



**SwissBioisostere** 



**SwissTargetPrediction** 





**SwissSimilarity** 



## Swiss Institute of Bioinformatics

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Library screened Screening method Run parameters

ZINC\_lead ECFP4

Date September 30, 2024, 11:41 am UTC

If you publish these results, please, cite the following paper:

Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., *J. Chem. Inf. Model.*, **2016**, *56*(8), 1399-1404.

## **Query Molecule**

## Results

ZINC000004496145 Score: 0.647

#### ZINC000001018834 Score: 0.647

#### ZINC000000148274 Score: 0.640

# Retrieve data:

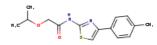


# • • D \(\Sigma\)



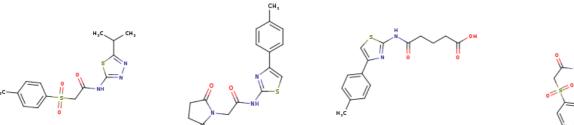


ZINC000040177119 Score: 0.635

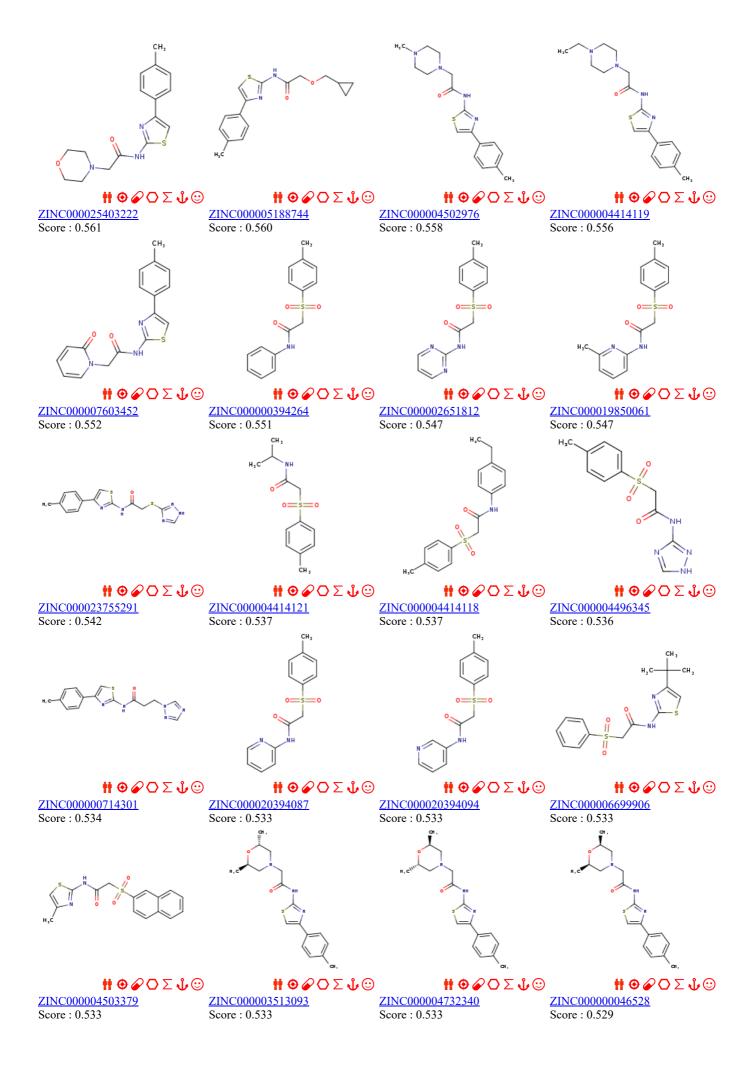


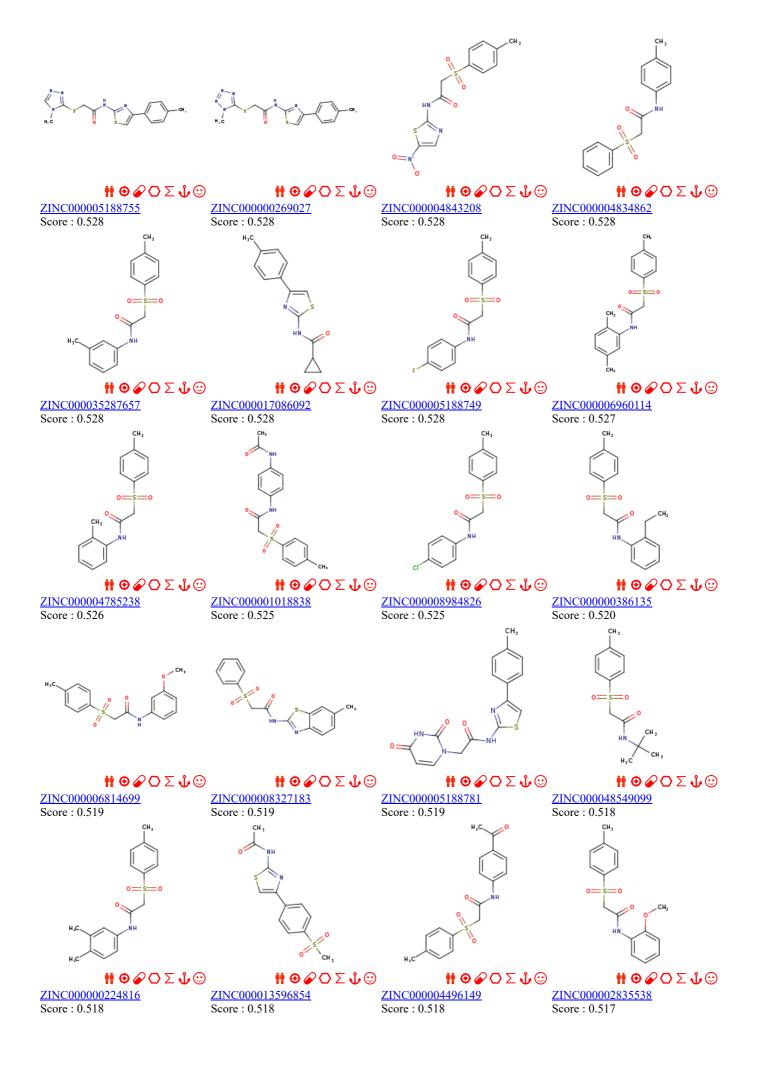
 $\mathsf{H} \bullet \mathscr{P} \circ \Sigma \, \mathsf{J} \odot \qquad \qquad \mathsf{H} \bullet \mathscr{P} \circ \Sigma \, \mathsf{J} \odot \qquad \qquad \mathsf{H} \bullet \mathscr{P} \circ \Sigma \, \mathsf{J} \odot \qquad \qquad \mathsf{H} \bullet \mathscr{P} \circ \Sigma \, \mathsf{J} \odot$ ZINC000004502978 ZINC000003218404 ZINC000004668908 ZINC000409179855 Score: 0.627 Score: 0.615 Score: 0.611 Score: 0.611  $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$ # **⊕ ⊘** ○ ∑ **↓** ⊙ ZINC000009320350 ZINC000005715152 ZINC000001466264 ZINC000001077506 Score: 0.604 Score: 0.604 Score: 0.604 Score: 0.596  $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$  $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$  $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$  $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$ ZINC000019822755 ZINC000005188753 ZINC000003232344 ZINC000004496134 Score: 0.596 Score: 0.593 Score: 0.593 Score: 0.589

