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QSAR Study on a Series of Protein Tyrosine Phosphatase 1B Inhibitors

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As a therapeutic target, protein tyrosine phosphatase 1B (PTP1B) has received considerable attention for the treatment of diabetes mellitus. A QSAR study using substituted monocyclic and polycyclic thiophene derivatives, recently reported as potent PTP1B inhibitors, was carried out. More than 60 physicochemical descriptors were calculated which underwent rational selection before their use in derivation of QSAR models. Statistically significant equations were generated using multiple linear regression analysis. External validation of the derived models with test set compounds proved good predictability of the models. Interpretation of the results revealed lipophilicity as a key regulatory feature which affects PTP1B inhibition along with several electronic and steric parameters. The study provides an important platform upon which novel rationally designed molecules can be synthesized with cautious optimism.