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DATASHEET

ICI 182,780 (Fulvestrant)

Product overview

Name	ICI 182,780 (Fulvestrant)
Cat No	HB2501
Alternative names	Fulvestrant
Biological action	Antagonist
Purity	>99%
Description	Estrogen receptor (ER) antagonist and high affinity GPER agonist

Biological Data

Biological description	Estrogen receptor (ER) antagonist (K_i values are 1 and 3.6 nM at ER α and ER β respectively). Shows no agonist activity and is devoid of estrogenic activity. Also a high affinity agonist at GPER (GPR30). Down-regulates the ER and impairs nuclear shuttling and dimerization of the receptor. Shows anticancer activity. Active <i>in vivo</i> .
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Solubility & Handling

Storage instructions	Room temperature
Solubility overview	Soluble in DMSO (100 mM), and in ethanol (50 mM)
Important	This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use.

Chemical Data

Chemical name	7 α ,17 β -[9-[(4,4,5,5,5-Pentafluoropentyl)sulfinyl]nonyl]estra-1,3,5(10)-triene-3,17-diol
Molecular Weight	606.77
Chemical structure	
Molecular Formula	C ₃₂ H ₄₇ F ₅ O ₃ S
CAS Number	129453-61-8
PubChem identifier	104741
SMILES	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)[C@@H](CC4=C3C=CC(=C4)O)CCCCCCCCC(CS(=O)CCCC(C(F)(F)F)F)F
InChi	InChI=1S/C32H47F5O3S/c1-30-17-15-26-25-12-11-24(38)21-23(25)20-22(29(26)27(30)13-14-28(30)39)10-7-5-3-2-4-6-8-18-41(40)19-9-16-31(33,34)32(35,36)37/h11-12,21-22,26-29,38-39H,2-10,13-20H2,1H3/t22-,26-,27+,28+,29-,30+,41?/m1/s1
InChiKey	VWUXBMIQPBWFH-LQKBAPIOSA-N
MDL number	MFCD00903953
Appearance	White solid

References

Emerging data on the efficacy and safety of fulvestrant, a unique antiestrogen therapy for advanced breast cancer.

Scott SM *et al* (2011) Expert Opin Drug Saf 10(5)

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Antagonists selective for estrogen receptor alpha.

Sun J *et al* (2002) Endocrinology 143(3)

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Estrogen and its receptors in cancer.

Chen GG *et al* (2008) Med Res Rev 28(6)

PubMedID 18642351

Activation of the human estrogen receptor by the antiestrogens ICI 182,780 and tamoxifen in yeast genetic systems: implications for their mechanism of action.

Dudley MW *et al* (2000) Proc Natl Acad Sci U S A 97(7)

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