

A selective Review and Virtual Screening Analysis of Natural Product Inhibitors of the NLRP3 Inflammasome

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Table S1. Filter parameters used to filter ZINC20 natural products subset.

Parameter	Minimum value	Maximum value
Molecular weight	130	550
Number of hydrogen-bond acceptors	0	10
Number of hydrogen-bond donors	0	5
Number of oxygen & nitrogen atoms	0	10
Number O & N atoms with hydrogens	0	5
XLogP	2	5.5

Table S2. Docking score of the best compounds that bind to the cofactor site (compounds 1-6) using the structure of the NACHT domain of NLRP3 (PDB code 7ALV)[35].

Number	Zinc ID	Chemguass4 score
1	ZINC000604405316	-17.5
2	ZINC000253500112	-17.2
3	ZINC000253500236	-17.1
4	ZINC000253499536	-17.3
5	ZINC000253499916	-16.0
6	ZINC000049590453	-16.7