

## Supporting information

### Fluorescently Labeled Thioacetazone for Detecting the Interaction with *Mycobacterium* Dehydratases HadAB and HadBC

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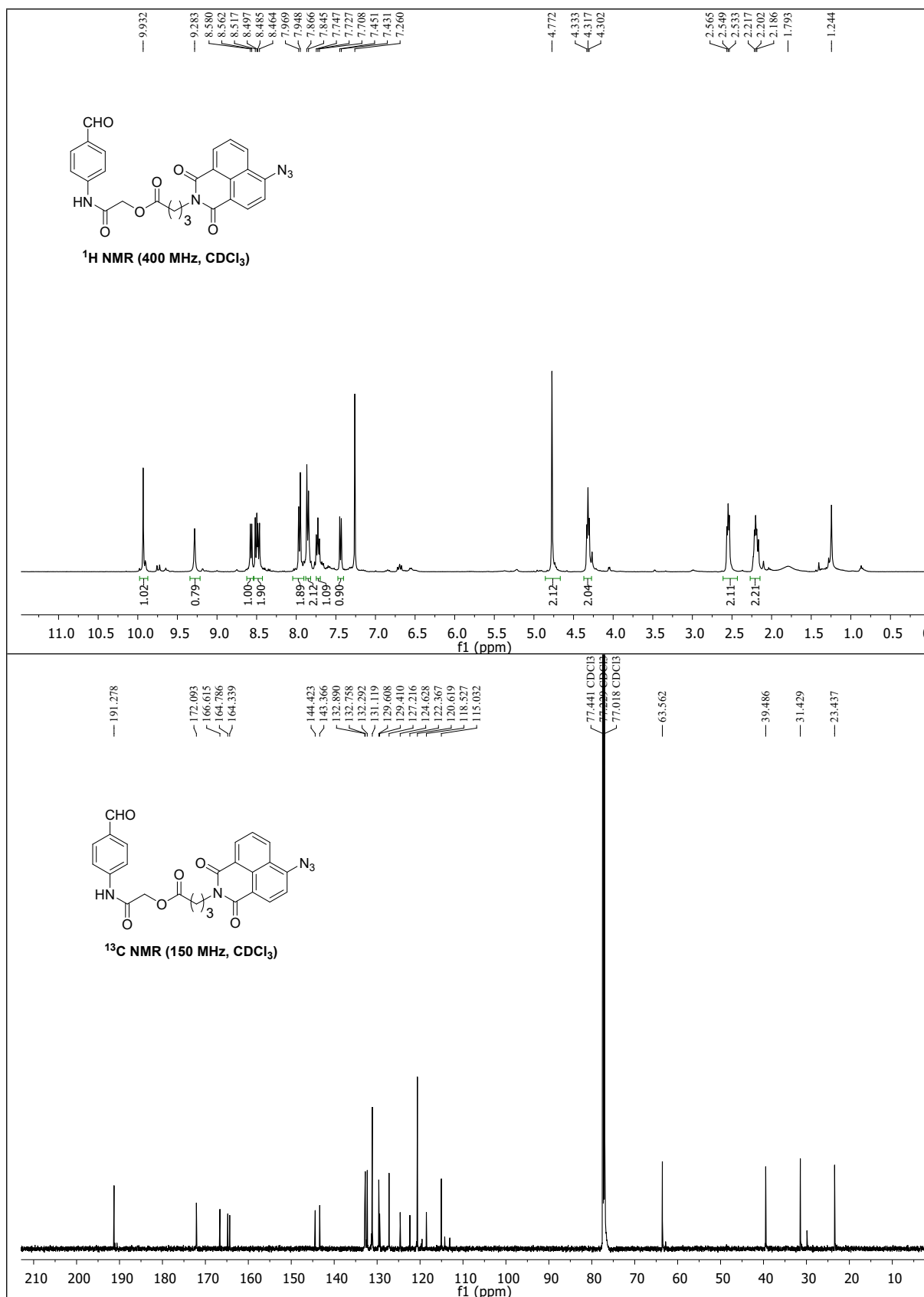
# Equal contribution      \*Corresponding authors

