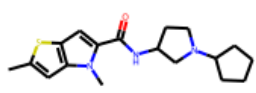
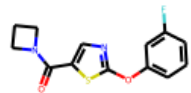


Supplementary Figure S1: **QED-based generated molecules.**

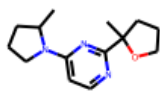
These compounds were randomly extracted from the library created. The value under the compound is the QEPI score.



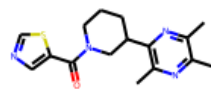
0.62



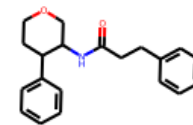
0.51



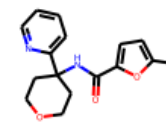
0.31



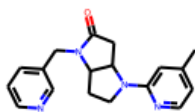
0.55



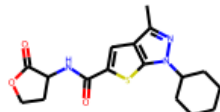
0.46



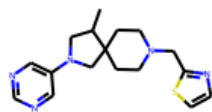
0.67



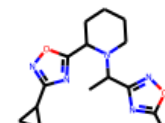
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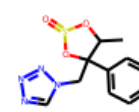
0.70



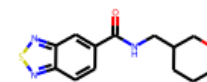
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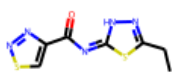
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0.47



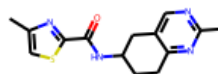
0.68



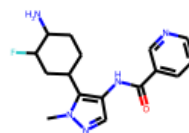
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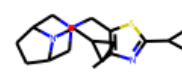
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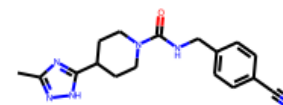
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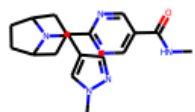
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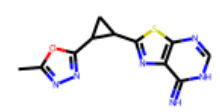
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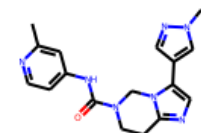
0.69



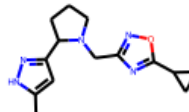
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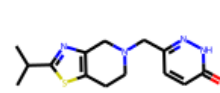
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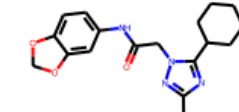
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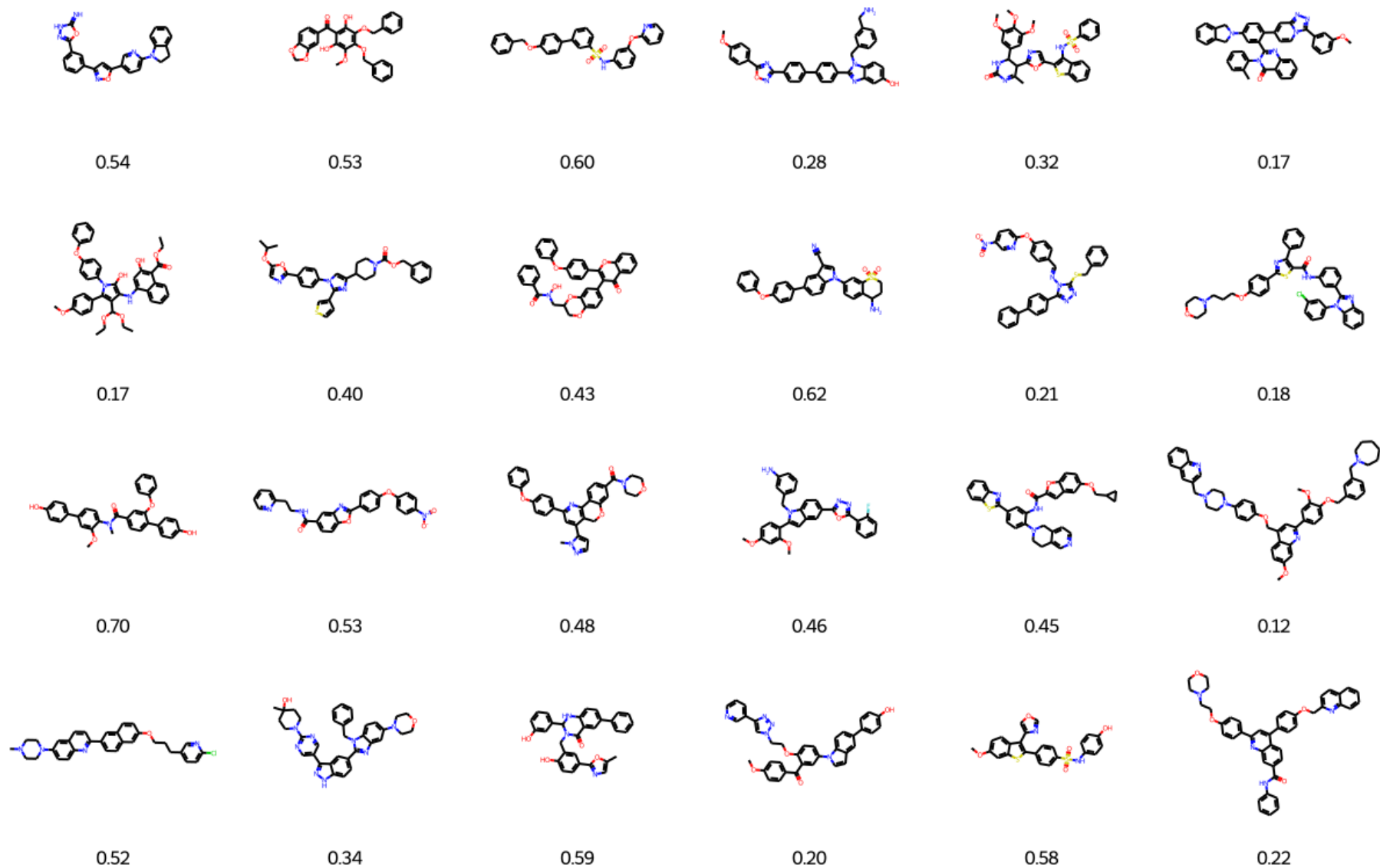
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0.68

