

# ACS Chemical Neuroscience

Date: 2024-08-15

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## 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:

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## List of figures (main text):

#	Title	Elab file	Data name file	Origin file	Data analysis/comments
1	ThT Assays 25C	<a href="#">231019 - Ac-PHF6-NH2 plate reader experiment - ThT Assays ClarioStar - 1.5 uM heparin added last</a>	<b>data.tsv</b> Fits: <b>fit_nucleation_elongation.tsv</b> <b>fit_secondary_nucleation.tsv</b>	-	$n_c=n_2=3$ for all fits

2	CD spectra	<p>1. Fresh solutions without heparin and 6 days aged with 1.5 uM Heparin  <a href="#">230921 - CD experiment: samples with heparin 6 days old</a></p> <p>2. Fresh solutions with heparin added immediately  <a href="#">230920 - Ac-PHF6-NH2: CD experiment, fresh samples with 1.5 uM Heparin</a></p>	See folder Figure 2 CD	-	-
4	TEM data	<p>TEM visualization of 25 uM sample, prepared after 4 days of ThT first and then removed from well plate and deposited on a TEM grid.  <a href="#">230911 - TEM visualization and grid preparation - Ac-PHF6-NH2 samples from well plate + PD2-WT</a></p>	-	-	-
5	IM-MS	<p>(A) and (B) are from <a href="#">2401012 - TIMS experiment: Ac-PHF6-NH2 20 uM time points (one capillary) - repeat, filter also 1580</a>  (C) and (D) are a summary of 5 independent measurements. Including one above+  <a href="#">240108</a>  <a href="#">240109 - new capillary each time</a>  <a href="#">240109 - one capillary</a>  <a href="#">240111</a></p>	<ol style="list-style-type: none"> <li><b>240112_exp1_ac-PHF6-NH2_T0_0001 (0 h)</b>  <b>240112_exp1_ac-PHF6-NH2_no_heparin_T24h_0001 (24 h)</b></li> <li><b>240112_exp1_ac-PHF6-NH2_T1_0001 (0 h)</b>  <b>240112_exp1_ac-PHF6-NH2_T24h_0001 (24 h)</b></li> <li>See corresponding folder Figure 4 C</li> <li>Data are from Figure 4 D</li> </ol>	<b>MS_data.opju</b>	MS averaged over 3 minutes

6	IMS data	2401012 - TIMS experiment: Ac-PHF6-NH2 20 uM time points (one capillary) - repeat, filter also 1580	1. <b>240112_exp1_ac-PHF6-NH2_T6_Q2_0001 - BPM</b> 2. <b>240112_exp1_AC-PHF6-NH2_T24h_Q2_000001_BPM</b>	-	Dimer was quadrupole at m/z 1580.9 +- 3
7	Discussion	-	Data for fibrils are from Figure 1 A (20 uM) Data for oligomers are from Figure 4 D		

## SI:

#	Title	Elab file	Data name file	Origin file	Data analysis/comments
1	Schematic overview of experiment				
2	ThT Assays 25C	231019 - Ac-PHF6-NH2 plate reader experiment - ThT Assays ClarioStar - 1.5 uM heparin added last	See folder Figure S2 AmyloFit misfits	-	$n_c = n_2 = 3$ for all fits
3	CD 33 days old sample	230914 - Ac-PHF6-NH2: CD first trial	<b>Ac-PHF6-NH2_100uM_11.08_10mMAA_1.5uM_heparin_20uM_ThT.xls</b>	-	-
4	Full MS	see Data from Figure 4 A and B (main text)	-	-	-
5	IMS and extracted MS	Data is from Figure 5 B	1. <b>240112_exp1_AC-PHF6-NH2_T24h_Q2_000001_BPM.d</b> 2. <b>221122_exp1_Ac-PHF6-NH2_Q1581_0001_TIC.d</b>	-	
TS 1	CCS values comparison	Current work 240112 - TIMS experiment: Ac-PHF6-NH2 20 uM time points (one capillary) - repeat, filter also 1580 previous data - 221122 - TIMS experiment: AC-PHF6-NH2 for calibration + 2 and 3+ filtering charge states.	<b>240112_exp1_ac-PHF6-NH2_T6_0001.d</b>		
6	CCS values vs isotropic curve	240112 - TIMS experiment: Ac-PHF6-NH2 20 uM time points (one capillary) - repeat, filter also 1580	<b>240112_exp1_ac-PHF6-NH2_T6_0001.d</b>	<b>CCS_values.opju</b>	

7	Fibrils and oligomers	-	Data for fibrils are from Figure 1 A (20 uM) Data for oligomers are from Figure 4 D		
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