

## Supplementary Information

### DRUG MOLECULE TARGETING WITH EXPLAINABLE ARTIFICIAL INTELLIGENCE IN FRIEDREICH'S ATAXIA

Kevser Kübra Kırboğa<sup>1\*</sup>, Ecir Uğur Küçüksille<sup>2</sup>, Utku Köse<sup>2</sup>

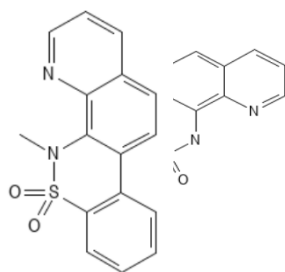
*1\* Suleyman Demirel University, Institute of Science, Bioengineering Department, 32260, Isparta, Turkey.*

*2 Suleyman Demirel University, Engineering Faculty, Computer Engineering Department, 32260 Isparta, Turkey*

*\*Kevser Kübra Kırboğa, E-mail: [kubra.kirboga@yahoo.com](mailto:kubra.kirboga@yahoo.com)*

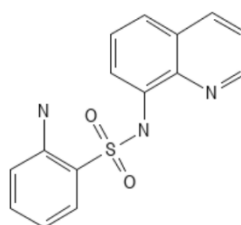
#### 1. Top 10 active and inactive compounds for Fe chelation.

**A**

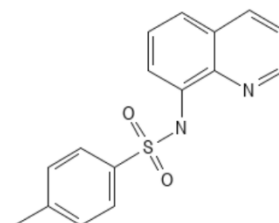


**1**

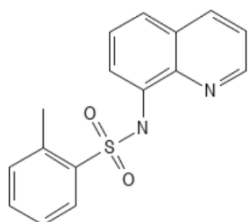
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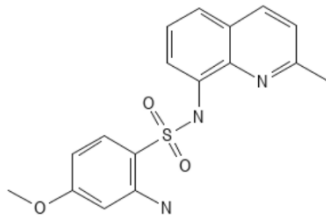
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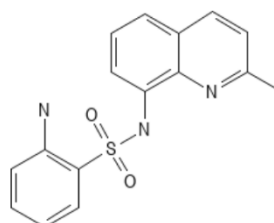
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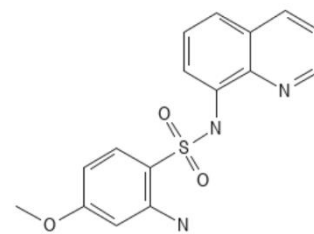
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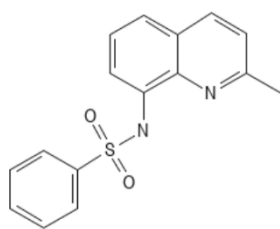
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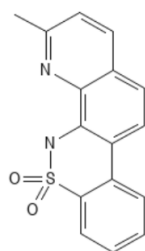
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**8**

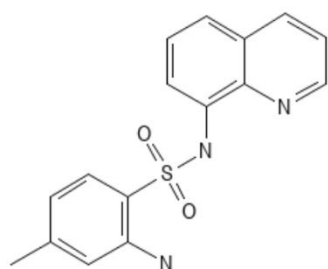


**9**

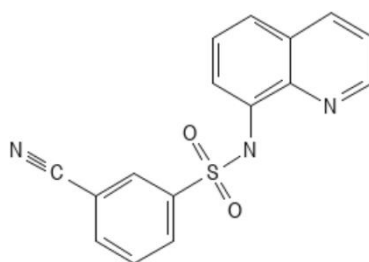


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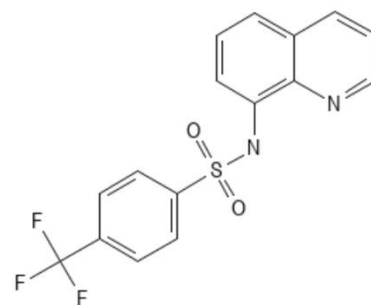
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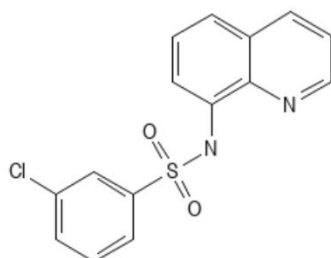
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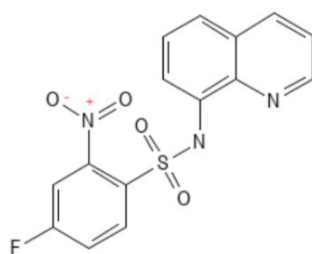
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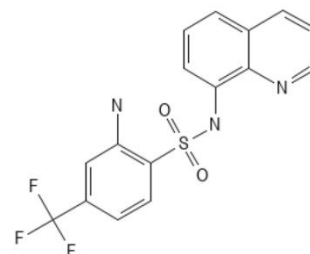
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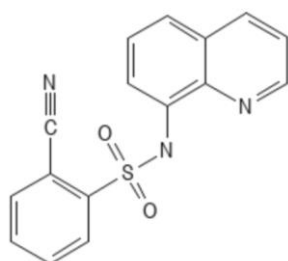
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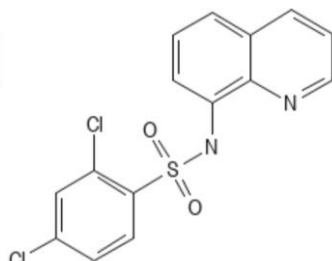
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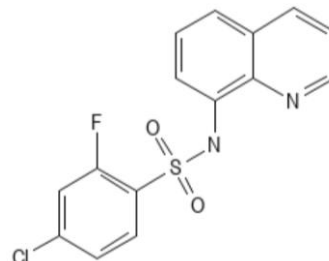
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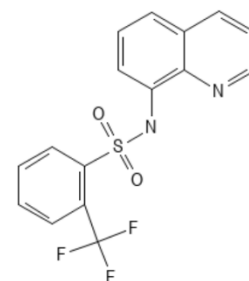
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**8**