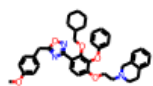


0.73

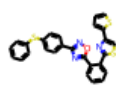


Supplementary Figure S2: **RO4-based generated molecules.**

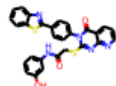
These compounds were randomly extracted from the library created. The value under the compound is the QEPPi score.



0.28



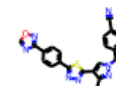
0.36



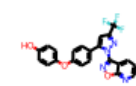
0.35



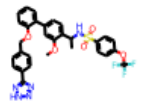
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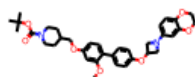
0.36



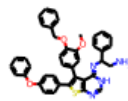
0.56



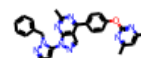
0.33



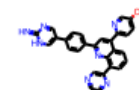
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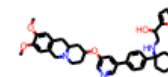
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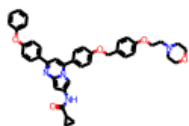
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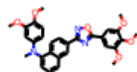
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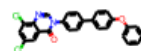
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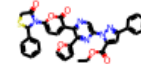
0.26



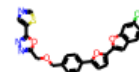
0.32



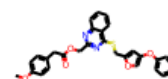
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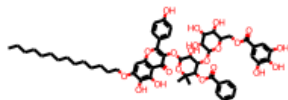
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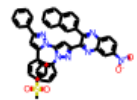
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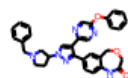
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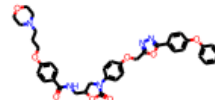
