

Supplementary Data C

(Dose-response curves for cellular assays)

Quantum Mechanics-Driven Structure-Activity Relationship Study of PEX5-PEX14 Protein-Protein Interaction Inhibitors Based On a Dibenzo[*b,e*]azepin-6(*6H*)-one Scaffold

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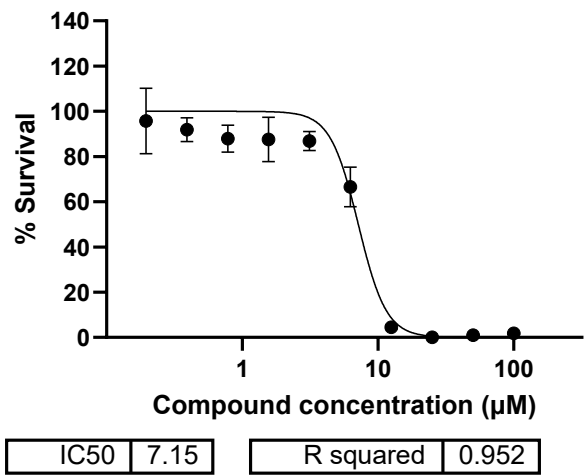
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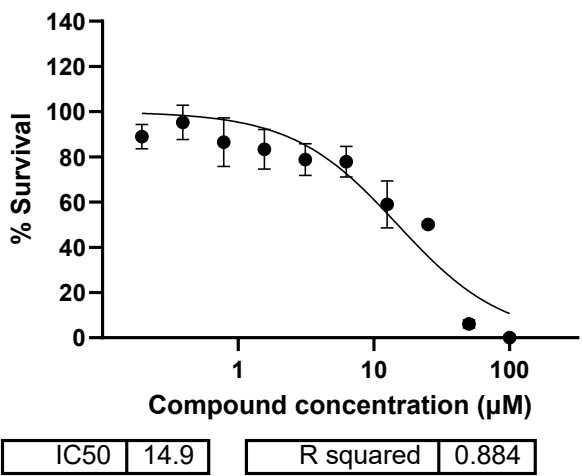
† Current affiliation: Institute of Biostructures and Bioimaging, National Research Council (CNR), Via Pietro Castellino, 111, 80131 Napoli, Italy.

Dose-response curves for *in vitro* trypanocidal activity of compounds 7-43 and Suramin (reference drug) against *T. brucei brucei* (bloodstream form). Error bars represent standard deviation from independent quadruplicate assays.

