ACKNOWLEDGEMENT

Just few days before writing this section of my thesis, I was going through the PhD thesis of a guy from Netherland and found his views regarding "acknowledgement" quite true to an extent. Actually he was not in favour of writing an acknowledgement. Not that he was not grateful to the people who helped him finishing his PhD thesis, but just because he did not like the causal reasons why acknowledgements are read. That is, the acknowledgement is one of the most read parts of a thesis, just to see (1) if your own name is mentioned, (2) if underlying feelings towards other persons can be discovered (as they are not just written down, but can be discovered in cryptograms), and (3) to talk about with the author in case nothing else of the PhD thesis was read. He thought he had a solution, by just saying:

"THANK YOU, to whom it concerns!!"

Although it solves some of the problems of acknowledgements (i.e., you do not forget to mention certain names, everybody can decide for him or herself whether [s]he is one of the "concerned"), it does not make up for everything that some people have done and meant for me during the process of writing this PhD thesis. So, as per the norms, I should acknowledge everyone which, however, is an impossible task given the many people that have helped to design, implement, apply, criticize, sponsor and evangelize the work. I am going to try anyway, and if your name is not listed, rest assured that my gratitude is not less than for those listed below.

First and foremost I want to thank my advisor at Bombay College of Pharmacy (BCP), Professor Evans Cliffton Coutinho. It has been an honour to be his PhD student. He has taught me, both consciously and subconsciously, how good computational chemistry is done. I appreciate all his contributions of time, ideas, and funding to make my PhD experience productive and stimulating. The joy and enthusiasm he has for his research was contagious and motivational to me, even during tough times in the PhD pursuit. I am also thankful for the excellent example he has provided as a successful molecular modeller and a good friend to seek an unbiased suggestion on virtually any thing.

I extend my gratitude to Dr. V.S.V. Vadlamudi Rao and Mr. Pravin Manker, our former Directors, for rendering the administrative formalities smooth and easy for the students. I also thank our present Director, Dr. S. K. Kulkarni and Principal, Dr. M. N. Saraf for providing college facilities for the successful completion of my research project. I want to express my deeply-felt thanks to Dr. Krishna Iyer and Dr. Mrs. Premlata Ambre for their warm encouragement and helpful chats.

I thank CSIR, New Delhi for the fellowship to support my research projects. I am grateful to the Bombay College of Pharmacy for allowing me to sustain myself financially by providing me the temporary lectureship for Computer Practicals of 2nd year B. Pharm. Students for two semesters. I am also thankful to the librarian Mrs. Desai and Mr. Sawant who always help
me getting my books. Thanks to Mr. Kawde, Mr. Gawde, Mr. Pramod, Mr. Shinde, Mr. Manjrekar, and the other staff of BCP for their help related to the office work.

I want to thank the past and present members of the CAMD lab in BCP: Dr. Arati, Dr. Alpesh, Dr. Santosh, Dr. Raghuvir, and Mushtaque for giving me an introduction into the lab and for sharing their knowledge. Thanks to Rakesh, Sonali, Vijay, Mahesh, Ravindra, Shubhangi and Devendra for providing a great work environment and spreading happiness on those scientifically dark days. I (and I am sure everyone of us) will never forget the laughing moments we all have shared during tea breaks and lunch time in the canteen, many a times along with Coutinho sir, Krishna sir, Premlata mam and Poonam Advani mam. I would also like to thank Dr. Mrs. Meena Kanyalkar and her family for the parties at their home in Mulund that most of the CAMD lab members have enjoyed with imported wines and delicious food items.

I would also like to thank all my past and present friends at BCP. Their constant support and encouragement had made my days at BCP unforgettable for life. Thanks to Dr. Kale, Dr. Rahul Dixit, Dr. Sanket, Dr. Nitin, Dr. Suresh, Dr. Tushar, Dr. Sidhaarth, Dr. Parag, Dr. Milind, Dr. Sarika, Dr. Poornam Patil, Dr. Date, Abhijit Dalvvi, Neha, Shruti, Sheetal, Shilpa, Reelma, Chandrashekar (CST), Nishant, Sameer, Pankaj, Rahul Shirole, Aashish, Rajendra Dhanve, Atul, Aagivesh, Aadi, Devendra, Bhupendra, Sharad Fender, Manon, Tapkir and many more. Some of them were my room mates also.

As you all know, work is not my entire life; there are more important things in life than a PhD thesis. Top of everything is our family. I thank my family for their love and unequivocal support in all my pursuits, for which my mere expression of thanks likewise does not suffice. Unfortunately, my father expired last year and that was a major setback not only to me but to the entire family. He was the person who always wanted to see me as a DOCTOR. This thesis is dedicated to him. Though he is not here to share this moment with me, I am sure he must be keeping an eye on me from the heaven. Huge appreciation goes to my loving mother who never let me know how much pain and suffering she has undergone, and yet always directed me to concentrate on my studies. Thanks a ton to my younger brother, Deepak, for supporting me financially after my fellowship was over. I owe my loving thanks to my caring, encouraging, understanding and patient wife, Kavita, for all the support that she gave me during the years I have been working on this thesis, especially all the holidays that she arranged to give me time to think and write about this subject. I really feel sorry for a sense of negligence that I have shown towards her during this period. Anyways, I am sure that she loves me a lot and will forgive me for that.

Finally, I thank the almighty GOD for the successful completion of my PhD thesis.

Perhaps, I forgot someone... so, just in case: thank you to whom it concerns!

For any errors or inadequacies that may remain in this work, of course, the responsibility is entirely my own.

Jitender Verma