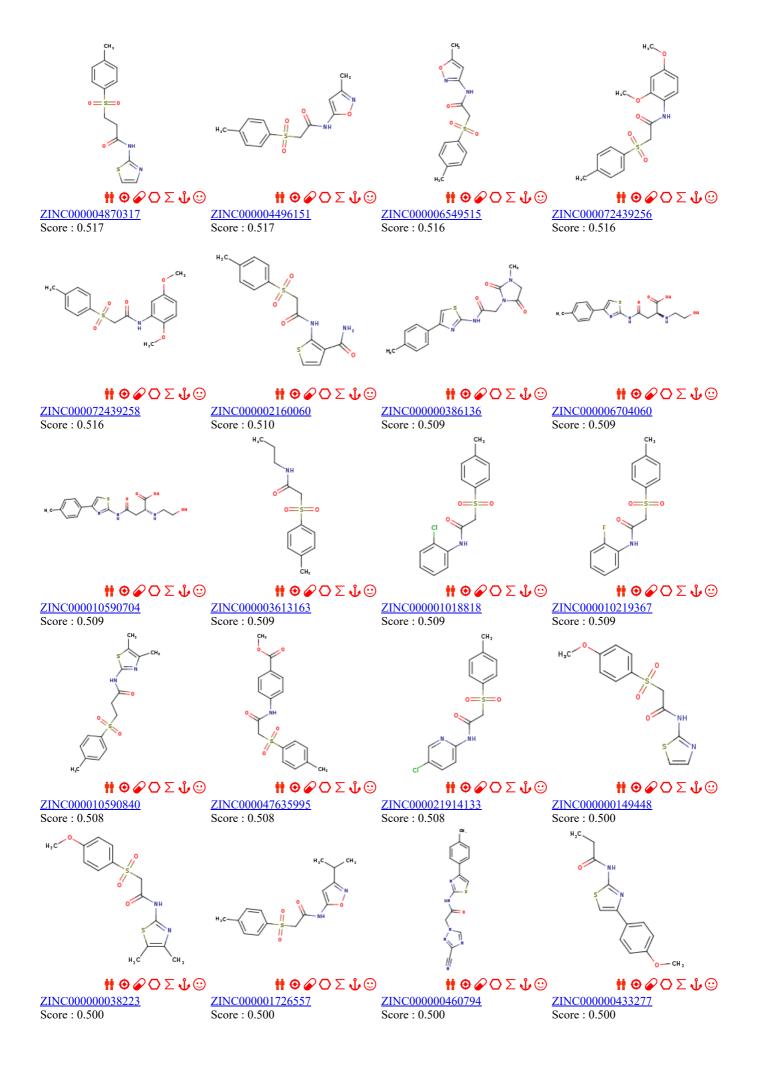
 $\begin{array}{c} \text{H} \oplus \bigcirc \bigcirc \Sigma \stackrel{\downarrow}{\downarrow} \odot \\ \text{ZINC0000004502987} \\ \text{Score}: 0.582 \\ \end{array} \begin{array}{c} \text{ZINC000000189271} \\ \text{Score}: 0.582 \\ \end{array} \begin{array}{c} \text{ZINC000001200254} \\ \text{Score}: 0.582 \\ \end{array} \begin{array}{c} \text{ZINC000004502991} \\ \text{Score}: 0.582 \\ \end{array} \begin{array}{c} \text{CH}, \\ \text{CH}, \\ \end{array}$ 