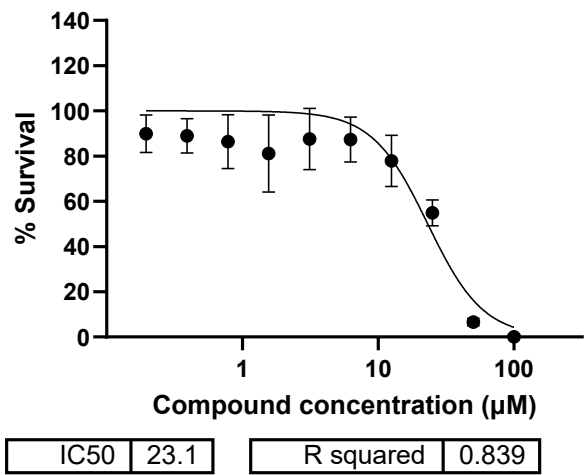
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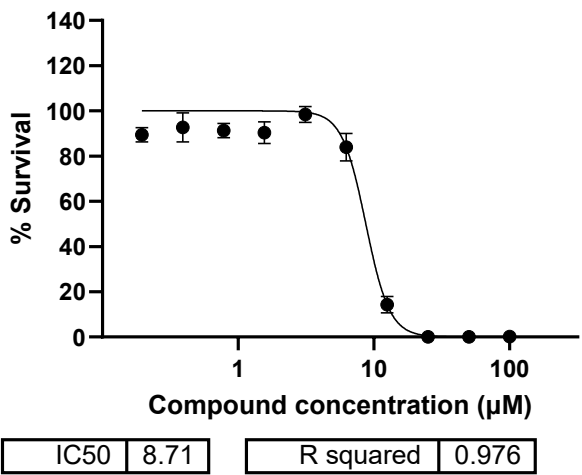
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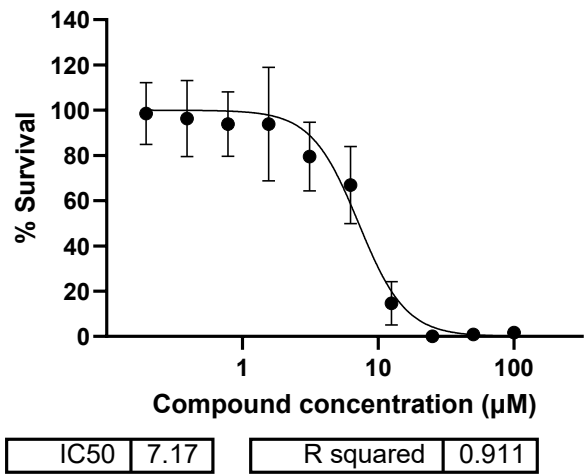
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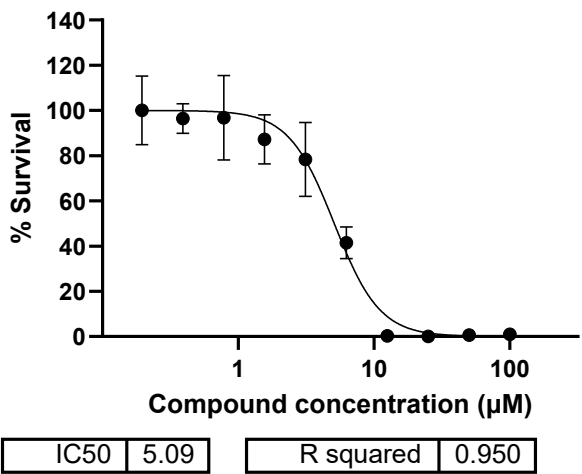
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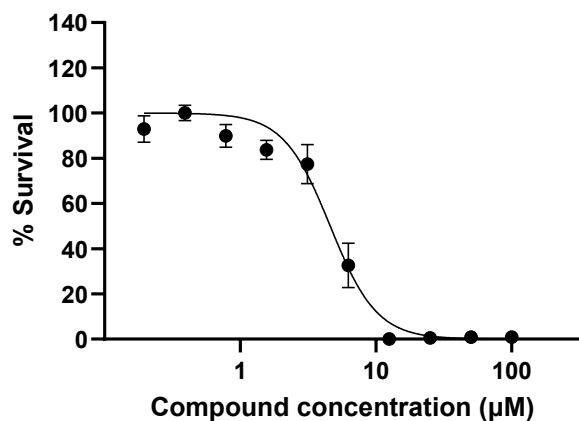
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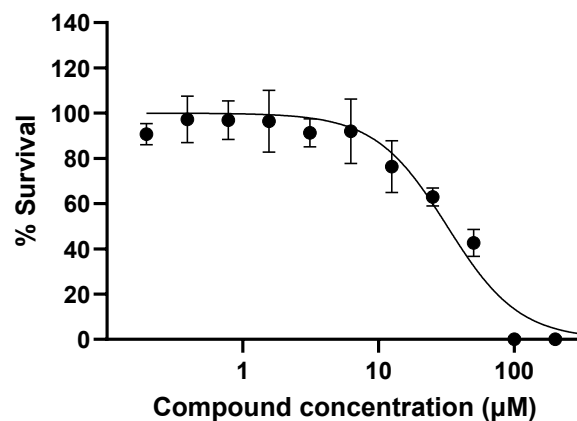


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IC50	4.60	R squared	0.972
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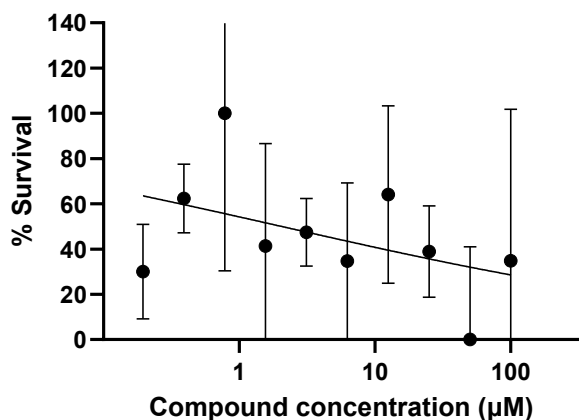
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IC50	32.0	R squared	0.941
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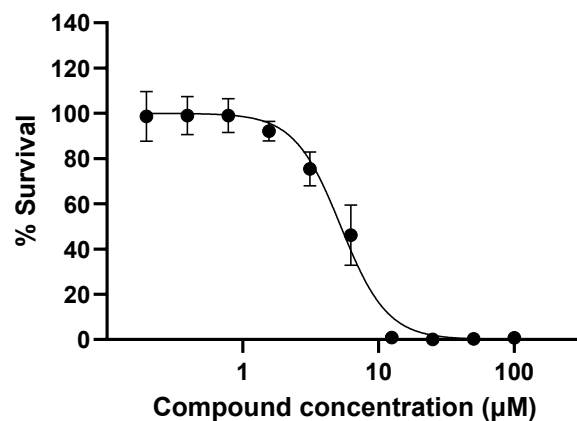
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Non-toxic



