

# A data-driven approach to construct a molecular map of *Trypanosoma cruzi* to identify drug and vaccine targets

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Website: <https://tinyurl.com/Tcruzipathwaymapx>

S. No.	Supplementary Figure no.	Description	Link
1.	Supplementary Figure 1	Supplementary Figure 1: The schematic diagram describing the flowchart to achieve the methodology.	<a href="https://tinyurl.com/suppfig1">https://tinyurl.com/suppfig1</a>
2.	Supplementary Figure 2	Supplementary Figure 2: The standard notations for the graphical representation of species and edges in cell designer v.4.4.2.	<a href="https://tinyurl.com/suppfig2">https://tinyurl.com/suppfig2</a>
3.	Supplementary Figure 3	Supplementary Figure 3: Docking of Tc24 protein with Benznidazole and Nifurtimox using AutoDock Vina. (a. Benznidazole, b. Nifurtimox). The top scoring pose of docking affinity against Tc24 for Benznidazole is -6.9 kcal/mol while the docking affinity for Nifurtimox is -6.7 kcal/mol.	<a href="https://tinyurl.com/suppfig3">https://tinyurl.com/suppfig3</a>
4.	Supplementary Figure 4	<p>Supplementary Figure 4A: <i>Trypanosoma cruzi</i> CL Brener Esmeraldo-like. Enriched GO terms of genes (a. Biological process, b. Cellular component, c. Molecular function). The size of the dots and their color gradient (according to the legend) reflects the log10 value of the p value of each GO term, larger dots represent higher significance (all p values &lt;0.05). X and Y axes represent semantic spaces which have no intrinsic meaning. REVIGO uses multi-dimensional scaling to reduce the dimensionality of a matrix of the GO terms' pairwise semantic similarities. This results in semantically similar GO terms remaining close together in the plot.</p> <p>Supplementary Figure 4B: <i>Trypanosoma cruzi</i> CL Brener Non-Esmeraldo-like. Enriched GO terms of genes (a. Biological process, b. Cellular component, c. Molecular function). The size of the dots and their color gradient (according to the legend) reflects the log10 value of the p value of each GO term, larger dots represent higher significance (all p values &lt;0.05). X and Y axes represent semantic spaces which have no intrinsic meaning. REVIGO uses multi-dimensional scaling to reduce the dimensionality of a matrix of the GO terms' pairwise semantic similarities. This results in semantically similar GO terms remaining close together in the plot.</p>	<a href="https://tinyurl.com/suppfig4">https://tinyurl.com/suppfig4</a>
5.	Supplementary Figure 5	Supplementary Figure 5A: <i>Trypanosoma cruzi</i> CL Brener Non-Esmeraldo-like. "Interactive graph" view of REVIGO (a. Biological process, b. Cellular component, c. Molecular function). Bubble color indicates the user-provided p-value. Highly similar GO terms are linked by	<a href="https://tinyurl.com/suppfig5">https://tinyurl.com/suppfig5</a>

		edges in the graph, where the line width indicates the degree of similarity.	
		<b>Supplementary Figure 5B: <i>Trypanosoma cruzi</i> CL Brener Esmeraldo-like.</b> "Interactive graph" view of REVIGO ( <b>a.</b> Biological process, <b>b.</b> Cellular component, <b>c.</b> Molecular function). Bubble color indicates the user-provided p-value. Highly similar GO terms are linked by edges in the graph, where the line width indicates the degree of similarity.	
6.	<b>Supplementary Figure 6</b>	<b>Supplementary Figure 6:</b> Gene ontology (GO) classification, KEGG/MetaCyc analysis of the <i>T. cruzi</i> genes ( <b>a.</b> ) <i>T. cruzi</i> CL Brener Esmeraldo like ( <b>b.</b> ) <i>T. cruzi</i> CL Brener Non-Esmeraldo like). The percentage regulated genes based on GO annotations and KEGG/MetaCyc pathways. ( <b>c</b> ) word cloud graph depicting enriched Metabolic Pathway ( <b>1</b> ) <i>Trypanosoma cruzi</i> CL Brener Esmeraldo-like ( <b>2</b> ) <i>Trypanosoma cruzi</i> CL Brener Non-Esmeraldo-like.	<a href="https://tinyurl.com/supfig6">https://tinyurl.com/supfig6</a>

\* % regulated genes are the percentage of the background or GO/pathway-related genes.