









# NSP3-MD Target meeting

Hadia Almahli

21st Oct 2024



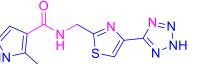


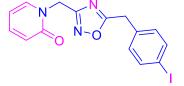
5E-5

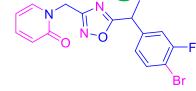


Okay density, binding observed in only one

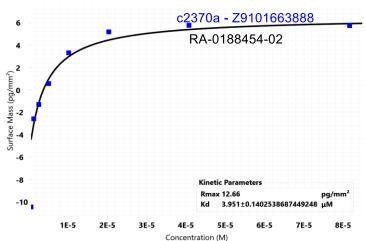
chain, different binding pose to fragment

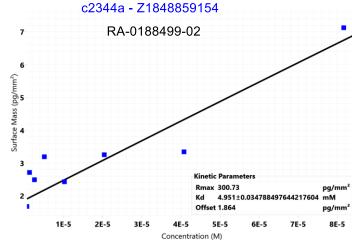


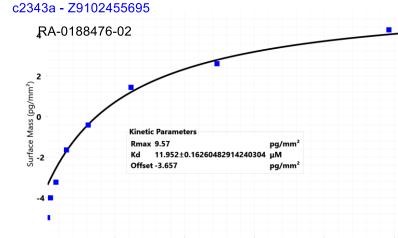


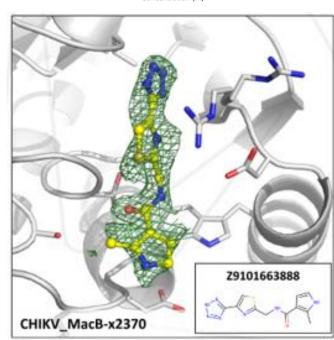


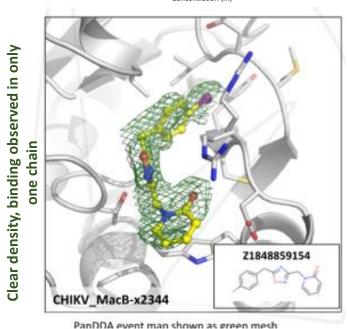
Clear density, binding observed in only

