

# Small molecule could have big impact on cancer

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Dr. Jung-Mo Ahn, associate professor of chemistry at The University of Texas at Dallas, has designed and synthesized a novel small molecule that might become a large weapon in the fight against prostate cancer.

In a study published online May 28 in the journal *Nature Communications*, Ahn and his colleagues at UT Southwestern Medical Center describe the [rational design](#) of the molecule, as well as [laboratory tests](#) that show its effectiveness at blocking the cancer-promoting function of proteins called androgen receptors.

Androgen receptors are found inside cells and have complex surfaces with multiple "docking points" where various proteins can bind to the receptor. Each docking point has a unique shape, so only a correctly shaped molecule will fit.

[Androgen hormones](#), such as testosterone, are the primary [molecules](#) that bind to androgen [receptors](#). Such binding sets off a chain of events that activates several different processes in the human body, including stimulating the development and maintenance of male characteristics.

Looking for a new approach to battle [prostate cancer](#), Ahn and his colleagues keyed in on blocking a critical docking point on the [androgen receptor](#).

"When a tumor is trying to grow, activation of this location provides what the tumor needs," Ahn said. "There are other surfaces on the

androgen receptor that are free to continue working with their respective proteins and to continue functioning. We sought to block only one set of interactions that contribute to prostate cancer growth. That's why we thought our approach might lead to potent efficacy with fewer side effects."

Using computer-assisted [molecular modeling](#), Ahn designed a helix-mimicking small molecule that fits precisely into a pocket on the androgen receptor that is associated with prostate cancer. Collaborating with senior study author Dr. Ganesh Raj, associate professor of urology at UT Southwestern and a specialist in treating urologic cancers, the researchers tested the compound in animal and isolated human tissue. Without exhibiting noticeable toxicity, the compound prevented the androgen receptor from recruiting its protein partners and it blocked the growth of prostate cancer cells.

"We have shown that our molecule binds very tightly, targeting the androgen receptor with very high affinity," Ahn said. "We also have confirmed that it inhibits androgen function in these cells, which is a promising finding for drug development. We showed that it does work through these mechanisms, and it is as effective in inhibiting the proliferation of prostate cancer cells as other compounds currently in clinical trials."

Ahn plans to continue his research to better understand how the small molecule and related compounds he developed work against cancer on a molecular level. He said much work is left to do before any potential drugs or treatment might be developed, but added "this is an exciting start."

About 239,000 men are expected to be diagnosed with prostate cancer in the U.S. in 2013 and about 30,000 will die of the disease, according to the American Cancer Society.

Provided by University of Texas at Dallas

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