**9**

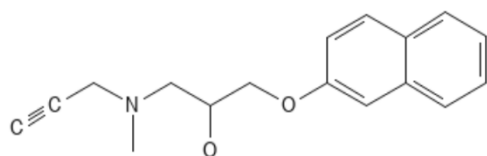


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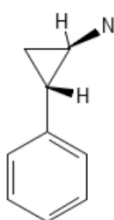
**Supplementary Figure S1.** Top 10 active and inactive compounds for Fe chelation. Chemical compounds of the top 10 inactive (A) and active (B) compounds for Fe chelation are shown.

## 2. Top 10 active and inactive compounds for HDAC.

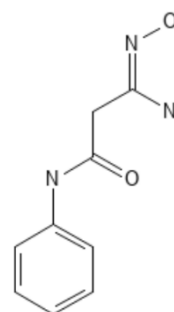
### A



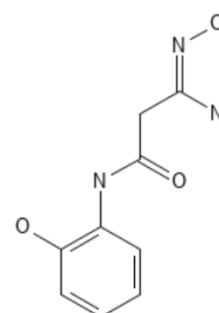
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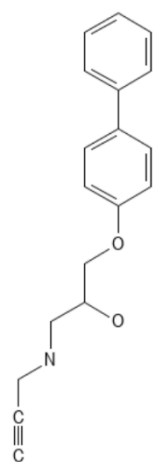
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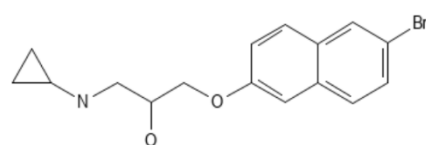
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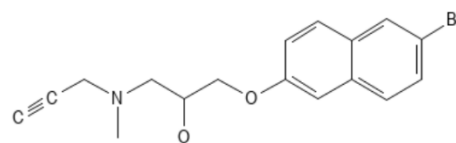
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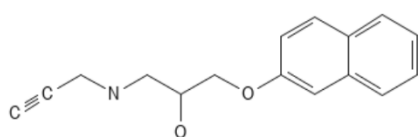
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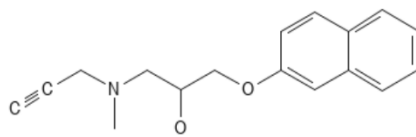
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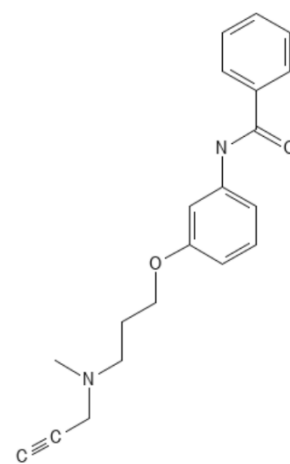
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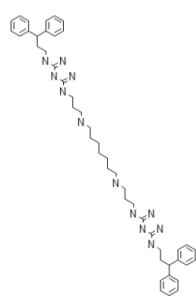


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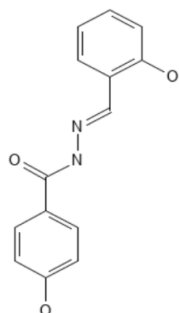


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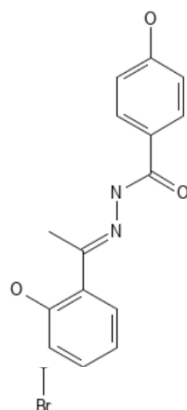
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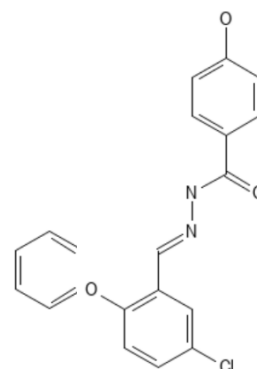
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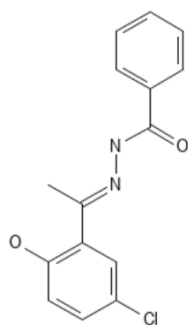
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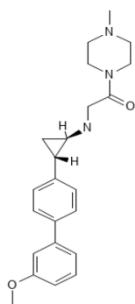
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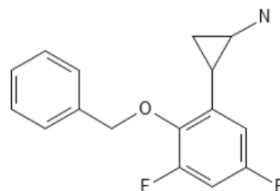
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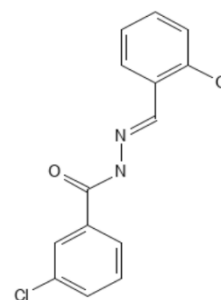
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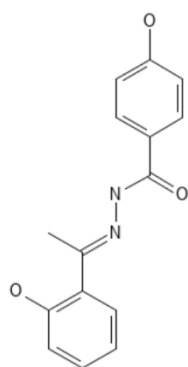
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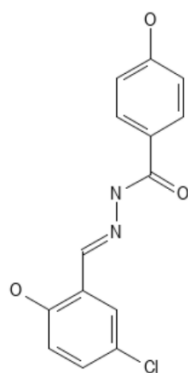
**7**



**8**



**9**



**10**

**Supplementary Figure S2.** Top 10 active and inactive compounds for HDAC. Chemical compounds of the top 10 inactive (A) and active (B) compounds for HDAC are shown.