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Immunomodulatory and Potent Anticancer Activity of Selective Steroidal Analogs

Machine-learning-designed synthetic small molecules show promise as potent, non-toxic, and metabolically stable drug leads against drug-resistant prostate cancer and metastasis.

Researchers at Purdue University have developed potent synthetic small molecules with high potential as drugs against castration-resistant prostate cancer (CRPC) that are non-toxic in normal human cell lines. To address the heterogeneity of cellular pathways in cancer, the source of a cancer's ability to become resistant to therapy, the investigators designed these molecules using a machine learning approach that targets the protein network implicated in the disease state to guide compound selection and synthesis. The series of compounds developed inhibits proliferation of C4-2 androgen-insensitive human prostate adenocarcinoma cells with IC50 as low as 0.72 nM, and the compounds are much more potent than a control, the current steroidal CRPC drug, abiraterone (ABI). The most potent compound and other active leads were also more metabolically stable than ABI in a mouse liver microsome assay. Further, these compounds promise to combat metastasis; they slow migration of cells relative to untreated cells in both LNCaP and C4-2 cell lines.

Advantages:

-Non-toxic

-Potent

-Addresses drug resistance

Potential Applications:

-Disease Research

-Cancer Therapy

TRL: 3

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Pharmaceuticals/Computational & Software Tools

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Intellectual Property:

Provisional-Patent, 2019-02-28, United States | NATL-Patent, 2020-02-28, China | PCT-Patent, 2020-02-28, WO | NATL-Patent, 2020-02-28, Canada | NATL-Patent, 2020-09-28, Europe | NATL-Patent, 2021-08-25, India | NATL-Patent, 2021-08-26, Japan | NATL-Patent, 2021-08-27, United States | DIV-Patent, 2025-11-07, Japan

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