Quantifying the Relationship Between Organic Aerosol Composition and Hygroscopicity/CCN Activity

Objective: Predict organic aerosol CCN activity for a complex organic aerosol mixture from functional group chemical composition

Climate Relevant SOA Property(s) Investigated: CCN Activity

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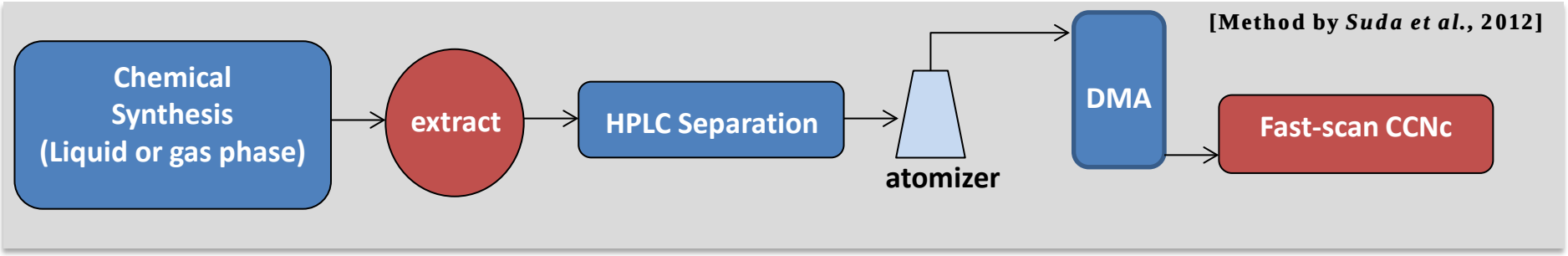
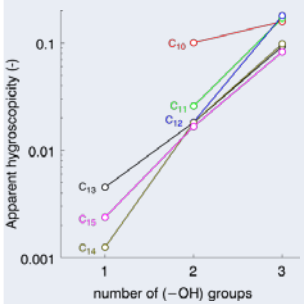
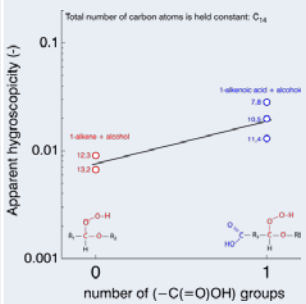
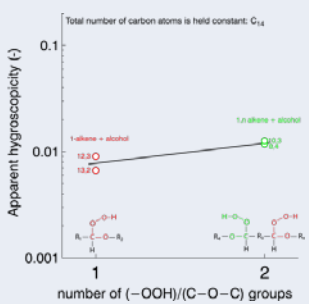
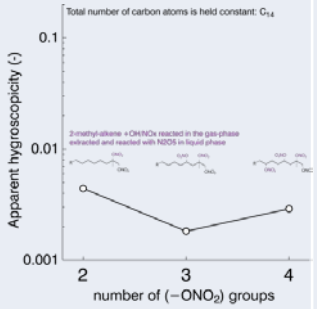
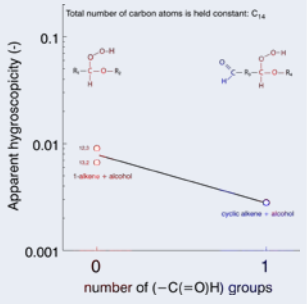
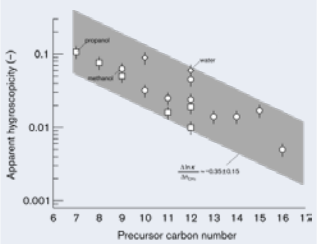
Summary of progress:

- Quantification of SOA functional group composition using HPLC and spectrophotometry
- Chemical synthesis to control number and location of relevant SOA functional groups (−OH), (C(=O)OH), (−C(=O)OH), (−OOH) + (C−O−C), (−ONO2), (−CH2−)
- Experimental determination of the slopes $\frac{\Delta\, Organic\ Aerosol\ CCN\ Activty}{\Delta\, Number/type\ of\ functional\ groups}$

Challenges or needed resources/collaborators:

- Need to test implications of predictions for SOA CCN activity evolution in different oxidation regimes using chemical mechanisms (e.g., MCM, GECKO-A) to provide guidance for modelers to better parameterize aging in simulations.

$\frac{\Delta\ Organic\ Aerosol\ CCN\ Activty}{\Delta\ Number/type\ of\ functional\ groups}$



Hydroxyl >>	Carboxylic acid >	Hydroperoxide >	Nitrate >	Aldehyde >	Methylene
(−OH)	(−C(=O)OH)	(−OOH) + (C−O−C)	(−ONO_2)	(−C(=O)H)	(−CH_2−)
$\frac{\Delta(O:C)}{\Delta n} = 1$	$\frac{\Delta(O:C)}{\Delta n} = 2$	$\frac{\Delta(O:C)}{\Delta n} = 3$	$\frac{\Delta(O:C)}{\Delta n} = 3$	$\frac{\Delta(O:C)}{\Delta n} = 1$	$\frac{\Delta(O:C)}{\Delta n} < 0$
$\frac{\Delta \ln \kappa}{\Delta n} = 3 - 11$	$\frac{\Delta \ln \kappa}{\Delta n} = 1.6$	$\frac{d \ln \kappa}{\Delta n} = 0.56$	$\frac{d \ln \kappa}{\Delta n} \sim 0$	$\frac{\Delta \ln \kappa}{\Delta n} \sim 0$	$\frac{\Delta \ln \kappa}{\Delta n} = -0.35$