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Supervisor Review of the Bachelor Thesis of Kareem Jeiroudir

It was a great pleasure to supervise the bachelor thesis of Kareem Jeiroudi on "Interpretability of Neural Networks in drug design".
This work is concerned with a highly relevant topic. It explores the possibility to explain the predictions of neural networks in the field of Drug Discovery, focusing on the method of "Integrated Gradients".

The interdisciplinary nature of this topic makes it particularly challenging. That challenge was met by Kareem with remarkable discipline and perseverance. He independently researched the necessary literature and showed an extraordinary ability to familiarize himself with new topics in a precise and comprehensive manner. He was not deterred by their difficulty and scope. On the contrary, with great interest and commitment he developed a profound understanding of the advantages and weaknesses of "Integrated Gradients" in Drug Discovery.
Under our guidance he implemented neural networks as well as the "Integrated Gradients" method. He compared several baselines for the latter, and proposed a method to evaluate the different approaches, which is arguably the most difficult and important part of this thesis.

During all of his work we were very impressed with Kareem: He acquired the necessary knowledge and skills to deal with the subject in depth with great motivation and independence. However, he regularly discussed the current status of his work with us and sought and valued our feedback.
His work exceeds what is commonly expected from a bachelor student. We can state with confidence that Kareem is more than worthy of the Bachelor of Science degree, given the excellent work he performed for this thesis.

Sepp Hochreiter