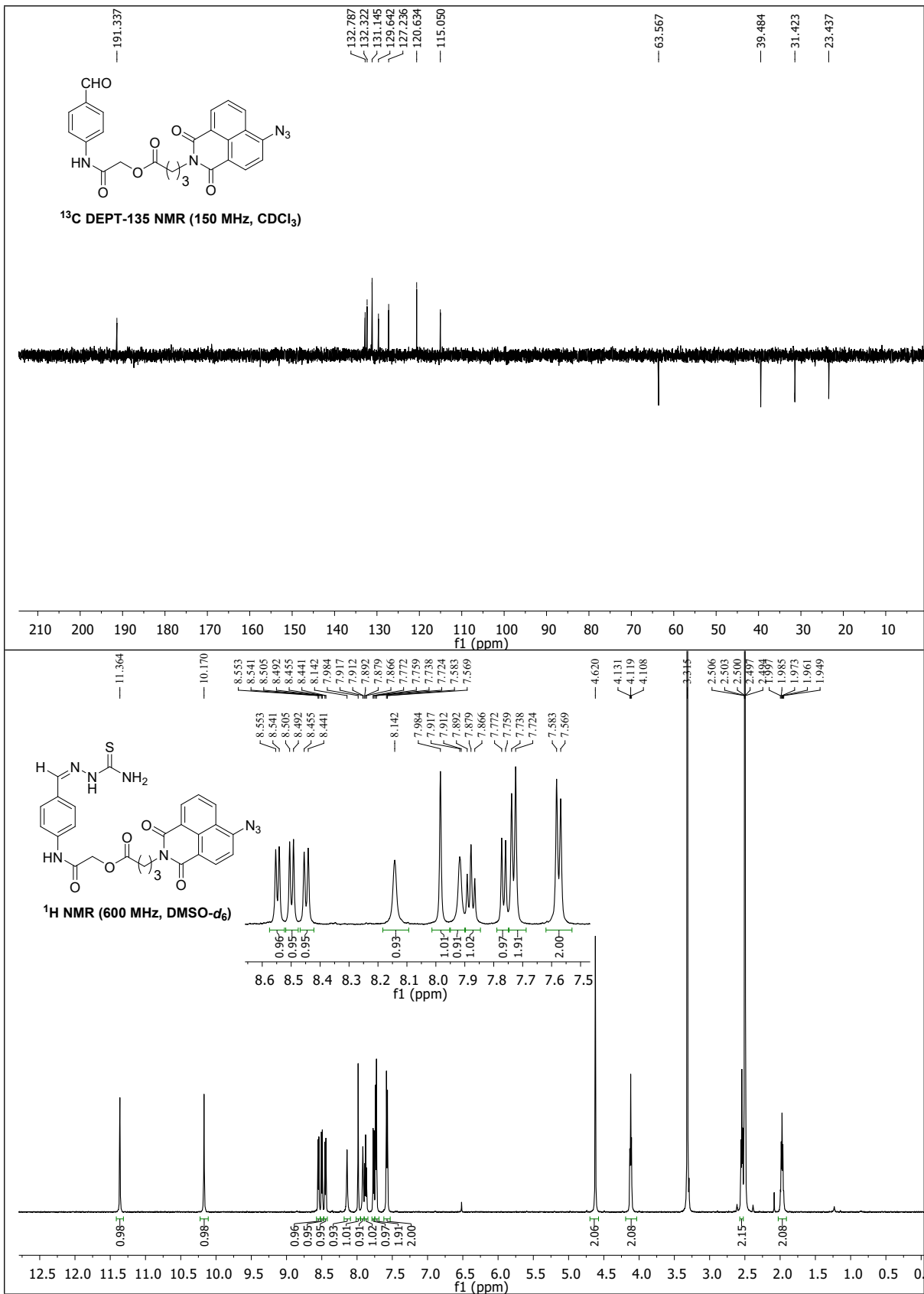
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Kolkata, India

