NETWORK OF POSSIBLE TARGETS WITH CLINICAL-PHARMACOLOGICAL POTENTIAL AROUND THE COMPOUNDS IDENTIFIED IN SYZYGIUM CUMINI

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INTRODUCTION

The prediction of targets for bioactive compounds identified in medicinal plants traditionally used in the world and their potential correlations with the diseases reported in this use or prospected by *in silico* target prediction research help in the evolution of studies involving these diseases and accelerate the discovery of drugs. They also reveal the potential for new effects of these compounds. Among the countless medicinal species, we have *Syzygium cumini* (L.) Skeels, a tropical tree (Myrtaceae) popularly known as "Jambolao" (Brazilian Portuguese).

OBJECTIVE

Our aim was to provide more information about *Syzygium cumini*, such as the pharmacological effects of its compounds and a better understanding of related diseases.

INTRODUCTION

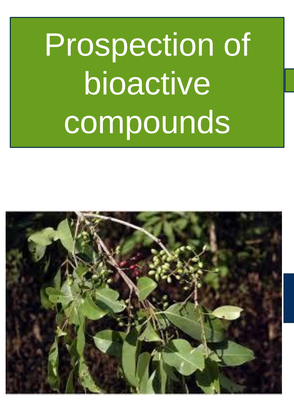


Figure 1. Prospection of *S.cumini* bioactive compounds, virtual screening and correlation of genes corresponding to diseases.

RESULTS AND DISCUSSION

SwissTargetPredicion | Virtual Screening

	A	B	C	D	E	F
1	SwissTargetPrediction					
2	Source	Target	Common name	Uniprot ID	ChEMBL ID	Target Class
3	1,2,6-Trigalloylglucose	Squalene monooxygenase (E	SQLE	Q14534	CHEMBL3592	Enzyme
4	1-galloylglucose	Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme
5	Beta-Sitosterol	Niemann-Pick C1-like protein	NPC1L1	Q9UHC9	CHEMBL2027	Other membrane protein
6	Betulinic acid	SUMO-activating enzyme subu	SAE1	Q9UBE0	CHEMBL2095174	Enzyme
7	Betulinic acid	SUMO-activating enzyme subu	UBA 2	Q9UBT2	CHEMBL2095174	Enzyme
8	Betulinic acid	DNA polymerase beta (by ho	POLB	P06746	CHEMBL2392	Enzyme
9	Betulinic acid	Aldo-keto reductase family 1	AKR1B10	O60218	CHEMBL5983	Enzyme
10	Caffeic Acid	Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase
11	Caffeic Acid	Arachidonate 5-lipoxygenase	ALOX5	P09917	CHEMBL215	Oxidoreductase
12	Caffeic Acid	Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase
13	Caffeic Acid	Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase
14	Caffeic Acid	Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase
15	Caffeic Acid	Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease
16	Caffeic Acid	Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase
17	Caffeic Acid	Matrix metalloproteinase 1	MMP1	P03956	CHEMBL332	Protease
18	Caffeic Acid	Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease
19	Caffeic Acid	Protein-tyrosine phosphatase	PTPN1	P18031	CHEMBL335	Phosphatase
20	Caffeic Acid	Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase
21	Caffeic Acid	Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase
22	Caffeic Acid	Carbonic anhydrase VB	CA5B	Q9Y2D0	CHEMBL3969	Lyase
23	Caffeic Acid	Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase
24	Chlorogenic acid	Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme

Figure 2. Target list of *S. cumini* compounds resulting from target prediction.

- This number represents the 125 different targets found by predicting targets for a probability equal to or greater than 80%.

