

Supplementary Information

Solidagenone from *Solidago chilensis* Meyen protects against acute peritonitis and lipopolysaccharide-induced shock by regulating the NF- κ B signaling pathway

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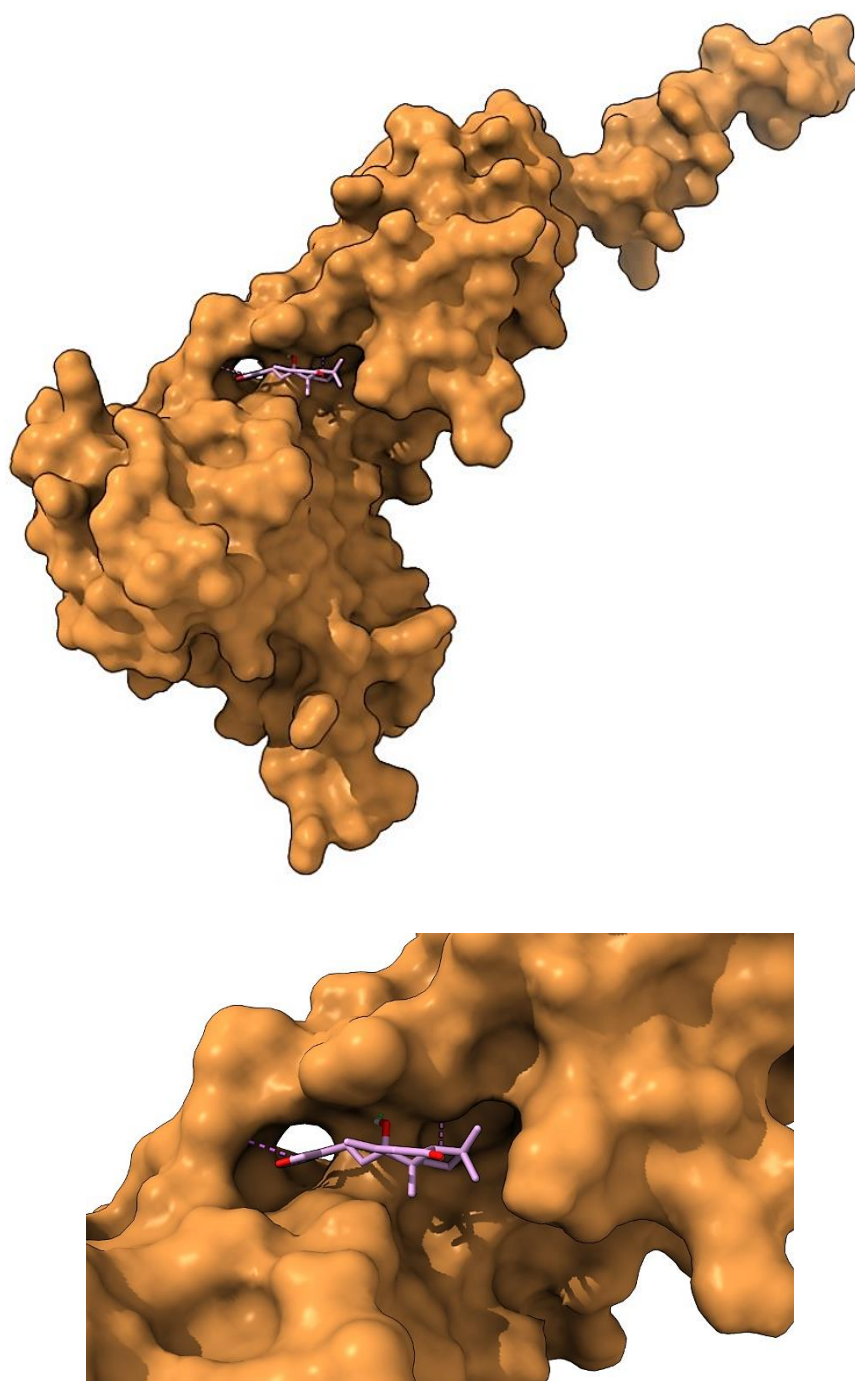


Figure S1. Solidagenone docked into the p65 subunit of NF-κB.

