



METABOLIC SITE AND METABOLITES PREDICTION OF 2-[(1E)-N-{2-[(2-{(Z)-[1-(2-HYDROXYPHENYL) ETHYLIDENE] AMINO}ETHYL) AMINO]ETHYL} ETHANIMIDOYL] PHENOL SCHIFF BASE LIGAND

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Abstract

The aim of the present work was to evaluate *In silico* the metabolic sites and metabolites of the ligand 2-[(1E)-N-{2-[(2-{(Z)-[1-(2-hydroxyphenyl) ethylidene] amino}ethyl) amino]ethyl} ethanimidoyl] phenol by online computer software programs such as ACD/I-Lab, Metaprint2D.

Keywords: metabolic sites, metabolism, online

MATERIAL AND METHODS

MetaPrint2D (<http://www.metaprint2d.ch.cam.ac.uk/metaprint2d/>) was employed to predict the metabolic site and the metabolites produced (Carlsson *et al.*, 2010).

METABOLIC SITE AND METABOLITES PREDICTION

Metabolism prediction is a research priority in many areas, including pharmaceutical, food safety, and environmental studies (Egan *et al.*, 2000). The metabolism sites (SOMs) in a drug are the positions of different metabolism reactions. Identification of SOMs is a significant factor in the development of a drug discovery process. MetaPrint2D is a fast, efficient, and accurate online tool for the prediction of the sites and the products of metabolism in small molecule drugs. The approach adopted is a development of the method of

(Boyer et al., 2007). The different metabolism sites prediction and the resultant metabolites of the ligand from MetaPrint2D are shown in the (Figures 1 and 2), respectively. The oxygen atoms of the hydroxyl function (O17, O24) are the most that will be metabolized and were predicted as the site of the major type of metabolism reactions, such as acetylation, acylation, glucuronidation, methylation, sulfation, and phosphorilation. In addition, C14 and C21 are the most atoms that will be metabolized in glucoxidation and hydroxylation reactions. On the other hand, C15 and C22 are the site of methoxylation reaction. Moreover, C3 and C7 are the major sites for the reaction of oxidation. Thus, the Schiff base ligand has several sites of metabolism.