METHODS

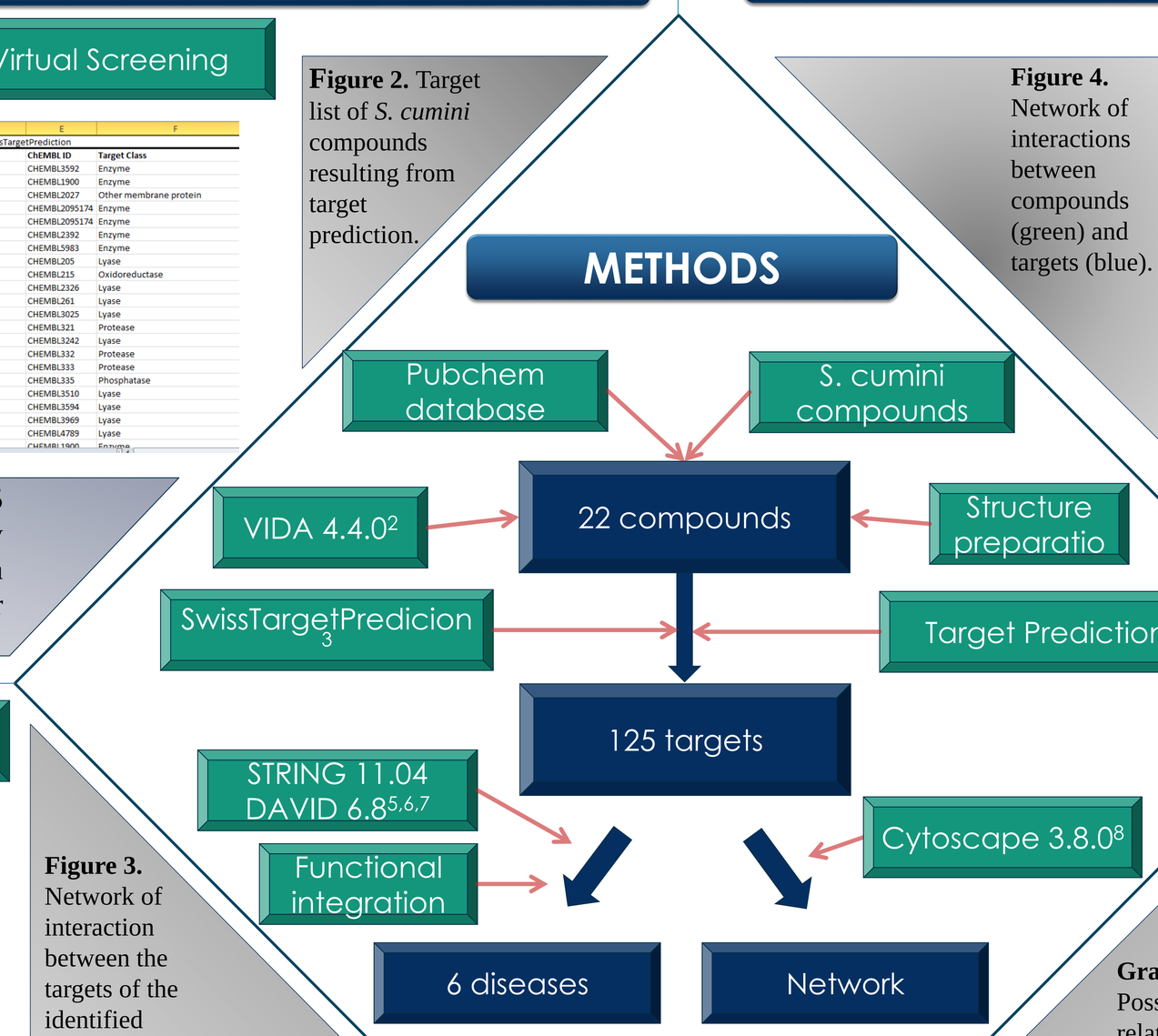
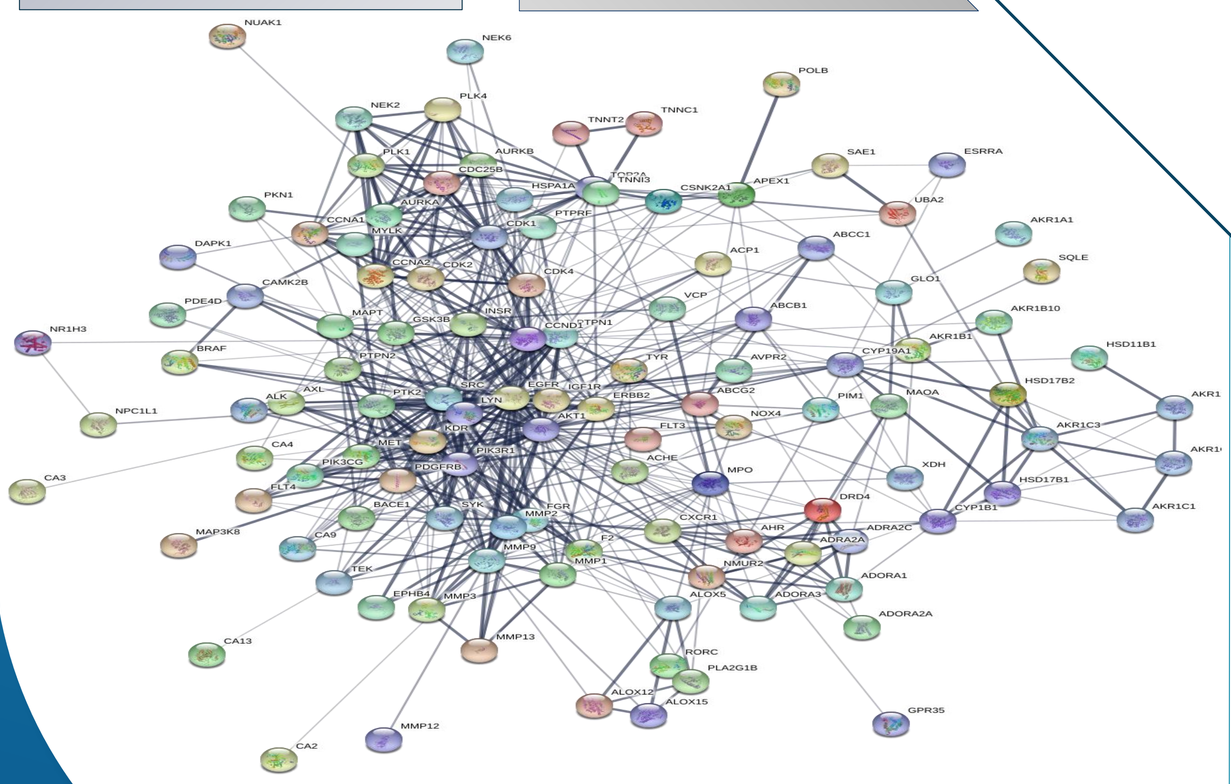