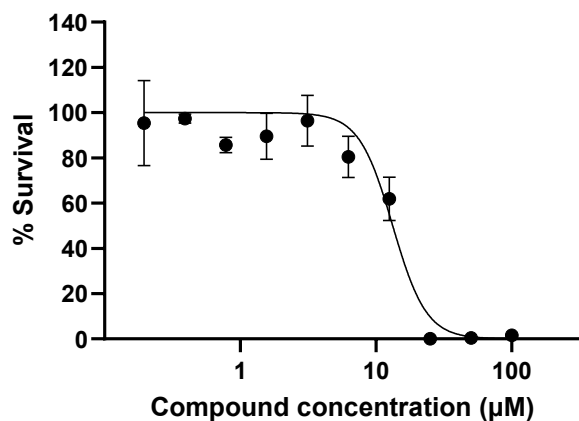
R squared	0.0658
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16



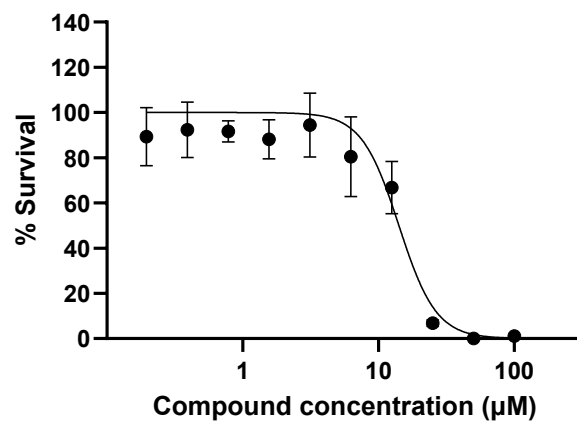
IC50	5.27	R squared	0.973
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17



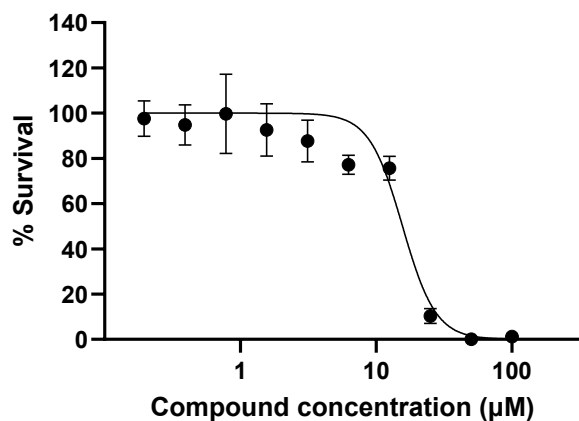
IC50	13.3	R squared	0.927
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18



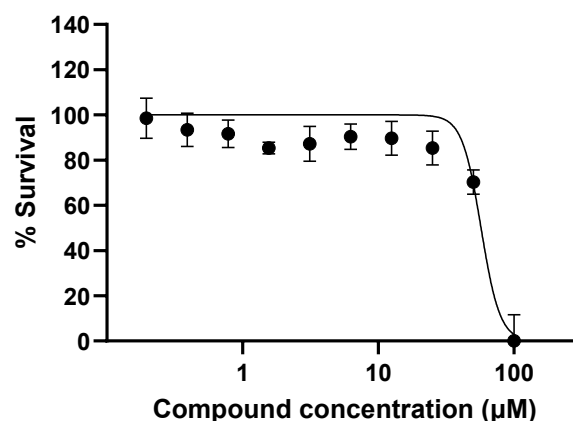
IC50	14.1	R squared	0.909
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19