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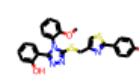
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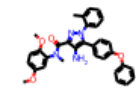
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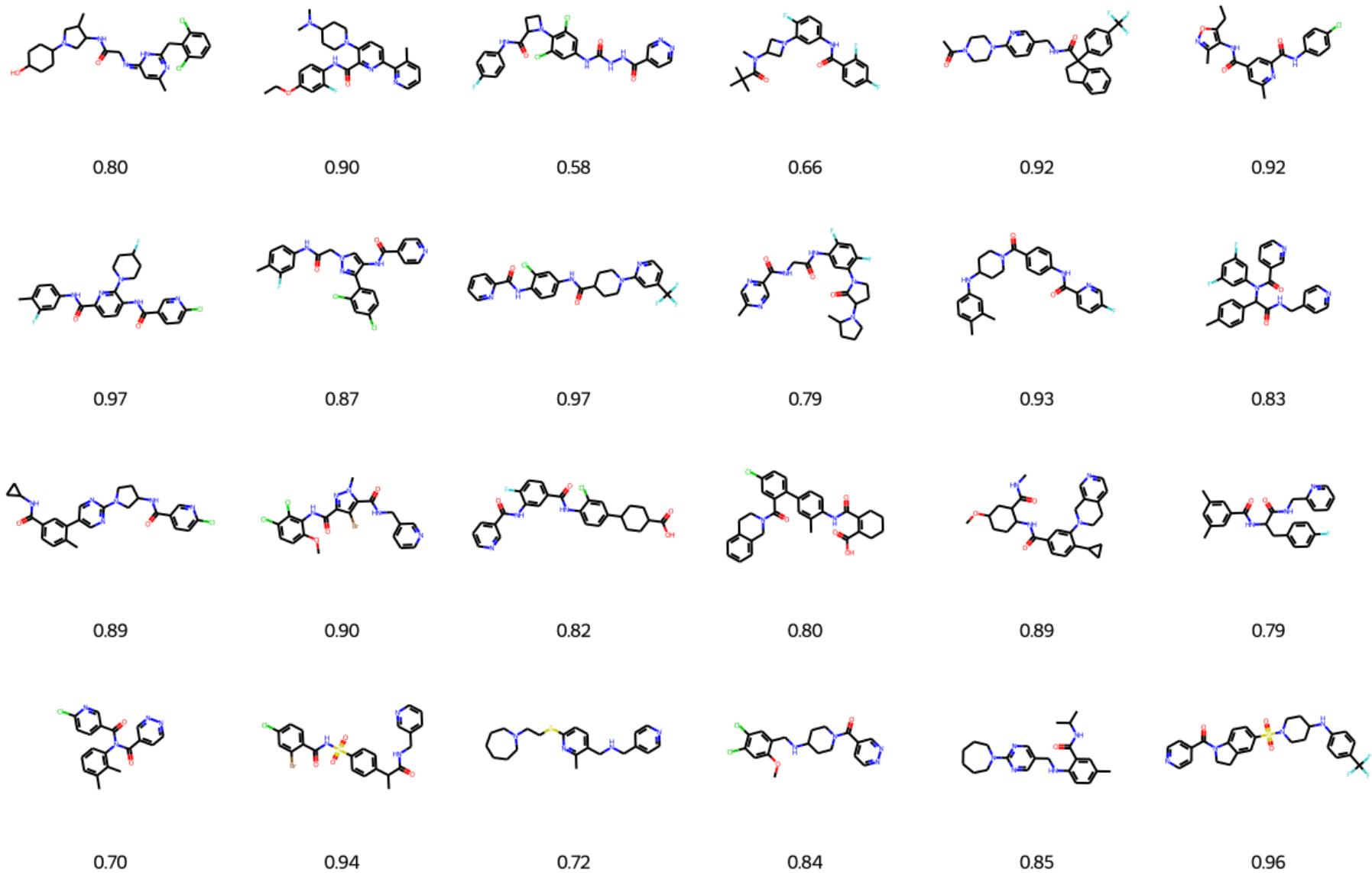
0.21



0.44

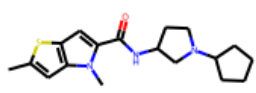


0.55

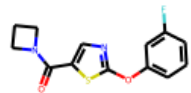


Supplementary Figure S3: **QEPPi-based generated molecules.**

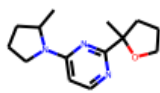
These compounds were randomly extracted from the library created. The value under the compound is the QEPPi score.



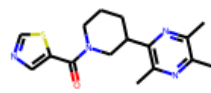
0.62



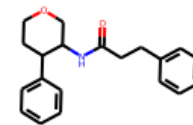
0.51



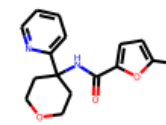
0.31



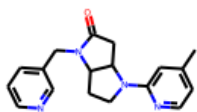
0.55



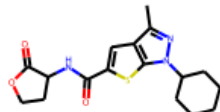
0.46



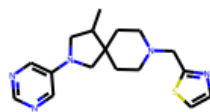
0.67



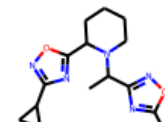
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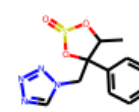
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0.53



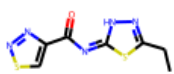
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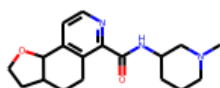
0.47



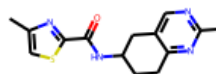
0.68



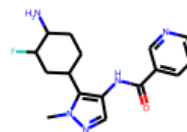
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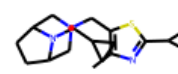
0.43



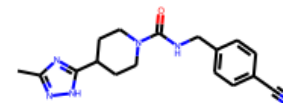
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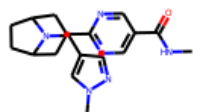
0.72



