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INVESTIGATION OF SYNTHETIC PATHWAY OF VARIOUS 2-(3-SUBSTITUTED

PROP-2-YNYLTHIO) IMIDAZOLES via ELECTROPHILIC CYCLIZATION

REACTIONS

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Imidazo[2,1-b][1,3]thiazine (2) and imidazo[2,1-c][1,4]thiazine (3) fragments are found in compounds which exhibit potential pharmaceutical properties as tumor cell growth inhibitors, cytotoxic [1], cardiotonic [2] or antibacterial [3] agents. One of the new routes to imidazothiazine compounds could be through electrophile initiated heteroatom cyclization reaction of alkynes which is used in synthesis of other types of heterocycles [4]. Thus we present the new way to synthesize imidazothiazine ring system *via* electrophilic cyclization of propargylic substrates. This synthetic route also enables variation of substituents in thiazine ring and possible halogen substitution in the system.

For our study 2-(3-substituted prop-2-ynylthio)benzimidazoles were chosen as model reactants in investigation of electrophile induced cyclization reactions. It was found that, cyclization of 2-(prop-2-ynylthio)benzimidazole (R= H) went through 5-exo-dig path (1) with selected electrophiles. While, 2-(3-substituted prop-2-ynylthio)benzimidazoles (R= Et, Ar) induced 6-endo-dig cyclization (2) and products were isolated in good yields. Some synthetized compounds 2 were chosen for further modification. However, cyclization of 2-(3-substituted prop-2-ynylthio)methylbenzimidazoles (n=1) resulted only in 6-exo-dig intramolecular cyclization (3) and in lower yields, as it appears due to the more labile sulphur. More details about reaction selectivity, scope, limitations and used reagents will be discussed in presentation.

References

- a) M.Thompson, A.J.Marshall, L. Maes, N.Yarlett, E. Gaukel, S.A. Wring, D. Launay, S. Braillard, E. Chatelain, C.E.Mowbray, W.A.Denny *Bioorg.Med.Chem.Lett.* 2018, 28, 207–213. b) M.A. Jarosinski, P.S.Reddy, W.K. Anderson *J. Med. Chem.* 1993, 36, 23, 3618 3627.
- V. Garaliene, L. Labanauskas, A. Brukstus Arzneimittel-Forschung/Drug Research 2006, 56, 4, 282 287.
- M.A. Salama, L.A. Almotabacani Phosphorus, Sulfur and Silicon and the Related Elements, 2004, 179, 2, 305 – 319.
- 4. B. Godoi, R.F. Schumacher, G. Zeni, Chem. Rev., 2011, 111, 2937-2980.