot
Position Frequency Data
Peptide Coverage Data
Comparison Plot Data
Theoretical Comparison Plot Data
Woods Plot Data
Theoretical Woods Plot Data
Kinetic Plot Data
Theoretical Kinetic Plot Data
Elements chosen for report have the same parameters as chosen in panel e.g. axis range and title. Adjust parameters for plots as needed in the report.
Create report!

Summary and availability

Summary:

- rapidly developing technologies require a flexible framework,
- the methods of data analysis should follow the development of both technology and expectations of its users.

Availability:

- a web-server (`http://mslab-ibb.pl/shiny/HaDeX/`),
- the R package (`https://CRAN.R-project.org/package=HaDeX`),
- a standalone software (`https://sourceforge.net/projects/HaDeX/`).

Acknowledgements

- Mass Spectrometry Lab, Institute of Biochemistry and Biophysics, PAS.
- MI² Data Lab, Faculty of Mathematics and Information Science, Warsaw University of Technology.

Funding: Foundation of Polish Science TEAM TECH CORE FACILITY/2016-2/2 Mass Spectrometry of Biopharmaceuticals - improved methodologies for qualitative, quantitative and structural characterization of drugs, proteinaceous drug targets and diagnostic molecules.

Acknowledgements

HaDeX developers:

- Weronika Puchala (main developer),
- Dominik Rafacz (frontend developer),
- Michał Burdukiewicz.