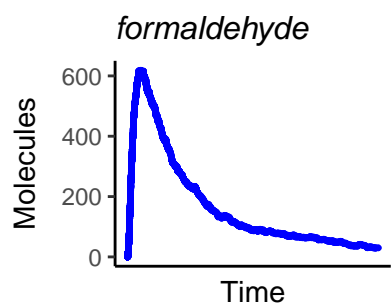
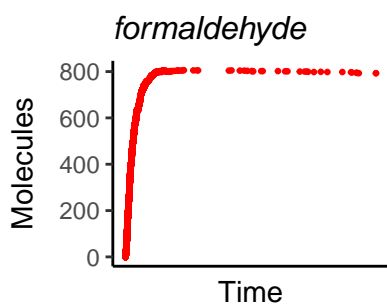
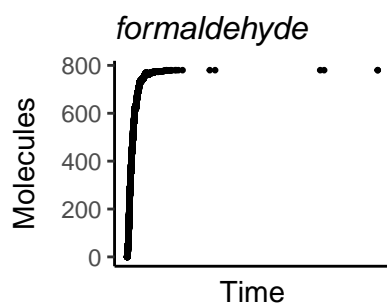
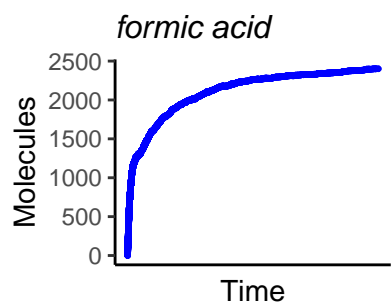
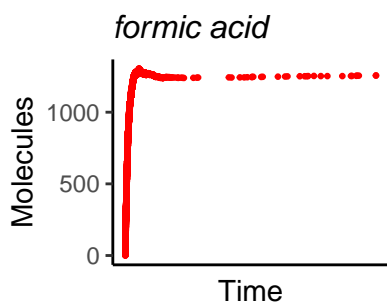
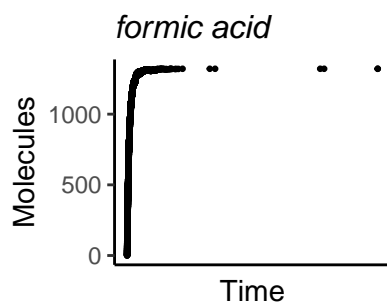
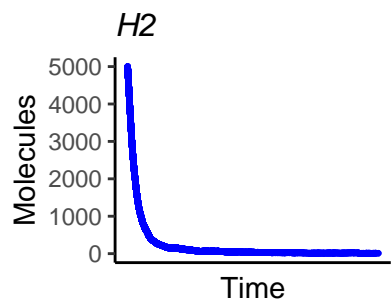
