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ESTIMATION OF ADMET PROPERTIES OF DFH4 AND ITS NOVEL DERIVATIVES

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Computer assisted prediction of absorption, distribution, metabolism, excretion and toxicity (ADMET) was performed using the SwissADME online tool, for the dihydroxyfumaric acid (DFH_4) and its synthesized derivatives, which showed good antiradical activities in previous studies (Fig. 1).

The colored part of the radar shows the desired physico-chemical surface suitable for oral bioavailability of the compound: LIPO (lipofilicity): -0,7 < XLOGP3 < +5,0; SIZE: 150g/mol < molecular weight < 500g/mol; POLAR (polarity): 20Å^2 < TPSA < 130Å^2; INSOLU (insolubility): -6 < log S (ESOL) < 0; INSATU (insaturation): 0.25 < ration of sp3 C atoms < 1; FLEX (flexibility): 0 < number of rotatable bonds < 9.

All studied compounds satisfy *Lipiski's* rule of five, and have a good estimated bioavailability (0.56), while Fig.1. also shows a good drug-likeness.



a) DFH_4



b) dimethyl 2,3-dihidroxifumarate



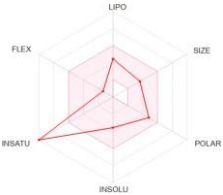
c) (*E*)-methyl 2,3-dihydroxy-4-oxo-4-(phenylamino)but-2-enoate



d) 2,3-dihydroxy-N^1,N^4-di(pyridin-2- il)fumaramide



e) (*E*)-3-(1H-benzo [*d*]imidazol-2-il)- 2,3-dihydroxiacrylic acid



(a) (*E*)-1,2-di(1H-benzo [d]imidazol-2-il)etene-1,2-diol

Fig.1. Bioavailability radars for the studied compounds.

Keywords: dihydroxyfumaric acid, DPPH• assay, functional groups, newly obtained derivates, kinetic behaviors.