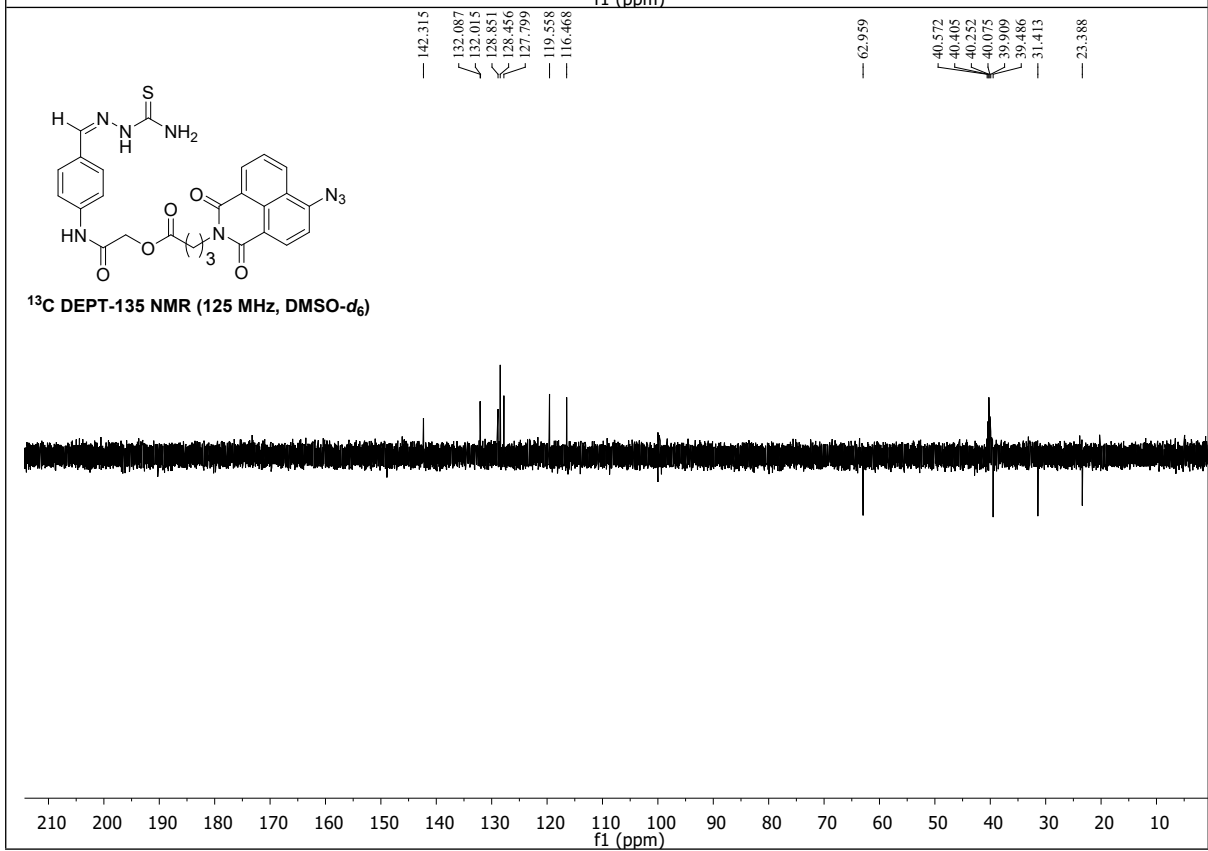
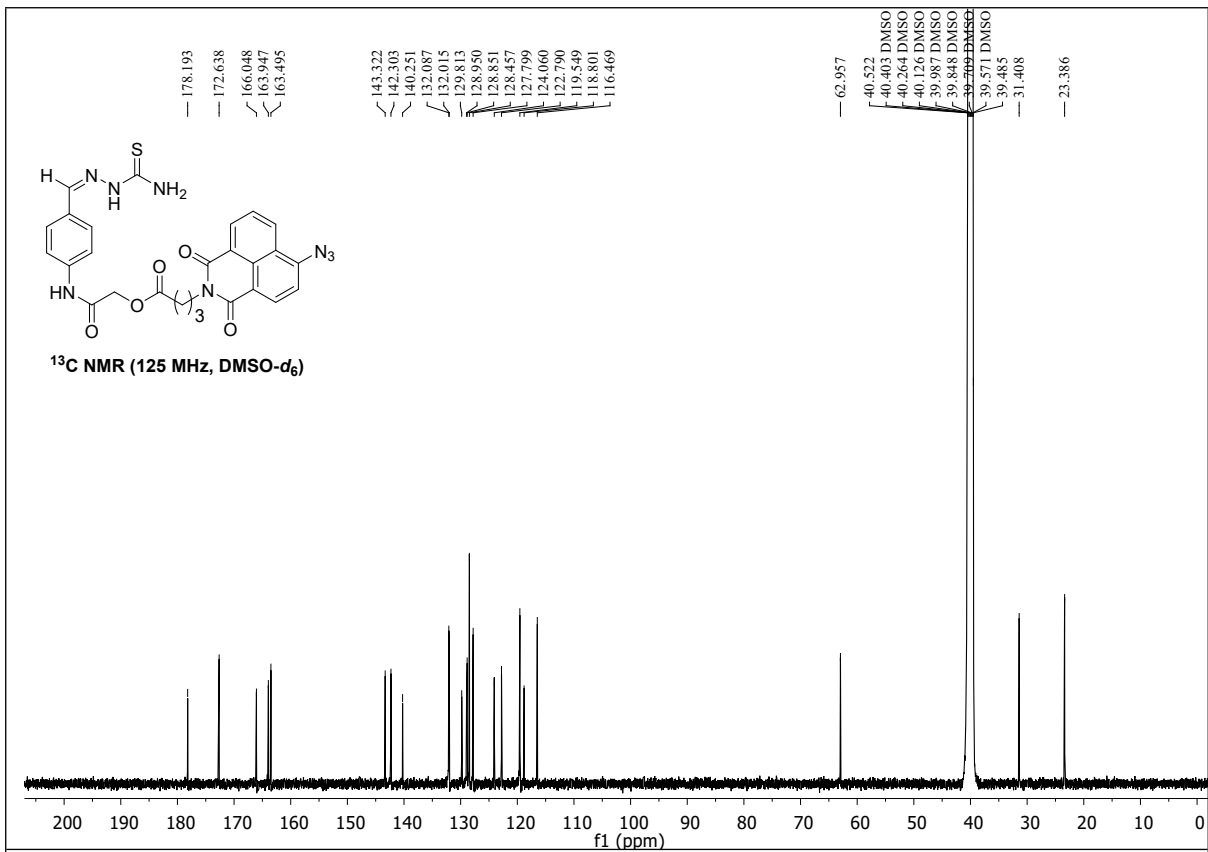
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# <sup>1</sup>H, <sup>13</sup>C, DEPT-135 NMR spectra of the synthesized compounds:

