Experimental report

17/09/2018

Proposal: 8-05-434 **Council:** 4/2018

Title: Vibrational spectroscopy on aspartate-alpha-decarboxylase enzyme withand without ligand to compare withinfrared/Thz spectroscopy

Research area: Biology

This proposal is a new proposal

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Local contacts: Monica JIMENEZ RUIZ

Samples: Aspartate-alpha-decarboxylase powder hydrated with D2O
Aspartate-alpha-decarboxylase powder hydrated with D2O with ligand

Instrument	Requested days	Allocated days	From	To
IN1 LAG	2	1	07/09/2018	08/09/2018
IN6-SHARP	1	0		
IN5	1	1	17/09/2018	18/09/2018

Abstract:

The Aspartate-alpha-decarboxylase (ADC) enzyme is responsible for the assimilation of L-aspartate in bacteria and fungi. D-Serine is an inhibitor of ADC which binds at the active centre and prevents the reaction from completion and causes a conformational change in the C-terminal loop within ADC. This conformational change can be assumed to be associated with a change in the vibrational dynamics as indicated by molecular dynamics simulations carried out by our group.

With the proposed experiment we aim to record neutron vibrational spectra on ADC samples with and without the inhibitor to explore the effect of this inhibitor on the vibrational dynamics and compare with infrared and THz spectroscopy as well as with MD simulations.

By combining neutron spectroscopy with molecular dynamics simulations and complementary infrared and Thz spectroscopy, we will obtain a conclusive answer to whether a dynamic change exists. Moreover, we will establish the well studied model system ADC as a reference to compare neutron and photon inelastic scattering on biological systems.

This proposal is part of the ILL-Hamburg PhD project of T.Raskar.