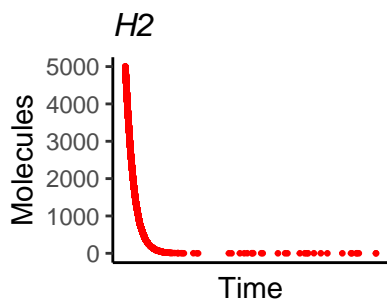
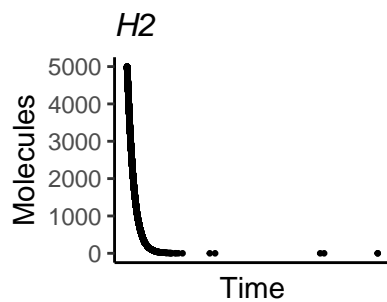
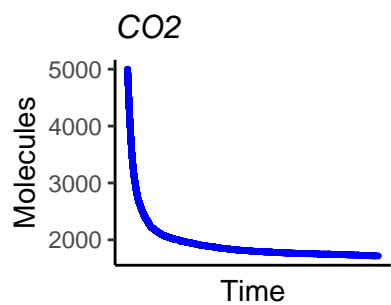
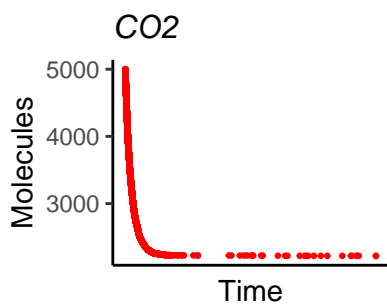
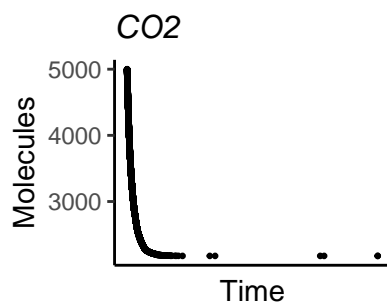
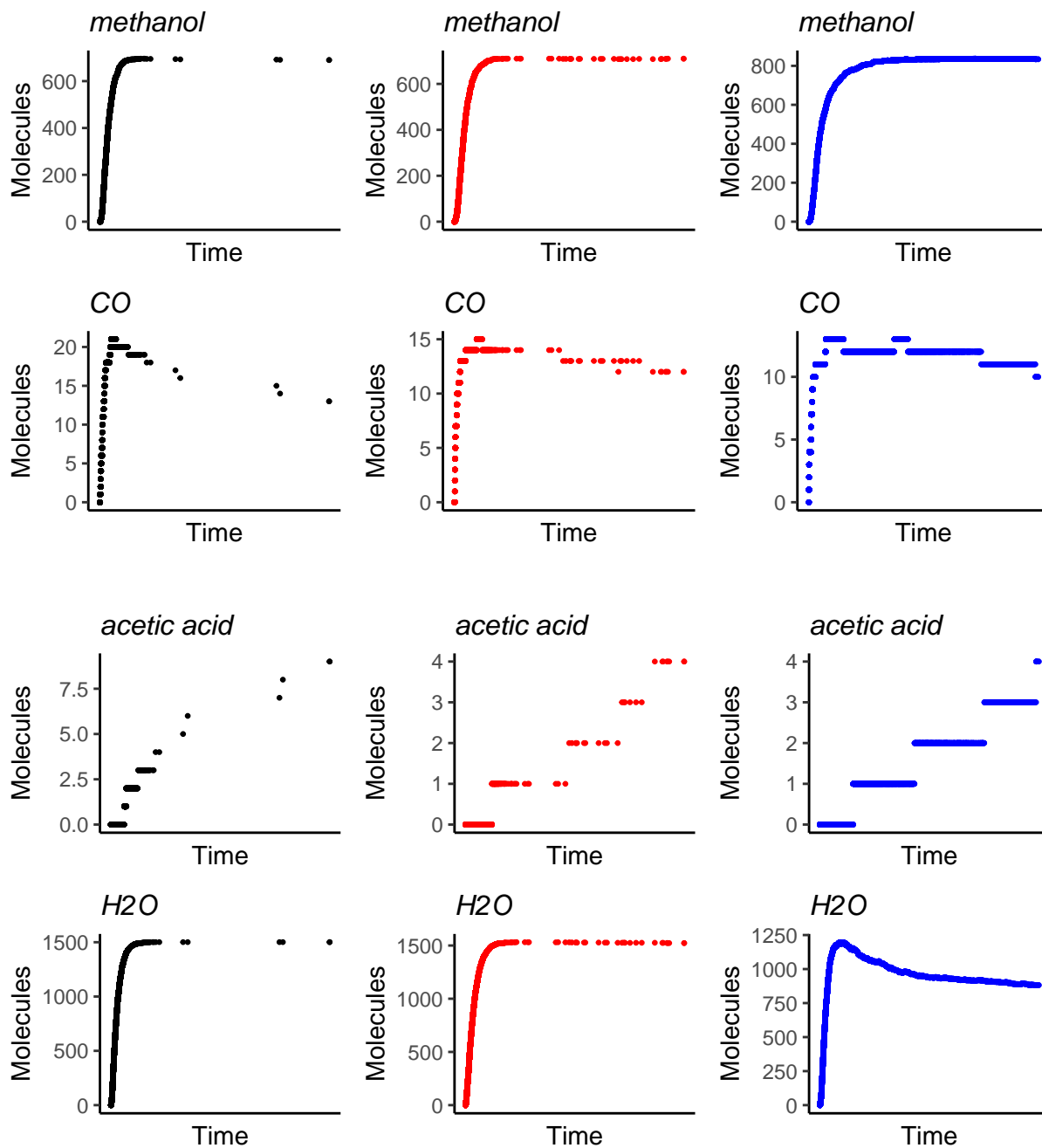