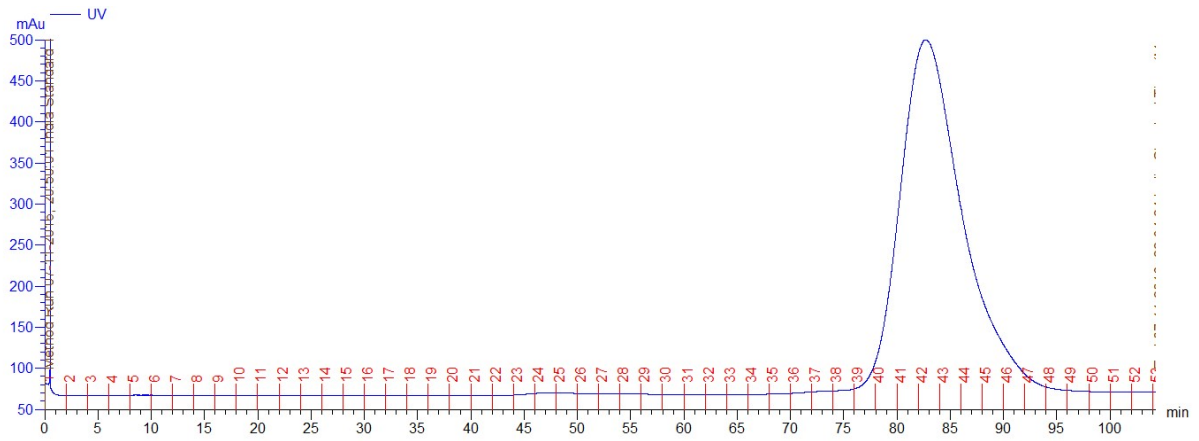




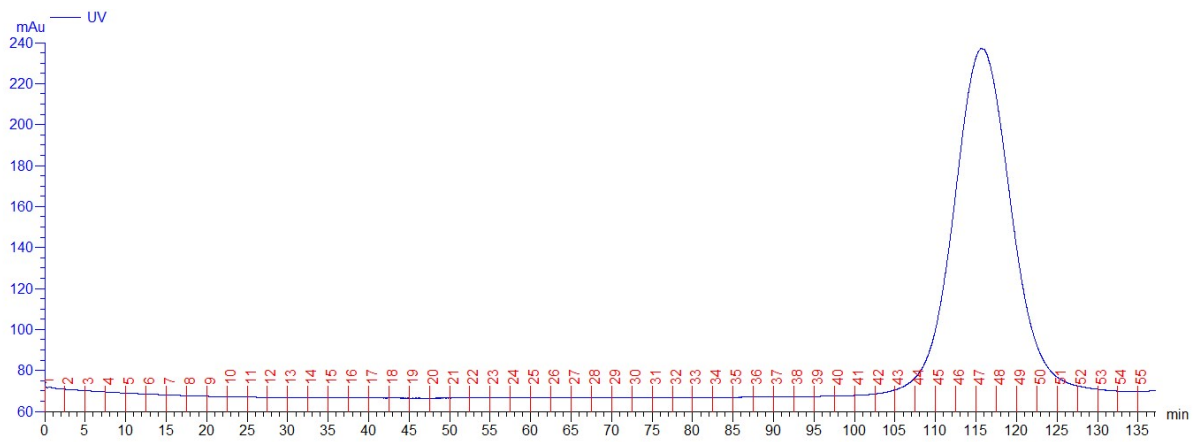


# Purification profile of the proteins used in this study using Size Exclusion Chromatography

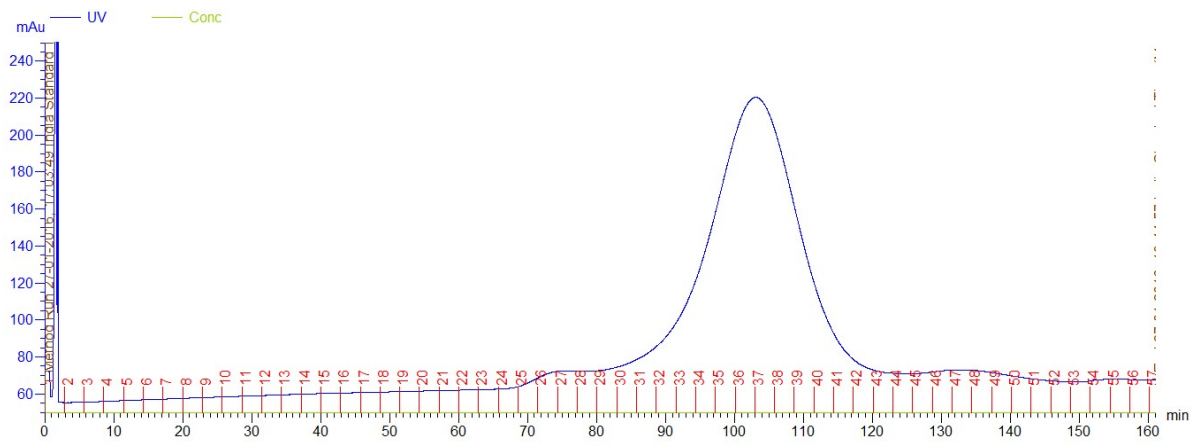