Figure 3. Network of interaction between the targets of the identified compounds of *S. cumini*.

STRING 11.0 | Functional integration

- The opacity of the links between the targets refers to the level of trust that is related to the reliability of the analysis.
- This complex network reveals 602 connections between the targets.



RESULTS AND DISCUSSION

Cytoscape 3.8.0 | Network

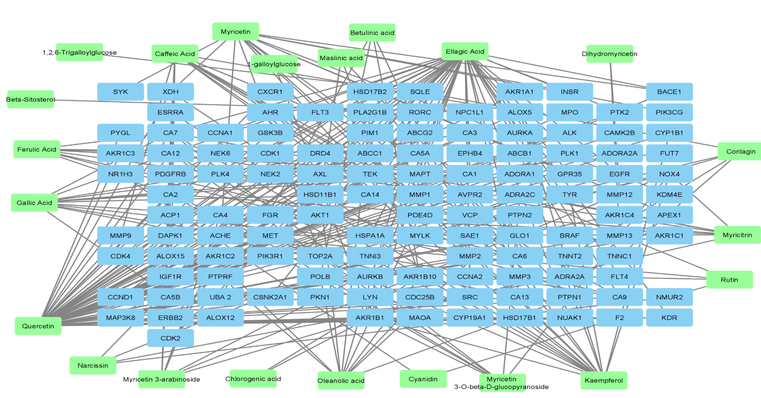
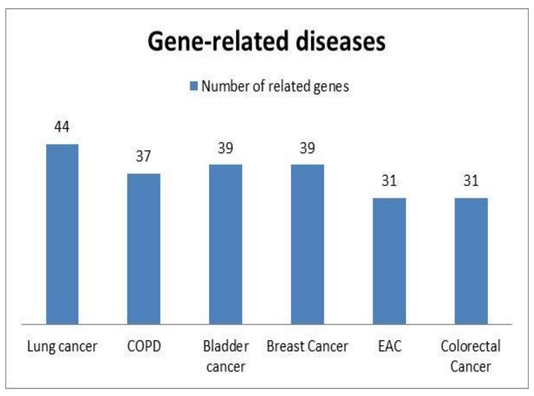


Figure 4. Network of interactions between compounds (green) and targets (blue).

- This complex network reveals 242 connections between compounds and targets.

DAVID 6.8 | Functional integration



Graphic 1. Possible diseases related to targets quantified in descending order of reliability.

- This graph reveals the influence of *S. cumini* compounds, through the targets found in virtual screening, with diseases such as: lung cancer, chronic obstructive pulmonary disease (COPD), bladder cancer, breast cancer, adenocarcinoma esophagus (EAC) and colorectal cancer.

CONCLUSION

Our results suggest a wide application of the identified compounds of *S. cumini*. The analyzes carried out revealed as targets, some types of cancer and COPD. Therefore, the bioactive compounds of *S.cumini* possibly have pharmacological and clinical interest effects.

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