Electronic Supplementary Material (ESI) for Analyst

Supplementary Information

A Nanoparticle-Coated Chemiresistor Array as a Microscale Gas Chromatograph Detector for Explosive Marker Compounds: Flow Rate and Temperature Effects

L. K. Wright,[1,3] *and E. T. Zellers*[1-3*]

[1]Department of Chemistry, [2]Department of Environmental Health Sciences

[3]Center for Wireless Integrated MicroSensing and Systems,

University of Michigan, Ann Arbor, MI, USA 4819-2029

* Corresponding author: e-mail: ezellers@umich.edu

Table S1. 90-day stability test results showing the extent of drift in average sensitivities for an MPN-coated CR array between Day 1 and Day 90 (see Figure S1).

Analyte	Avg. Sensitivity Change	Correlation Coefficient (r^2)[a]
Toluene	+11.7%	0.99
n-Propanol	+34.6%	0.97
2-Butanone	+16.0%	0.99
Octane	+12.0%	0.99
Nitromethane	+1.6%	0.99

[a] determined from linear regression of the sensitivities of all 4 sensors in the array on Day 90 onto to those on Day 1.

Table S2. Peak asymmetry factors (*AF*) for the marker compounds from each sensor at the lowest and highest temperatures and a flow rate of 1.2 mL/min.

MPN	DMNB		2,6-DNT		2,4-DNT	
	55°C	80°C	55°C	80°C	55°C	80°C
C8	1.8	1.7	1.5	1.3	3.1	2.6
DPA	1.9	1.7	2.2	2.0	3.4	2.6
OPH	2.6	2.2	3.0	2.5	4.3	3.0
HME	1.8	1.5	2.5	2.3	3.9	3.0

Table S3. Peak asymmetry factors (*AF*) for the marker compounds from each sensor at the lowest and highest flow rates and an array temperature of 70°C.

MPN	DMNB		2,6-DNT		2,4-DNT	
	1.1 mL/min	3.7 mL/min	1.1 mL/min	3.7 mL/min	1.1 mL/min	3.7 mL/min
C8	1.4	1.2	2.5	2.0	2.3	2.0
DPA	1.5	1.4	2.5	2.1	3.2	2.6
OPH	2.1	1.7	4.2	3.0	4.2	3.1
HME	1.7	1.5	2.8	2.5	4.0	3.3

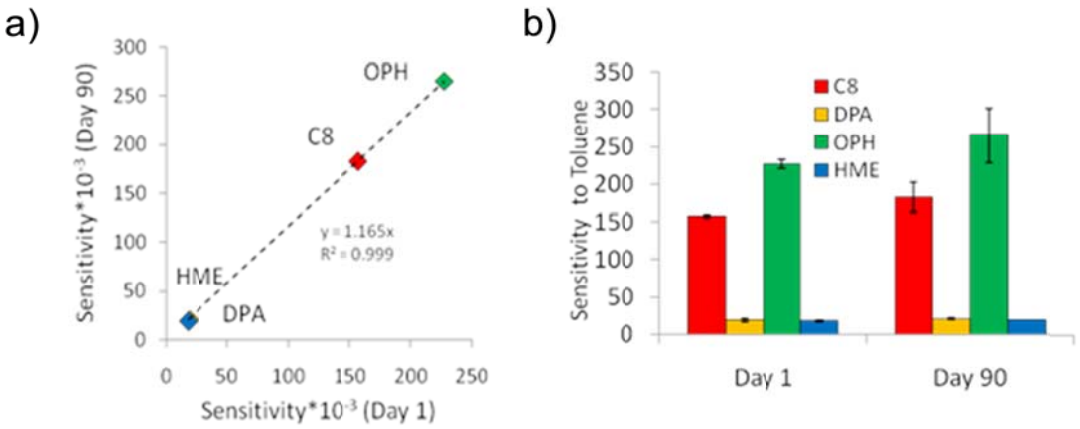

Figure S1. (a) Correlation of responses to toluene vapor on Day 1 vs. Day 90. Slope of 1.16 reflects the positive drift in sensitivities, but the large correlation coefficient indicates a common-mode source of such drift and the retention of relative sensitivities among the sensors in the array; (b) absolute response patterns among the sensors, confirming the stability of relative sensitivities over time. Similar results were found for the other vapors in Table S1.

