Target Name	TNF-alpha converting enzyme (TACE)
Target TTD ID	TTDR00847

Target Species	Human
Chemical Type	Anthranilic acid derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = 0.637(\pm 0.229)I_{4,Br} - 0.163(\pm 0.084)\log P + 7.156(\pm 0.248)$ $n = 16, r = 0.898, r^2_{cv} = 0.69, s = 0.20, F_{2,13} = 27.14(6.70)$
QSAR Model 2	$\log(1/IC_{50}) = 0.763(\pm 0.188)I_{4,Br} - 0.100(\pm 0.063)\log P + 6.767(\pm 0.121)$ $n = 19, r = 0.907, r^2_{cv} = 0.75, s = 0.16, F_{2,14} = 37.28(6.51)$
QSAR Model 3	$\log(1/IC_{50}) = 0.491(\pm 0.258)I_{1,CC} + 0.429(\pm 0.280)I_{4,Br}$ $- 0.891(\pm 0.309)I_{1,N} - 0.284(\pm 0.122)\log P + 7.457(\pm 0.342)$ $n = 18, r = 0.905, r^2_{cv} = 0.64, s = 0.19, F_{4,13} = 14.79(5.20)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** I1 stands for R1-substituents and has a value of unity for R1 = OCH2Ph and zero for others, I2 stands for R2-substituents and has a values of unity for R2 = CH2-3-pyridyl group and zero for others, I3 stands for R3-substiutents and is equal to 1 for R3 = an aromatic substituent and zero otherwise, I4, which stands for R4-substituents also has a value of unity for R4 = an aromatic moiety and zero for others.
Reference	A quantitative structure–activity relationship study on some series of anthranilic acid-based matrix metalloproteinase inhibitors. *Bioorganic & Medicinal Chemistry* 13 (2005) 5454–5462