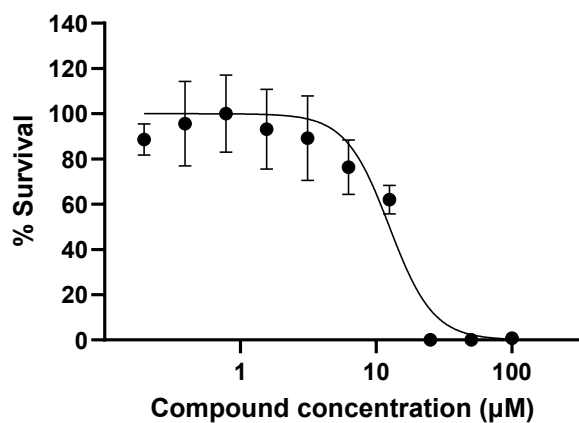
IC50	15.6	R squared	0.926
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20



IC50	57.0	R squared	0.834
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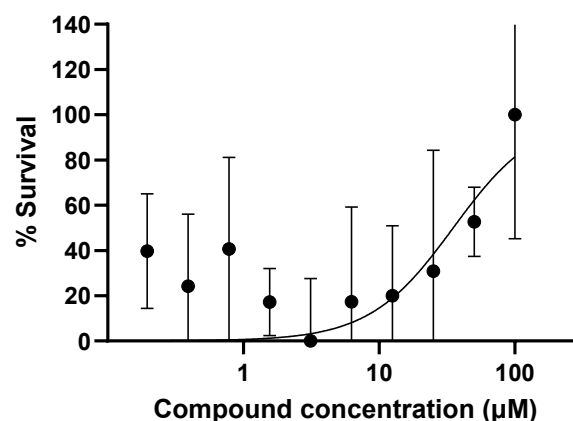
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IC50	12.5	R squared	0.896
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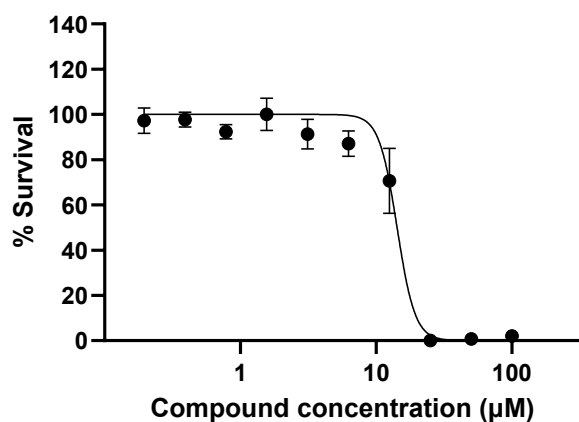
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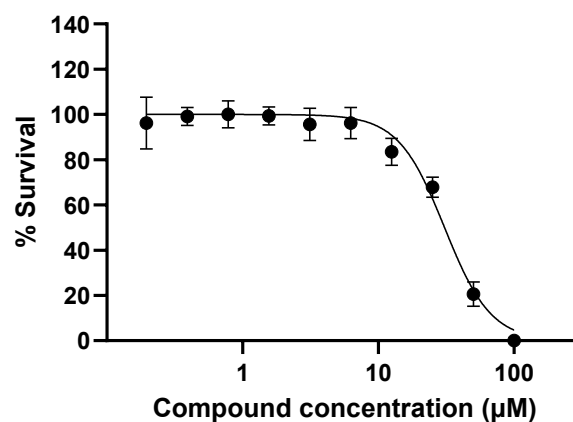
R squared	0.131
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23

