Supplementary Online Material

Air and surface sampling method for assessing exposures to quaternary ammonium compounds using liquid chromatography tandem mass spectrometry

Ryan F. LeBouf, M. Abbas Virji, Anand Ranpara, Aleksandr B. Stefaniak

Field Studies Branch, Respiratory Health Division, National Institute for Occupational Safety and Health

In the MRM method, a single ion (parent ion) is selectively allowed to pass through the collision cell where an additional fragmentation occurs. A single ion is again chosen, the daughter ion, such that the transition from parent to daughter is unique and provides a sensitive and selective response to the compound of interest. This targeted analysis virtually eliminates many matrix interferences and focuses on the analyte of interest. In the SIR method, only one quadrupole is used and focused on the molecular ion of the analyte of interest.

Calibration curves were linear across a wide dynamic range (0.35 to 100 ng/mL) (Table S1). Correlation coefficients were greater than 0.997.

Table S1. Calibration curve regression parameters

Method	Compound	Slope	Intercept	R^2
MRM	BEC	0.0433	0.0068	0.9991
	BAC12	0.0336	-0.0014	0.9991
	BAC14	0.0353	0.0127	0.9993
	DDAB	0.0784	0.0181	0.9991
	BAC16	0.0414	0.0554	0.9979
SIR	BEC	0.0530	0.0034	0.9988
	BAC12	0.0302	0.0023	0.9997
	BAC14	0.0309	0.0055	0.9998
	DDAB	0.0361	0.0027	1.0000
	BAC16	0.0273	0.0016	0.9992

Note: Calibration range 0.35-100 ng/ml

Calculated method detection limits (MDLs) for sampling media ranged from 0.3 to 2 ng/mL for the different quats compounds using MRM and 0.1 to 2.0 ng/mL using SIR (Table S2). GFF generally had the lowest MDLs of all media types except for BEC on GFF. MDLs were calculated as 3×RMSE/slope for all media and quats compounds except for DDAB on PTFE and PW using MRM, which were set to the lowest measured concentration used in the assessment.

Table S2: Method Detection Limits for Quats on Sampling Media using MRM and SIR

Method	Compound	GFF MDL (ng/mL)	PTFE MDL (ng/mL)	PW MDL (ng/mL)
MRM	BAC12	0.3	0.7	0.5
	BAC14	0.5	0.8	1.0
	BAC16	0.5	0.6	2.0
	BEC	0.5	0.4	0.4
	DDAB	0.6	1.0	0.5
SIR	BAC12	0.2	0.5	0.5
	BAC14	0.4	0.4	2.0
	BAC16	0.2	0.5	0.9
	BEC	0.1	0.4	0.5
	DDAB	0.2	0.6	0.2

PW moistened with 2-propanol was the best at recovering quats from a surface. Recoveries of all three BAC analytes were greater than 90% when sampling from an ideal, glass surface after a single wipe (Table S3).

Table S3. Recoveries of Quats from Surfaces

Analytes	Glass		Epoxy Resin		Metal	
	% Recovery	% RSD	% Recovery	% RSD	% Recovery	% RSD
BAC 12	96	6	94	9	94	5
BAC 14	95	4	83	5	89	5
BAC 16	92	5	73	5	89	3
BEC	70	7	45	7	72	5
DDAB	78	9	53	6	82	7

Storage stability of quats on GFF and PW sampling media using SIR method were outside the ±10% bias criterion for most storage days when compared to day zero (Figure S1). For GFF, BAC compounds at room temperature and BEC at refrigerated temperature were greater than 10% bias. For PW, BAC12 and BAC14 for both storage conditions and BEC at room temperature were greater than 10% bias.

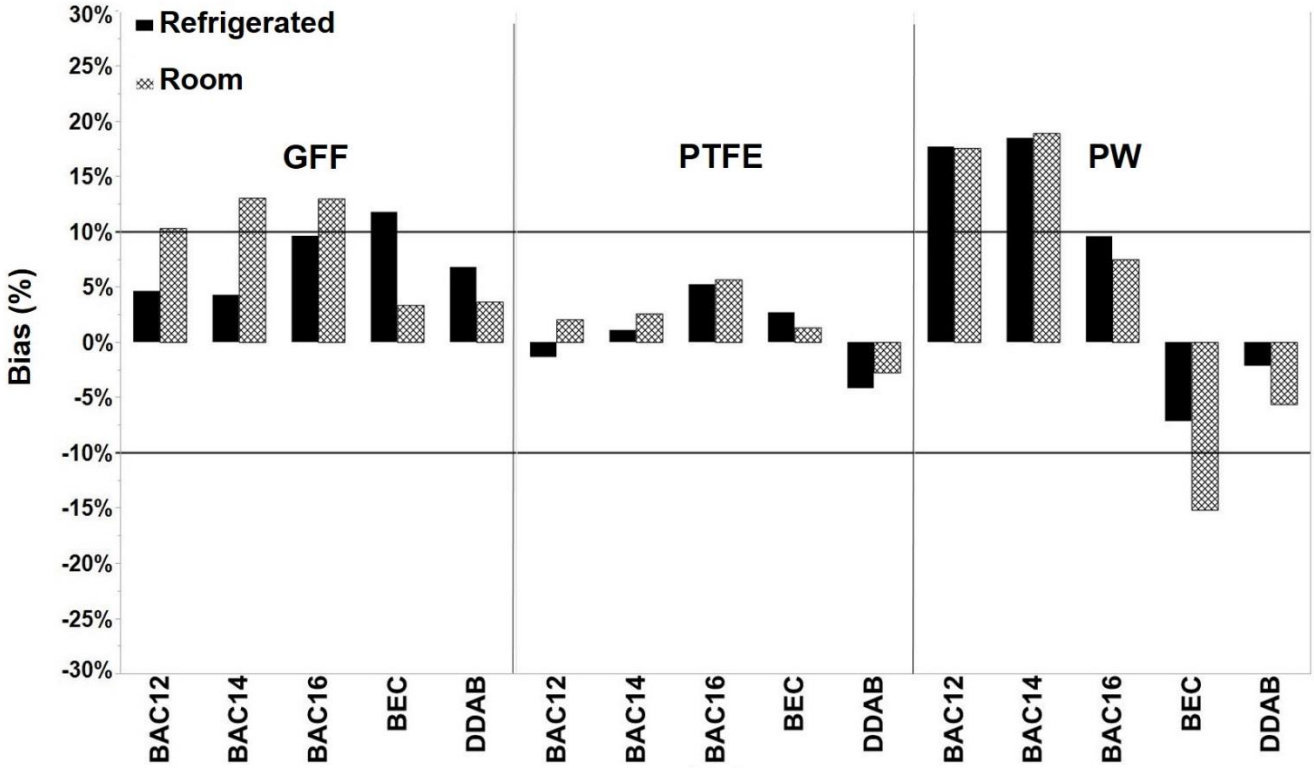

Figure S1. Storage Stability of Quats (%bias) on Media using SIR compared to day zero measurements