

# RECEPTOR AND SOURCE PROFILING BY GC/MS ANALYSIS OF TEMPORALLY AND SPATIALLY RESOLVED PM SAMPLES.

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**Introduction.** The ability of combined gas chromatography/mass spectrometry (GC/MS) techniques to provide detailed information about the chemical composition, provenance and potential threat of complex environmental samples has been widely recognized for more than 40 years. Over the past decade, or so, Rogge et al.<sup>1</sup> have demonstrated the power of GC/MS techniques for particulate matter (PM) source characterization. Yet, acceptance of GC/MS techniques in PM receptor modeling studies has been relatively slow and, thus far, no standard GC/MS methods for PM source or receptor characterization have been approved by the EPA.

**Methods.** For a recent exploratory study of PM compositions, origins and impacts in the Paso del Norte airshed under the auspices of the EPA funded SCERP (Southwest Center for Environmental Research and Policy) Paso del Norte Air Research Program, the authors relied on solvent extraction (SX) GC/MS procedures developed by Rogge et al.<sup>1</sup> to characterize 24-hr quartz fiber filter (QFF) samples obtained from 9 spatially-distributed Hi-Vol PM10 samplers as well as on thermal desorption (TD) GC/MS methods developed by Dworzanski et al.<sup>2</sup> to characterize over 50 time-resolved (2-hr) QFF samples obtained with modified 1m<sup>3</sup>/hr dichotomous PM10 samplers. Principal component analysis (PCA) and related chemometric techniques were used for data reduction and multispectroscopy data fusion as well as for component extraction (deconvolution) and multiway data correlation.

**Results.** In several instances the presence of highly specific organic marker compounds permitted direct, unambiguous source attribution. More often, characteristic compound patterns helped identify putative sources, sometimes aided by multiway correlation with inorganic PM data. A high degree of correspondence was found between the rapid TD-GC/MS (which can be carried out on 2-hr QFF slices containing only microgram amounts of sample) and conventional SX-GC/MS procedures. Moreover, combined PCA of temporally resolved TD-GC/MS data and spatially resolved SX-GC/MS data can be used to predict approximate source locations for specific PM components observed in time-resolved receptor profiles.

**Conclusions.** Time-resolved PM receptor profiles obtained by 2-hourly TD-GC/MS analysis can be correlated with conventional 24-hr SX-GC/MS data on spatially resolved Hi-Vol samples to help detect and characterize sources in complex urban environments.

## References.

1. Rogge, W.F. et al *Environ. Sci. Technol. Parts I-IX* 1991-1998.
2. Dworzanski, J.P.; McClennen, W.H.; Cole, P.A.; Thornton, S. N.; Arnold, N.S.; Snyder, A.P.; Meuzelaar, H.L.C. *Field Anal. Chem. Technol.* 1997, 1, 295-305.

Table 1. Factor Loadings for the Combined Data Matrix of TC-GC/MS and SX-GC/MS

Class	Compounds	Factor2	Factor3
n-Alkanes	C18	-0.77	0.11
	C19	-0.84	0.06
	C20	-0.18	-0.16
	C21	-0.56	0.07
	C22	-0.66	0.16
	C23	-0.15	0.76
	C24	-0.00	0.73
	C25	-0.00	0.81
	C26	-0.00	0.87
	C27	-0.00	0.87
	C28	-0.00	0.88
	C29	-0.00	0.89
	C30	-0.00	0.87
Hopanes	27nco	0.66	0.35
	27a	-0.07	0.39
	29a	0.63	0.29
	30a	-0.05	0.31
	31a S	-0.08	0.34
	31a R	0.07	0.36
	32a S	-0.07	0.34
	32a R	-0.06	0.33
	33a S	-0.00	0.32
	33a R	-0.02	0.32
n-Alkanoic acids	nonanoic acid	-0.95	-0.15
	decanoic acid	-0.78	-0.04
	dodecanoic acid	-0.85	-0.01
	undecanoic acid	-0.94	-0.11
	tetradecanoic acid	-0.94	0.13