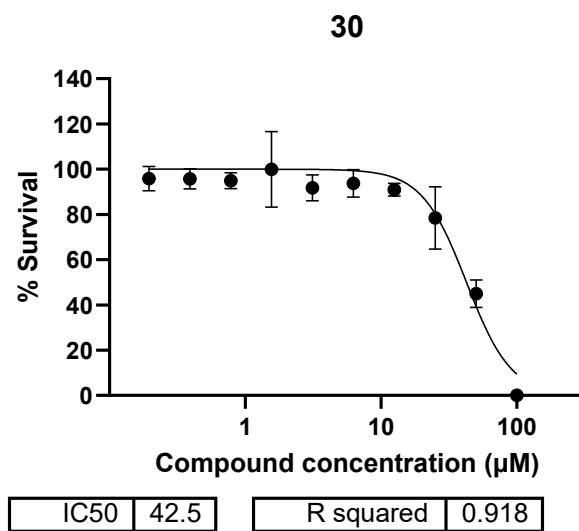
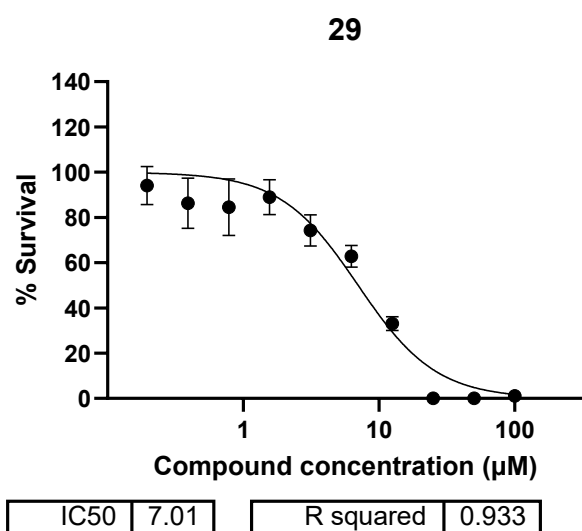
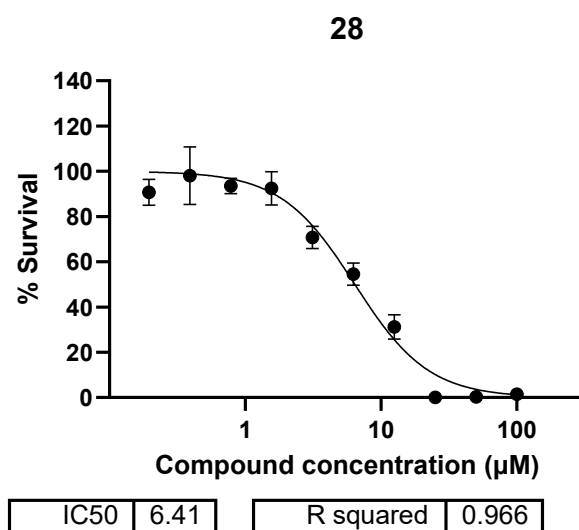
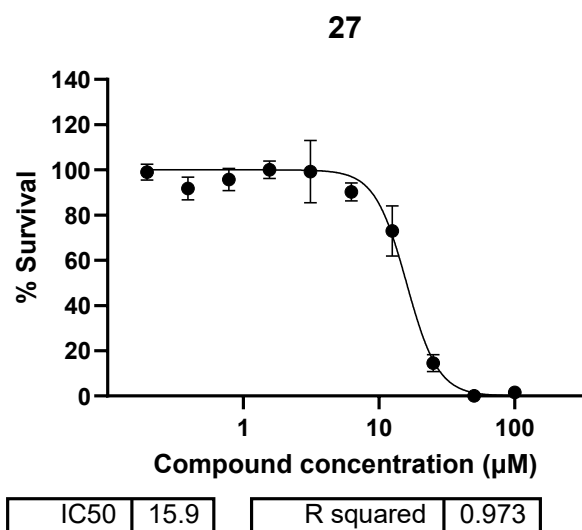
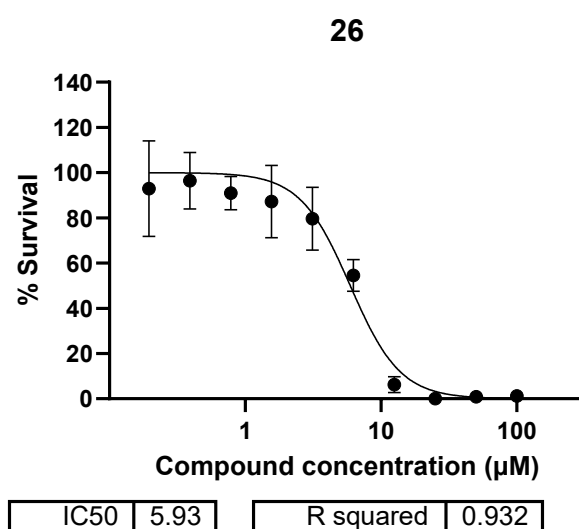
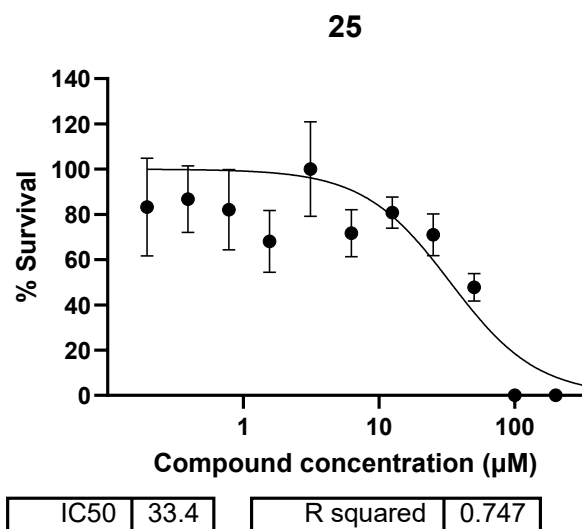