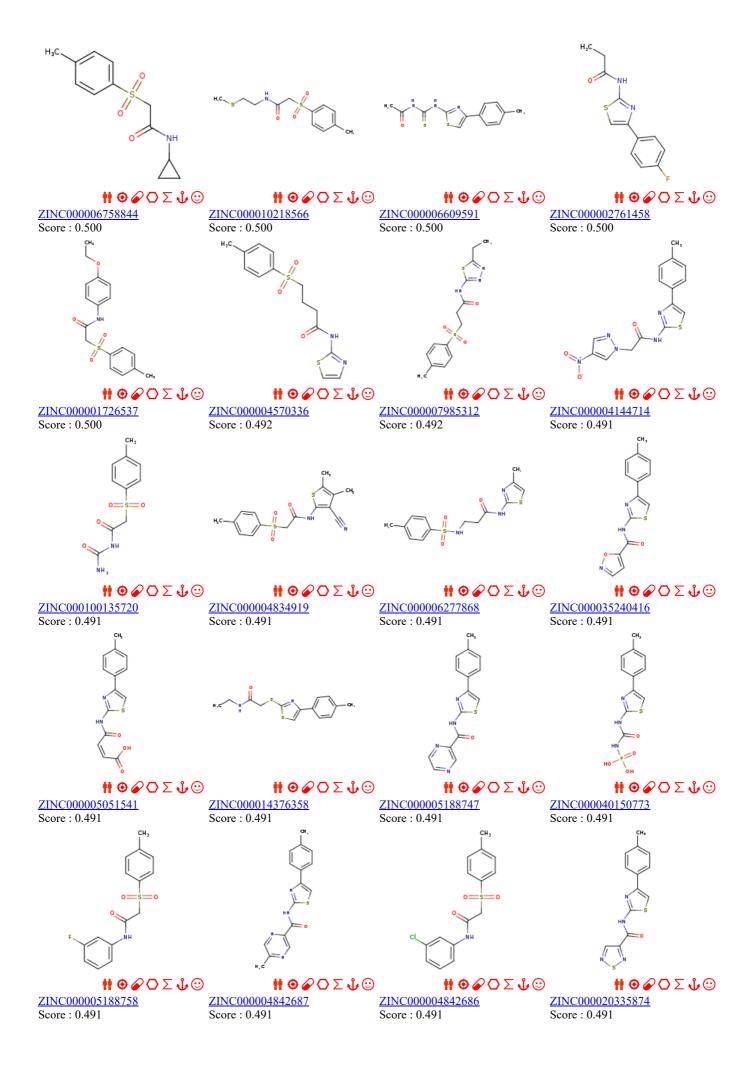


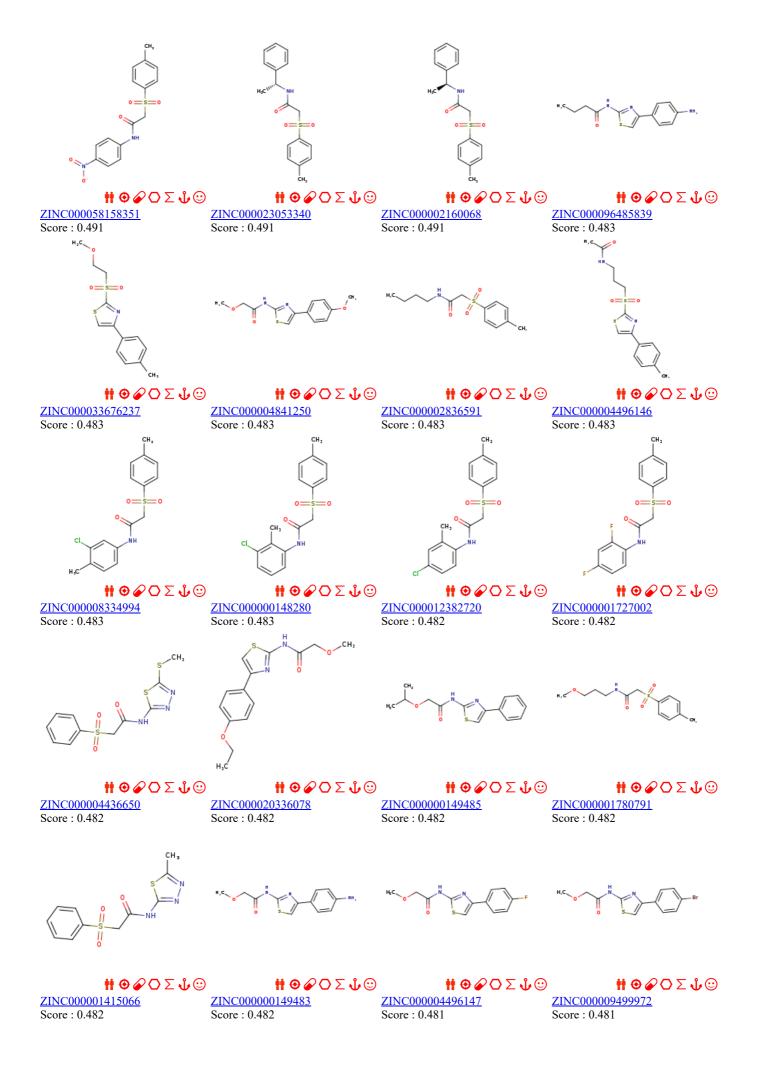
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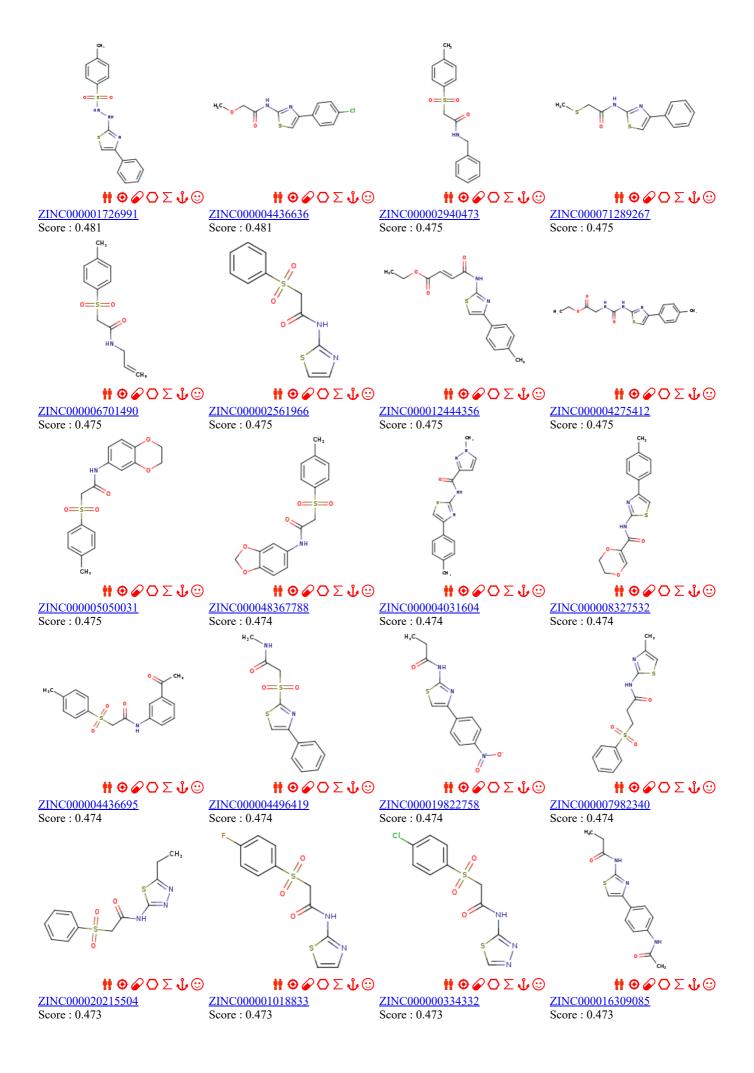


