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Consolidated Recommendation of the Board on the Ph.D. Thesis
Submitted by *Mr. R.R. Saravanan*

Title of the Thesis: Spectroscopic, Crystallographic & Hirshfeld surface analysis and Molecular docking studies on some Thiosemicarbazone derivatives

The Ph.D. thesis submitted by the candidate Mr. R.R. Saravanan is a report of the research work carried out extensively on some Thiosemicarbazone derivatives viz., Single crystal X-ray Crystallography, FT-IR, FT-Raman spectroscopic methods, Conformational analysis, Molecular electrostatic potential, quantum chemical calculations and Molecular docking studies are carried out for the chosen Thiosemicarbazone derivatives (i) (E)-2-(1-(4-fluorophenyl)ethylidene)hydrazine carbothioamide (EFEHC), (ii) (E)-1-(1-(4-Chlorophenyl)ethylidene)thiosemicarbazide (ECET), (iii) (E)-2-(1-(4-bromophenyl)ethylidene)hydrazine carbothioamide (EBEHC), (iv) (E)-2-(1-(3-methoxyphenyl)ethylidene)hydrazine carbothioamide (MET) and (v) (E)-2-(1-(4-hydroxy-3-ethoxyphenyl)ethylidene)hydrazinecarbothioamide (EHEHC). The characterizations of the Thiosemicarbazone derivatives are carried out by a well-planned manner and the observed crystallographic and spectroscopic data were in good agreement with the calculated data. The results obtained are consistent and remarkable. This is a good piece of work in the field of Medical and Pharmaceutical Physics.

Summary of the citations given by the Examiners in appreciation of the Thesis

1. Commendations by Prof. Dr. Jens – Uwe Grabow, Institut Für Physikalische, Chemie and Elektrochemie, Lehrgebiet A, Gottfried – Wilhelm-Leibniz Universität, Hannover, Germany.

- The candidate has shown great expertise in theoretical understanding and experimental techniques.
- The work described in the thesis is very adorable and the candidate has proven experimental skills and theoretical understanding and taken utmost care in analyzing the data.
- The work contained in the thesis contributes to the advancement of science.

- The topic is very relevant and is aimed at academic achievement and practical utility.
- The thesis clearly shows the researchable problems, issues and relevance.
- The objectives and methodology and usefulness are clearly indicated.
- The distribution of chapters is excellently one and the scholar has shown great ability in discussing the problem and interpreting the results.
- The Summary gives conclusions of the results and suggestions for future work.
- The topic chosen for research has importance in the field and it has wide academic significance.
- The title of the thesis is adequately chosen and relevantly indicates the work undertaken.
- The thesis clearly states the researchable problems, issues, relevance, objectives, methodology, data, analysis and usefulness are adequately addressed.
- In short, the thesis adds a significant contribution to scientific knowledge and research methodology.
- **I recommend the thesis for the award of the Ph.D. degree of the University of Madras. The merit of the candidate is highly commended.**

2. *Commendations by Dr. Debasish Bhattacharyya, Deputy Director, CSIR Indian Institute of Chemical Biology, 4, Raja S.C. Mallick Road, Jadavpur, Kolkatta – 700 032, India.*

- The thesis is well written and the conclusions are supported by a wealth of physical data.
- Tables and figures are properly placed, adequate in number. They are distinct and clear.
- Experiments were performed carefully taking care of control sets.
- No extrapolations of inference were drawn based on assumptions.
- We hope that the information generated will be useful in the pharmaceutical industry in the future.

- References cited are adequate and an updated literature survey has been done.
- Overall, the thesis is of a high standard. The supervisor is an established investigator in the area of spectroscopy and quantum chemistry.
- Segments of the thesis has either been published in peer reviewed international journals or communicated for publication.
- I congratulate the candidate and his supervisor for presenting a decent high quality thesis where a substantial volume of contemporary information is loaded.
- **I recommend the award of Ph.D. degree to the candidate by the University without reservation. Further, the thesis is acceptable in the current form for the award of the degree. The merit of the candidate is highly commended.**

3. *Commendations by Dr. S. Gunasekaran, Supervisor and Guide, Convener of the Ph.D. Board.*

- The thesis establishes the potentiality of the crystallographic and spectroscopic techniques as a powerful diagnostic and monitoring device.
- The theoretical methods, spectroscopic techniques and molecular docking studies are adopted for analysis of some thiosemicarbazone derivatives to find the anti-cholesterol drug property.
- The results presented in this research show the candidate's thorough understanding of the produced scientific information along with his excellent foundations to use those data to describe and characterization of the target molecules, which includes a clear view of the connection between the experimental and theoretical methods.
- The candidate has understood the intricacies of the experimental procedure very well and proceeded with his Thiosemicarbazone derivatives taken for the studies.

- The theories of the spectroscopic methods and quantum mechanical calculations have been elaborated along with the construction of the instruments used.
- The thesis consists of adequate numbers of Tables, good quality of Figures and images of compounds derived from the calculations.
- The candidate has published part of the quality works reported in the thesis in journals and therefore the candidate is appreciated and admired for the quality of reported work in this thesis.
- Finally, the analysis performed by the candidate contributes to improving the knowledge of the chosen compounds and in this way, it allows for further and future research on the applicability of such chemical systems.
- **The thesis is highly commended for the award of Ph.D degree in Physics.**

Based on the highly commended recommendations of the examiners of the Ph.D. board constituted in the case of the candidate Mr. R.R. Saravanan, I, Dr. S. Gunasekaran, as the convener of the board, strongly recommends the award of the Ph.D. degree to the candidate from the University of Madras.

**Signature of the Supervisor
(with Seal)**