Association rule mining to help detect plant phenolic compounds putatively involved in decreased ruminal methane production *in vitro*

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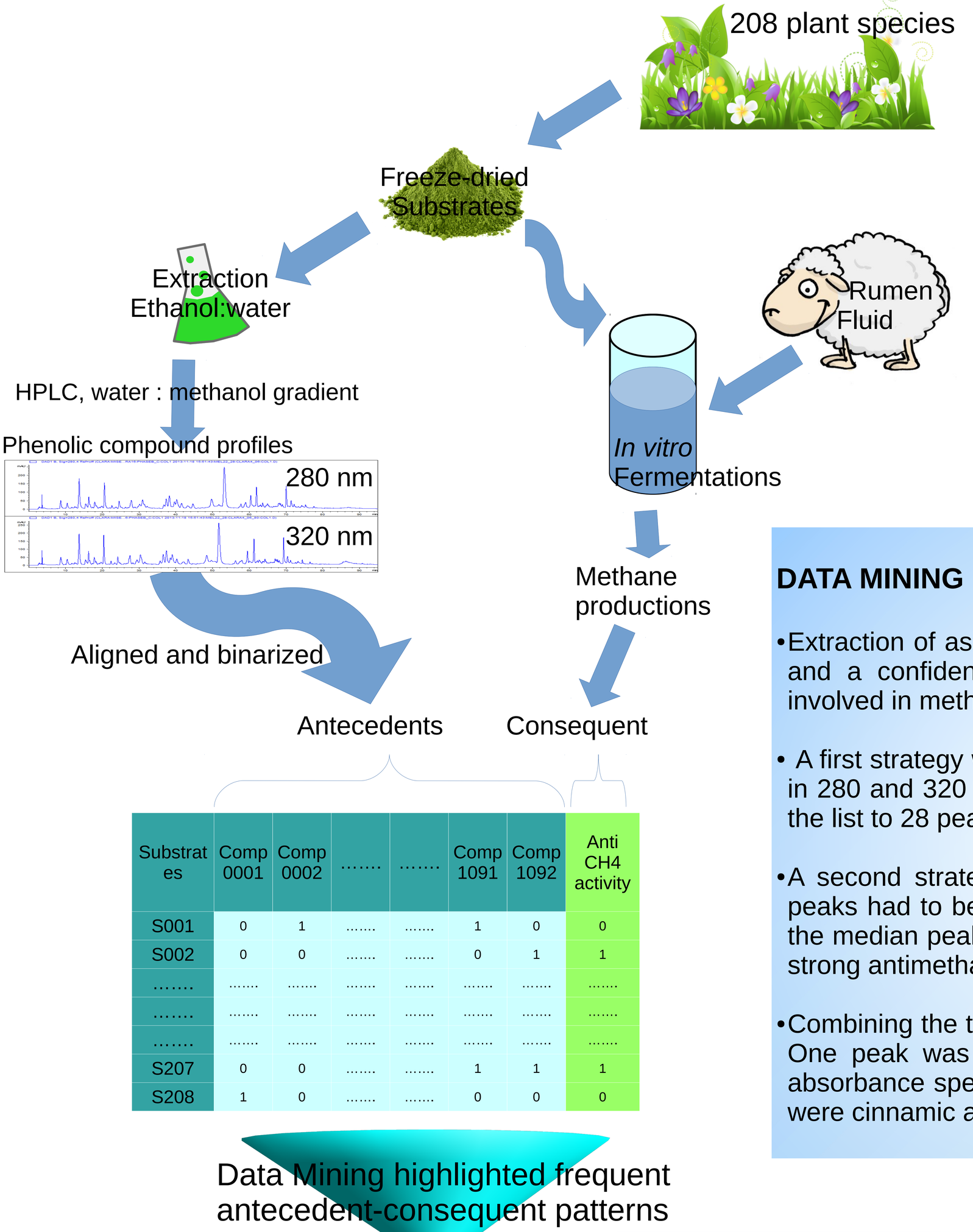
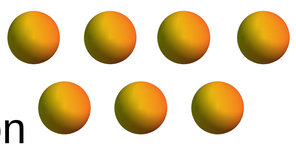
- To mitigate methane emission by ruminants, phenolic compounds of bioactive plant could be valuable candidates.
- However, these phytochemicals come in myriad chemical structures, and a given plant may contain more than hundred of them.
- We use a data mining technique, association rules to emerge compounds involved in the antimethanogenic activity of plants during ruminal fermentation.



Substrates	Comp 0001	Comp 0002	…….	…….	Comp 1091	Comp 1092	Anti CH4 activity
S001	0	1	…….	…….	1	0	0
S002	0	0	…….	…….	0	1	1
…….	…….	…….	…….	…….	…….	…….	…….
…….	…….	…….	…….	…….	…….	…….	…….
…….	…….	…….	…….	…….	…….	…….	…….
S207	0	0	…….	…….	1	1	1
S208	1	0	…….	…….	0	0	0

Data Mining highlighted frequent antecedent-consequent patterns

7 peaks submitted to identification



DATA

- Data were 2 matrices (280 and 320 nm) 208 plants x 1092 peaks (UV absorbing compounds)
- Very frequent peaks (>0.5) were discarded before data mining to avoid false-positives.
- The plants had on average 100 peaks
- The consequent item included 64 significant anti-methanogenic activities of which 15 strong effects

DATA MINING

- Extraction of association rules with a minimum support of 5 and a confidence > 0.5 gave 205 peaks that could be involved in methane reduction
- A first strategy with the contraints of co-occurence of peaks in 280 and 320 nm matrices and confidence >0.65 reduced the list to 28 peaks
- A second strategy in which the constraints were that the peaks had to be major (i.e. more than 10 times the area of the median peak) and present in the plants that showed the strong antimethanogenic effect, reduced the list to 24 peaks
- Combining the two strategies resulted in 7 candidate peaks. One peak was easily identified as gallic acid. Based on absorbance spectra between 200 and 400 nm, three others were cinnamic acid derivatives and two were flavonols.

CONCLUSION

In the virgin forest of bioactive plant phenolic compounds, association rules work like bushcutters clearing pathways to help discover active compounds

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