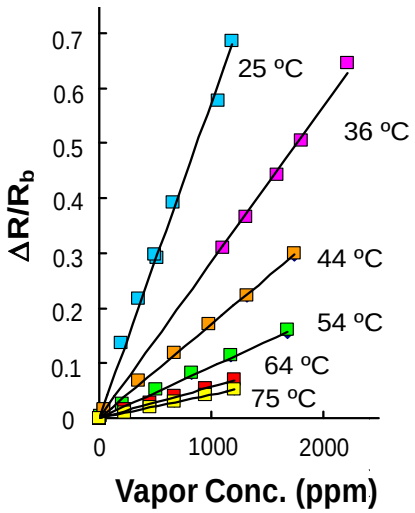

Figure S2. Calibration curves for 2-propylbenzene from a representative C8-MPN coated CR sensor showing a reduction in sensitivity with increasing temperature but retention of linearity (stability).

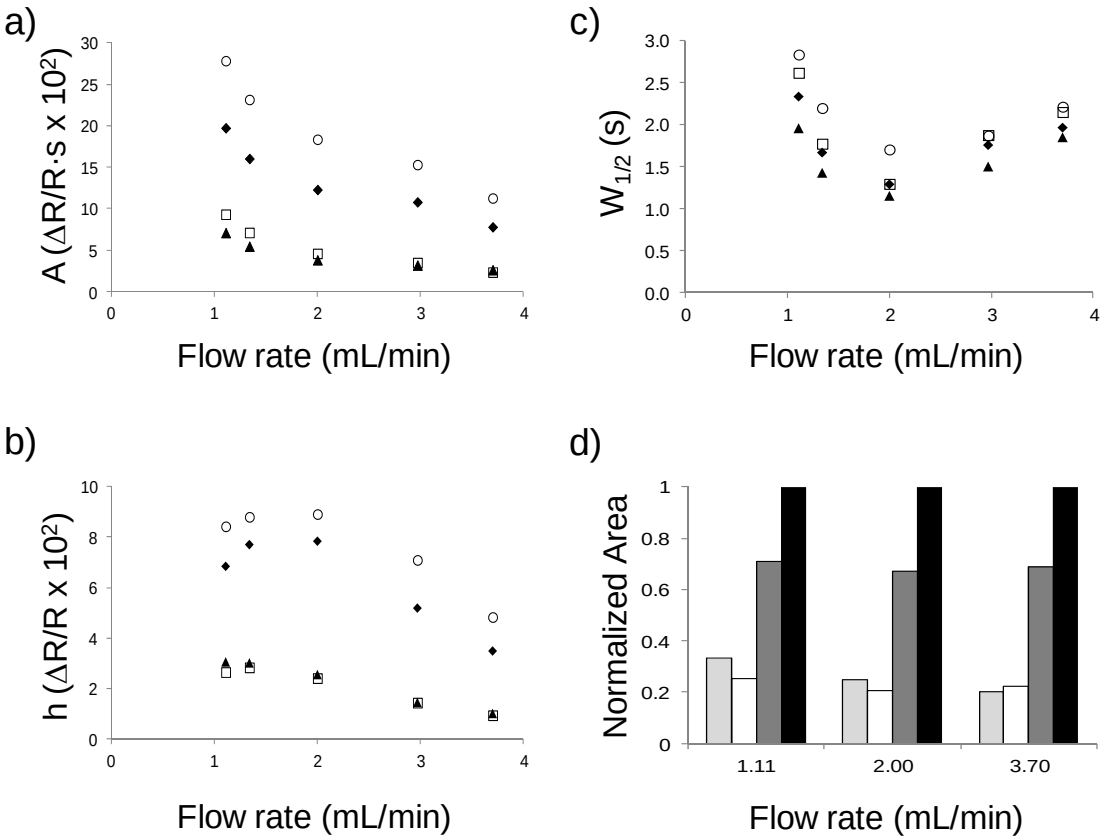

Figure S3. Effects of flow rate on peak parameters for DMNB: (a) *A*; (b) *H*; (c) $W_{½}$; (d) relative response patterns (from peak areas). Legend: C8 (□), DPA (▲), OPH (♦), HME (○); bar chart, from left to right: C8, DPA, OPH, HME.

