Supporting Information for "Limits of Recognition for Binary and Ternary Vapor Mixtures Determined with Multi-Transducer Arrays" by *C. Jin and E. T. Zellers*

The results tabulated below are from analyses performed with the 5-sensor MT array and 5-sensor CAP ST-array related to the LOR determinations of 12 binary mixtures. The analyses are similar to those performed for the 8-sensor MT-U array in the main body of the article.

Table SI-1. LOR evaluations of 12 binary mixtures using simulated data from the 5-sensor MT-U array.

Components A	B	RR(%)[a]	LOR_{95}	LOD_A[b]	LOD_B[b]	S_A[c]	S_B[c]	E_{AB}[d]	e_A/e_B[e]	A[f]	P_A[g]	P_B[g]	P_A/P_B[h]
HEP	CHL	99.8	84	890	190	0.26	0.28	0.91	0.14	0.16	230	52	4.4
OCT	CHL	99.8	80	150	190	0.66	0.28	1.2	0.25	0.2	100	52	2.0
OCT	EAC	99.6	46	150	480	0.66	0.27	1.0	2.3	2.5	102	130	0.8
HEP	TCE	98.4	96	890	180	0.26	0.21	0.91	0.09	0.13	230	37	6.2
OCT	TCE	98.2	100	150	180	0.66	0.21	1.1	0.22	0.26	100	37	2.8
EOH	CCL	98.0	52	410	430	0.26	0.09	0.48	0.26	0.21	110	39	2.8
HEP	EAC	97.8	56	890	480	0.26	0.27	0.60	0.11	0.15	230	130	1.8
CHL	CCL	97.0	56	190	430	0.28	0.09	0.86	0.35	0.38	52	39	1.3
EOH	PCE	96.8	76	410	70	0.26	0.43	0.95	0.22	0.18	110	29	3.7
CHL	PCE	96.6	70	190	70	0.28	0.43	0.86	0.18	0.22	52	29	1.8
TOL	EOH	96.4	10	130	410	0.20	0.26	0.94	5.3	7.5	26	110	0.2
POH	PCE	95.0	74	80	70	0.73	0.43	0.66	0.40	0.41	58	29	2.0

[a] average recognition rate determined at an RCR = 1:1 over a concentration range of 5-10LOD for each component;
[b] units = ppm; [c] array sensitivity in units of response/ppm; [d] E_{AB} is the Euclidean distance between normalized vectors for vapors A and B; [e] e_A and e_B are the Euclidean distances between the vectors for components A and B and the vector for their 1:1 mixture, respectively; [f] *A* is an index of asymmetry defined as the ratio of $lor_{95\text{-}A}/lor_{95\text{-}B}$ (see Figure 1a in text);
[g] *P* is the product of the LOD and S for a given mixture component. [h] Linear regression of *A* vs. $(P_A/P_B)^{-1}$ yields an $r^2 = 0.835$.

Table SI-2. Range and asymmetry of relative concentration ratios evaluated at a minority-component concentration of 10LOD (RCR_{10}) for 5-sensor MT array determined with 12 binary mixtures over which the recognition rate of the mixture is ≥95%.[a]

Mixture Components		RCR_{10}	Range of RCR_{10} (8:1, 7:1, 6:1, 5:1, 4:1, 3:1, 2:1, 1:1, 1:2, 1:3, 1:4, 1:5, 1:6, 1:7, 1:8, 1:9, 1:10, 1:11, 1:12)
A	B		
HEP	CHL	22	(2:1) – (1:10)
OCT	CHL	20	(2:1) – (1:12)
OCT	EAC	5	(2:1) – (1:3)
HEP	TCE	36	(2:1) – (1:15)
OCT	TCE	36	(3:1) – (1:14)
EOH	CCL	5	(1:1) – (1:5)
HEP	EAC	6	(2:1) – (1:3)
CHL	CCL	6	(2:1) – (1:14)
EOH	PCE	18	(1:1) – (1:18)
CHL	PCE	16	(3:1) – (1:6)
TOL	EOH	2	(2:1) – (1:3)
POH	PCE	18	(2:1) – (1:7)

[a] the column of entries for RCR_{10} is the fold-range of relative concentration ratios for each mixture for which RR ≥95%. Each line spans that RCR range and shows the degree of asymmetry relative to the RCR = 1:1 value when concentrations are expressed as multiples of the LOD for each component. Values in parentheses at the end of a line are the corresponding RCR values in units of ppm.

