

Drugging the undruggable Trypanosoma Brucei 1CGrx1

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Supplementary Information

Figure S1. Overview of the calculated properties of the fragment library. All the descriptors were calculated by using MOE2020.

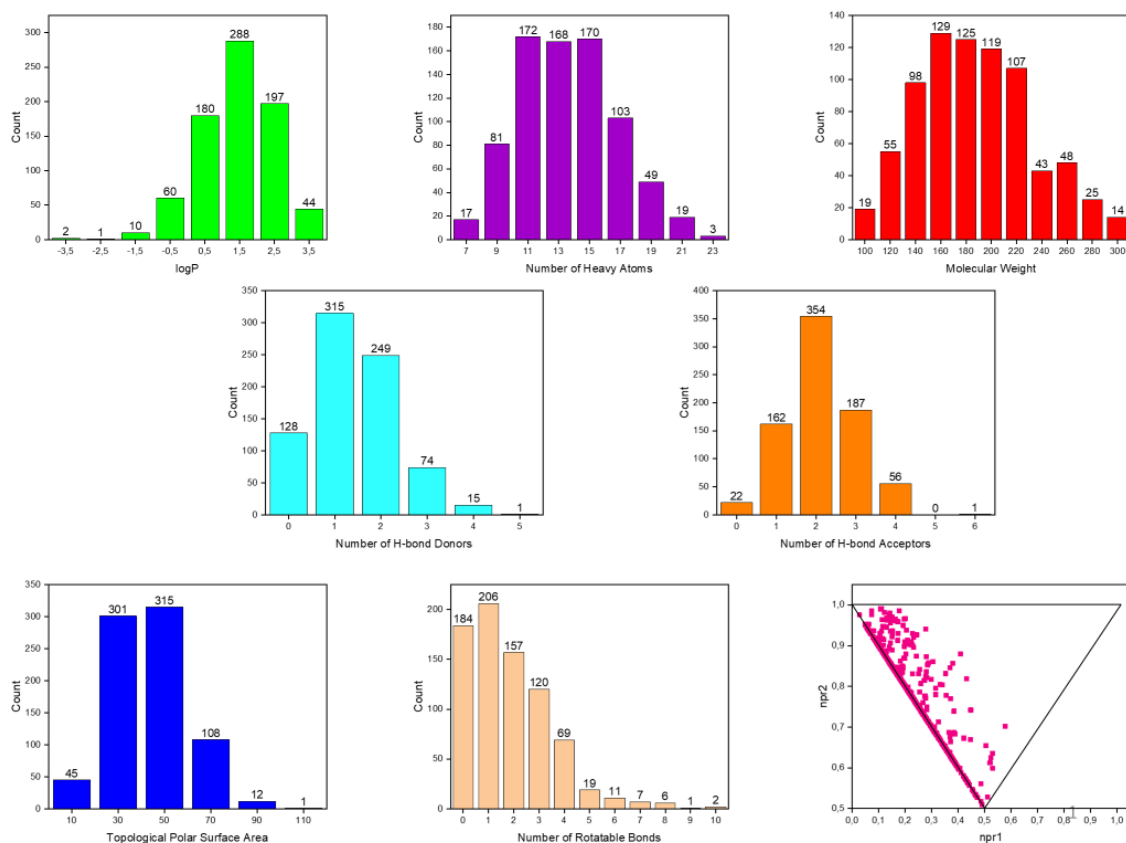


Figure S2. Alignment and comparison of the sequence for Grx1 (Trypanosoma Brucei) and Grx4 (Escherichia Coli). The residues that are close to the co-enzyme glutathione are circled in red. As it can be observed, the site is well conserved between the two.