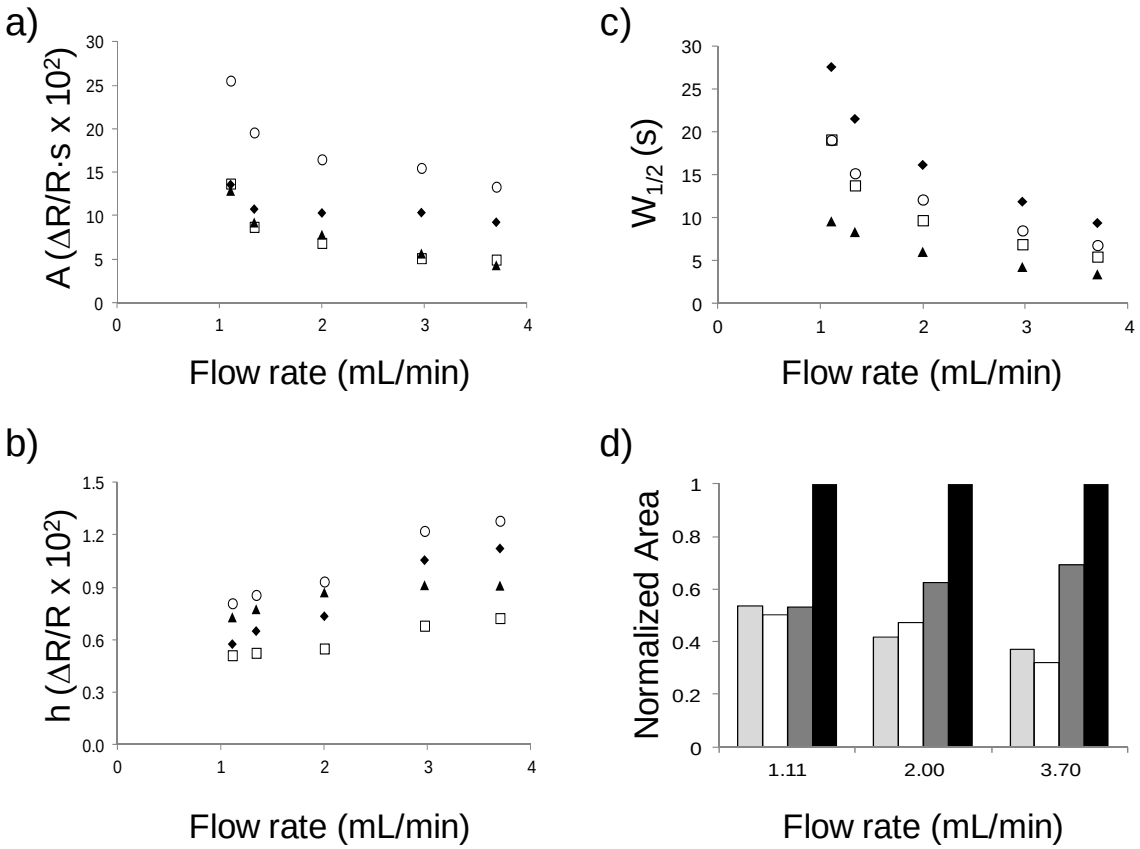

Figure S4. Effects of flow rate on peak parameters for 2,6-DNT: (a) *A*; (b) *H*; (c) $W_{½}$; (d) relative response patterns (from peak areas). Legend: C8 (□), DPA (▲), OPH (♦), HME (○); bar chart, from left to right: C8, DPA, OPH, HME.

