

Feasibility of a selective epoxidation technique for use in quantification of peracetic acid in air samples collected on sorbent tubes

Data Dictionary

Field Name	Field Contents
PAA	Peracetic acid
HP	Hydrogen peroxide
AA	Acetic Acid
CHO	Cyclohexene oxide
ppb	Concentration of analyte in parts per billion
liquid-phase	Denotes method of collection: Vial experiment comprising of 1 mL of acetonitrile, 2 μ L of peracetic acid solution, 100 μ L of cyclohexene
liquid + sorbent	Denotes method of collection: Vial experiment comprising of 1 mL of acetonitrile, 2 μ L of peracetic acid solution, 100 μ L of cyclohexene, and 350 mg XAD-7 sorbent material
Chamber	Denotes method of collection: Teflon chamber with 80 L of air at 50% relative humidity containing 2 μ L of PAA solution. Air pulled from chamber via vacuum pump over XAD-7 sorbent tube at 250 mL/min for 4 hours.
Fortified Sampler	Denotes method of collection: Teflon chamber with 80 L of air at 50% relative humidity. 2 μ L of PAA solution added to XAD-7 sorbent tube. Clean air pulled from chamber via vacuum pump over XAD-7 sorbent tube at 250 mL/min for 4 hours.
XIC (83-ion) (kCounts)	Extracted-ion peak area (m/z 83)
IS	Internal Standard
RT	Room temperature
LOD	Limit-of-detection
LOQ	Limit-of-quantitation
N	Number of replicates averaged
PAA 0/ AA 0	Concentrations of peracetic acid and acetic acid in sample. Ratio of 0 ppb PAA / 0 ppb AA.
PAA 0/ AA 1000	Concentrations of peracetic acid and acetic acid in sample. 0 ppb PAA and 1000 ppb AA.
PAA 0/ AA 10000	Concentrations of peracetic acid and acetic acid in sample. 0 ppb PAA and 10000 ppb AA.
PAA 100 / AA 1000	Concentrations of peracetic acid and acetic acid in sample. 100 ppb PAA and 1000 ppb AA.

PAA 100 / AA 10000	Concentrations of peracetic acid and acetic acid in sample. 100 ppb PAA and 10000 ppb AA.
PAA 100	100 ppb of PAA
PAA 0 / HP 0	Concentrations of peracetic acid and hydrogen peroxide in sample. 0 ppb PAA and 0 ppb HP.
PAA 0 / HP 1000	Concentrations of peracetic acid and hydrogen peroxide in sample. 0 ppb PAA and 1000 ppb HP.
PAA 0 / HP 10000	Concentrations of peracetic acid and hydrogen peroxide in sample. 0 ppb PAA and 10000 ppb HP.
PAA 100 / HP 1000	Concentrations of peracetic acid and hydrogen peroxide in sample. 100 ppb PAA and 1000 ppb HP.
PAA 100 / HP 10000	Concentrations of peracetic acid and hydrogen peroxide in sample. 100 ppb PAA and 10000 ppb HP.
PAA_5mL	Peracetic acid sample using 5 mL of acetonitrile
CHO_5mL	Cyclohexene oxide sample using 5 mL of acetonitrile
XIC (83-ion) (storage)	Extracted-ion peak data corresponding to PAA samples that were stored either at room temperature or -20°C for 72 h.
IS (storage)	Internal standard peak data from PAA samples that were stored either at room temperature or -20°C for 72 h.
XIC (83-ion) (no storage)	Extracted-ion peak data corresponding to PAA samples that were not stored for 72 h that served as control experiments.
IS (no storage)	Internal standard peak data from PAA samples that were not 72 h that served as control experiments.
Blank Chamber	Denotes method of collection: Teflon chamber with 80 L of air at 50% relative humidity. No PAA solution added to XAD-7 sorbent tube. Air pulled from chamber via vacuum pump over XAD-7 sorbent tube at 250 mL/min for 4 hours. Served as negative control.
Tube_1_350_mg	The first tube in the sample train for PAA collection in breakthrough experiments. Contents: 350 mg of XAD-7 sorbent.
Tube_2_175_mg	The second tube in the sample train for PAA collection in breakthrough experiments. Contents: 175 mg of XAD-7 sorbent.
XAD-7	Describes the type of sorbent in sorbent tubes in the study. Purchased from SKC Inc.

1 hr	1 hour collection of PAA onto sorbent tube
3 hr	3 hour collection of PAA onto sorbent tube
4 hr	4 hour collection of PAA onto sorbent tube
Storage (5mL)	Denotes samples that were stored for 72 hours either at -20°C or room temperature
No storage (5mL)	Denotes samples that weren't stored prior to processing and serves as control
Time (h)	The storage time (in hours) of the sorbent tube containing collected PAA