General structure of the data for the PHF6 paper

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Created by: Iuliia Stroganova

Short project description:

Data associated with publication "Exploring the Aggregation Propensity of PHF6 Peptide Segments of the Tau Protein using Ion Mobility Mass Spectrometry Techniques"

People involved in the project:

Iuliia Stroganova[1,2], Hannah Willenberg[1,†], Thaleia Tente[1], Agathe Depraz Depland[1,2], Sjors Bakels[1,2], and Anouk M. Rijs[1,2*].

Division of Bioanalytical Chemistry, Department of Chemistry and Pharmaceutical Sciences, Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, De Boelelaan 1105, 1081 HV Amsterdam, the Netherlands.
Centre for Analytical Sciences Amsterdam, 1098 XH, Amsterdam, the Netherlands
†Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 1, Nijmegen, 6525 ED, The Netherlands.

List of figures (main text):

#	Title	Elab file	Data name file and TuneMix file for calibration	Origin file	Data analysis
1	Typical MS of Ac-PHF6-NH2 on TIMS.	22-11-16 4 PHF6 peptides 24h room temp incubated	221116_exp1_Ac-PHF6-NH2_000001.d **221116_exp1_TM_004.d**	***<221116_Ac-PHF6-NH2_001_Figure1.opju>***	Chromatogram for total MS averaged over 5 minutes.
2	Extracted ion mobility and extracted MS of m/z 1580	221116Ac-PHF6-NH2 fresh sample	221116_exp1_Ac-PHF6-NH2_000001.d **221116_exp1_TM_004.d**	***<221116_exp1_Ac-PHF6-NH2_000001_EIM_EIM 1579.9580-1581.9600 +All MS_Figure2.opju>***	• Figure 2A extracted ion mobility (EIM) from m/z 1579.9580-1581.9600 • Figure 2B extracted MS from ion mobility peaks: ◦ 1.956±0.018 ◦ 1.602±0.019 ◦ 1.416±0.016 ◦ 1.295±0.016 ◦ 1.023±0.016

3;4	Quadrupole filtered m/z 1580 with fragments	Figure 3B 22 11 22 TIMS experiment: AC-PHF6-NH2 for calibration + 2 and 3+ filtering charge states. Figure 4B 221116Ac-PHF6-NH2 fresh sample (for intact mobilities)	221122_exp1_Ac-PHF6-NH2_Q1581_000001.d • **Figure 3B - Total MS** • **Figure 4A - Total IMS** **221122_exp1_TM_009.d** 221116_exp1_Ac-PHF6-NH2_000001.d **221116_exp1_TM_004.d**		• Figure 3B - chromatogram for total MS averaged over 5 minutes (from 221122_exp1_Ac-PHF6-NH2_Q1581_000001.d). • Figure 4A - total ion mobility averaged over all m/z 50-3000 (from 221122_exp1_Ac-PHF6-NH2_Q1581_000001.d). • Figure 4B-E - intact ions are from 221116_exp1_Ac-PHF6-NH2_000001.d • Figure 4B-E - fragment ions are from 221122_exp1_Ac-PHF6-NH2_Q1581_000001.d ◦ Intact 1^{1+} EIM from m/z 790.4800-793.4900 ◦ Fragment 1^{1+} EIM from m/z 790.3719-792.8347 ◦ Intact 9^{4+} EIM from m/z 1777.3260-1780.0800 ◦ Fragment 9^{4+} EIM from m/z 1777.2409-1780.3079 ◦ Intact 8^{3+} EIM from m/z 2106.9440-2108.6100 ◦ Fragment 8^{3+} EIM from m/z 2105.9835-2109.8317 ◦ Intact 11^{5+} EIM from m/z 1738.0500-1740.2580 ◦ Fragment 11^{5+} EIM from m/z 1737.7652-1740.1551 • Figure D4 (Supplementary Information) - - fragments are from 221122_exp1_Ac-PHF6-NH2_Q1581_000001.d ◦ Fragment 3^{2+} EIM from m/z 1184.9684-1187.4365 ◦ Fragment 7^{3+} EIM from m/z 1842.9779-1846.2595 ◦ Fragment 5^{2+} EIM from m/z 1974.5506-1977.9098 ◦ Fragment 6^{2+} EIM from m/z 2369.2495-2372.6027
5	TIMS vs. TWIMS (selected mobilities m/z 2370)	**TWIMS:** • **Normal settings** 221101_Thaleia's method • **Soft settings** 230518: PS shifted arrival times **TIMS:** 230103 Ac-PHF6-NH2 fresh sample	**TWIMS:** • **Normal settings** 221101_AC-PHF6-NH2_IMS_TEST.raw • **Soft settings** 230518_Ac-PHF6-NH2_new_test5_IMSF_50.raw **TIMS:** 230103_Ac-PHF6-NH2_0001.d 230103_Tune_exp1_000002.d		• Figure 5A - EIM from m/z 2369.406-2372.399 • Figure 5B - EIM from m/z 2370.031-2371.734 • Figure 5C - EIM from m/z 2370.2300-2371.2200
6	4 peptides together	TIMS experiment: 4 PHF6 peptides 24h room temp incubated	1. **221116_exp1_Ac-PHF6-NH2_002.d (221116_exp1_TM_006.d)** 2. **221116_exp1_Ac-PHF6_001.d (221116_exp1_TM_006.d)** **3. 221116_exp1_PHF6-NH2_003.d (221116_exp1_TM_010.d)** **4.221116_exp1_PHF6_001.d (221116_exp1_TM_011.d)**	***<221116_4 peptides_Figure6.opju>***	Mass spectra were averaged over 5 minutes (full acquisition time) Data were processed in Excel table

