Review
of the domestic scientific advisor
on the dissertation of Mrs. Anel Kapar
"Modeling of solid-phase microextraction of volatile organic compounds from environmental objects"
presented for the defense of Ph.D. degree
on educational program "8D05301 - Chemistry"

Monitoring the environment is essential for assessing risks and making decisions to manage environmental pollution effectively. Traditional environmental analyses are costly primarily due to time-consuming sample preparation. Headspace (HS) solid-phase microextraction (SPME) is a promising sample preparation method for organic pollutants in environmental samples due to its simplicity, greenness, automation, and ability to achieve low detection limits at a minimal cost. Nevertheless, optimizing SPME parameters requires extensive experimental effort and expense. Achieving the right balance between detection limits and accuracy involves thorough optimization numerous extraction parameters such as fiber coating type, extraction temperature, time, pH, sample/headspace ratio, agitation rate, desorption temperature and time. This process is time-consuming, expensive, and complex, with method developers often prioritizing maximizing analyte responses over accuracy during optimization. Simulation of the SPME process is a valuable tool for developing and optimizing analytical methods.

The dissertation of Anel Kapar is aimed at the development of computational models of solid-phase microextraction of volatile organic compounds (VOCs) from environmental objects. The developed models allow to enhance the optimization process and predict optimal parameters for various analytes and samples without extensive experimental optimization. To this end, new computational models for simulating SPME of VOCs from air, water, and soil have been developed.

The PhD project of Anel Kapar involves development of mathematical and physical models of processes taking place in the multi-compartment extraction system with mass transfer of volatile organic compounds between air, water, soil, and polymeric extraction coating. The methods of assessment and prediction of multiple parameters of extraction systems such as diffusion of analytes in the gas phase and inside the coating, distribution constants are evaluated based on lowest deviations between simulated and experimental extraction profiles. Thus, the work of Anel Kapar is of high importance and relevance in the field of green sample preparation and analysis.

During the study, Anel Kapar showed herself as independent and hard-working young scientist with a strong theoretical and practical background. She was able to generate creative ideas and hypotheses for solution of complex tasks and obtaining new knowledge.

As a result of her PhD project, Anel Kapar has published two articles in the international peer-reviewed journals indexed in Q1, one article journal recommended by the Committee for Control in Education and Science of the Ministry of Science and

Higher Education of the Republic of Kazakhstan, and one abstract of international scientific conference.

The PhD study of Anel Kapar was conducted under the project AP08052684 "Effective development of methods for analyzing environmental objects based on headspace solid-phase microextraction using computer modeling" (2020-2022) both funded by the Ministry of Education and Science of Kazakhstan.

In my opinion, on the importance of the topic, scientific novelty, practical value and volume of the research, the dissertation of Kapar Anel "Modeling of solid-phase microextraction of volatile organic compounds from environmental objects" fulfills all requirements of the Ministry of Science and Higher Education of the Republic of Kazakhstan to the Ph.D. dissertations, and Kapar Anel deserves the Ph.D. degree on educational program "8D05301 - Chemistry".

Domestic scientific advisor:
PhD D.S. Orazbayeva

әл-Фараби атындағы ҚазҰУ Ғылыми кадрларды даярлау және аттестаттау басқармасының басшысы
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