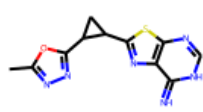
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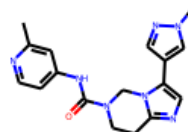
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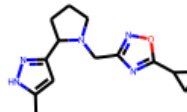
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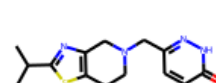
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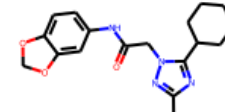
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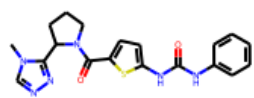
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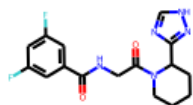
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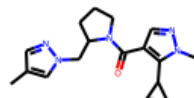
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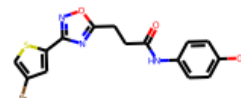
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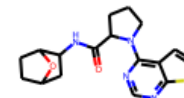
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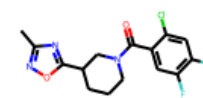
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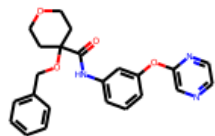
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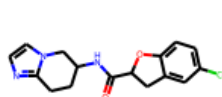
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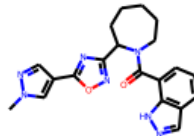
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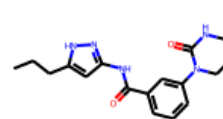
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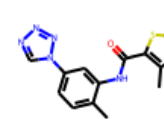
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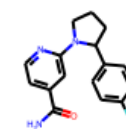
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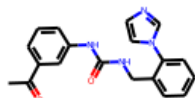
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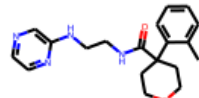
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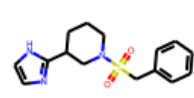
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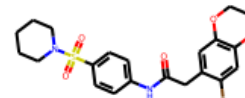
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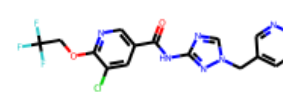
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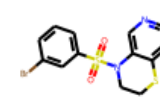
0.62



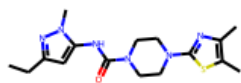
0.87



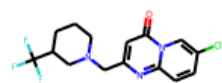
0.77



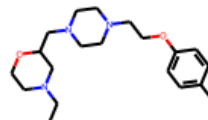
0.54



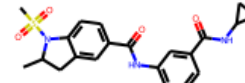
0.69



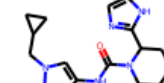
0.49



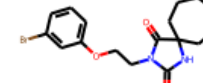
0.39



0.81



0.74



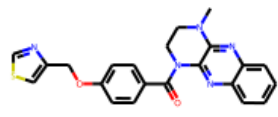
0.47

Supplementary Figure S4: **Compounds from Enamine PPI library.**

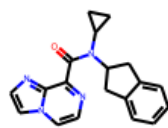
These compounds were randomly extracted from the library. The value under the compound is the QEPPi score.



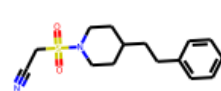
0.88



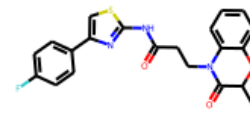
0.57



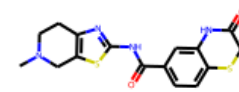
0.61



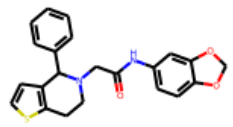
0.37



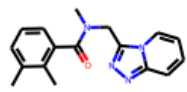
0.94



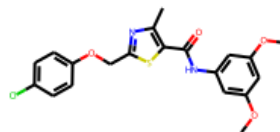
0.66



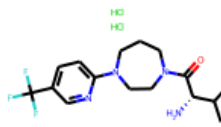
0.85



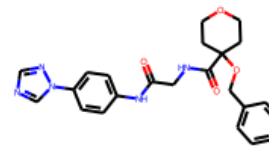
0.59



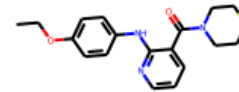
0.89



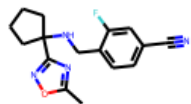
0.53



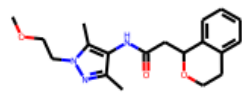
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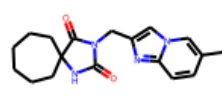
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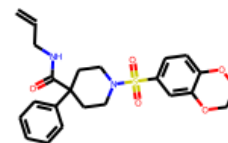
0.75



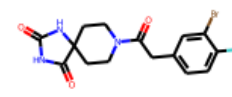
0.80



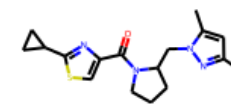
0.65



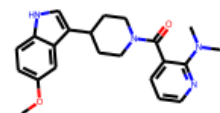
0.86



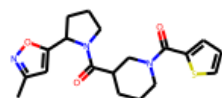
0.42



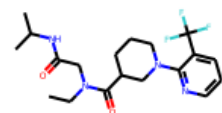
0.61



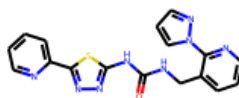
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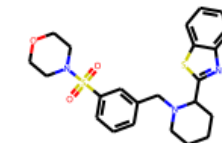
0.64



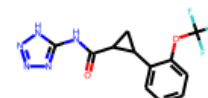
0.57



0.57



0.74



0.75