List of figures (Supplementary information):

#	Title	Elab file	Data name file	Files with proceessed data	Data analysis remarks
1	Effect of capillary voltage	230223 - TIMS experiment: Ac-PHF6-NH2 , harsher capillary and deltas for the paper	See data names 230223_exp1_Ac-PHF6-NH2_C_XXXX_000001.d 2500 V was taken from 230223_exp1_Ac-PHF6-NH2_000001.d Tuning files are: **230223_exp1_TM_0001.d** **230223_exp1_TM_0002.d** **230223_exp1_TM_0003.d**	***<230223_Capillary_voltage_TIMS.opju>***	• m/z 1843 EIM from m/z 1843.1172-1845.7892 • m/z 1580 EIM from m/z 1579.9580-1581.9600 • m/z 2106 EIM from m/z 2106.9442-2108.6102
2	Effect of D2	230223 - TIMS experiment: Ac-PHF6-NH2 , harsher capillary and deltas for the paper	See data names 230223_exp1_Ac-PHF6-NH2_D2_XXV_000001.d 0 V was taken from 230223_exp1_Ac-PHF6-NH2_000001.d	***<230223_D2_D3_D6_TIMS.opju>***	• m/z 1843 EIM from m/z 1843.1172-1845.7892 • m/z 1580 EIM from m/z 1579.9580-1581.9600 • m/z 2106 EIM from m/z 2106.9442-2108.6102
3	Effect of D3	230223 - TIMS experiment: Ac-PHF6-NH2 , harsher capillary and deltas for the paper	See data names 230223_exp1_Ac-PHF6-NH2_D3_XXV_000001.d 20 V was taken from 230223_exp1_Ac-PHF6-NH2_000001.d	- (see above)	- (see above)
4	Effect of D6	230223 - TIMS experiment: Ac-PHF6-NH2 , harsher capillary and deltas for the paper	See data names 230223_exp1_Ac-PHF6-NH2_D6_XXV_000001.d 10 V was taken from 230223_exp1_Ac-PHF6-NH2_000001.d	- (see above)	- (see above)
5	Effect of ion energy and collision energy	220819 TIMS experiment: further optimization of the method based on the discussion with Christopher	• 220819_exp1_Ac-PHF6-NH2_1580.9_000003.d (ion/col energy 15/0), • 220819_exp1_Ac-PHF6-NH2_1580.9_000004.d (ion/col energy 9/0), • 220819_exp1_Ac-PHF6-NH2_1580.9_000009.d(ion/col energy 6/3) • 220819_exp1_TM_000001.d	Screen shot from DataAnalysis	MS averaged over full acquisition time - 3 minutes
Section 1	CCS calibration procedure PS	-	-	-	-
6	ThT assays 4 different capping groups PHF6	221130: ThT Assay heparin, NaCl, buffer	**20221130_Fluorescence_method_AcPHF6NH2_buffer_NaCl_heparin_long_iuliia.xls** (raw data) **PHF6_all_processed.txt** (processed data)	**PHF6_all_processed.txt**	The xls file contains all the long time points as well. Averaging procedure is described in the text. The processed and averaged data are in the file **PHF6_all_processed.txt**
7	ThT assays for Ac-PHF6-NH2 with different buffer concentrations	230201 ThT assay with Ac-PHf6-NH2 high AA buffer concentration	**100, 500, 1000 mM AA are from 20230201_Fluorescence_method_peptides.xls** **10 mM from 20221130_Fluorescence_method_AcPHF6NH2_buffer_NaCl_heparin_long_iuliia.xls**	***<230201_fluprescence_Ac-PHF6-NH2_buffer_concentrations.opju>***	10 mM with Ac-PHF6-NH2 are from 20221130_buffer
8	TEM images Ac-PHF6-NH2 different conditions	(Ac-)PHF6(-NH2) Sample Preparation for TEM (buffer, NaCl or heparin) and MS (buffer)			
9	TEM images of 4 PHF6 peptides	Ac-)PHF6(-NH2) Sample Preparation for TEM (buffer, NaCl or heparin) and MS (buffer)			
10	Ion mobility assignment of fragment ions due to neutral loss of monomer	Fragment ions: 22 11 22 TIMS experiment: AC-PHF6-NH2 for calibration + 2 and 3+ filtering charge states. 230103 Intact oligomers, 230104 Intact oligomers	• Fragment 8^{3+} 221122_exp1_Ac-PHF6-NH2_Q1581_EIM 2105.9835-2109.8317 +All MS, 0.0-5.0 min.xy • Fragment 11^{5+} 221122_exp1_Ac-PHF6-NH2_Q1581_EIM 1737.7652-1740.1551 6+ All MS, 0.0-5.0 min.xy • Fragment 9^{4+} 221122_exp1_Ac-PHF6-NH2_Q1581_EIM 1777.2409-1780.3079 5+ All MS, 0.0-5.0 min.xy • Intact 13^{3+} 230104_Ac-PHF6-NH2_exp1_Q2054.82_000002_BPM +All MS.xy • Intact 16^{6+} 230103_ac-PHF6-NH2_Q2107.6_0003_BPM +All MS.xy • Intact 17^{6+} 230104_Ac-PHF6-NH2_exp1_001_EIM 2238.3500-2240.3590 +All MS.xy		See raw data fiels for fragments in folder for Figure 4 Main text Intact oligomers raw data are in included in this folder.
11	MS with different settings on the PS	A. Normal settings 221101_Thaleia's method B. Soft settings 230518: Ac-PHF6-NH2	Figure S11 A - 221101_AC-PHF6-NH2_IMS_TEST.raw Figure S11 B - 230518_AC-PHF6-NH2_NEW_TEST_IMSF_50.raw	Screen shot from MassLynx	Both are MS from TIC averaged over 10 minutes (the same acquisition time).
Table S3	CCS table from TIMS measurements (average over 3 days)	1. 221116Ac-PHF6-NH2 fresh sample 2.221115 Ac-PHF6-NH2 fresh sample 3. 230104 Ac-PHF6-NH2 fresh sample	1. 221116_exp1_Ac-PHF6-NH2_000001.d ◦ 221116_exp1_TM_000004.d 2. 221115_exp1_Ac-PHF6-NH2_000001.d ◦ 221115_exp1_TM_000003.d 3. 230104_Ac-PHF6-NH2_exp1_000001.d ◦ 230104_Tune_exp1_000004.d Tuning files are highlighted in blue	Data are processed in Excel table:	-
	CCS table from TWIMS measurements (average over 3 measurements)	230518: Ac-PHF6-NH2	1. 230518_AC-PHF6-NH2_NEW_TEST5_IMSF_50.raw 2. 230518_AC-PHF6-NH2_NEW_TEST6_IMSF_50.raw 3. 230518_AC-PHF6-NH2_NEW_TEST7_IMSF_50.raw ◦ 230518_TM_TEST7_IMSF_50.raw ◦ 230518_UBIQ_TEST7_IMSF_50.raw Tuning files are highlighted in blue	Data are processed in Excel table: ***<230518_Ac-PHF6-NH2_CCS_values.xls>***	-
12	Correlation between TIMS and TWIMS		see above		**Data are taken from Excel table with comparison of 2 instruments**