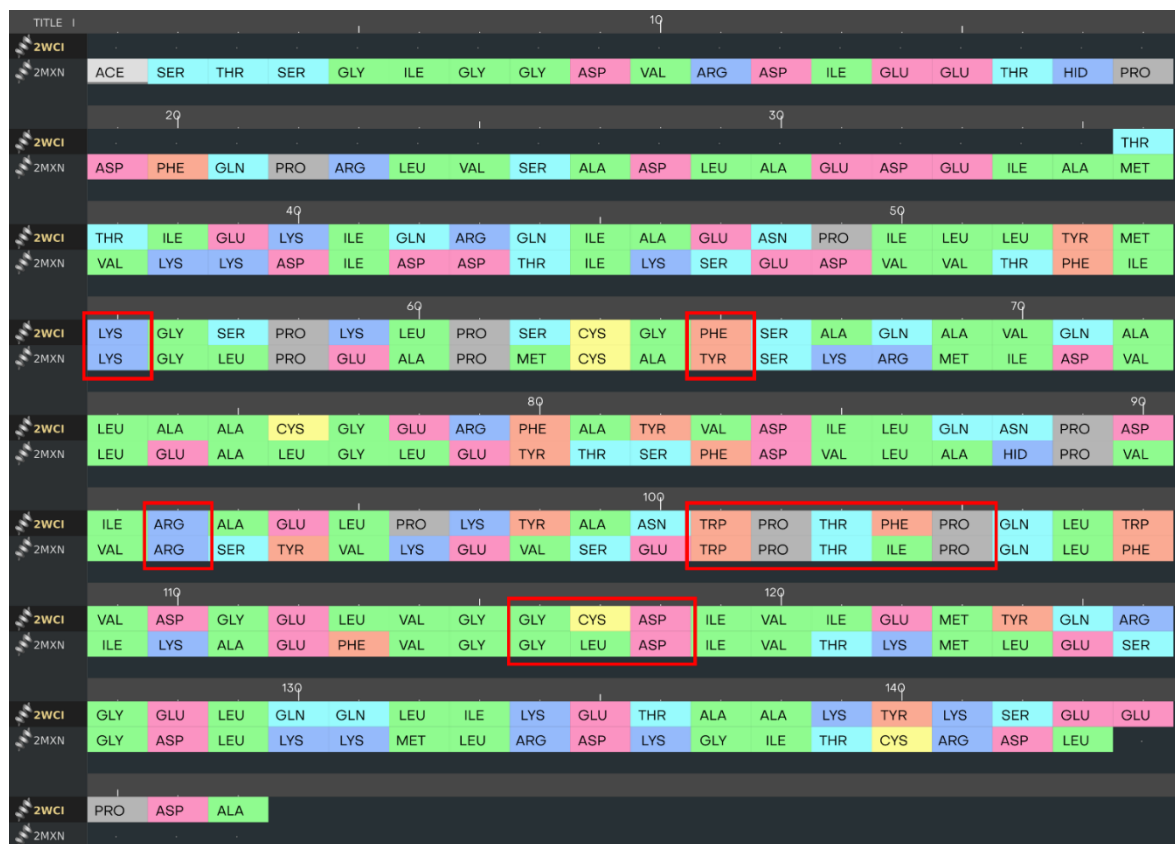
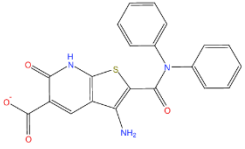
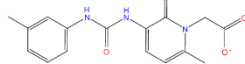
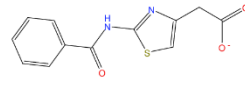
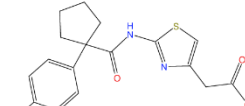
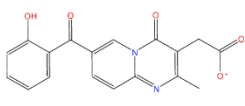
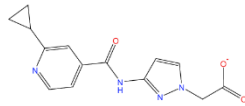
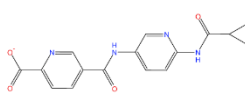
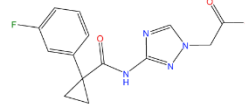


Figure S3. List of the compounds originated from VS.

<p>1</p>  <p>MolPort-002-404.4260 Weight: 404.4260</p>	<p>2</p>  <p>MolPort-035-314.3210 Weight: 314.3210</p>	<p>3</p>  <p>MolPort-002-261.2810 Weight: 261.2810</p>	<p>4</p>  <p>MolPort-005-347.3900 Weight: 347.3900</p>
<p>5</p>  <p>MolPort-009-337.3110 Weight: 337.3110</p>	<p>6</p>  <p>MolPort-046-285.2830 Weight: 285.2830</p>	<p>7</p>  <p>MolPort-047-325.3040 Weight: 325.3040</p>	<p>8</p>  <p>MolPort-045-303.2730 Weight: 303.2730</p>