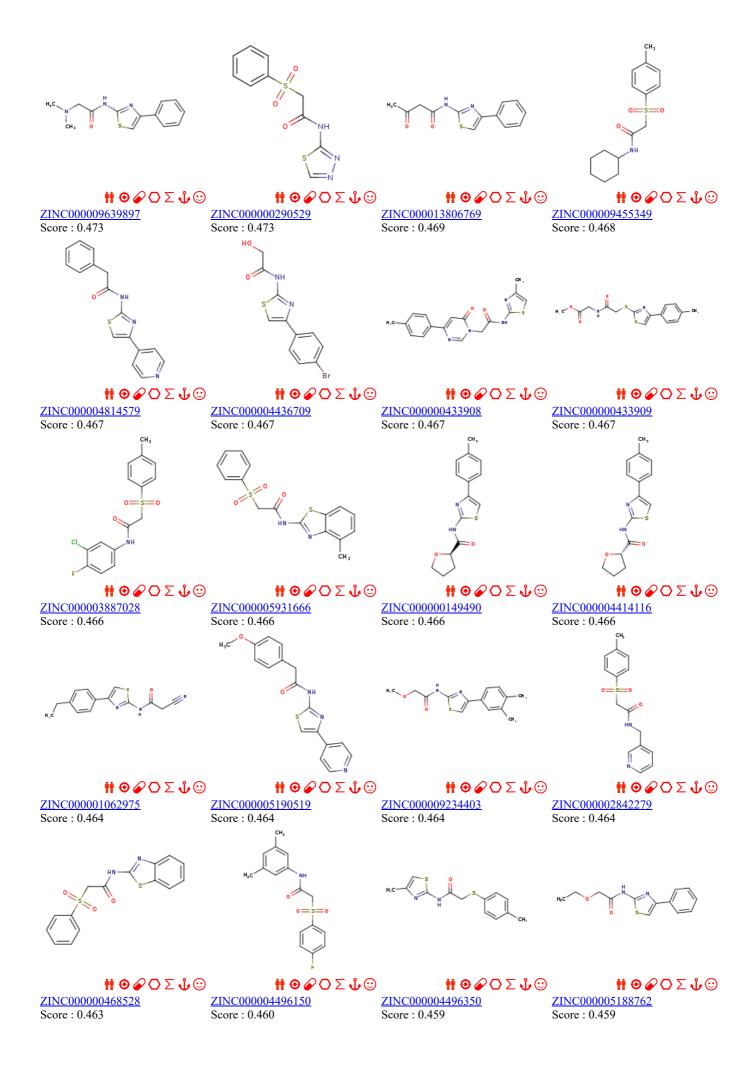


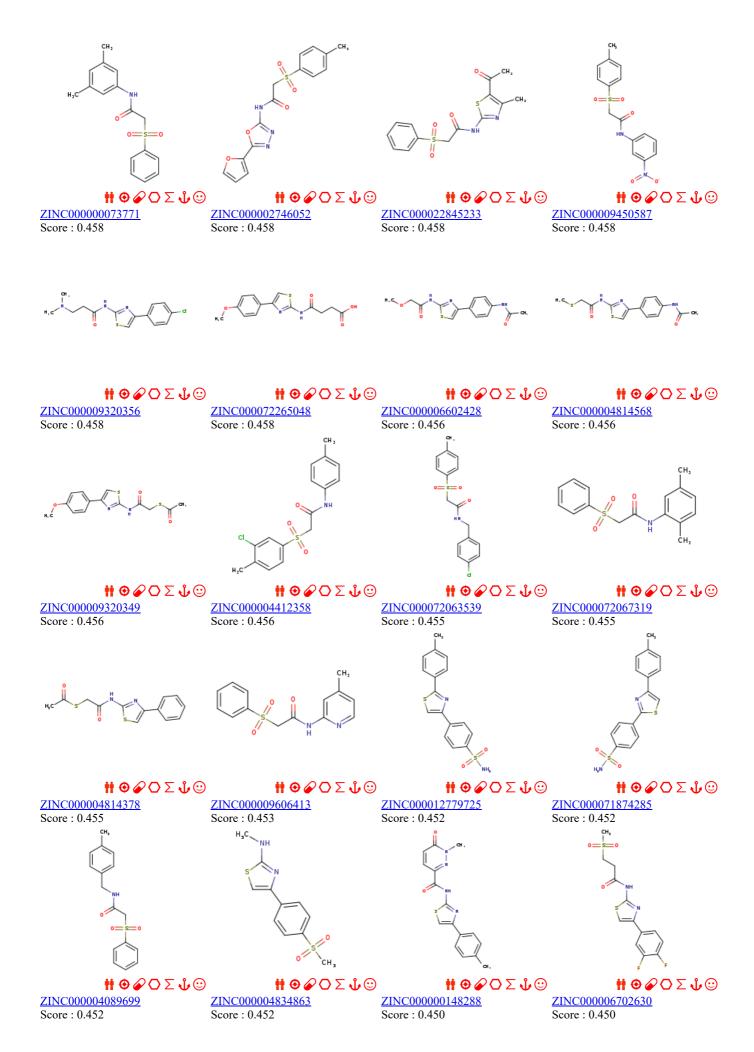


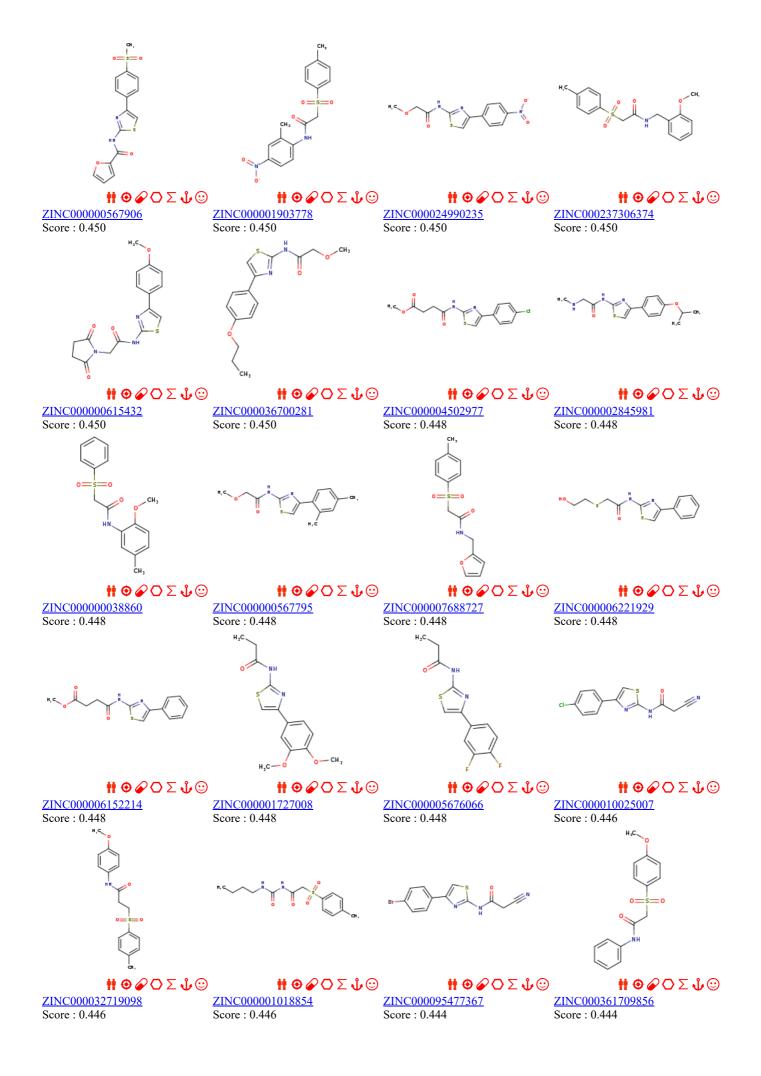


