Searching for reaction pathways in formose data

1. Generate reaction network:

Contains reactions for:

- enolate formation,
- enolate protonation,
- aldol addition of formaldehyde to enolates,
- Cannizzaro reactions and
- enolate reactions with sugars of $C_{<4< sub>}$.

2. Remove nodes

Formaldehyde, hydroxide and water are ignored as nodes in pathways searches ($CaCl_2$ is not included in the framework).

3. For each data set:

- Make a list of detected compounds, include which compounds cannot be detected.
- This list is ordered by amplitude (highest amplitude first)
- Only reactions which include compounds in this list as reactants are included in the pathway search.
- Remove reactions in which inputs are products

4. Connect inputs (reactants) to products

Find the shortest pathways from the carbon input to the compound with the highest amplitude .

5. [Version 2] Connect products to each other.

iterate down the amplitude list, find shortest pathways to every compound downstream
of the node.

6. Check that all products have reactions leading to them

If they do not, cycle backwards from them in the sorted amplitude list until a connection is found.