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QSAR modeling of arylsulfonylhydrazones as potential anti-breast cancer agents

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Breast cancer is the most common cancer among women worldwide. Despite progress in early detection and treatment, there is still a pressing need for more effective drugs with fewer side effects. Arylsulfonylhydrazones exhibit a range of pharmacological properties, with their anticancer potential being of particular interest. Computational approaches, such as in silico analysis, play a crucial role in the early stages of drug discovery, significantly reducing the time and resources required for preliminary evaluations. In this study, a Quantitative Structure–Activity Relationship (QSAR) analysis, a widely used ligand-based drug design (LBDD) method, was applied to a series of arylsulfonylhydrazone derivatives to investigate the relationship between their chemical structures and anticancer activity against human breast cancer. The developed models can support the design of novel, promising compounds for further research and development as potential anticancer agents.

Keywords: QSAR, arylsulfonylhydrazones, anti-breast cancer agents