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Realização

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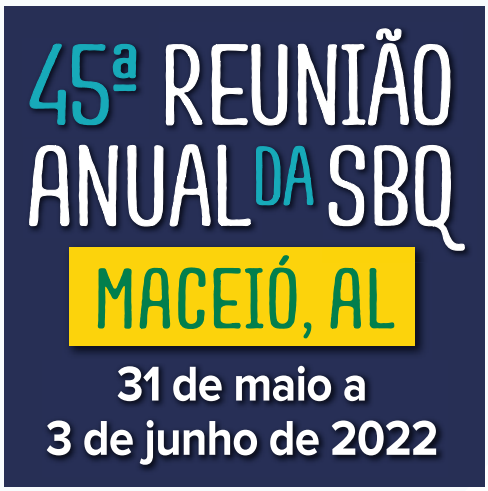
FERNANDO DE CARVALHO DA SILVA

Anais da 45ª Reunião Anual da SBQ



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Synthesis of 1,2,3-triazole selenides with anti-*T. cruzi* activity

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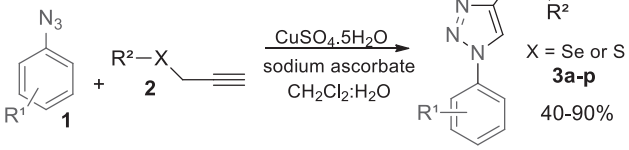
Key words: *antiprotozoan, chalcogen, heterocycle, organochalcogen.*

Highlights

This work presents the synthesis of new 1,2,3-triazole selenides and their evaluation as a potential drug for Chagas disease.

Abstract

Chagas disease (CD) is classified by the UN as a neglected tropical disease, caused by the protozoan *Trypanosoma cruzi* and causes more than 50,000 deaths a year. There are no major investments to improve the current treatment, which are only two medicaments available in the clinic since the 1940s.[1] Thus, research involving more efficient drugs for the treatment of CD is relevant to public health. In this work, we used a hybridization strategy combining organoselenium and 1,2,3-triazoles to design new 1,2,3-triazole selenides and evaluate their biological potential against T. cruzi. These two classes of compounds showed several biological activities such as antitumor, bactericidal, and antiprotozoal[2] and the combination of these two scaffolds appears as an alternative in the discovery of new drugs for the treatment of CD. The synthesis of the 1,2,3-triazole selenides (**3a-p**), was achieved by a 1,3-dipolar addition cycle with the copper and ascorbate catalytic system - as described in the scheme 1 - with aromatic azides **1** and terminal alkynes **2**, previously prepared.[2,3] A series of 16 new compounds were obtained with yields ranging from 40 to 90% and confirmed by ^{1}H-NMR.



Scheme 1. Synthesis of new 1,2,3-triazole selenides

Table 1. Yields and structures of 3a-p molecules and their respective antiprotozoal activity

	R¹	R²	R%	IC_{50} (μM)		R²	R²	R%	IC_{50} (μM)
3a	4-CH_3-C_2H_4	H	75	9,3	**3i**	H	4-Cl-C_2H_4	60	16,8
3b	4-Cl-C_2H_4	H	90	11,5	**3j**	H	4-CH_3-C_2H_4	70	7,4
3c	H	H	52	8,2	**3k**	H	4-F-C_2H_4	76	11,6
3d	4-NO_2-C_2H_4	H	42	>64	**3l**	H	2,4,6-CH_3-C_2H_2	50	39,2
3e	4-OCH_3-C_2H_4	H	84	12,7	**3m**	H	3-CF_3-C_2H_4	63	5,4
3f	2-Cl-C_2H_4	H	56	15,2	**3n**	H	Naphtyl	80	3,1
3g	2-CH_3-C_2H_4	H	85	9,8	**3o***	H	Ph	40	21,2
3h	3-CH_3-C_2H_4	H	82	9,2	**3p**	H	Tiophenyl	50	15,6

* X = S; Benznidazole [positive control] = 2,1 (μM)

The ability of these compounds to kill the protozoan *T. cruzi* was demonstrated through IC_{50} values described in Table 1. Seven of them were considered active, with derivatives **3m** and **3n** being the best in the series, considered potential candidates against CD. Since the effectiveness of a drug is related to its ability to penetrate biological barriers to reach the target site and induce its activity, the oral bioavailability of these compounds was predicted by Swissadme Web Tool and a moderate outcome was predicted for all compounds. In addition, other tests are being finalized, mainly to determine the mode of action of **3m-n**, and cytotoxicity results showed high selectivity of these hybrids. In conclusion, the series of new hybrid molecules with triazoles and chalcogen moieties fractions were synthesized and presented excellent results as possible new drugs against CD.

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