Target Name	5-α-Reductase
Target TTD ID	TTDS00240

Target Species	Human
Chemical Type	Benzoquinolinones
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50})=6.56(\pm0.19)+1.21(\pm0.37)pi$ n=14 r=0.69 F=10.75 p=0.01
QSAR Model 2	$\log(1/IC_{50})=6.37(\pm0.35)+1.08(\pm0.63)pi$ n=5 r=0.70 F=2.94 p=0.19
QSAR Model 3	$\log(1/IC_{50})=6.64(\pm0.22)+1.42(\pm0.45)pi$ n=9 r=0.77 F=10.08 p=0.02
QSAR Model 4	$\log(1/IC_{50})=6.41(\pm0.19)+4.07(\pm1.53)pi - 3.57(\pm1.86)pi^2$ n=14 r=0.78 F=8.42 p=0.01
QSAR Model 5	$\log(1/IC_{50})=6.14(\pm0.37)+4.14(\pm2.51)pi - 3.66(\pm2.93)pi^2$ n=5 r=0.85 F=2.53 p=0.28
QSAR Model 6	$\log(1/IC_{50})=6.50(\pm0.22)+4.30(\pm1.93)pi - 3.68(\pm2.41)pi^2$ n=9 r=0.84 F=7.17 p=0.03
QSAR Model 7	$\log(1/IC_{50})=6.63(\pm0.19)+0.878(\pm0.32)pi$ n=16 r=0.59 F=7.46 p=0.02
QSAR Model 8	$\log(1/IC_{50})=6.74(\pm0.24)+0.81(\pm0.39)pi$

	n=11 r=0.57 F=4.25 p=0.07
QSAR Model 9	$\log(1/IC_{50})=6.44(\pm0.17)+3.28(\pm0.97)pi-2.58(\pm1.00)pi^2$ n=16 r=0.75 F=8.59 p=0.00
QSAR Model 10	$\log(1/IC_{50})=6.53(\pm0.20)+3.64(\pm1.11)pi-2.94(\pm1.10)pi^2$ n=11 r=0.80 F=7.12 p=0.02
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** The QM parameters included the LUMO (E LUMo)and HOMO (E HOMO) energies. The CLOGP program provided a value for the octanol/water partition coefficient (clogp). 10 Published substituent constants were used for the groups on the phenyl ring.ll These parameters included values for sigma, pi, F, R, and substituent MR obtained from a database of parameters. the substituent descriptor pi (Equations l-6) representing the lipophilic property of the substituent.
Reference	QSAR STUDY OF BENZOQUINOLINONES AS INHIBITORS OF HUMAN TYPE 1 5-α-REDUCTASE. Bioorganic& Medicinal Chemistry Letters, Vol.3, No.6. pp.1157-1162, 1993