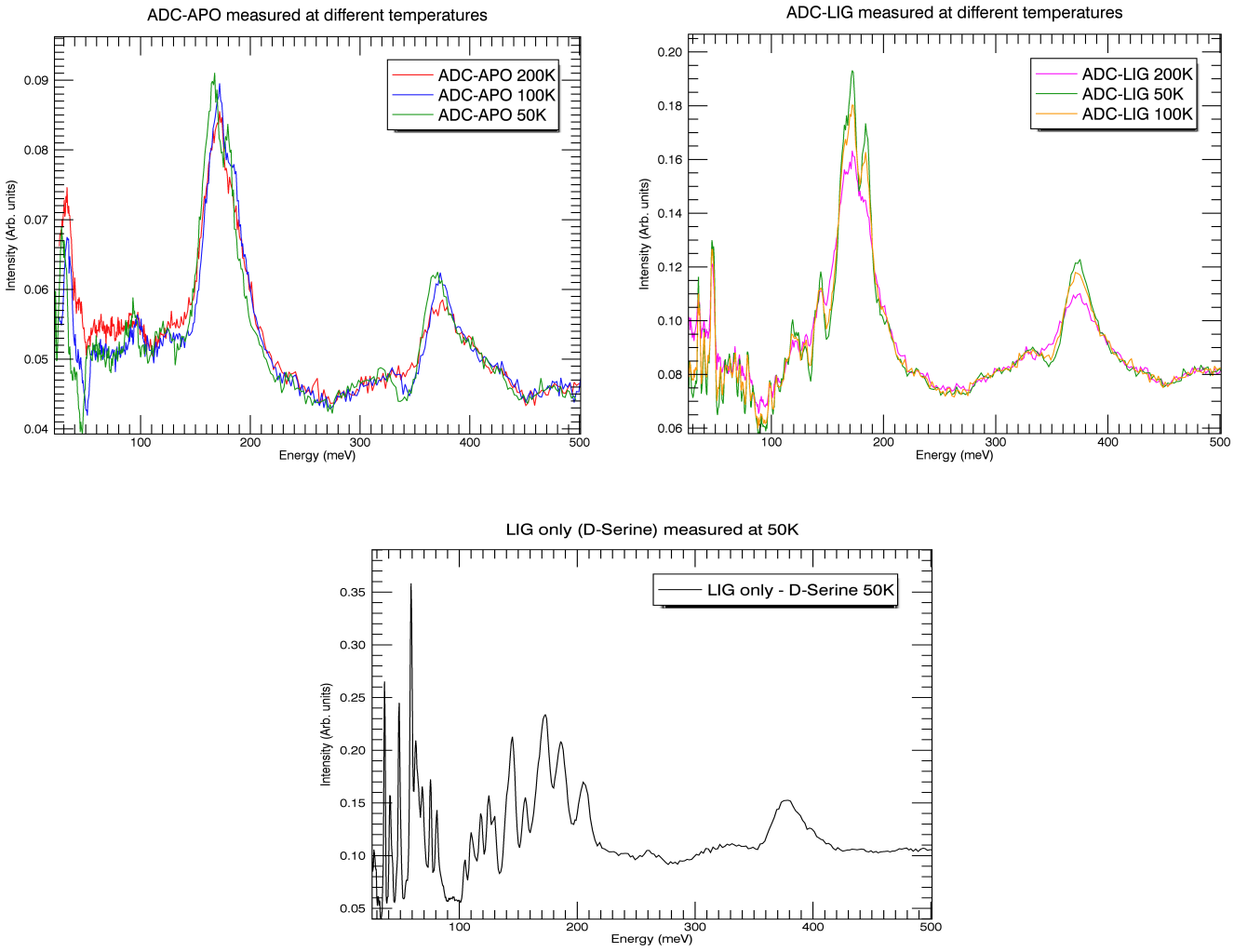

Figure 1. IN1 deep inelastic spectra upto 500 meV for A. ADC-APO, B. ADC-LIG at 50, 100 and 200K and C. LIG only (D-Serine) at 50K.

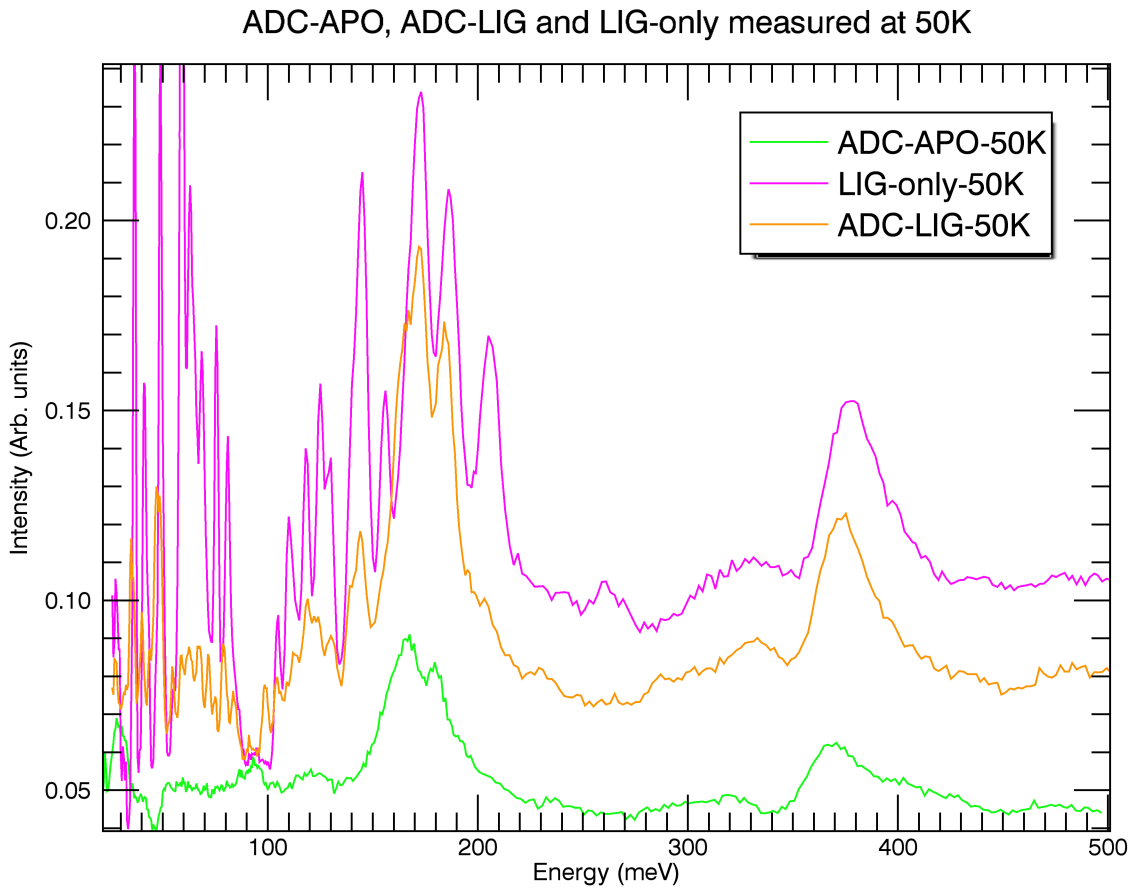

Figure 2. IN1 deep inelastic spectra upto 500 meV for ADC-APO, ADC-LIG and LIG only (D-Serine) at 50K.

