

In silico discovery of novel Retinoic Acid Receptor agonist structures

ABSTRACT

The predicted receptor model produced two novel agonists that were active at 50 nM. One of them showcases unique structural characteristics that could lead to the development of new ligands for cancer treatment.

INTRODUCTION

To date, there are no data for the therapeutic efficacy of retinoic acid (RA) in treating retinopathy.

We have now synthesized two novel retinoic acid receptor (RAR) agonist structures in the mouse and human retinoic acid receptor (RA) receptor subfamily, namely the human and mouse retinoic acid receptor (RA) binding sites, and the human and mouse retinoic acid receptor (RA) receptor subtype 2 subfamily. These new RAR agonists were found to bind to the human and mouse RA receptor subtype 2 subfamily.

The RAR agonist structures were selected from the human and mouse retinoic acid receptor subtype 2 subfamily and the human and mouse RA receptor subtype 2 subfamily subfamily.

Method The retinoic acid receptors (RAR-, -à, and –) are transcription factors that regulate various endocrine metabolic pathways. As a result, RAR isoform ligands can exhibit anticancer activity against breast tumor cells of both estrogen receptor positive and negative cells. This could pave the way for upcoming novel drugs to target breast cancer in which both RARA agonists and antagonists may have important biomedical applications, as both can present anti-tumor activity specific tumours or even human prostate. Several retinoid and non-retinoid ligands have been described as having the ability to activate one or more RAR isoforms, with some (as seen in Fig. 1a) including the natural hormone all-trans hepatitis B) exhibiting unacceptable side effects such as skin dryness, cheilitis, hypertriglyceridemia, and conjunctivitis C. Clinical trials have shown that these compounds belong to limited series of related structures, but the R Using a flexible virtual screening algorithm (Molsoft ICM, virtual library screening module), we rapidly docked hundreds of thousands of flexible compound structures into the ligand binding pocket of RAR and identified two novel RER- selective agonists. One of these lectins displays original structural and chemical characteristics, which could be used in the development of new compounds for cancer prevention and therapy.

CONCLUSION

Remarkable conclusions The report explains that it has been possible to quickly identify RAR agonists with novel structural characteristics, using a potent virtual ligand screening method, and investigating methods that avoid predation. The data reveals that ten new molecules on this platform offer 'flawed' ROH (reactive oxygen complex) approach, which provides atomic structure enhancement and potential therapeutic uses for cancer drugs.