## HadAB



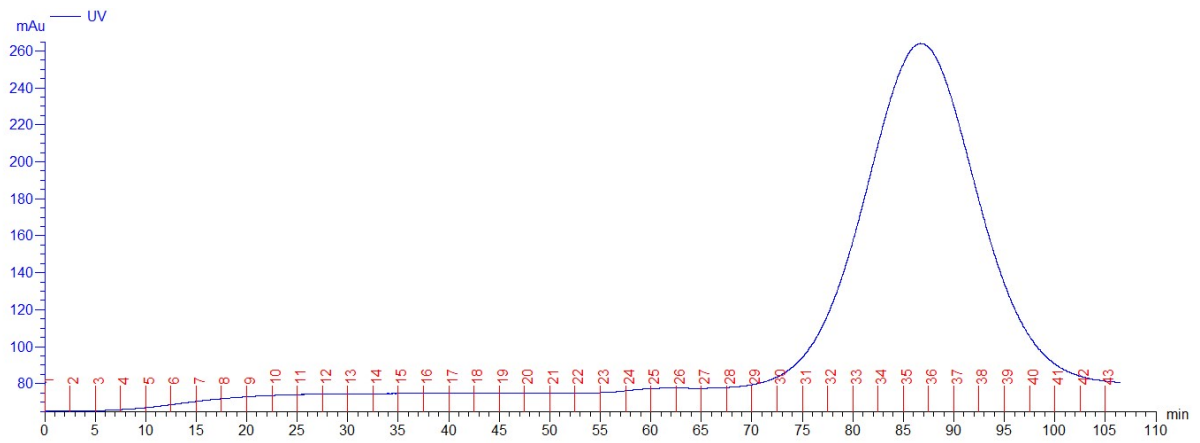
## HadBC



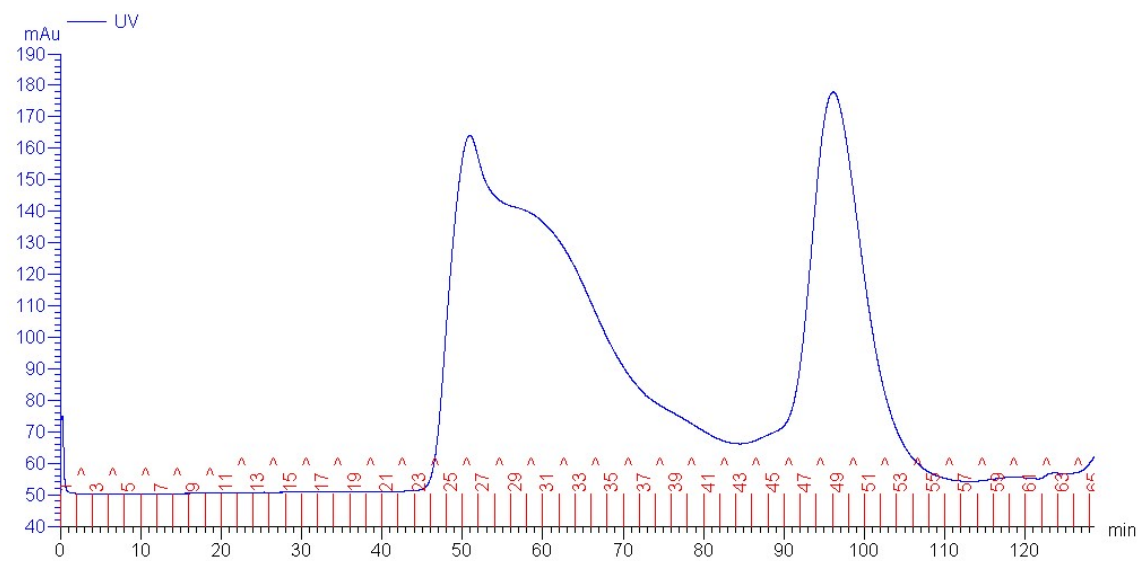
### EthA



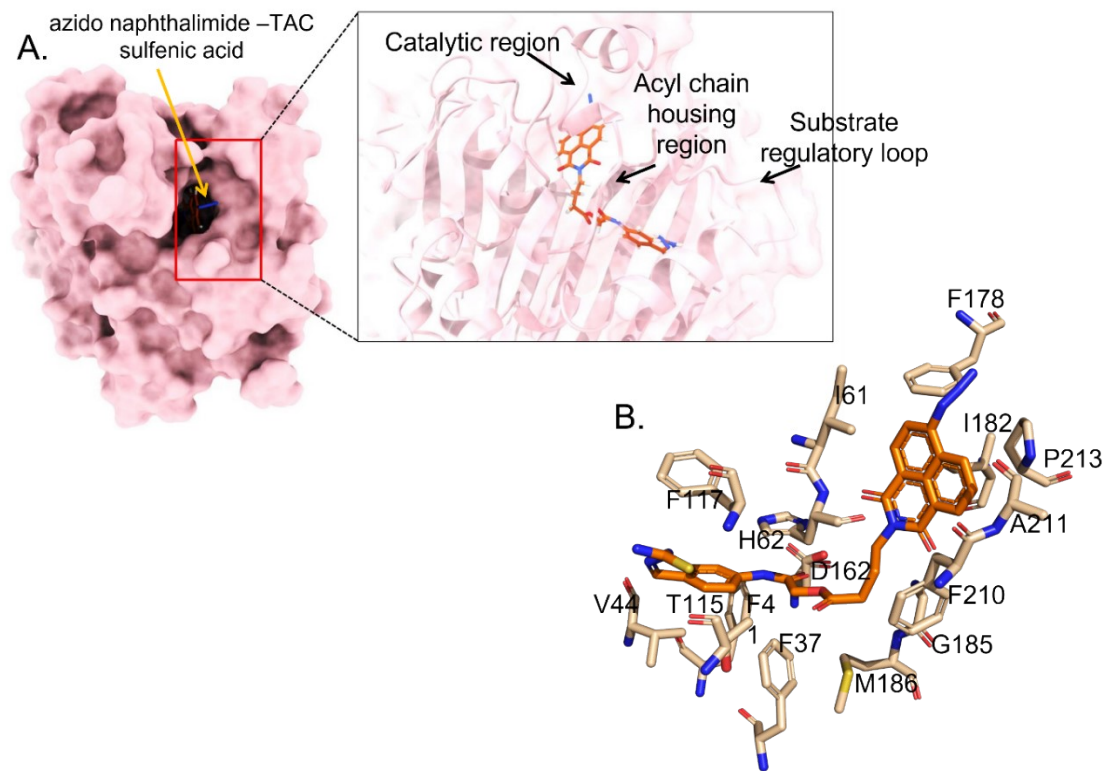
### MymA



### HtdX



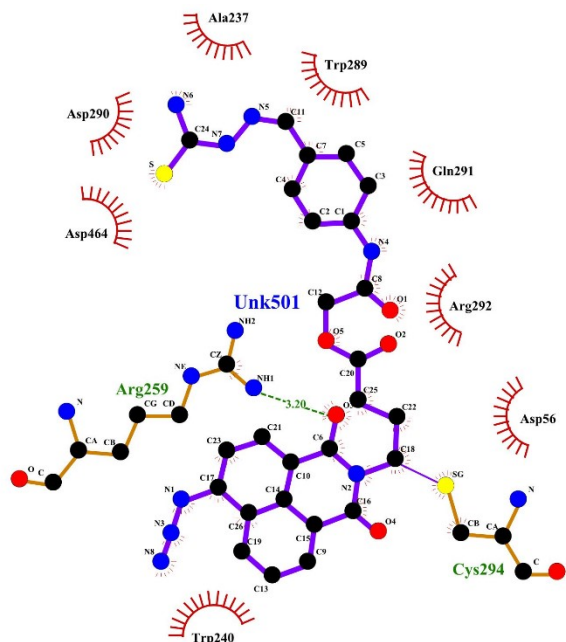
