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Wien, am 04.05.2022

Attn: Thesis review JYOTI

Dear Professor Gregorowicz,

First, let me express my appreciation and gratitude for inviting me to act reviewer of the PhD thesis “Carbazole and acrylate molecularly imprinted polymers and their application as recognition units in electrochemical chemosensors for selective determination of chosen drug substances” submitted by Jyoti. The thesis comprises a body of work on electrosynthesizing molecularly imprinted polymers (MIP) focusing on two different analytes, namely cilostazol and duloxetine. Both these compounds are potent drugs which makes them attractive targets for point-of-care diagnostics and analysis. Overall, Jyoti included five publications and manuscripts into her thesis, of which two are published in high-ranking journals, namely “Biosensors and Bioelectronics” and “Journal of Materials Chemistry B”, respectively. The other three are either submitted or prepared. Three of them are more sensing-oriented studies aiming at designing electrochemical sensors for the two analytes mentioned. The other two contain physicochemical work aiming at elucidating the influence of certain substituent groups on the polymerization ability and electrochemical behavior of different 3,6-dithienylcarbazole derivatives. In fact, all those studies include not only the (expected) experimental data, but also substantially rely on modelling to underpin and explain the corresponding experimental findings.

This short summary already highlights the most fundamental strong point for the present thesis: it integrates physicochemical experiments, systematic modelling work, and applying the final monomers and polymers in designing electrochemical sensors aiming at real-life application in a clinical setting. Therefore, this work is much more interdisciplinary and systematic than many other studies in the area of molecular imprinting/electropolymerization that often focus on one of these aspects. Within her work, Jyoti thus clearly demonstrates that she is capable and willing on carrying out

scientific research that requires combining experimental and theoretical skills as well as a range of measuring and characterization techniques. Her thesis thus delivers a full story from selecting suitable monomers – partly *in silico* – to actually synthesizing the corresponding imprinted and non-imprinted polymers and characterizing them for their sensor responses mainly with voltammetry and electrochemical impedance spectroscopy. On the other hand, this also required her to use a range of (in-situ) characterization techniques, such as AFM, SEM and PM-IRRAS, with the latter being a very powerful tool for spectrometrically characterizing electrode processes in situ. Aside of this larger sensor-related part, the PhD thesis also contains work aiming at elucidating the influence of molecular structure of different 3,6-dithienylcarbacoles on their polymerization behavior. This requires thorough modeling of the electron densities of the respective native molecules and the corresponding radical ions that finally polymerize. This part of the thesis is not yet published, but on the way of getting there.

The quality of the work becomes of course obvious from the two papers already published in renowned journals. However, a PhD thesis of course should comprise more than “just” a collection of papers: it needs to demonstrate that the candidate is proficient in researching a larger “story” in the course of that process. The present thesis fulfils this requirement in a highly appreciable way, as it covers the whole “value chain” of MIP synthesis and the corresponding sensing.

There are some minor shortcomings of the monography shown, especially regarding presentation, when sometimes language becomes a bit complicated, some statements regarding the theoretical background seem a bit too generalized or when the experimental part contains descriptions of the spectrometries etc. used (which I would expect in introduction). However, these are minor details, indeed, that by no means diminish the high scientific quality of the overall work.

In summary, I have very much appreciated reading the thesis and learning about the science behind it. Without any doubt, the work done, the papers, and the content generated make for a good PhD thesis. Jyoti has clearly demonstrated her ability to carry out research in a very broad field of science. This shows that she deserves the PhD degree beyond any doubt even when applying very strict standards to such graduations. If you have any further questions regarding this report, I am of course at your disposal.

With kind regards,