

## Supplementary Information

# The protective effect of solidagenone from *Solidago chilensis* Meyen against lipopolysaccharide-induced shock by regulating the NF- $\kappa$ B signaling pathway

Ivanilson Pimenta Santos<sup>1</sup>, Laís Peres Silva<sup>1</sup>, Dahara Keyse Carvalho Silva<sup>1</sup>, Bruna Padilha Zurita Claro do Reis<sup>1</sup>, Temistocles Barroso de Oliveira<sup>2</sup>, Andressa Maia Kelly<sup>2</sup>, Edivaldo dos Santos Rodrigues<sup>3</sup>, Claudia Valeria Campos de Souza<sup>3</sup>, José Fernando Oliveira-Costa<sup>4</sup>, Simone Sacramento Valverde<sup>2</sup>, Osvaldo Andrade Santos-Filho<sup>3</sup>, Milena Botelho Pereira Soares<sup>1,5,\*</sup>, and Cássio Santana Meira<sup>1,5,\*</sup>

<sup>1</sup> Gonçalo Moniz Institute, Oswaldo Cruz Foundation, FIOCRUZ, Salvador, BA, 40296-710, Brazil;

<sup>2</sup> Pharmaceutical Technology Institute - FarManguinhos, Natural Products Department, Oswaldo Cruz Foundation, FIOCRUZ, Rio de Janeiro, RJ, 21041-250, Brazil;

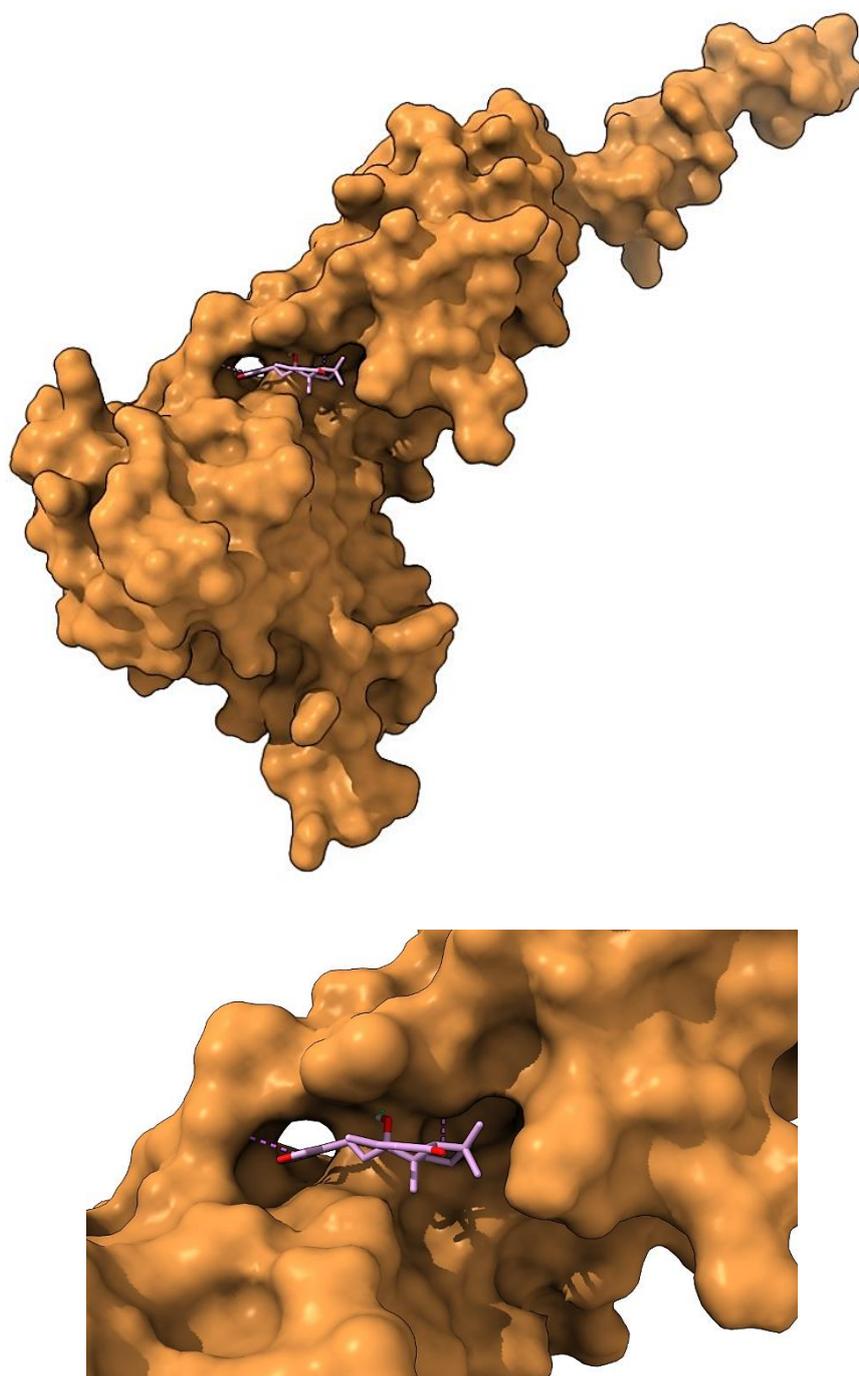
<sup>3</sup> Molecular Modeling and Computational Structural Biology Laboratory, IPPN, Health Sciences Center, Federal University of Rio de Janeiro, RJ, 21941-599, Brazil;