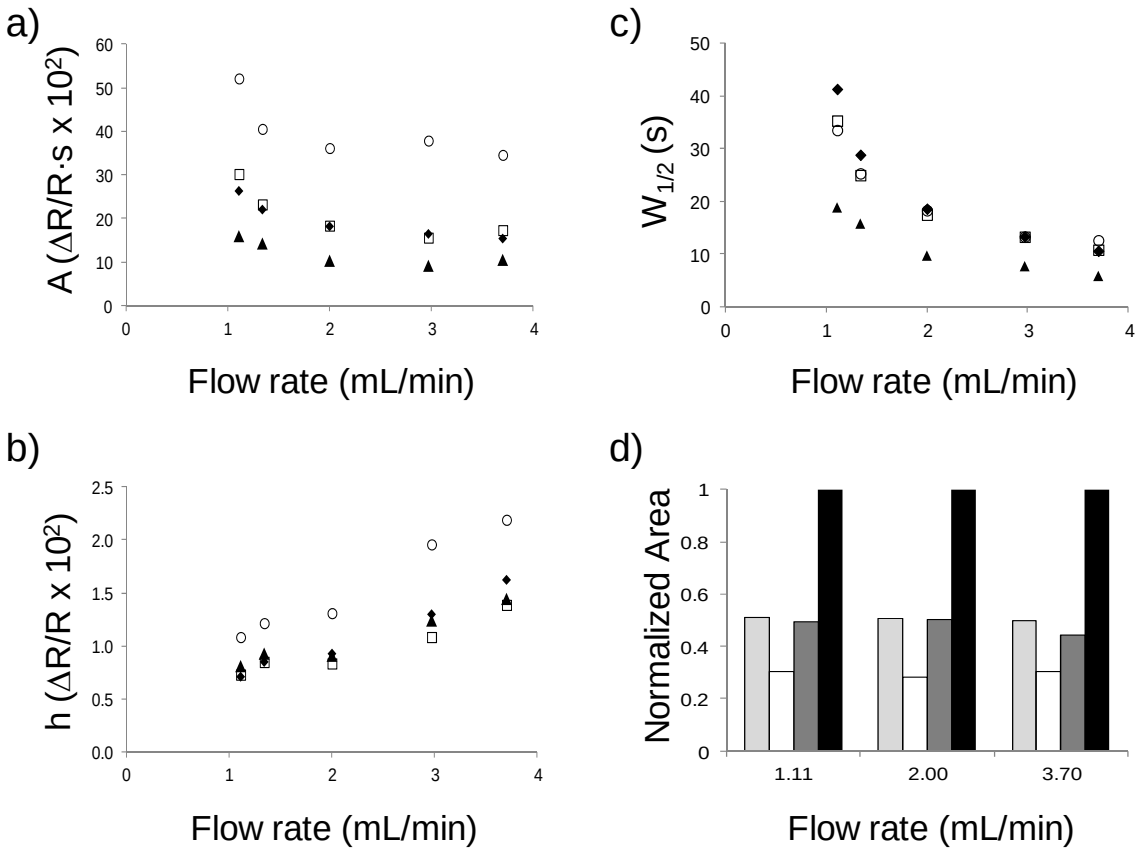

Figure S5. Effects of flow rate on peak parameters for 2,4-DNT: (a) *A*; (b) *H*; (c) $W_{½}$; (d) relative response patterns (from peak areas). Legend: C8 (□), DPA (▲), OPH (♦), HME (○); bar chart, from left to right: C8, DPA, OPH, HME.

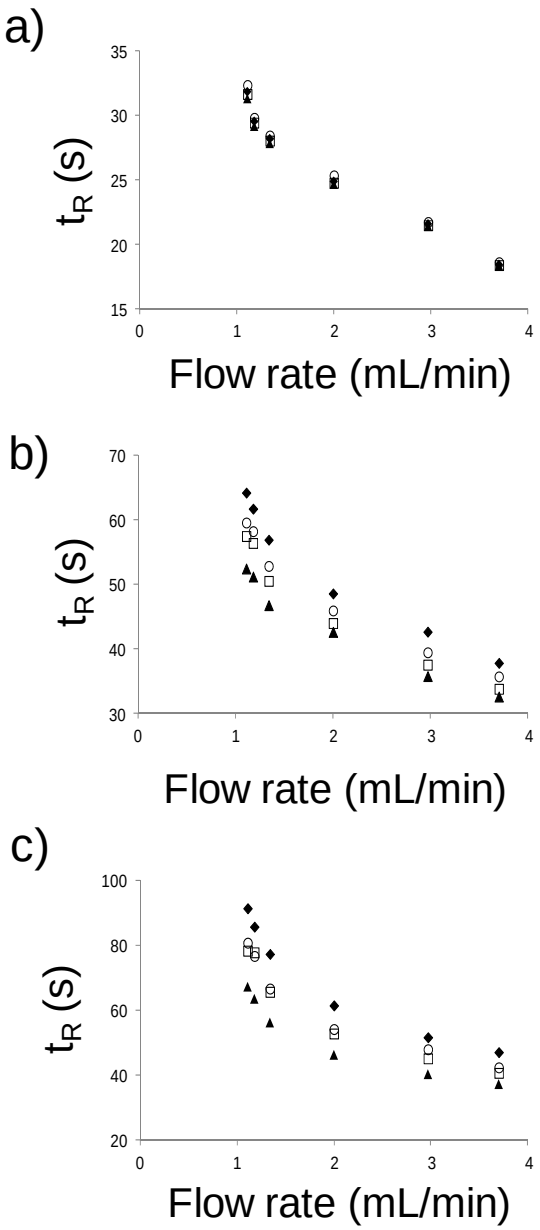

Figure S6. Effect of flow rate on t_R for (a) DMNB, (b) 2,6-DNT, and (c) 2,4-DNT. Legend: C8 (□), DPA (▲), OPH (♦), HME (○).