Pectin methylesterase does amazing things with its pectin substrate

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Pectin methylesterase (PME) plays a major role in the softening of fruit that accompanies ripening. It is also involved in processing fruit pulp and fruit juices. PME removes methyl ester groups from methyl galacturonic acid residues of pectin chains to produce increasingly acidic polysaccharides. As a consequence the plant cell walls (dietary fibre) are altered chemically and physically and the fruit texture changes. If one methyl group was removed at a time deesterification would be a slow and random process. However, it is known that deesterification occurs in adjacent residues to give blocks of galacturonic acids.

**Objective:** To explain how pectin methylesterase acts on pectin.

**Method:** Molecular dynamics simulations with a range of methylated model substrates

**Results and Discussion:** We have shown that PME does not release the pectin between each deesterification step but acts in a progressive manner with pectin moving through the active site one residue at a time. However, the process is not simple because the product of each deesterification has to be reorientated before the pectin can slide forward to move the next methyl galacturonic residue into the active site.

**Conclusion:** PME operates in a progressive manner in spite of the product of each deesterification step not being aligned to be the next substrate.