

Fig. 1: concentration-response curves of isolated compounds (1-7) and amphotericin B on *Leishmania (Viannia) braziliensis* expressing firefly luciferase as a reporter gene. Compounds 1, 2, and 5 were more active, with IC_{50} values of 21.4, 28.3, and 24.8 μ M, respectively. Compounds 4 and 7 showed IC_{50} values of 78.5 and 72.6 μ M, respectively, and amphotericin B showed IC_{50} of 0.12 μ M. Luciferase activity was measured by luminescence detection after 72 h treatment. IC_{50} values were calculated using GraphPad Prism (Version 6.0c).

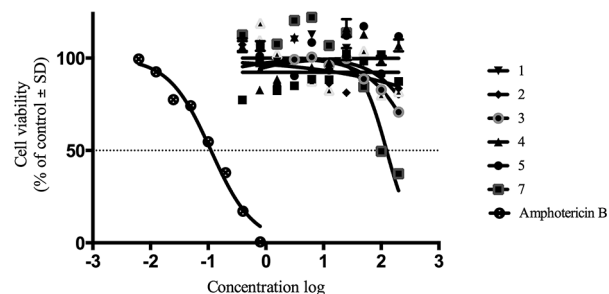


Fig. 2: concentration-response curves of isolated compounds (1-7) and amphotericin B on THP-1 cells. None of these compounds were considered toxic to THP-1 cells. Amphotericin B showed IC_{50} of 12.0 μ M in the assay on THP-1 cells. Cell viability was quantified by MTT after 72 h treatment and IC_{50} was calculated using GraphPad Prism (Version 6.0c).

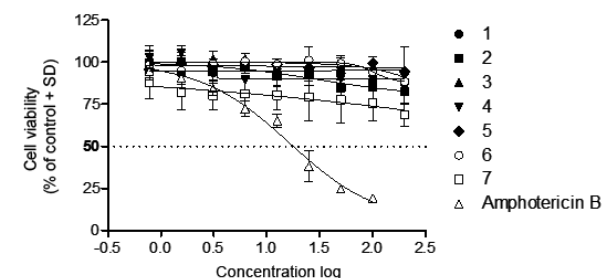


Fig. 3: concentration-response curves of isolated compounds (1-7) and amphotericin B on Vero cells. None of these compounds were considered toxic to Vero cells. Amphotericin B showed IC_{50} of 18.2 μ M in the assay on Vero cells. Cell viability was quantified by MTT and IC_{50} was calculated using GraphPad Prism® Version 5.01.

TABLE

Table of log *P* values and predicted bioactivity scores

Log P	Bioactivity calculated score [C]									
Compound	[A]	[B]	[C]	[D-F]	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1	2.63	1.35	1.24	-	low	0.24	low	0.45	low	0.41
2	2.37	2.80	2.28	-	low	low	low	0.29	low	0.34
3	2.17	3.00	1.95	-	low	low	low	low	low	0.20
4	2.69	3.38	2.63	2.83 ^D	low	low	low	low	low	0.24
5	0.78	0.58	0.74	-0.83 ^D	low	low	low	0.52	low	0.53
6	1.13	1.65	1.13	1.63 ^D	low	0.34	low	low	low	0.54
7	2.89	2.64	2.89	3.04 ^D	low	low	low	low	low	0.34
Pentamidine	-	-	-	4 ^E ; 2.32 ^F ; 1.32 ^F	-	-	-	-	-	-
Miltefosine	-	-	-	2.68 ^F ; 2.25 ^F	-	-	-	-	-	-
Amphotericin B	-	-	-	0.8 ^E ; -0.66 ^F ; -2.3 ^F	-	-	-	-	-	-

A: Tetko et al. (2005); B: Advanced Chemistry Development Inc., 2016. (ACD/Labs) ACD/PERCEPTA Version 2015. Frankfurt am Main. Available from: www.acdlabs.com; C: Molinspiration Cheminformatics 2017. Available from: <http://www.molinspiration.com/cgi-bin/properties>; D: SciFinder Database. Available from: <https://scifinder.cas.org>; E: DrugBank Database, DrugBank Version 5.0. Available from: <https://www.drugbank.ca/>. Experimental property; F: drugBank Database, DrugBank Version 5.0. Available from: <https://www.drugbank.ca/>. Predicted property.