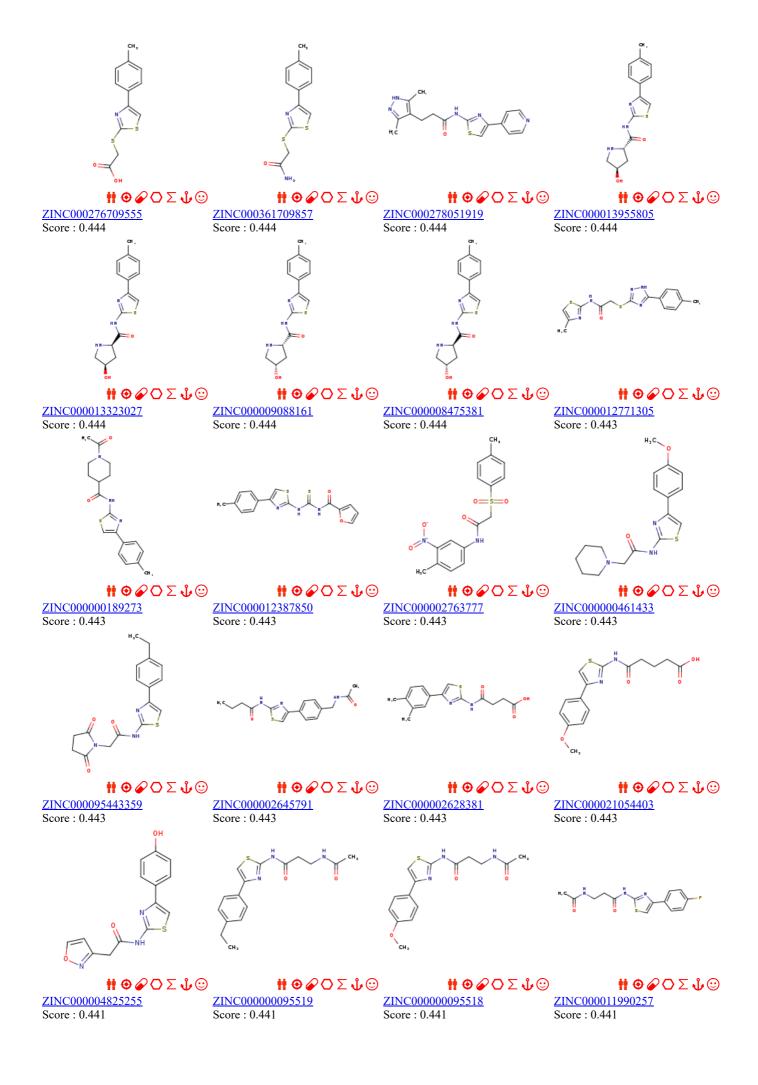


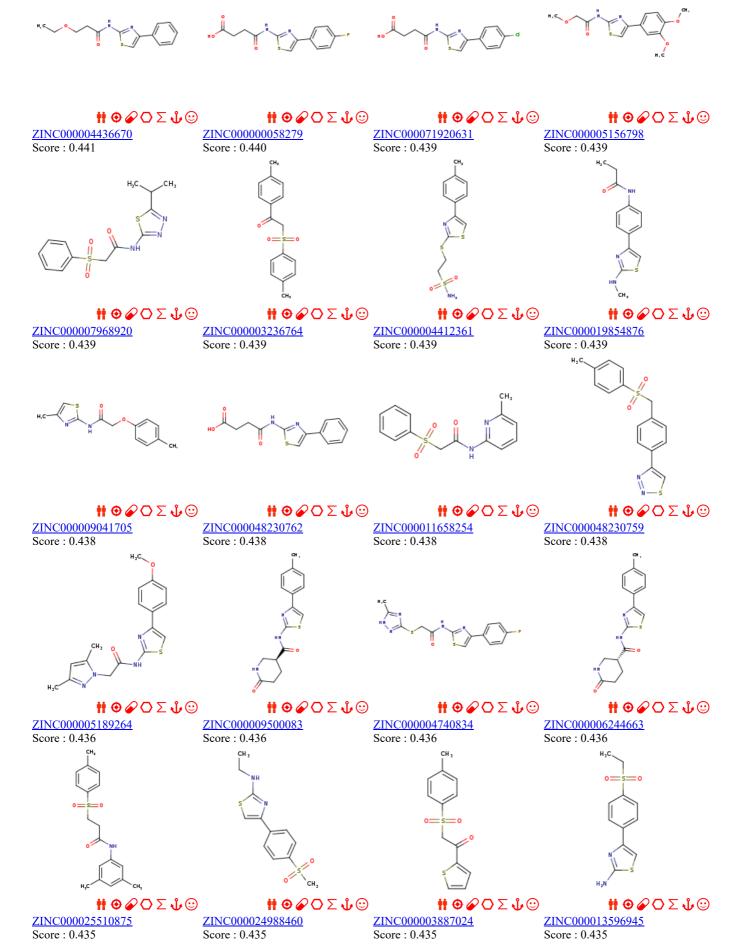


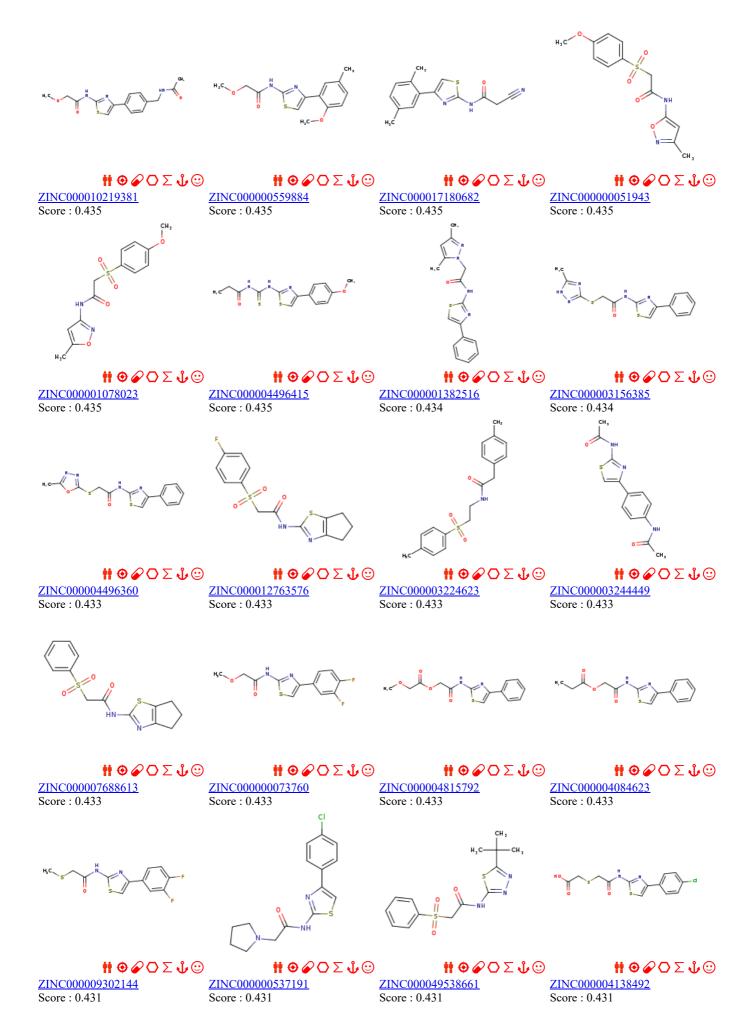


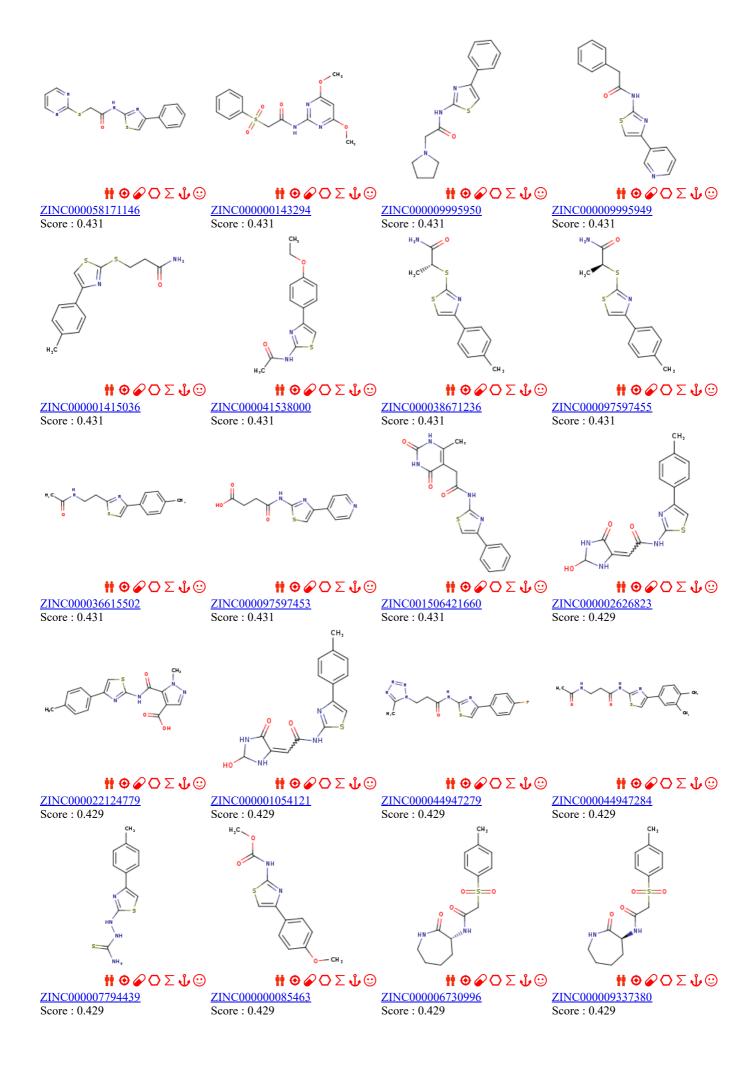