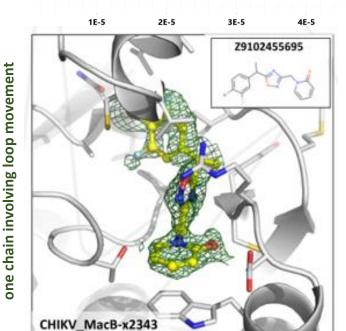












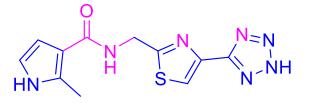




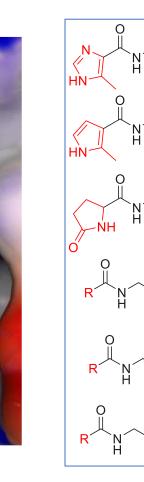
#### **Top rated compound**

c2370a - Z9101663888

RA-0188454-02



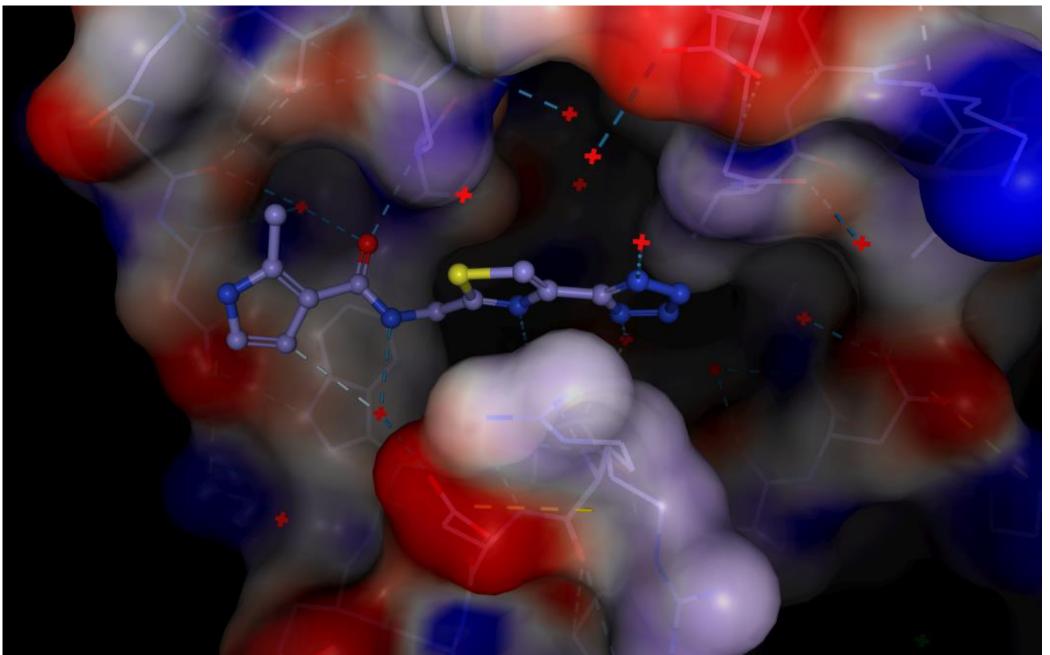
#### **Planned SAR expansion**



#### **Purchased reactants**

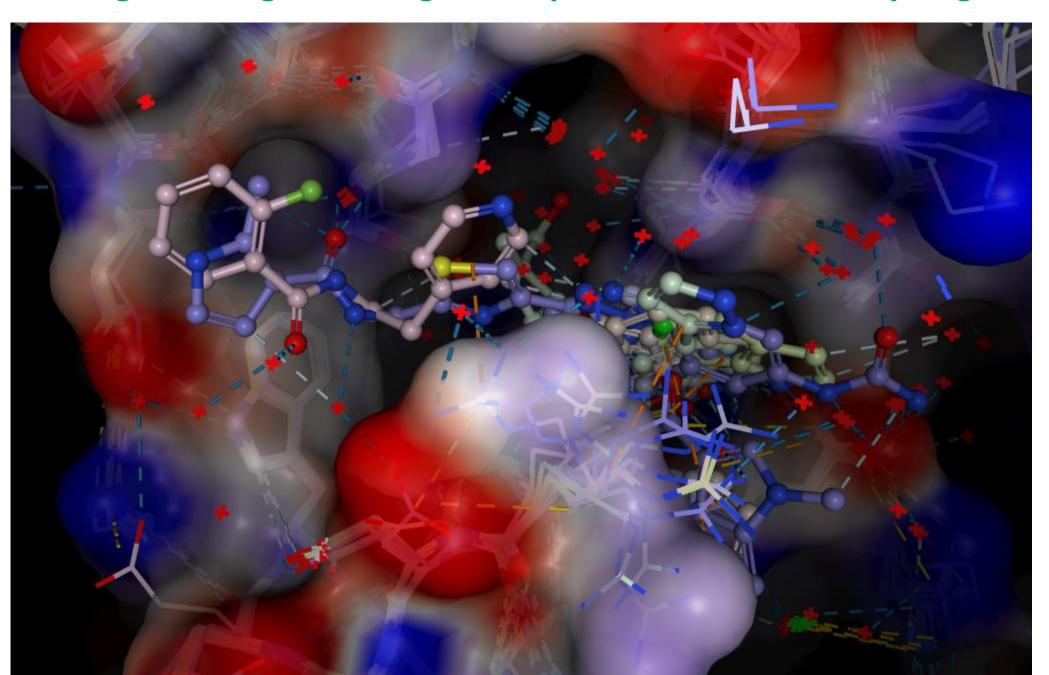
## The original merged catalogue compound





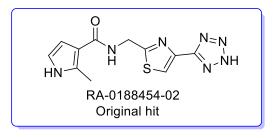
### The original merged catalogue compound with the nearby fragments

