









# **Growing beyond the Merged Fragments**

3 hits Synthesis of expansion for SAR (reactants already ordered)
Beyond above expansion (Expansion based on nearby fragments)

Hadia Almahli



Pure catalogue compounds/ Analogues design



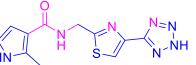


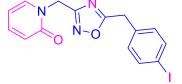
5E-5

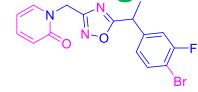


Okay density, binding observed in only one

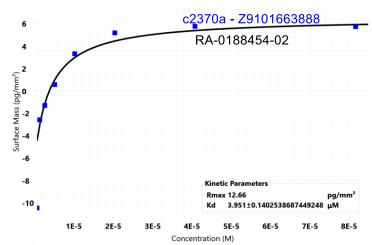
chain, different binding pose to fragment

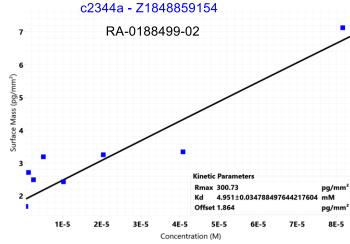


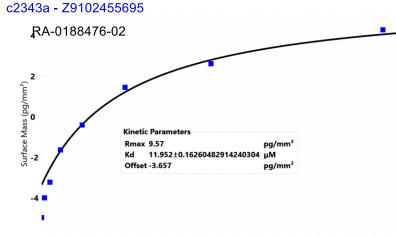


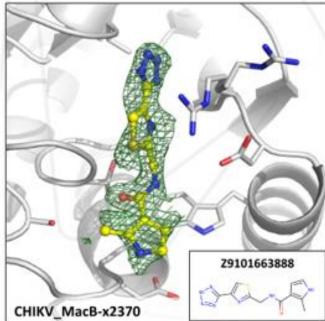


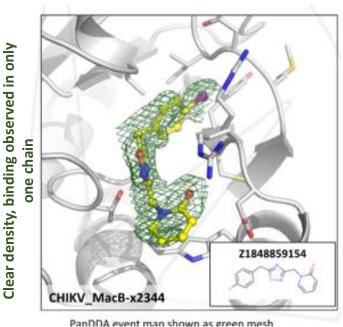
Clear density, binding observed in only

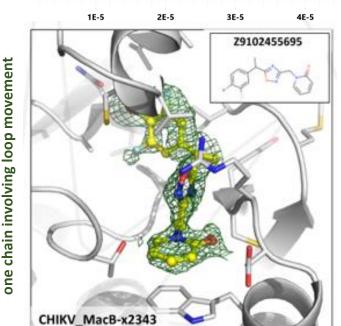












### Synthesis of expansion for SAR (reactants already ordered)

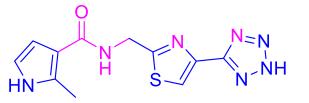




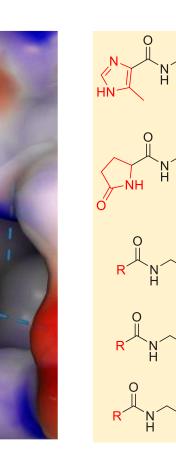
#### **Top rated compound**

c2370a - Z9101663888

RA-0188454-02

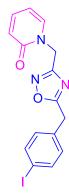


### **Planned expansion**



#### **Ordered reactants**

OH H<sub>2</sub>N 
$$\stackrel{N-NH}{>}$$
N  $\stackrel{N-NH}{>}$ N  $\stackrel{N-N$ 

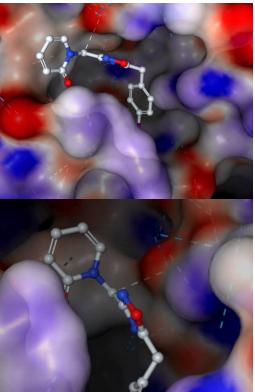


## Synthesis of expansion for SAR (reactants already ordered)



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





### **Planned expansion**

#### **Ordered reactants**

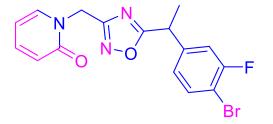
## Synthesis of expansion for SAR (reactants already ordered)