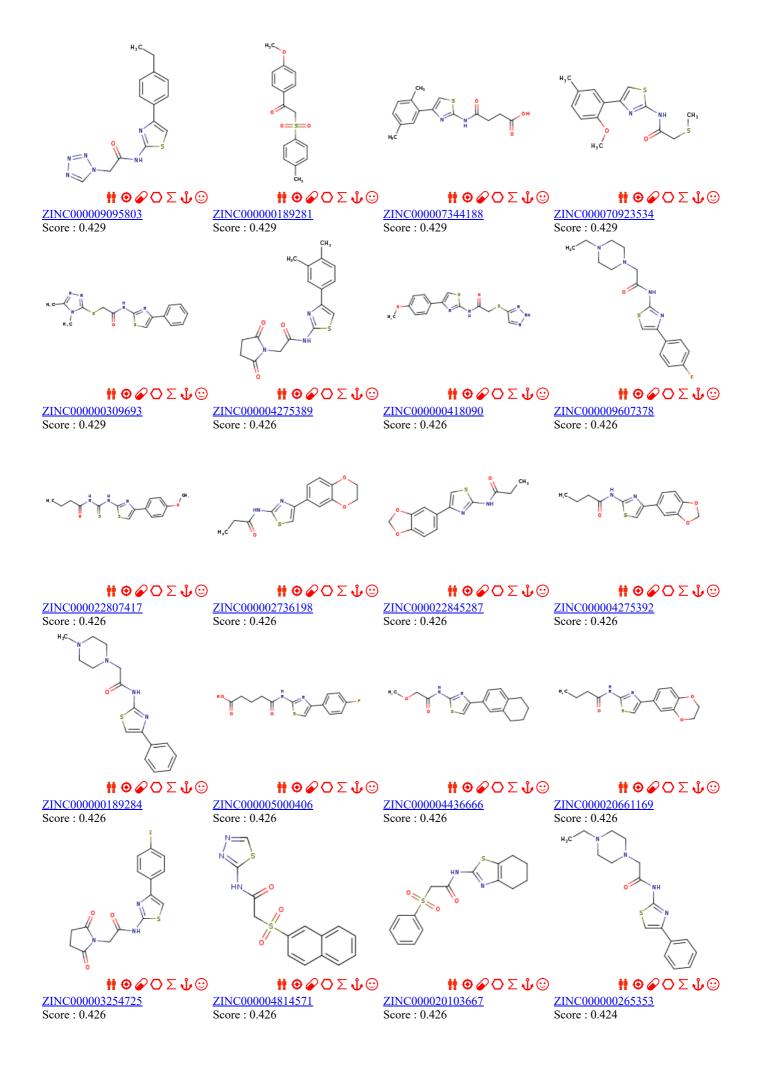


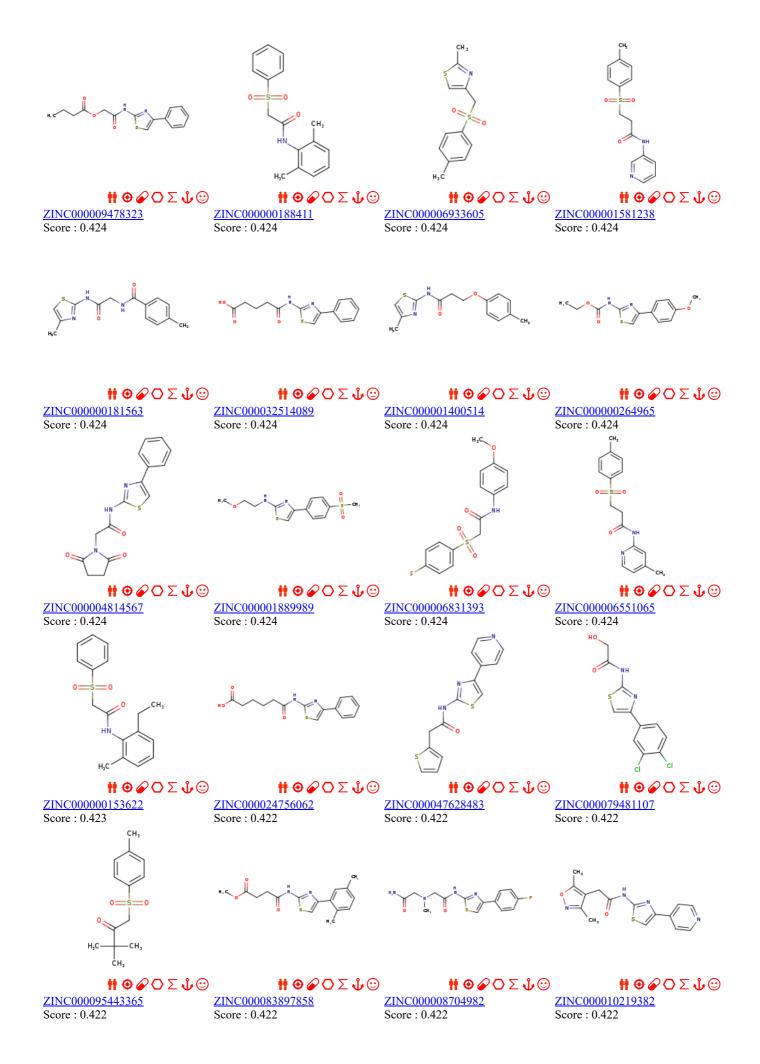


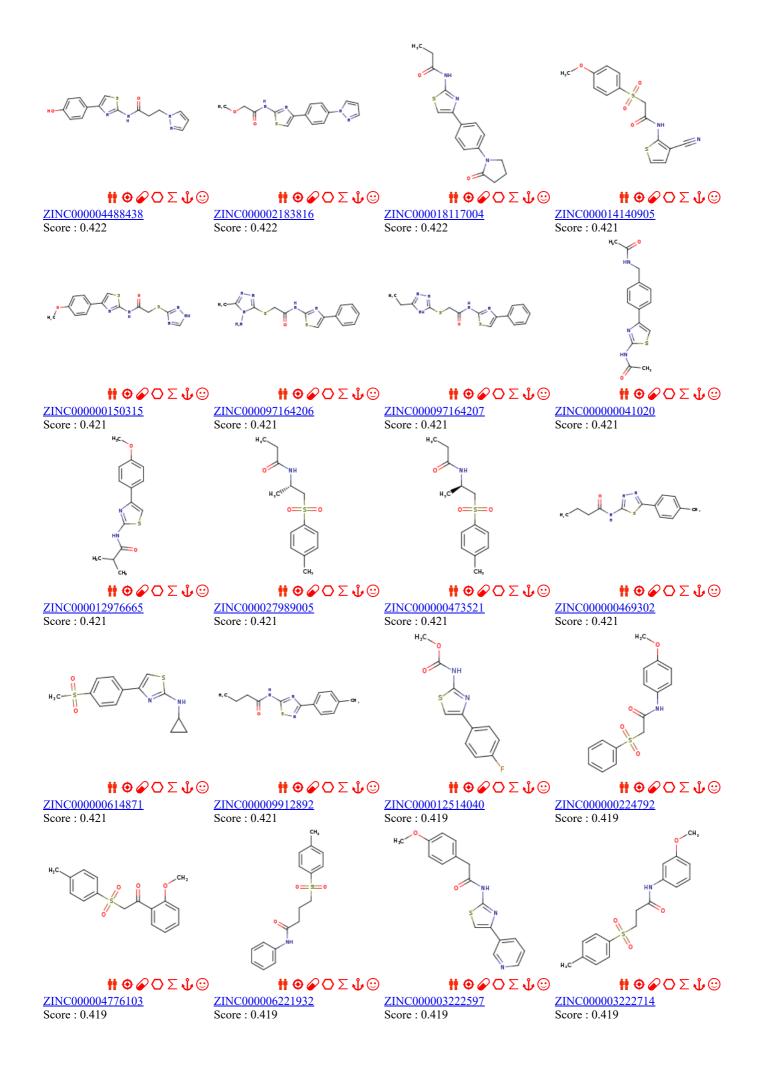


