

Pinic Acid – A Missing Piece in the Puzzle

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Motivation:

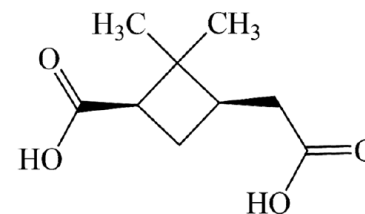
- Pinic acid is a major product of monoterpene oxidation.[1]
- Highly water soluble – present in cloudwater.[2]
- Lack of systematic investigation.[3]

Objectives:

- A mechanistic investigation of its OH oxidation mechanism in the aqueous phase.
- Product identification. pH dependence?

Approaches:

- Synthesis of *cis*-pinic acid. [3]
- Batch photooxidation in the lab.
- Offline analysis: HR-ESI-MS (elemental composition, yield).
- Online analysis: Particle-into-liquid sampler- (PILS-) MS.



Pinic Acid (PA)
 $C_9H_{14}O_4$

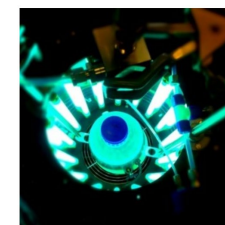


Jessica Vejdani Amorim

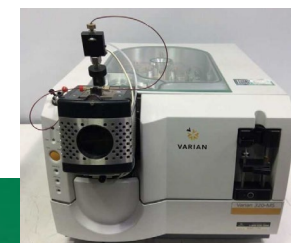


Timothy Guo

Photoreactor



ESI- triple-quad MS



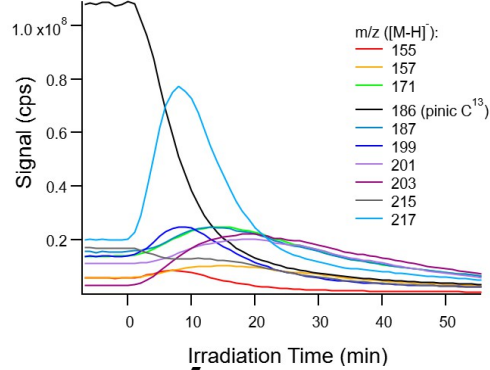
atomizer



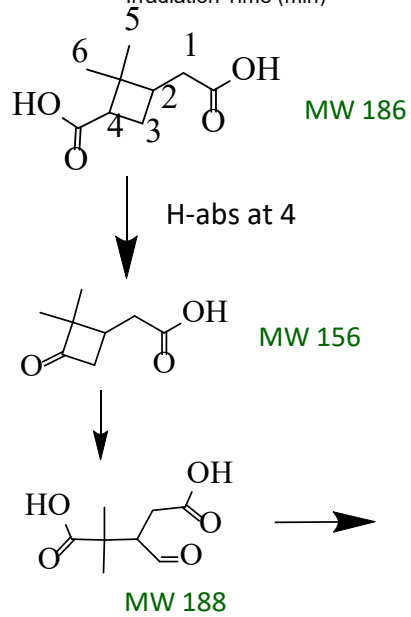
PILS



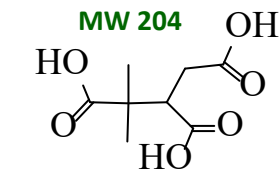
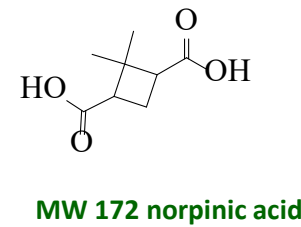
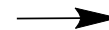
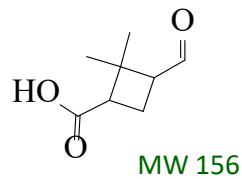
Preliminary Results



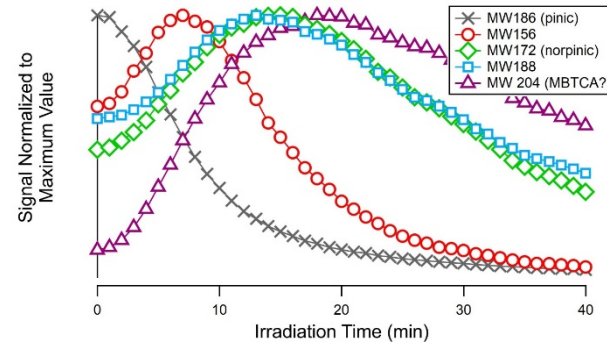
Highlighting a few product



H-abs at 1

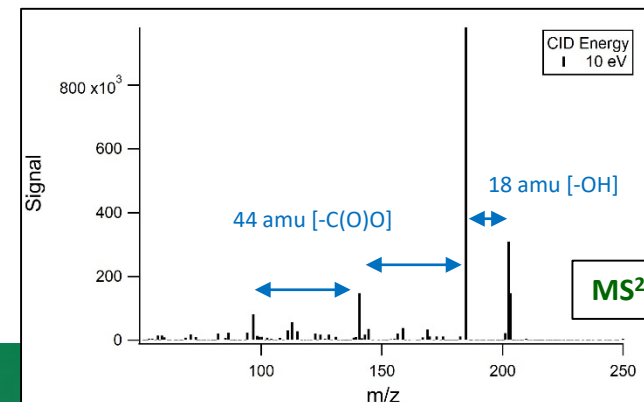
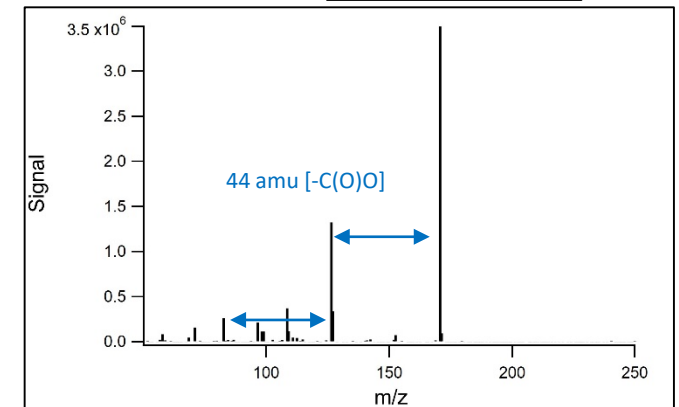


1,2,3-methyltricarbalic acid (MBTCA?)



Multi-generational OH oxidation is occurring

MS² for m/z171



Fragmentation pattern of norpinic is consistent with a diacid. m/z203 may be a diacid instead of MBTCA

MS² for m/z203