<sup>4</sup> Center for Infusions and Specialized Medicines of Bahia, Bahia State Health Department, Salvador, BA, 41745-900, Brazil;

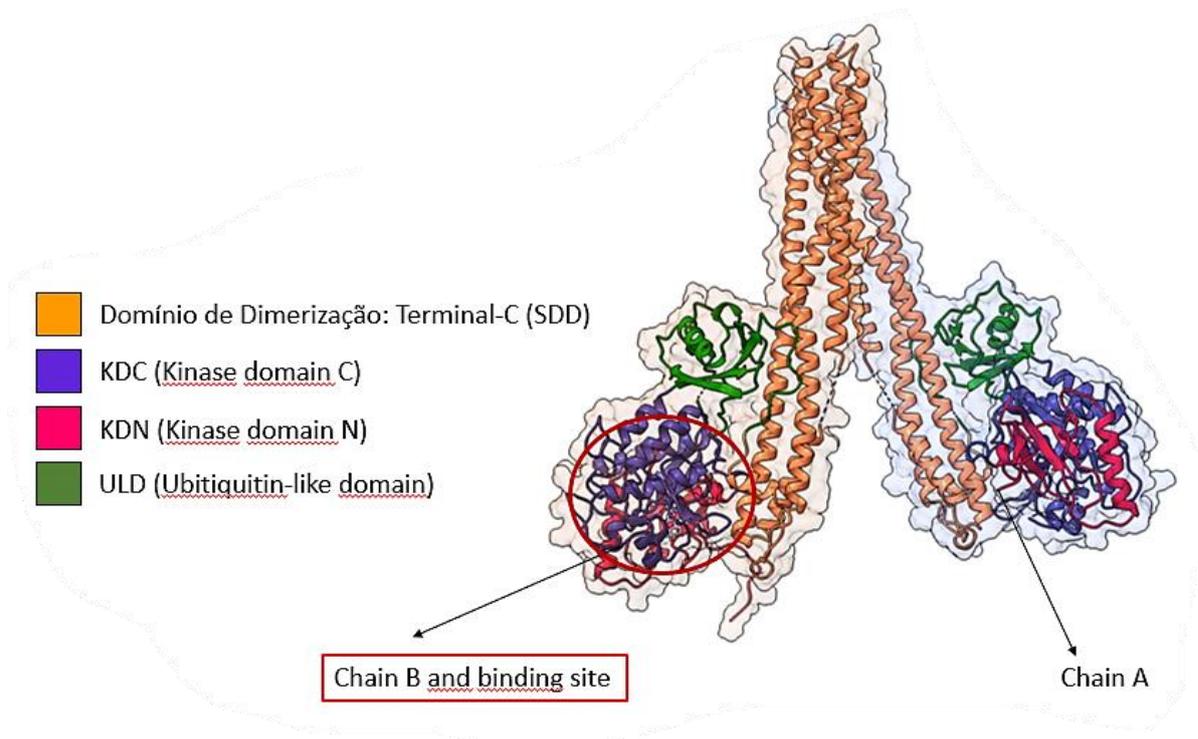
<sup>5</sup> Institute of Innovation in Advanced Health Systems (ISI SAS), University Center SENAI/CIMATEC, Salvador, BA, 41650-010 Brazil.

