Structural dynamics in plant receptor ETR1 after binding of ethylene and 1-methylcyclopropene

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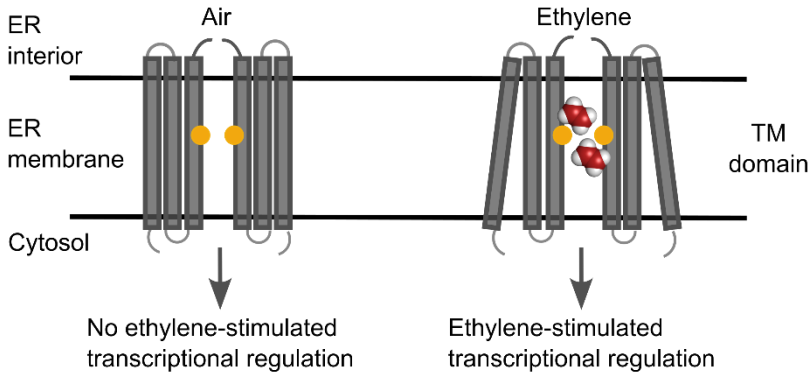
The small molecule ethylene is a gaseous plant hormone known to induce various developmental processes in plants such as seed germination, senescence, and fruit ripening after binding to the plant receptor ETR1 (ethylene response 1) in its transmembrane sensor domain (TMD).[1] The TMD obtains its high affinity and specificity for the chemically simple ethylene molecule through an essential copper cofactor, which also binds in the TMD. It is known that receptors bound to ethylene undergo conformational changes and therefore fail to activate downstream targets, which finally triggers the ethylene response of the plant and initiates the ripening of fruits. Additionally, many strained alkenes, such as 1-methylcyclopropene (1-MCP) are proven to be effective antagonists of ethylene responses that target ethylene receptors and therefore prevent fruit ripening. [2] However, it remains elusive, how ethylene binding deactivates ETR1, how the signal is transduced to downstream elements, and why 1-MCP functions as an ethylene antagonist.

Here, we show initial insights into how ethylene may deactivate ETR1 and how 1-MCP maintains ETR1 activity. Based on our predicted and experimentally validated model of the ETR1 TMD [3,4] and the characterized ethylene binding site [5], we generated an ETR1:Cu(I):ethylene TMD model [3] and developed parameters of ethylene or 1-MCP binding to Cu(I) employing a bonded model. Both the distances and force constants obtained indicate that 1-MCP interacts more strongly with copper than ethylene. The obtained trajectories of the ethylene-bound ETR1 TMD suggest directional movements of amino acids known to be associated with ethylene binding or signal transduction. These movements are less pronounced or absent in the unbound- or 1-MCP-bound states. Overall, these studies provide initial insights into how ethylene binding affects ETR1 structural dynamics, and how antagonists, such as 1-MCP, maintain ETR1 activity and will ideally provide an experimentally validated view of the structural dynamics of full-length ETR1 at the atomistic level. The latter is a prerequisite for understanding how ethylene binding is signaled to downstream elements.



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