1. Title of the Invention

Estrogen Receptor (ESR) superfamily inhibitor to control tumor growth in breast cancer patients

2. Field of the Invention

The present invention relates to the field of healthcare, specifically to the development of a novel drug molecule that acts as an inhibitor of the estrogen receptor (ESR) superfamily. This drug is designed for hormonal/endocrine therapy of estrogen-sensitive breast cancers, aiming to effectively bind with estrogen receptors and induce cell death/apoptosis or suppress cancer cell growth.

3. Background of the Invention

Breast cancer is a significant health concern globally, affecting a large number of individuals, primarily women. It accounts for approximately 12-14% of all cancer cases worldwide, with an estimated 670,000 deaths attributed to breast cancer in 2023. A key factor in the development of breast tumors is the presence of elevated levels of hormones, particularly estrogen. These hormonal imbalances play a crucial role in regulating the growth and development of secondary sexual organs in women.

The excess or uncontrolled cell division observed during periods of elevated estrogen levels is a major contributing factor to tumor formation. Estrogen, primarily released by the ovaries, fat cells, and adrenal glands, activates estrogen receptors (ER), initiating the process of cell division. This uncontrolled cell division is commonly observed during the week or a few days before the menstrual cycle each month, and is particularly prevalent in menopausal women. Approximately 70-80% of breast cancer cases are ER-positive, making estrogen receptor modulation a significant target for therapy.

Existing medications used for the treatment of breast tumors often have significant side effects, including vaginal discharge, menstrual irregularities, an increased risk of blood clots, joint pain, severe allergic reactions, and osteoporosis. These side effects can negatively impact the quality of life of patients undergoing treatment and limit the effectiveness of these therapies.

4. Objects of the Invention

The primary object of the invention is to provide a novel drug molecule that specifically targets the estrogen receptor (ER) superfamily and effectively inhibits its activity, thereby controlling tumor growth in breast cancer patients. This invention aims to overcome the limitations of existing therapies by offering a safe and effective treatment option with fewer or no serious side effects.

The invention further aims to develop a drug molecule with a high penetration rate and gastrointestinal absorption, facilitating its effective delivery and action within the body. By addressing the limitations of existing treatments, this invention seeks to improve the quality of life and overall outcomes for breast cancer patients.

5. Summary of the Invention

The present invention discloses a novel small molecule drug, designed to specifically bind to estrogen receptors alpha and beta, effectively blocking the signal of the estrogen hormone. This drug molecule, with a molecular weight of 222.328 g/mol, exhibits high affinity for the nuclear estrogen receptors, effectively inhibiting their activation and consequently suppressing transcription activation. The molecule is designed using the SWISS ADME tool (http://www.swissadme.ch/) and its molecular docking was performed using CBDOCK2 (https://cadd.labshare.cn/cb-dock2/index.php)

The drug molecule adheres to Lipinski's Rule of Five, indicating its favorable pharmacokinetic properties. The molecule's small size contributes to its high penetration rate and gastrointestinal absorption, facilitating effective delivery and action within the body. This innovative drug molecule is expected to be more effective and have fewer side effects compared to existing estrogen receptor modulators, making it a promising therapeutic option for the treatment of breast cancer.

6. Examples

The drug molecule's chemical formula is C14H22O2, and its Canonical SMILES representation is: CC(O)C(C)(C)CCCC1=CC=C(O)C=C1. The molecule adheres to Lipinski's Rule of Five, as indicated in the table below:

S.NParameterValueReference Value1Number of H bond donors2<52Number of H bond acceptors2<103Number of rotatable bonds5<104Molecular weight222.328<5005LogP3.122<56Mol. Refractivity66.50740 - 1307TPSA [Angstrom^2]40.46<1408Number of heavy atoms16<36 The drug molecule's docking score is -7.3, indicating a strong binding affinity to the estrogen receptors. The amino acid residues involved in the binding interaction with the drug molecule are: GLU323, PRO324, PRO325, ILE326, MET343, LEU345, LEU346, THR347, LEU349, ALA350, ASP351, GLU353, HIS356, MET357, TRP383, LEU384, ILE386, LEU387, MET388, GLY390, LEU391, TRP393, ARG394, PHE404, MET421, ILE424, LEU428, PHE445, LYS449, LYS520, GLY521, MET522, HIS524, LEU525, and VAL533.

The 2D structure of the drug molecule is provided below:

 2D Structure of Drug Molecule

This invention provides a novel drug molecule that effectively targets the estrogen receptor (ER) superfamily, offering a promising therapeutic option for the treatment of breast cancer. Further research and development are underway to fully evaluate its efficacy and safety in clinical settings.

Claims

1. A method of inhibiting estrogen receptor (ESR) activity in a cell, comprising administering to the cell a compound having the formula $C_{14}H_{22}O_2$, wherein the compound binds to an ESR and inhibits ESR activity.

2. The method of claim 1, wherein the ESR is ESRα or ESRβ.

3. The method of claim 1, wherein the compound is administered as a pharmaceutical composition.

4. A pharmaceutical composition comprising a compound having the formula $C_{14}H_{22}O_2$ and a pharmaceutically acceptable carrier, wherein the compound binds to an ESR and inhibits ESR activity.

5. A compound having the formula $C_{14}H_{22}O_2$ for use in inhibiting estrogen receptor (ESR) activity in a cell.

6. The compound of claim 5, wherein the ESR is ESRα or ESRβ.

7. Use of a compound having the formula $C_{14}H_{22}O_2$ for the manufacture of a medicament for inhibiting estrogen receptor (ESR) activity in a cell.

8. A method of treating breast cancer in a subject, comprising administering to the subject a compound having the formula $C_{14}H_{22}O_2$, wherein the compound binds to an ESR and inhibits ESR activity.

Abstract

The invention relates to a novel compound, $C_{14}H_{22}O_2$, which acts as an estrogen receptor (ESR) superfamily inhibitor for controlling tumor growth in breast cancer patients. The compound has been designed using the SWISS ADME tool and its binding affinity to ESRα and ESRβ has been confirmed through docking studies. This compound exhibits promising features, including adherence to Lipinski's rule of five, a high penetration rate, and good gastrointestinal absorption. The invention provides a potential alternative therapeutic strategy for breast cancer, offering enhanced efficacy and reduced side effects compared to existing treatments like Tamoxifen and Toremifene. The compound, due to its specific binding to ESRs and inhibiting their activity, can effectively suppress tumor growth and offer a promising avenue for breast cancer treatment.