IC50	14.2	R squared	0.966
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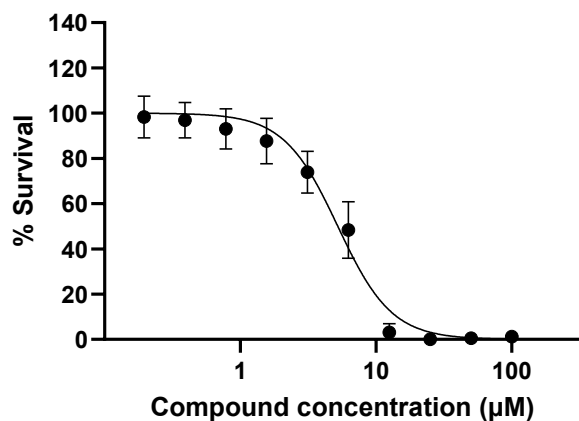
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IC50	30.7	R squared	0.965
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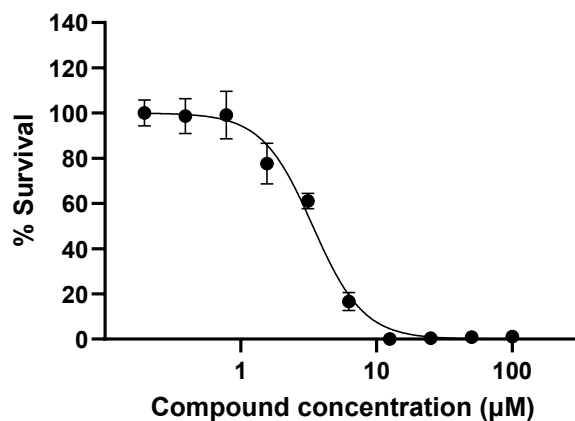


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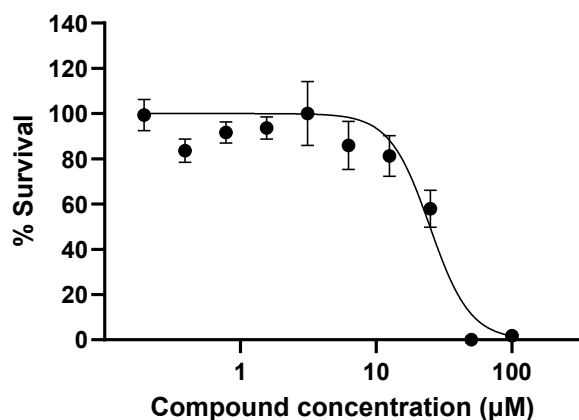
IC50	5.22	R squared	0.963
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32



IC50	3.39	R squared	0.980
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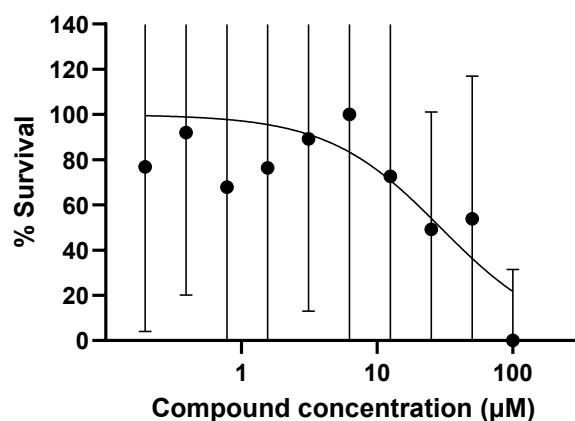
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IC50	24.8	R squared	0.910
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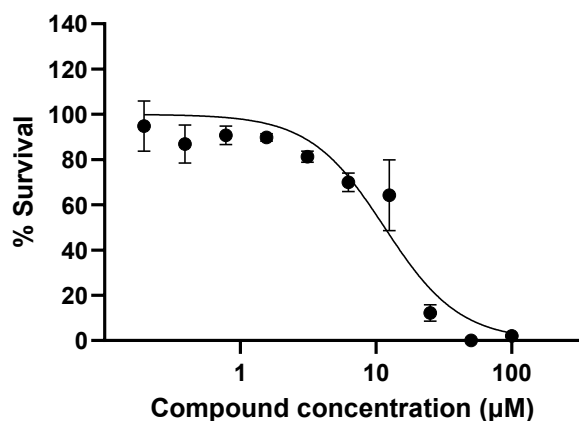
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Non-toxic



