Target Name	Transcription factor $NF-\kappa B$
Target TTD ID	TTDR00250

Target Species	Human
Chemical Type	Sesquiterpene lactones
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{100} = 0.239\ (\pm 0.054)\ UNC + 0.431\ (\pm 0.164)\ ML + 0.648\ (\pm 0.143)\ EA + 0.050\ (\pm 0.023)\ SH3 - 2.861\ (\pm 0.169)$ $n = 103, R = 0.772, R^2 = 0.596, s = 0.381, F = 36.2, P < 0.0001$
QSAR Model 2	$pIC_{100} = 0.271\ (\pm 0.068)\ UNC + 0.452\ (\pm 0.226)\ ML + 0.518\ (\pm 0.163)\ EA - 2.597\ (\pm 0.224)$ $n = 60, R = 0.779, R^2 = 0.607. s = 0.329. F = 28.8, P < 0.0001$
QSAR Model 3	$pIC_{100} = 1.001\ (\pm 0.256)\ ML + 0.327\ (\pm 0.082)\ UNA + 0.977\ (\pm 0.162)\ EA - 2.913\ (\pm 0.261)$ $n = 44, R = 0.848, R^2 = 0.718, s = 0.251, F = 34.0, P < 0.0001$
QSAR Model 4	$pIC_{100} = 0.239\ (\pm 0.061)\ UNC + 0.913\ (\pm 0.262)\ ML + 0.599\ (\pm 0.218)\ EA - 2.983\ (\pm 0.262)$ $n = 44, R = 0.846, R^2 = 0.715, s = 0.252, F = 33.5, P < 0.0001$
QSAR Model 5	$pIC_{100} = 1.012\ (\pm 0.206)\ ML + 0.347\ (\pm 0.071)\ UNA + 0.933\ (\pm 0.134)\ EA - 2.893\ (\pm 0.210)$ $n = 37, R = 0.904, R^2 = 0.812, s = 0.201, F = 49.06, P < 0.0001$
QSAR Model 6	$pIC_{100} = 1.060\ (\pm 0.141)\ ENONE + 0.731\ (\pm 0.126)\ SH2 - 0.628\ (\pm 0.132)\ ATOM - 3.462\ (\pm 1.101)$ $n = 16, R = 0.933, R^2 = 0.870, s = 0.233, F = 26.8, P < 0.0001$
QSAR Model 7	$pIC_{100} = 0.303\ (\pm 0.088)\ UNC + 0.639\ (\pm 0.174)\ CN2 - 0.109\ (\pm 0.027)\ MR - 0.346\ (\pm 0.114)\ OH + 0.053\ (\pm 0.577)$ $n = 22, R = 0.818, R^2 = 0.669, s = 0.282, F = 8.58, P = 0.0006$
QSAR Model 8	$pIC_{100} = 0.984\ (\pm 0.097)\ UNC - 1.233\ (\pm 0.286)\ HOM - 26.574\ (\pm 3.052)$ $n = 9, R = 0.975, R^2 = 0.950, s = 0.128, F = 57.30, P = 0.0001$
QSAR Model 9	$pIC_{100} = -1.067\ (\pm 0.325)\ SH1 + 1.862\ (\pm 0.531)\ SH2 + 0.804\ (\pm 0.286)\ ATOM + 1.195\ (\pm 1.153)$ $n = 10, R = 0.860, R^2 = 0.740, s = 0.145, F = 5.70, P = 0.0343$

Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** The Calculated Descriptors and the Abbreviation Used for the Calculations: Structural descriptor (**Abbreviation**): Total number of α,β-unsaturated carbonyl structures in the molecule (sum of ML, ENON and ACYL) (**UNC**); α-methylene-γ-lactone (**ML**); Conjugated ester groups (**UNA**); Conjugated keto or aldehyde functions (**ENONE**); Number of oxygen atoms (**ATOM**); Number of hydroxyl groups (**OH**); Octanol water partition coefficient (**LOGP**); Electron affinity (**EA**); Dipole moment (**DIPOL**); Molar refractivity (**MR**); Connectivity Indices (**CN0-2**); Shape Indices (**SH1-3**); Highest occupied molecular orbital (**HOMO**); Lowest unoccupied molecular orbitals (**LUMO1-3**).
Reference	Quantitative Structure-Activity Relationship of Sesquiterpene Lactones as Inhibitors of the Transcription Factor $NF-\kappa B$. *J. Med. Chem.* 2004, 47, 6042-6054