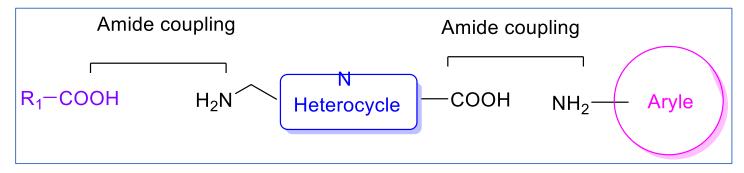


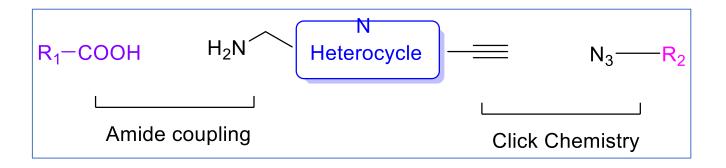


### Synthesis beyond currently ordered reagents











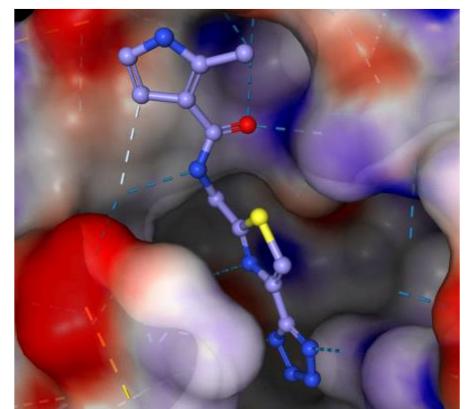


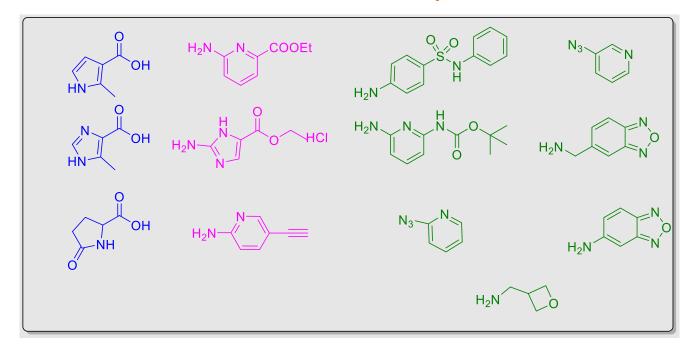
#### **Top rated compound**

c2370a - Z9101663888

RA-0188454-02

#### Ordered reactants for the 1st expansion

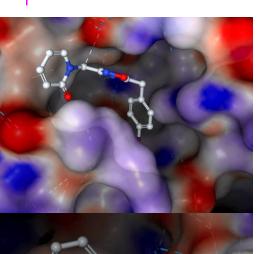






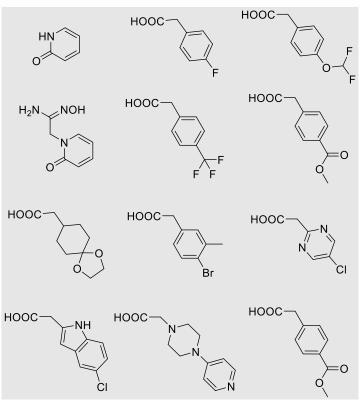
2nd rated compound c2344a - Z1848859154 RA-0188499-02





#### **Planned expansion**

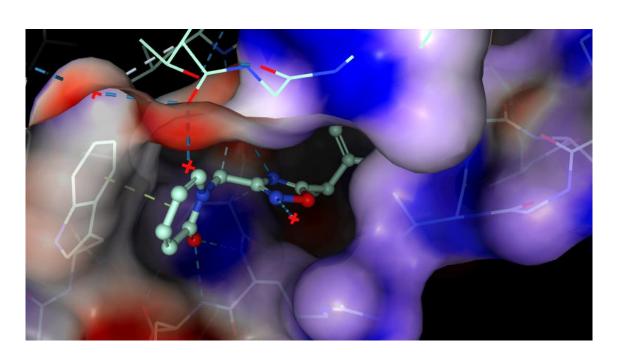
#### **Purchased reactants**



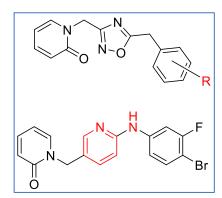






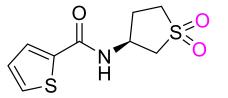


### **Planned expansion**



#### **Ordered reactants**





c2350a - Z86430593