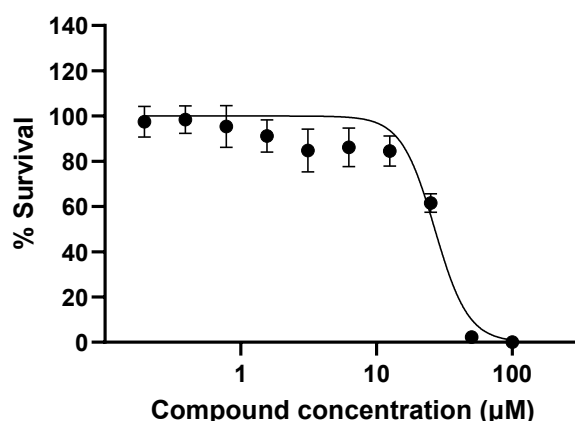
R squared	0.0848
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35

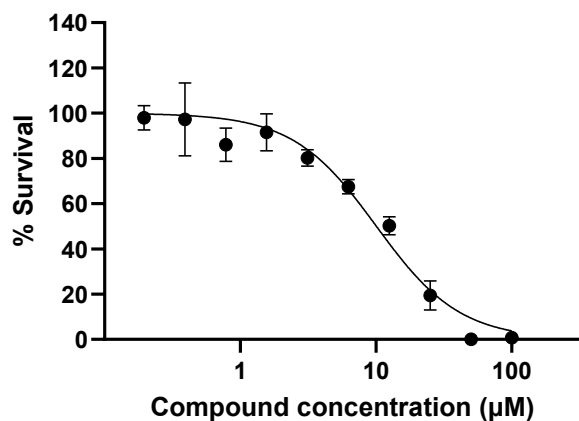


IC50	11.5	R squared	0.913
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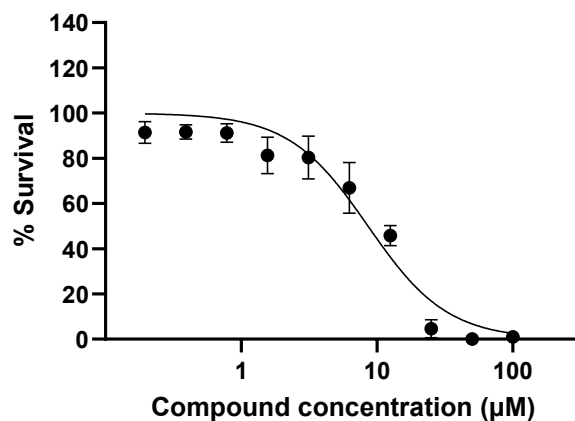
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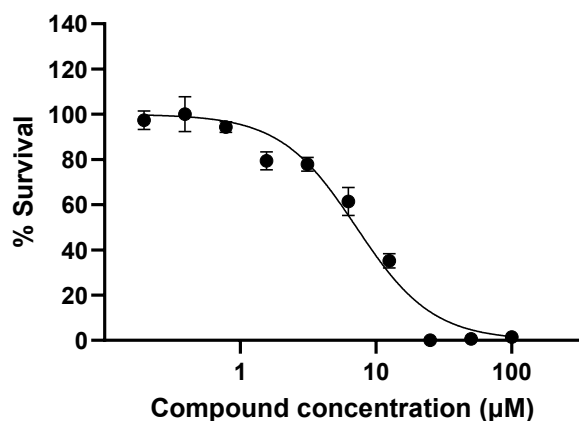
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37

