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Computational Assessment of Biological Activities of Estrogenic Compounds

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Estrogen receptor α (ERα) is associated with numerous diseases, including breast cancer, osteoporosis, endometrial cancer, and prostate hypertrophy. In addition to the biochemical and physiological importance of the natural ER ligands, in recent years considerable concern has emerged about the possible deleterious effects of xenoestrogens, particularly exogenous ER agonists. It appears that the ER shows affinity for a remarkably wide range of structurally diverse compounds, such as polyaromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), phytoestrogens, phthalates, and pesticides. Everyday foodstuffs are another source of estrogen-like compounds. Given the diverse range of compounds that may bind to the ER and exert an effect on human and animal health, there is considerable medical interest in understanding the details of ligand-ER affinity and developing techniques to predict the affinity of compounds for ERα. Previous computational efforts in this area have concentrated mainly on empirical regression-based (quantitative structure-activity relationship (QSAR)) approaches. In the previous study, we explored the ligand-ERα interactions using the knowledge-based multiple-conformation docking method with an improved scoring scheme. Here a Naïve Bayesian method is proposed for the classification of estrogenic compounds in a high throughput speed.

Keyword: Erstrogen receptor, xenoestrogen, QSAR, Bayesian classification, toxicity