ABSTRACT

Medicinal plants provide an extensive array of bioactive agents and an impressive extent of modern drugs has been isolated, established from the traditional system of medicine. *Scoparia dulcis* L. is a distinguished ethnomedicinal plant immensely distributed in tropical and subtropical regions of Asia, Africa, America and Europe and extensively assayed for its diverse pharmacological possessions such as analgesic, anti-inflammatory, neurotrophic, antiviral, antimalarial, anticancer and antidiabetic activities. Although many researches have already been documented for the incredible therapeutic efficacies of *Scoparia dulcis* L. in various parts of the world, very little work has been evaluated from North East India, especially from Assam. The present state of affair was an attempt made to isolate and characterize some of the bioactive secondary metabolites as well as *in silico* evaluation of the probable therapeutic potentialities of the isolated metabolite(s) by following standard protocol and application of bioinformatics tools, databases and software. The effort led to the isolation of a novel ketonic compound, (E)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one. Further effort regarding *in silico* therapeutic screening of the isolated metabolite revealed the potentiality of the compound to inhibit 2-Hydroxy-6-Oxo-6-Phenylhexa-2,4-Dienoate Hydrolase BPHD (HsaD) enzyme of *Mycobacterium tuberculosis* H37Rv strain. On studying binding efficacy of the isolated compound with the active site of HsaD enzyme of *Mycobacterium tuberculosis* H37Rv strain, exhibited good binding affinity compared to 10 out of 23 standard inhibitors. From the regression analysis, the QSAR equation was generated and finally the activity (IC$_{50}$) of the isolated compound was predicted and found to be satisfactory compared to all the 23 standard inhibitors.
Thus, this piece of endeavour led to the isolation of a novel metabolite from *Scoparia dulcis* L. which exhibited the potentiality to become a lead molecule for treatment of tuberculosis. However, this *in silico* assessment demands further exploration in *in vivo* model to endorse the findings which may provide a new dimension to the discovery of a novel antitubercular drug in near future.