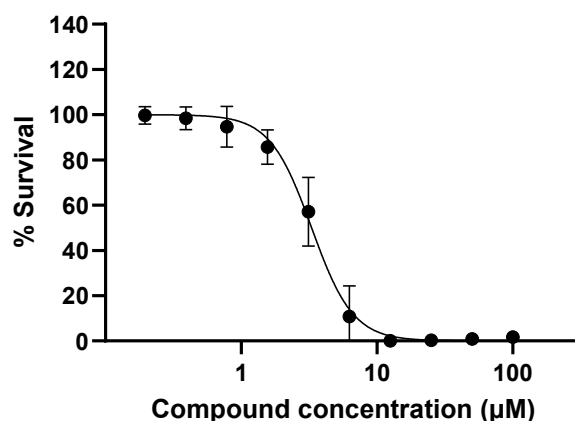
IC50	10.0	R squared	0.952
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38

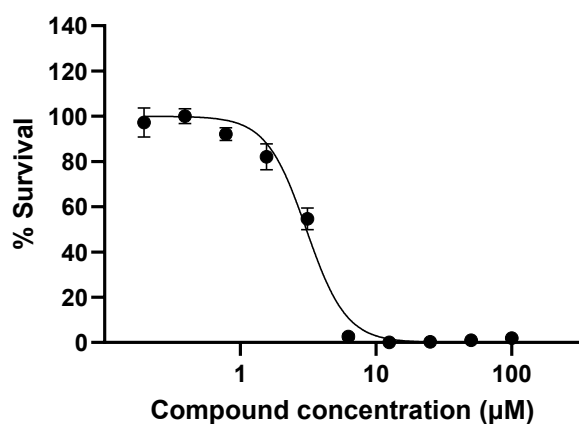
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39

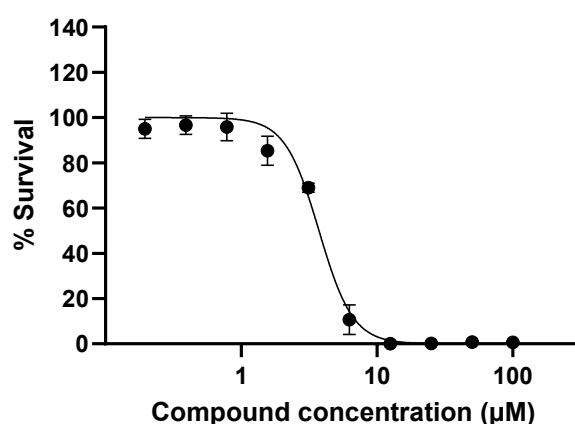
IC50	7.16	R squared	0.967
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40

IC50	3.29	R squared	0.974
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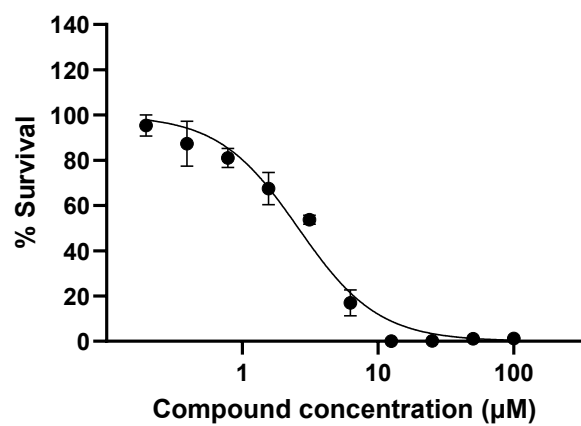
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IC50	3.06	R squared	0.985
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42

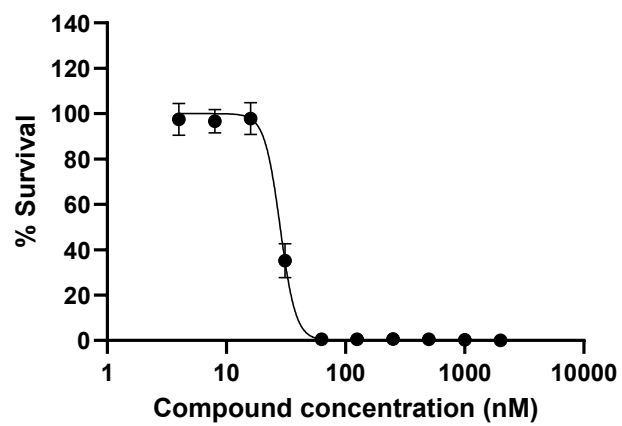
IC50	3.73	R squared	0.984
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43



IC50	2.58	R squared	0.969
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Suramin



IC50	28.3	R squared	0.992
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Dose-response curves for *in vitro* cytotoxic activity of compounds 7-43 and Blasticidin (reference cytotoxic compound) against human HepG2 cell line. Error bars represent standard deviation from independent triplicate assays.