Comparing simulations of irreversible and reversible CO_2 fixation reactions (simplified CO_2 fixation)

The output on the next page is generated after manually tweaking Lia's CO_2 fixation simulation from the summer. The original simulation is the irreversible CO_2 fixation network (output in **black**). In **red**, reversible reactions with negligible backward rates yield simulations which are very similar to the irreversible reaction simulations. In **blue**, the reversible reactions with equal forward and backward reaction rates result in a distinct trajectory.

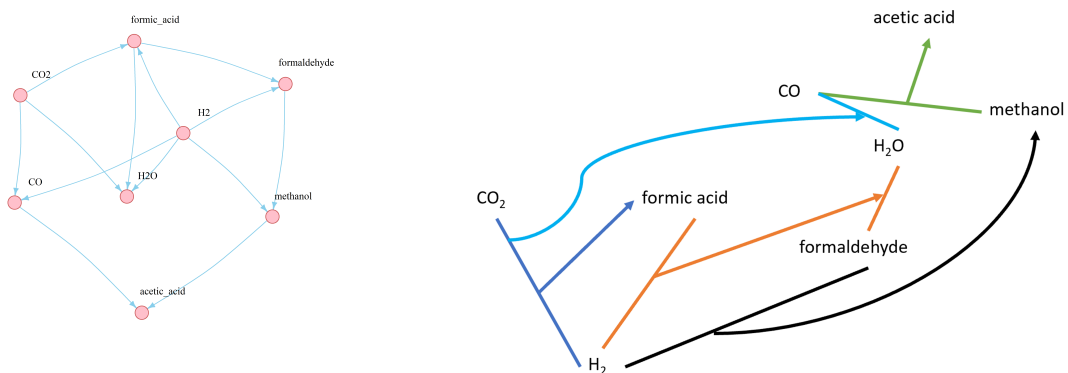
Forward reactants	Forward products	Propensity function	Parameters
CO_2, H_2	<i>formic acid</i>	$k_1 * CO_2 * H_2$	$k_1 = 10$
<i>formic acid</i> , H_2	<i>formaldehyde</i> , H_2O	$k_2 * \textit{formic acid} * H_2$	$k_2 = 19.9$
<i>formaldehyde</i> , H_2	<i>methanol</i>	$k_3 * \textit{formaldehyde} * H_2$	$k_3 = 23.5$
<i>methanol</i> , CO	<i>acetic acid</i>	$k_4 * \textit{methanol} * CO$	$k_4 = 0.869$
CO_2, H_2	CO, H_2	$k_5 * CO_2 * H_2$	$k_5 = 0.061$



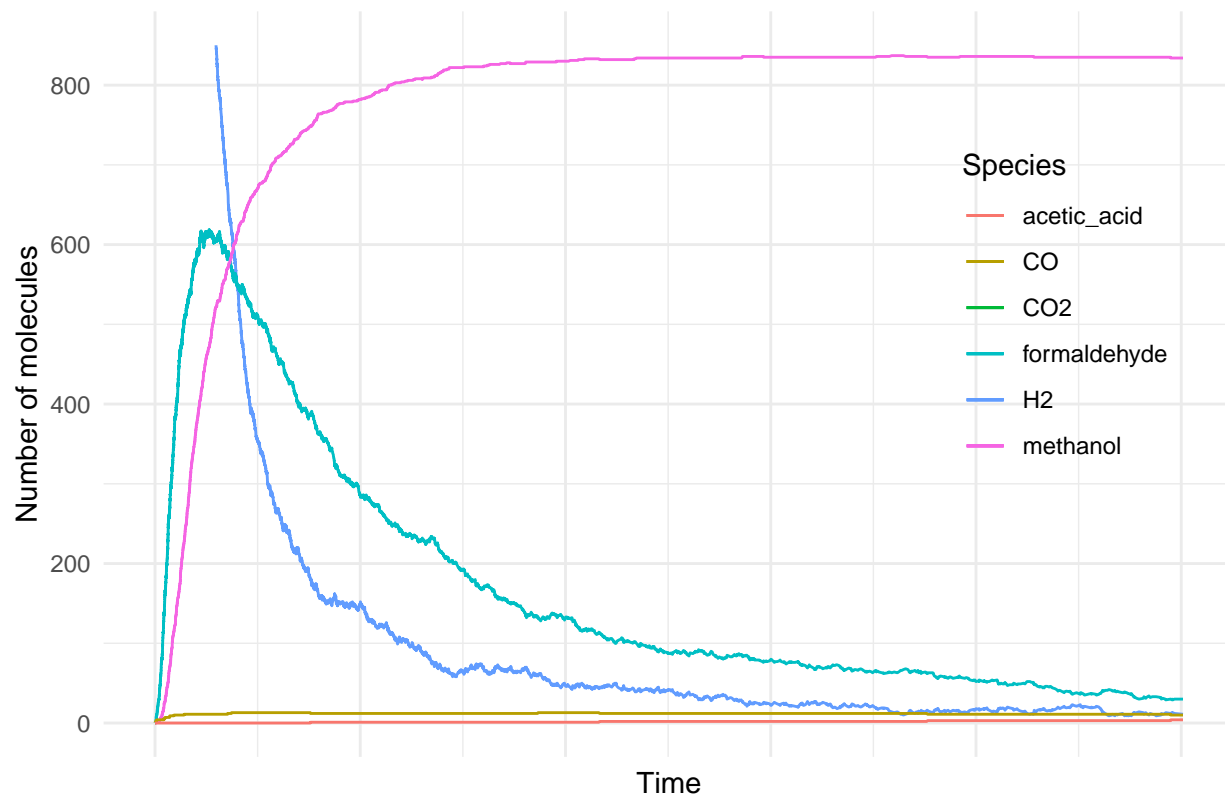


Inspecting the reversible network

The network diagram below shows the relationship between the different reactants and products.



Reversible C fixation



Compare to Lia's simulations