Table SI-3. LOR evaluations of 12 binary mixtures by a 5-sensor CAP ST array.

Components A	Components B	RR(%)[a]	LOR_{95}	LOD_A[b]	LOD_B[b]	S_A[c]	S_B[c]	E_{AB}[d]	e_A/e_B[e]	A[f]	P_A[g]	P_B[g]	P_A/P_B[h]
HEP	CHL	97.4	70	60	40	0.73	0.60	0.85	0.10	0.13	46	23	2.0
OCT	CHL	97.4	64	30	40	1.8	0.66	1.0	0.16	0.17	46	25	1.8
OCT	EAC	99.0	44	30	40	2.2	0.61	1.1	0.32	0.31	57	25	2.3
HEP	TCE	96.8	76	60	70	1.4	0.35	0.94	0.09	0.09	91	23	4.0
OCT	TCE	95.2	78	30	70	3.5	0.38	1.0	0.26	0.1	91	25	3.6
EOH	CCL	93.6	0	90	160	0.46	0.64	0.69	5.3	---	44	100	0.4
HEP	EAC	98.4	44	60	40	0.90	0.56	0.98	0.35	0.35	57	23	2.5
CHL	CCL	96.4	50	40	160	1.2	0.29	0.81	0.93	1.1	44	46	1.0
EOH	PCE	96.0	76	90	40	0.80	2.6	0.98	3.1	4.9	76	100	0.7
CHL	PCE	97.2	38	40	40	2.0	1.2	0.96	0.64	0.89	76	46	1.7
TOL	EOH	95.0	5.2	130	90	0.78	3.0	1.1	3.7	5.3	100	280	0.4
POH	PCE	95.2	56	30	40	2.4	2.5	0.82	2.5	3.0	76	98	0.8

[a] average recognition rate determined at an RCR = 1:1 over a concentration range of 5-10LOD for each component; [b] units = ppm; [c] array sensitivity in units of response/ppm; [d] E_{AB} is the Euclidean distance between normalized vectors for vapors A and B; [e] e_A and e_B are the Euclidean distances between the vectors for components A and B and the vector for their 1:1 mixture, respectively; [f] A is an index of asymmetry defined as the ratio of $lor_{95\text{-}A}/lor_{95\text{-}B}$ (see Figure 1a in text); [g] P is the product of the LOD and S for a given mixture component. [h] Linear regression of A vs. $(P_A/P_B)^{-1}$ yields an $r^2 = 0.894$.

Table SI-4. Range and asymmetry of relative concentration ratios evaluated at a minority-component concentration of 10LOD (RCR_{10}) for the 5-sensor CAP ST array determined with 12 binary mixtures.[a]

Mixture Components		RCR_{10}	Range of RCR_{10}	
A	B		12:1 11:1 10:1 9:1 8:1 7:1 6:1 5:1 4:1 3:1 2:1 1:1 1:2 1:3 1:4 1:5 1:6 1:7 1:8 1:9	
HEP	CHL	24	(20:1)	(1:1)
OCT	CHL	20	(7:1)	(1:3)
OCT	EAC	8	(6:1)	(1:2)
HEP	TCE	27	(9:1)	(1:3)
OCT	TCE	30	(8:1)	(1:4)
EOH	CCL	0		
HEP	EAC	8	(12:1)	(1:2)
CHL	CCL	15	(1:1)	(1:4)
EOH	PCE	27	(7:1)	(1:4)
CHL	PCE	16	(1:1)	(1:5)
TOL	EOH	5	(2:1)	(1:1)
POH	PCE	18	(1:1)	(1:7)

[a] the column of entries for RCR_{10} is the fold-range of relative concentration ratios for each mixture for which RR ≥95%. Each line spans that RCR range and shows the degree of asymmetry relative to the RCR = 1:1 value when concentrations are expressed as multiples of the LOD for each component. Values in parentheses at the end of a line are the corresponding RCR values in units of ppm.