\*Correspondence: [cassio.meira@fieb.org.br](mailto:cassio.meira@fieb.org.br); [milena@bahia.fiocruz.br](mailto:milena@bahia.fiocruz.br)

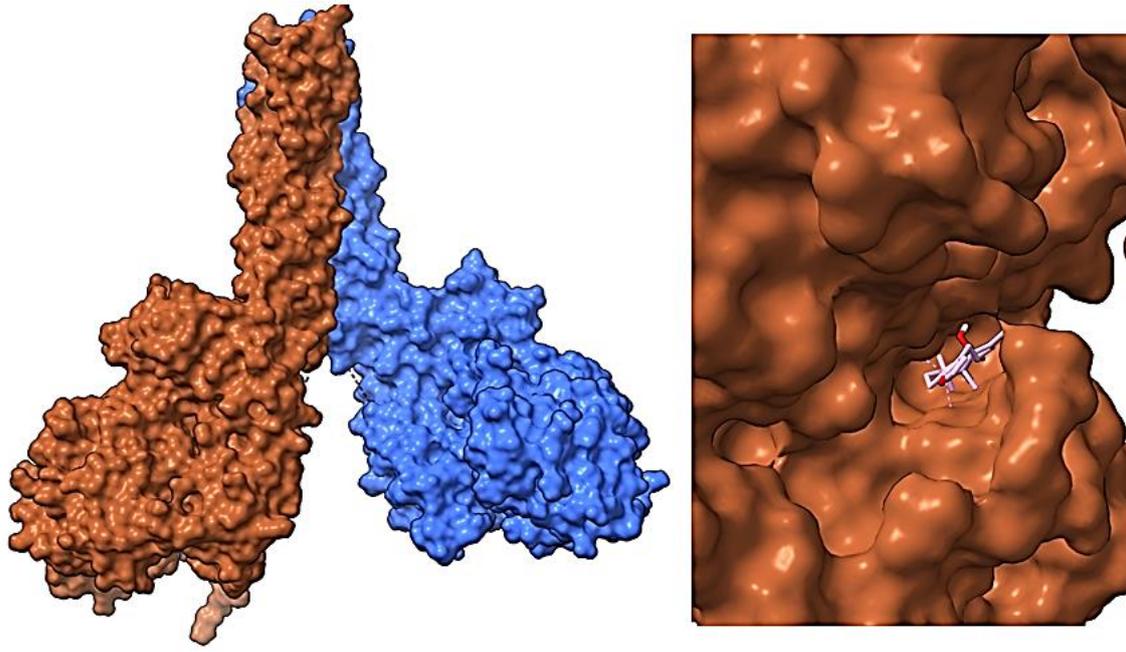
Supplementary Information



**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.

<b>Physicochemical Properties</b>	
Formula	C <sub>20</sub> H <sub>28</sub> O <sub>3</sub>
Molecular weight	316.43 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	5
Fraction Csp <sup>3</sup>	0.65
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	91.96
TPSA	50.44 Å <sup>2</sup>
<b>Lipophilicity</b>	
Log <i>P</i> <sub>o/w</sub> (iLOGP)	3.29
Log <i>P</i> <sub>o/w</sub> (XLOGP3)	3.63
Log <i>P</i> <sub>o/w</sub> (WLOGP)	4.30
Log <i>P</i> <sub>o/w</sub> (MLOGP)	2.71
Log <i>P</i> <sub>o/w</sub> (SILICOS-IT)	4.61
Consensus Log <i>P</i> <sub>o/w</sub>	3.71
<b>Water Solubility</b>	
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
<b>Pharmacokinetics</b>	
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> <sub>p</sub> (skin permeation)	-5.65 cm/s
<b>Druglikeness</b>	
Lipinski	Yes; 0 violation

Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

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**Medicinal Chemistry**

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

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