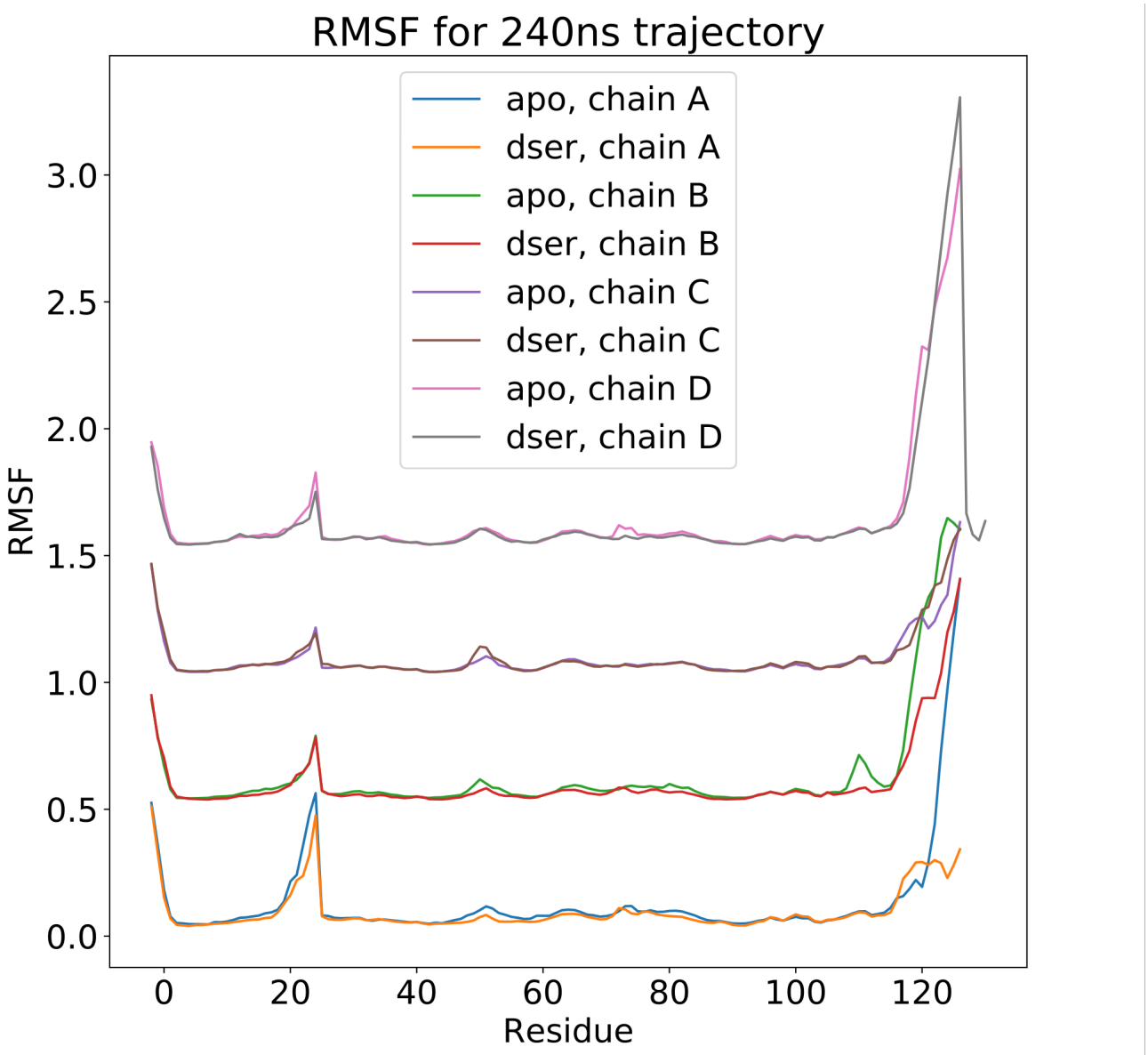

Figure 3. Root mean square fluctuation for the four chains of ADC in apo and D-Serine bound forms obtained from molecular dynamics simulations.