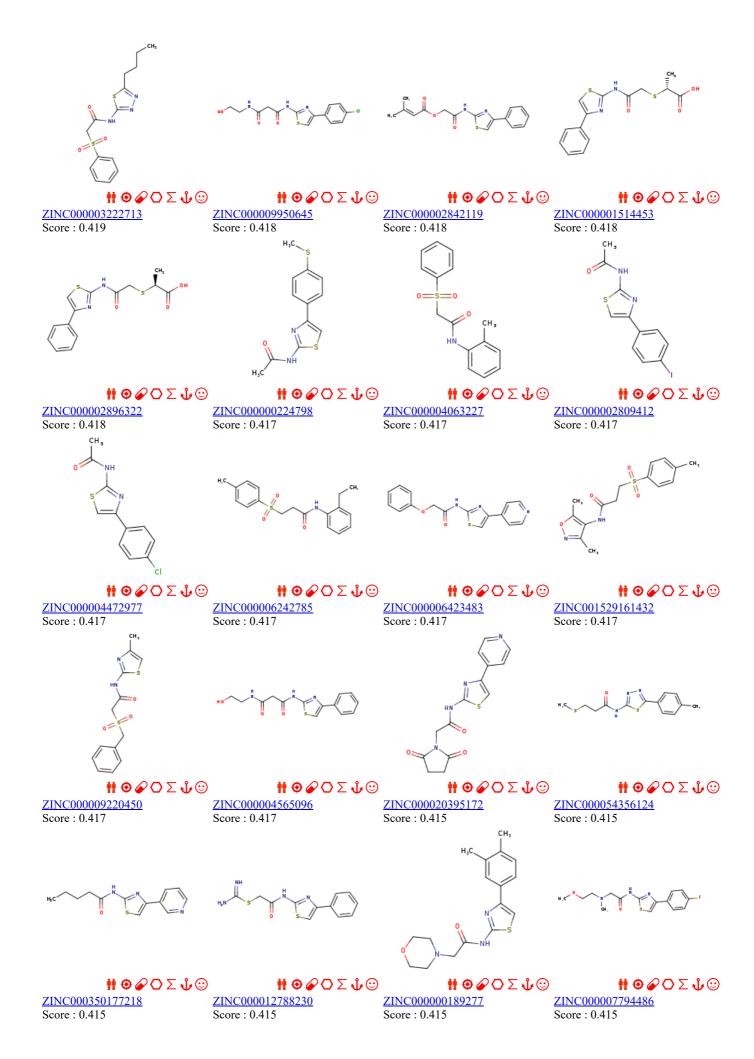


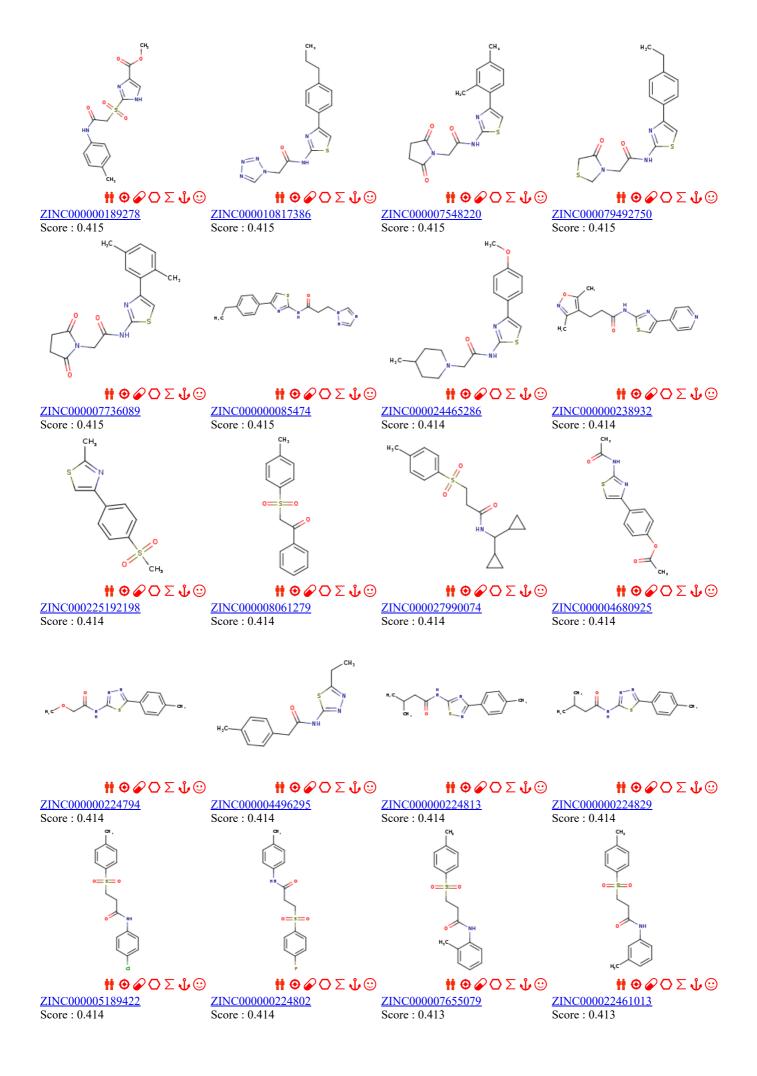


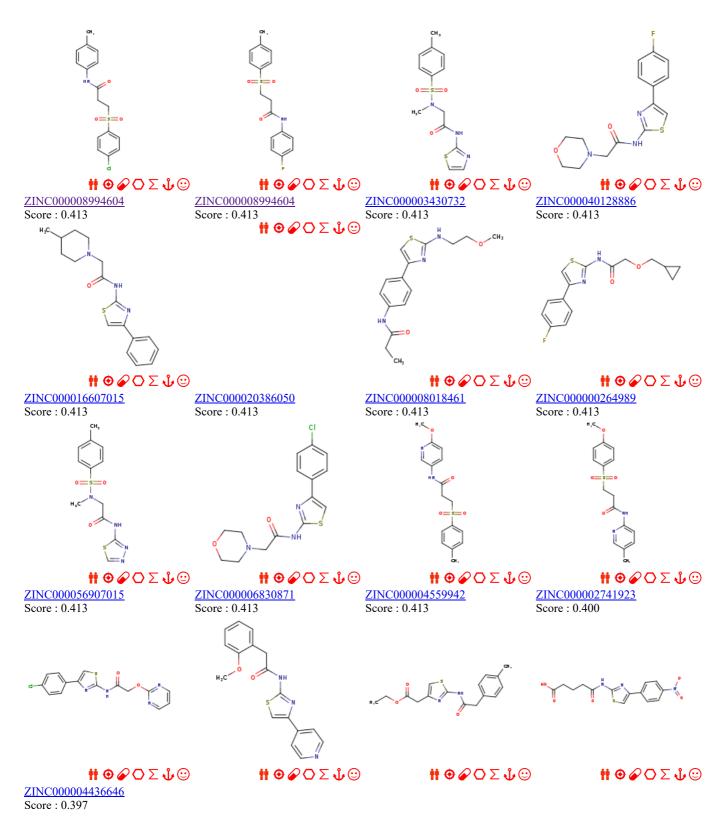












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# **⊕ ⊘ ○** ∑ **↓ ○** 



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