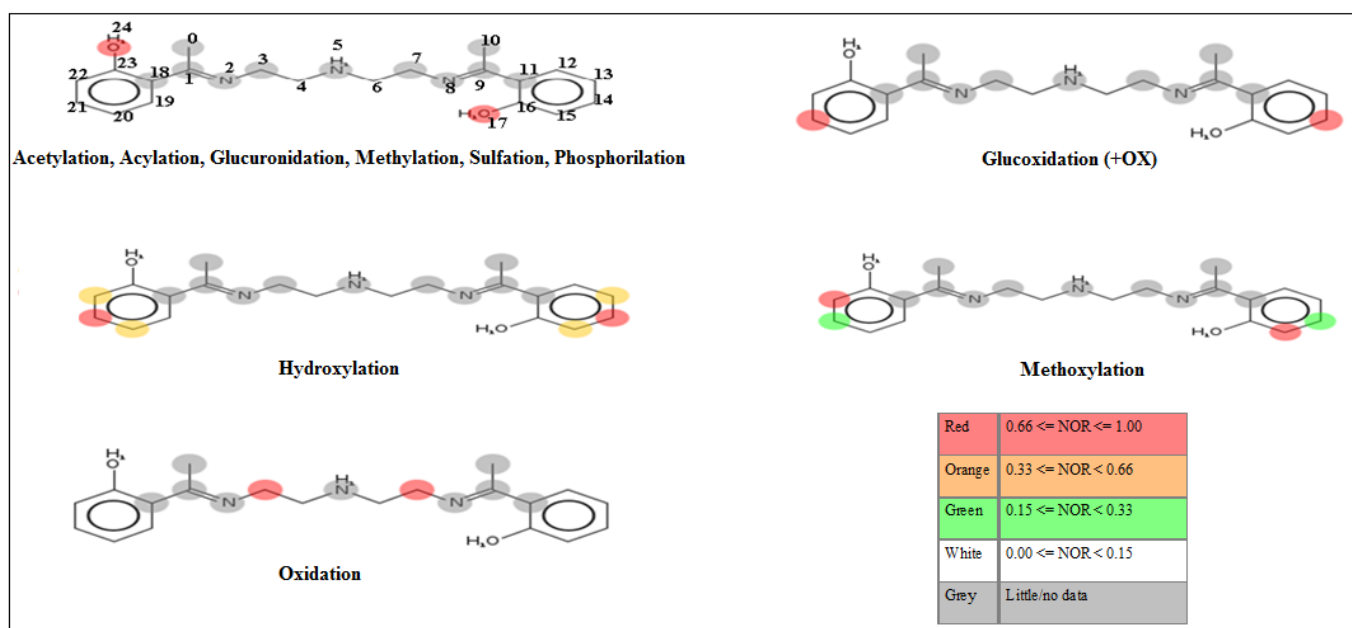


FIGURE 1: Reactions and Sites of metabolism. The atoms that most will be metabolized are colored according to the likelihood of a metabolic site; **High:** red, **Medium:** orange, **Low:** green, very low: not colored, and **No data:** grey. NOR indicates the Normalized Occurrence Ratio; a high NOR indicates a more frequently reported site of metabolism in the metabolite database.

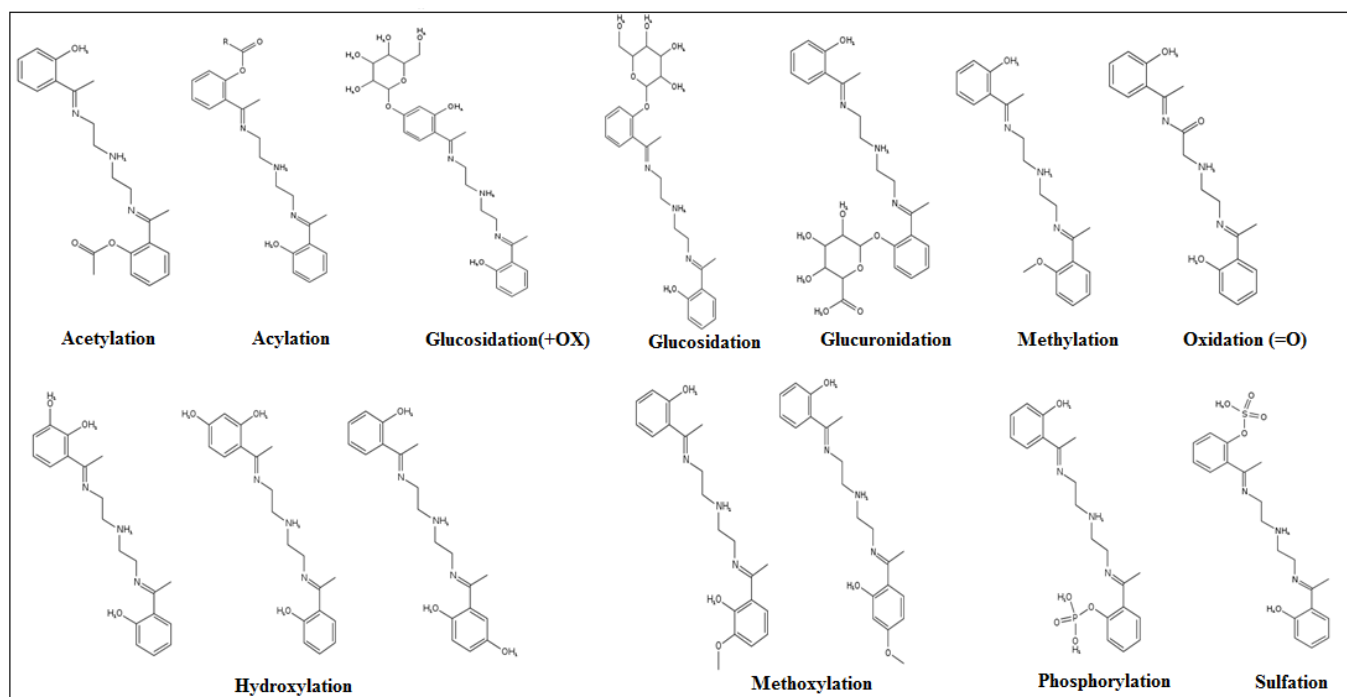


FIGURE 2. Different metabolites of the ligand at different metabolism reactions

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