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SYNTHESIS OF POTENTIAL IRE1α INHIBITORS

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Cancer has a major impact on society around the world and it is one of the leading causes of death. IRE1α is an enzyme that plays a part in the development of certain cancers, such as breast cancer, colon cancer, and prostate cancer. IRE1α inhibitors might be used to treat these types of cancer. [1]
The aim of this study was to find IRE1α inhibitors that would have a greater selectivity and bioavailability than the previously discovered ones. Based on computational data about the activity of compound 4f, it was chosen as the model compound for further synthesis.
The reaction used for the synthesis of compound 4f and its analogues was found to yield endocyclically acylated 1,2,4-triazol-5-amines instead of the anticipated exocyclically acylated compounds, but isomerization of endocyclically acylated 1,2,4-triazol-5-amines yielded exocyclically acylated compounds. However, the limited hydrolytic stability of compounds 3a-f suggested that the inhibitory activity of these compounds could be mainly due to the presence of compounds 2a-f in solution. Indeed, compound 2f had the greatest ability to inhibit IRE1α out of all the synthesized compounds.

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