Continued

	pentadecanoic acid	-0.97	0.01
	pentadecanoic acid	-0.97	0.01
	hexadecanoic acid	-0.91	0.29
Steranes	octadecanoic acid	-0.93	-0.16
	27D Ba 20S	-0.06	0.34
	27D Ba 20R	-0.07	0.24
	29 aaa R	0.02	0.43
Amyrins	27aBB R	-0.15	0.16
	27 aBB S	-0.07	0.33
	o Amyrin	-0.11	0.41
	a Amyrin	-0.07	0.73
	a Amyrin acetate	-0.05	0.74
PAH & Aromatics	178PAH	-0.22	0.45
	fluoranthene	-0.12	0.18
	pyrene	-0.11	0.35
	retene	0.34	0.37
	benzanthracene	-0.65	0.23
	chrysenes	-0.03	0.27
	benzo[fluoranthene]	0.03	0.20
	benzo[e]pyrene	-0.11	0.24
	benzo[a]pyrene	-0.02	0.26
	perylene	-0.03	0.29
	275PAH_1	-0.20	0.16
	275PAH_2	-0.28	0.11
	275PAH_3	-0.30	0.11
275PAH_4	-0.02	0.20	
302PAH_1	-0.44	0.09	
302PAH_2	-0.57	-0.13	
302PAH_3	-0.49	-0.15	
Phthalates	diallyl phthalate	-0.30	0.16
	dibutyl phthalate	-0.08	0.65
	35-(2-allylnonyl)phthalate	-0.33	0.39

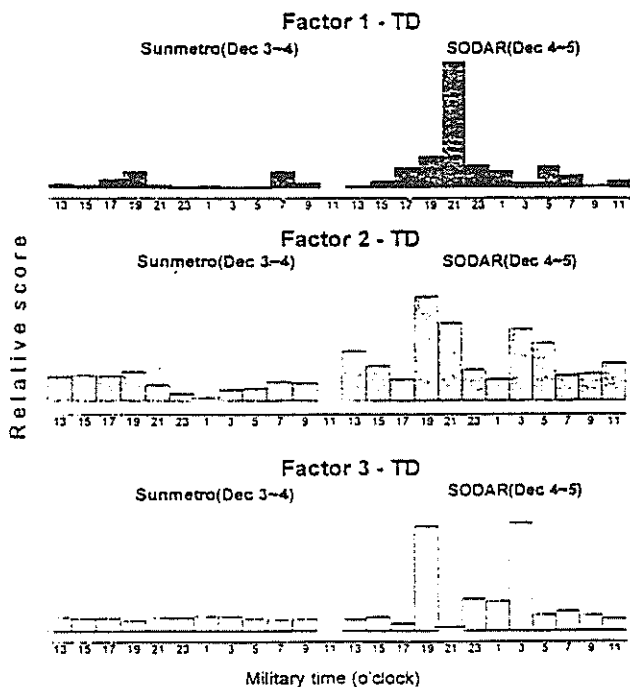


Fig. 1. Time-resolved principal component score profiles of 3 most significant factors in TD-GC/MS data.

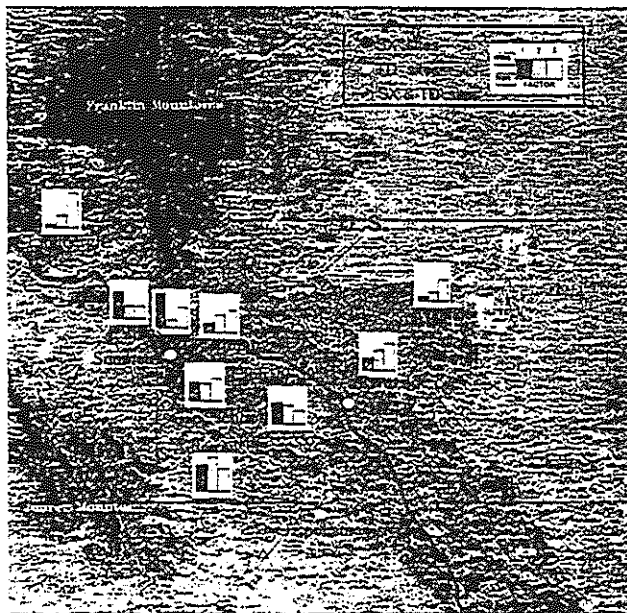


Fig. 2. Spatially-resolved principal component scores of 3 most significant factors in SX-GC/MS data.