Sketch for simulating chemodiversity

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(rough) sketch components responsible for chemodiversity

Genes

- define which enzymes are produced in which quantities
  - list in fig. 1 in [1]
- can be scaled down/inactivated (i.e. when predators leave for generations)
  - easy to ramp up production as long as the genes are still there
- plants can survive without problems with inactive PSM-cycles when no adversaries are present.

Inheritance & Mutation

- via whole-genome and local-genome duplication
- copies accumulate mutations that lead to neofunctionalization
- e.g. subtle differences in terpene synthases can yield vastly different products
  - i.e. these changes can appear easily
  - need to classify products by "chemical distance" for simulation
  - **TODO**: Map/Markov-Chain of mutations that may occur here?

Evolutional strategies

- "Bet-hedging": reduce variations of fitness over time
  - **TODO**: understand
  - different effects of intra-cohort-variation vs. inter-cohort-variation
- Plants with inactive PSM can survive if predators are deterred by other individuals due to automimicry-effect which *could* foster wider genetic variance

  - the more of those individuals are present in a population, the less their overall fitness becomes.
  - **TODO**: fitness must also be able to depend on relative appearance of adversarial traits in the population
    * Keyword: Frequency-dependent-selection (FDS)

Pathways to produce chemical compounds

- 40k+ compounds just stem from compounds of the calvin-cycle taking the MEP-pathway or from the krebs-cycle taking the MVA-pathway
  - both yield the same intermediate product that forms the basis.
- 10k+ compounds are amino-acid-derivatives
- Chapter VI in [1] exemplary describes 4 complete different pathways that yield compounds.
  - similar compounds/pathways should be found in the simulation

Consequences of producing compounds

- taking away parts of the calvin/krebs cycle puts pressure on those
  - **TODO**: find out what they do and on what they depend.
- **TODO**: where do amino-acids come from? How much impact has the diversion of these components?

Maintaining chemical diversity

+ screening hypothesis

- many PSM found have no *known* biological activity
- plants "keep them around" in case another mutation needs them to produce something "useful"
- creating things without use increase the need for photosynthesis and/or nutrient uptake.

- screening hypothesis

- it is suggested that local abiotic & biotic selection pressures are the main driver
- inactive molecules are not maintained long
- it was observed that some plants "rediscovered" some compounds in their evolution suggesting they got rid of them when no pressure to maintain them was applied

questions resulting from this that should be answered in the simulation

- details in chapter VIII of [1]
- how quick can lost diversity be restored?
- how expensive is it to keep producing many inactive substances while also producing active deterrents? Does this lead to a single point-of-failure due to overspecialisation? What must be done to prevent this?
- strong selection pressure *should* decrease quantity of compounds due to costs, but plants do not seem to care.
  - is this diversity needed in presence of multiple different adversaries?
  - does the simulation specialize when only presented with one adversary? What about adaptive adversaries?
  - adaptation in the qualitative & quantitative evolution in response to changed pressure? (i.e. those who cannot adapt quick enough die?)

Scenario

Plants

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data Foo = Bar
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Enzymes

Herbivores

Environment

Fitness

Mating & Creation of diversity