

Target Name	Peptide deformylase
Target TTD ID	TTDR00267

Target Species	Mammal
Chemical Type	Hydroxamic acid derivatives
Mode of Action	Inhibitor
QSAR Model 1	$-\log\text{IC}_{50 \text{ PDF-Fe}} = 0.075(\pm 0.022) \text{MR}^{\text{R1}} + 0.089(\pm 0.022) \text{MR}^{\text{R2}} - 3.424(\pm 0.828)$ $n = 19 \quad r = 0.81 \quad s = 0.46 \quad F = 15.6$
QSAR Model 2	$-\log\text{IC}_{50 \text{ PDF-Fe}} = 0.056(\pm 0.020) \text{MR}^{\text{R1}} + 0.985(\pm 0.198) \text{Fr}^{\text{R2}} - 3.386(\pm 0.727)$ $n = 19 \quad r = 0.86 \quad s = 0.41 \quad F = 21.7$
QSAR Model 3	$-\log\text{MIC}_{E. coli \text{ DC2}} = 1.024(\pm 0.373) \text{Fr}^{\text{R2}} - 0.964(\pm 0.198) \text{In} - 2.810(\pm 0.950)$ $n = 17 \quad r = 0.84 \quad s = 0.37 \quad F = 17.0$
QSAR Model 4	$-\log\text{MIC}_{M. cata. \text{ RA21}} = 0.075(\pm 0.022) \text{MR}^{\text{R1}} - 0.812(\pm 0.360) \text{In} - 2.188(\pm 0.891)$ $n = 10 \quad r = 0.85 \quad s = 0.34 \quad F = 9.4$
QSAR Model 5	$-\log\text{IC}_{50 \text{ NEP}} = 0.624(\pm 0.378) \text{Fr}^{\text{R1}} - 2.011(\pm 1.009)$ $n = 4 \quad r = 0.76 \quad s = 0.52 \quad F = 2.7$
QSAR Model 6	$-\log\text{IC}_{50 \text{ COL-1}} = 0.164(\pm 0.041) \text{Fr}^{\text{R1}} + 0.681(\pm 0.110)$ $n = 4 \quad r = 0.94 \quad s = 0.05 \quad F = 15.8$
QSAR Model 7	$-\log\text{IC}_{50 \text{ HME}} = -0.038(\pm 0.022) \text{Fr}^{\text{R1}} + 1.995(\pm 0.064)$ $n = 3 \quad r = 0.87 \quad s = 0.02 \quad F = 3.0$

<b>QSAR Model 8</b>	$-\log IC_{50COL-3} = 3.750(\pm 0.557) f^{R1} + 1.270(\pm 0.78)$ $n = 3 \quad r = 0.99 \quad s = 0.11 \quad F = 45.0$
<b>QSAR Model 9</b>	$-\log IC_{50MAT} = -2.571 (\pm 0.907) f^{R1} + 0.312(\pm 0.127)$ $n = 3 \quad r = 0.94 \quad s = 0.18 \quad F = 8.03$
<b>Molecular Descriptor</b>	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p><i>n</i> is the number of compounds; <i>r</i>, the correlation coefficient; <i>s</i>, the standard deviation; <i>F</i>, the F-ratio; <i>Fr</i>, hydrophobic parameter; <i>MR</i>, molar refractivity; <i>f</i>, the electronic parameter.</p>
<b>Reference</b>	<p>2D-QSAR in Hydroxamic Acid Derivatives as Peptide Deformylase Inhibitors and Antibacterial Agents. <i>Bioorganic &amp; Medicinal Chemistry</i> 10 (2002) 3713–3716</p>