## Docking Pose



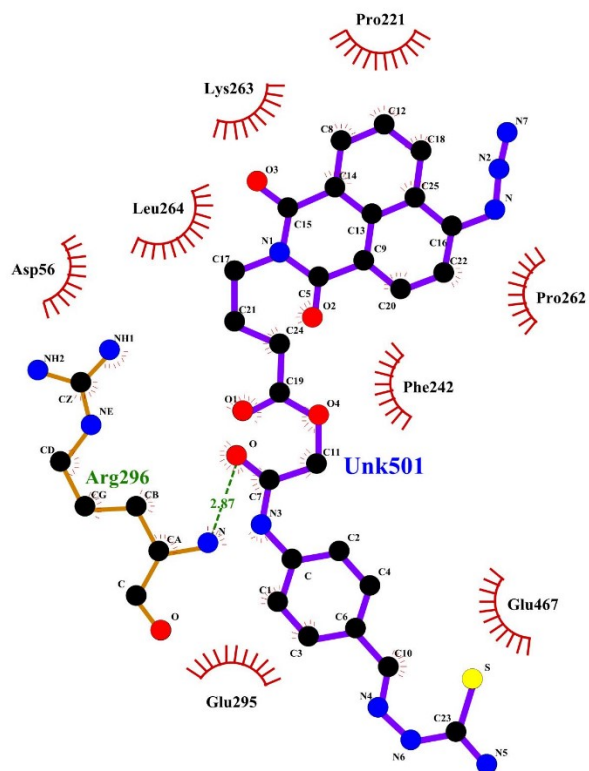
**HtdX docked with the TAC-probe.** (A) Surface representation image of HtdX depicts the docked TAC probe occupying its substrate binding pocket, (B) HtdX residues involved in interaction with the probe.