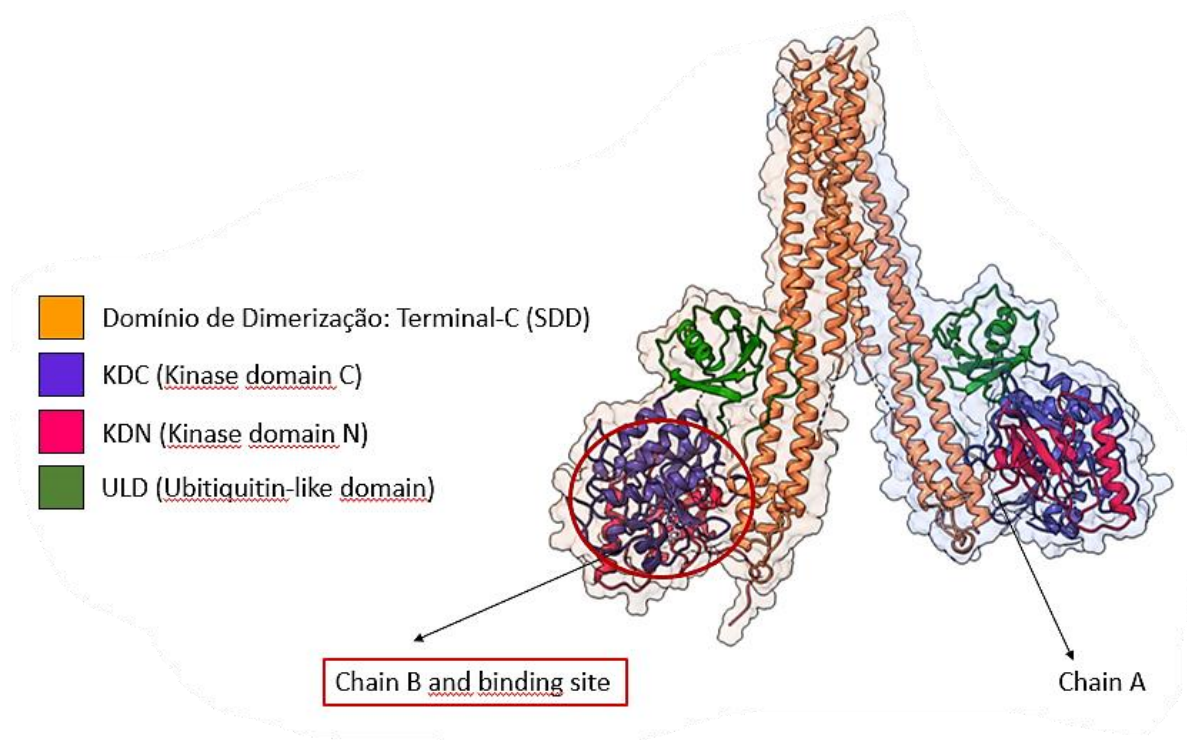


Figure S2. IKK system.

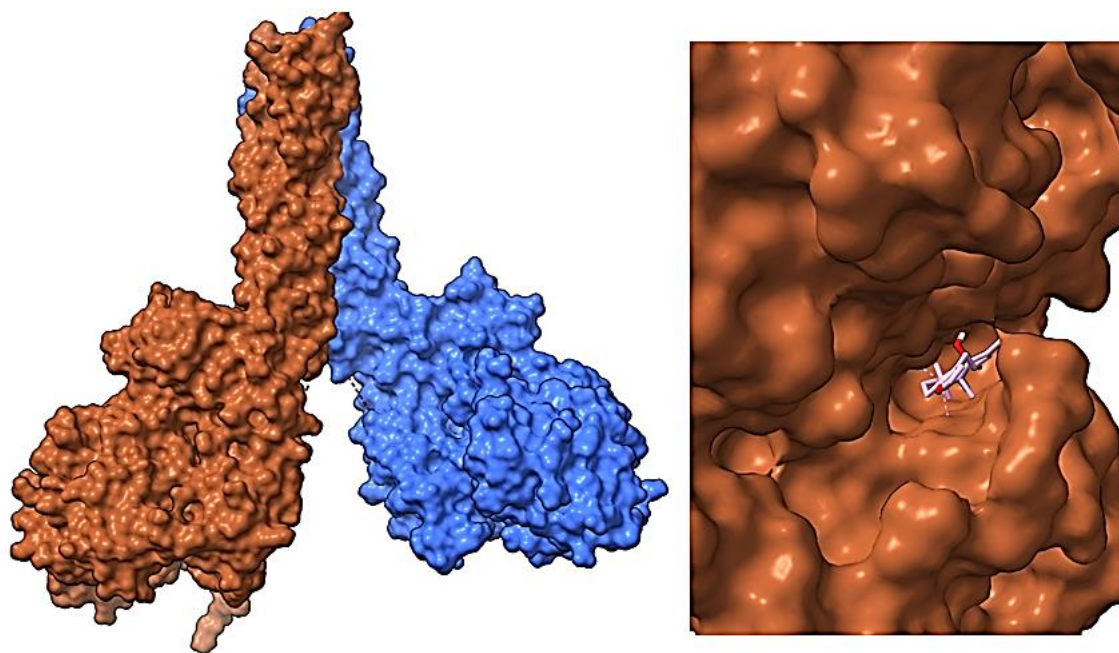


Figure S3. IKK system, and detail of solidagenone-IKK interaction.

Table S1. ADME parameters, druglikeness, and medicinal chemistry of solidagenone.

Physicochemical Properties	
Formula	C ₂₀ H ₂₈ O ₃
Molecular weight	316.43 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	5
Fraction Csp ³	0.65
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	91.96
TPSA	50.44 Å ²
Lipophilicity	
Log <i>P</i> _{o/w} (iLOGP)	3.29
Log <i>P</i> _{o/w} (XLOGP3)	3.63
Log <i>P</i> _{o/w} (WLOGP)	4.30
Log <i>P</i> _{o/w} (MLOGP)	2.71
Log <i>P</i> _{o/w} (SILICOS-IT)	4.61
Consensus Log <i>P</i> _{o/w}	3.71
Water Solubility	
Log <i>S</i> (ESOL)	-4.05
Solubility	2.81e-02 mg/ml; 8.88e-05 mol/l
Class	Moderately soluble
Log <i>S</i> (Ali)	-4.38
Solubility	1.33e-02 mg/ml; 4.19e-05 mol/l
Class	Moderately soluble
Log <i>S</i> (SILICOS-IT)	-5.53
Solubility	9.40e-04 mg/ml; 2.97e-06 mol/l
Class	Moderately soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log <i>K</i> _p (skin permeation)	-5.65 cm/s
Druglikeness	
Lipinski	Yes; 0 violation

Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry

PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	4.61
