Reviewer’s report

Title: Quantitative Structure-Activity Relationship of Molecules Constituent of Different Essential Oils with Antituberculosis Activity against Mycobacterium tuberculosis and Mycobacterium bovis.

Version: 2
Date: 21 May 2015
Reviewer: Vishwa M Katoch

Reviewer’s report:

1. This manuscript provides new information about anti-mycobacterial activity of selected constituents of essential oils, QSAR relationships and toxicity against cell lines. This information is novel and has immense scientific potential in terms of developing new anti-TB agents.

2. Objectives and design of this study are clearly stated. Methods selected for activity assessment, toxicity, descriptors, QSAR, molecular modelling etc are all robust and acceptable.

3. There are number of suggestions about improving the presentation: (i) This is not the first or one among few studies on anti-TB activity of plant based products. Even in this manuscript number of references – nos 10, 11, 12, 17, 31, 32, 33 are on the same subject. There are several studies from India on anti-TB activity of plant/herbal based products which merit consideration for being quoted. Thus language in the background of abstract and main body of manuscript needs appropriate modification.

4. In the Results (abstract and main paper) the words “more” active have been used ( eg. 5th sentence in results in abstract, 3.1, ). It needs to be clearly stated – more/higher than what ?. This is only language issue but very important from scientific point of view.

5. For identifying/screening molecules/agents, ratio of activity to toxicity is important. Authors have rightly focused on molecules with maximum activity. However, it would have been ideal to test all and then discuss with favourable ratio. This aspect needs justification and also mention in the discussion.

6. There is apparent contradiction in statement about toxicity – last concluding paragraph about higher activity and lower toxicity versus last paragraph of 3.2. These need clarification/appropriate modification

In view of above, I will recommend the publication of manuscript after adequate modification.

Level of interest: An article of outstanding merit and interest in its field

Quality of written English: Needs some language corrections before being published
Statistical review: No, the manuscript does not need to be seen by a statistician.

Declaration of competing interests:
I declare that I have no competing interests