UCL SCHOOL OF PHARMACY

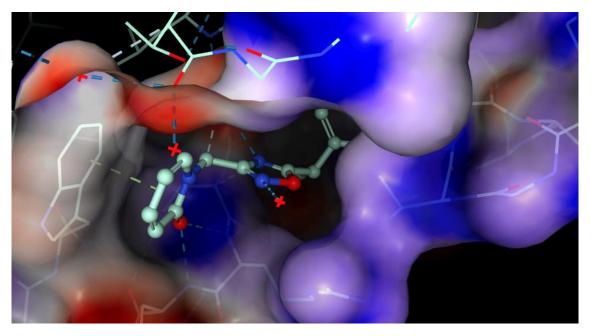
3<sup>rd</sup> rated compound

RA-0188476-02

c2343a - Z9102455695



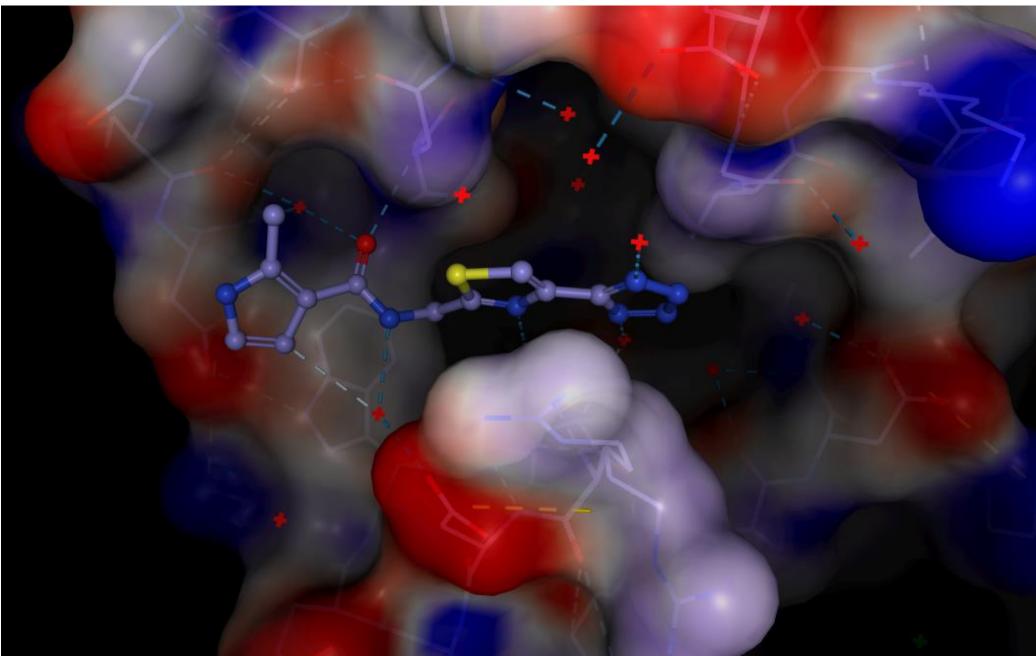




### **Planned expansion**

#### **Ordered reactants**

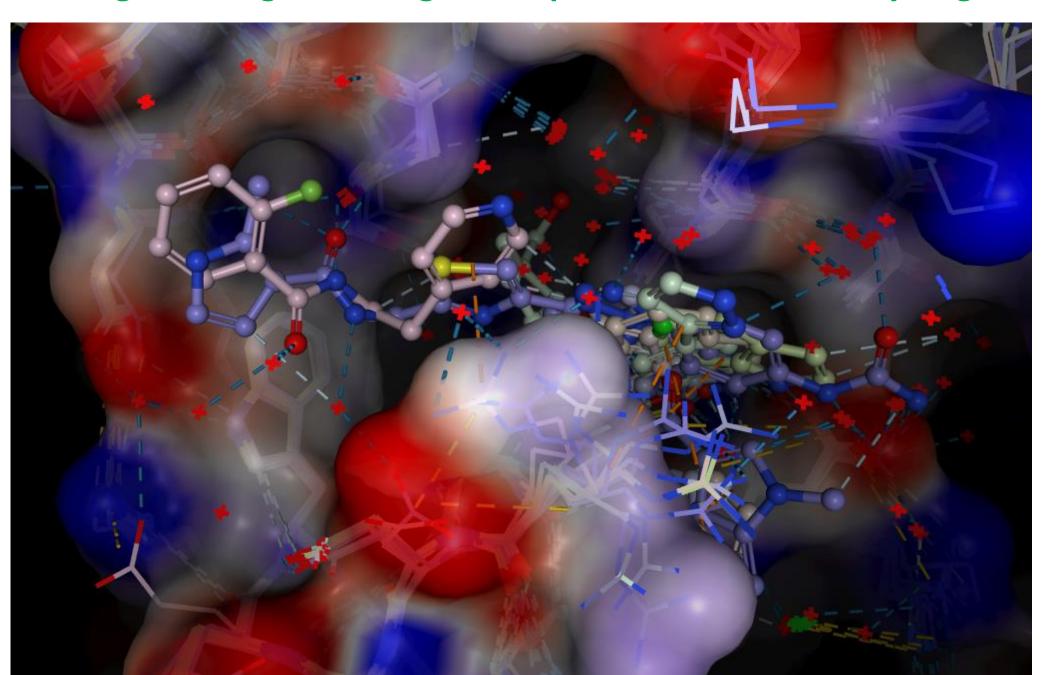
# The original merged catalogue compound





# The original merged catalogue compound with the nearby fragments





## Synthesis beyond currently ordered reagents