#	Title	Elab file	Data name file	Files with proceessed data	Data analysis remarks
Section 2	EIMS with and without quadrupole selection. Peak assignments	With quad selection: • 230103 - TIMS experiment: Ac-PHF6-NH2, quad filtered 2+ and 3+ and 4+ • 230104 - TIMS experiment: Ac-PHF6-NH2 5+ and 7^3+ • 230323 - TIMS experiment: checking settings for lower charged oligomers, like 3_1+ and re-measure quad on 10_4+, 17_6+, and 9_4+ Without quad selection: • All of the above + 22116 - TIMS experiment: 4 PHF6 peptides 24h room temp incubated	Without Quad selection, EIM from the files (stored in folder without quad selection): • 221116_exp1_Ac-PHF6-NH2_000001.d 221116_exp1_TM_000004.d • 230103_Ac-PHF6-NH2_exp1_000001.d 230103_Tune_exp1_000002.d • 230104_Ac-PHF6-NH2_exp1_000001.d 230104_Tune_exp1_000004.d • 230323_exp1_Ac-PHF6-NH2_000001.d 230323_exp1_TM_000001.d With quad selection, BPMs from the files in Yoda. All files are organized per m/z with qiad selection in a dedicated folder.	Stored in folder Origin files m/z 1580 - Quad_filtering_mz1580.opju All the other m/z are in EIMS_supplementary.opju	-

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