## Ligplot Analysis depicting the respective residues used in the study interacting with probe

### EthA-TAC probe

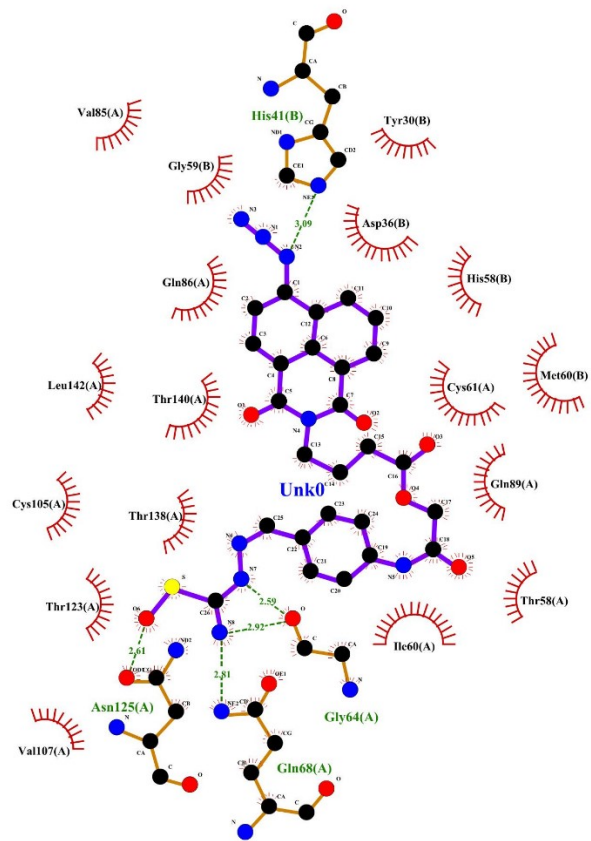


### MymA-TAC probe

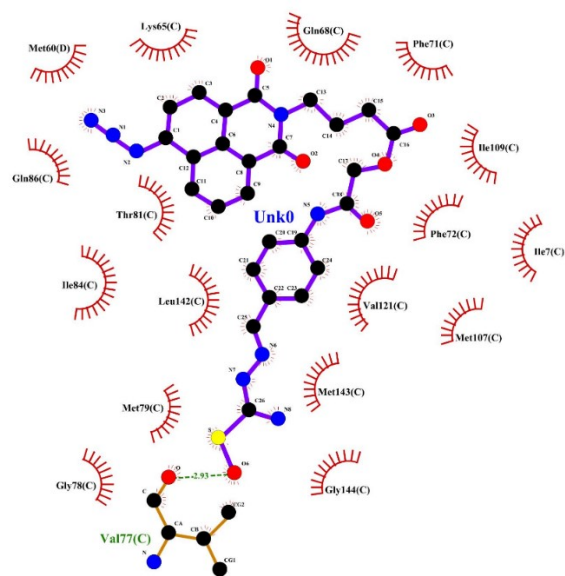




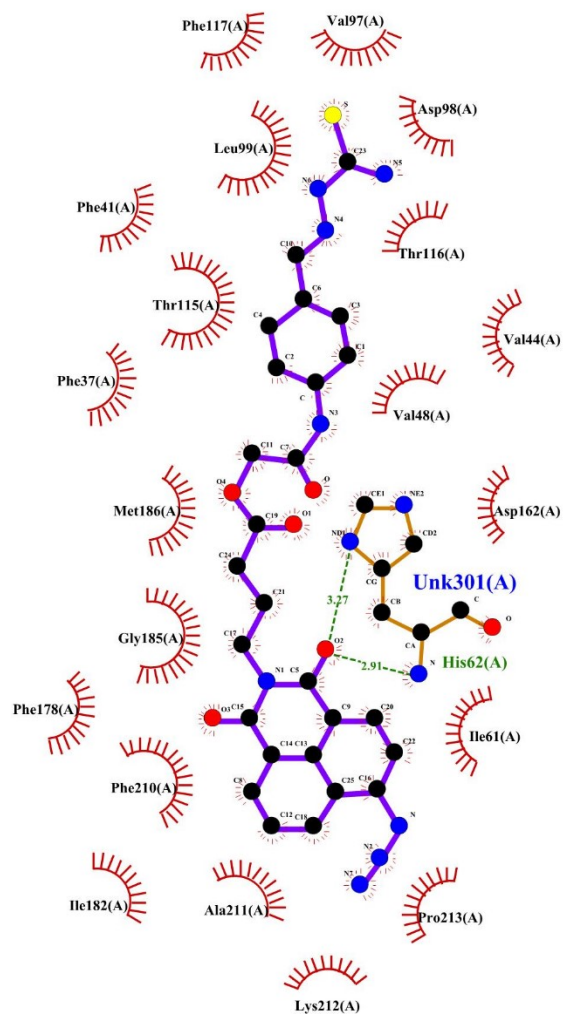
### HadAB-TAC sulfenic acid probe



### HadBC-TAC sulfenic acid probe



# HtdX-TAC probe



## Estimated Docking Results

**Table 1**

<b>S.no</b>	<b>Protein</b>	<b>Estimated free energy of binding</b>	<b>Estimated Inhibition constant (Ki)</b>
<b>1.</b>	<b>HadAB</b>	<b>-8.80 kcal/mol</b>	<b>0.35 <math>\mu</math>M</b>
<b>2.</b>	<b>HadBC</b>	<b>-8.27 kcal/mol</b>	<b>0.86 <math>\mu</math>M</b>
<b>3.</b>	<b>HtdX</b>	<b>-10.64 kcal/mol</b>	<b>1.50 <math>\mu</math>M</b>
<b>4.</b>	<b>EthA</b>	<b>-11.39 kcal/mol</b>	<b>5.18 <math>\mu</math>M</b>
<b>5.</b>	<b>MymA</b>	<b>-10.6 kcal/mol</b>	<b>7.36 <math>\mu</math>M</b>