

SUPPLEMENTARY MATERIAL

Quantifying BTEX in aqueous solutions with potentially interfering hydrocarbons using a partially selective sensor array

James S. Cooper^{a,*}, Harri Kiiveri^b, Lee. J. Hubble^a, Edith Chow^a, Melissa S. Webster^a, Karl-H. Müller^a, Andrea Sosa Pintos^a, Avi Bendavid^a, Burkhard Raguse^a and Lech Wiczorek^a

^aCSIRO Manufacturing Flagship, PO Box 218, Lindfield, NSW 2070, Australia

^bCSIRO Computational Informatics, 65 Brockway Road, Floreat WA 6014

*CORRESPONDING AUTHORS: PH: +61294137143, EMAIL: james.cooper@csiro.au

Table S-1 Components in the Synthetic Gasoline Mixture

		Name	Vol% of the component in the synthetic gasoline mixture	Solubility (mg/L)
straight	1	<i>n</i> -pentane	7.5%	40
	2	<i>n</i> -hexane	7.5%	9.5
	3	<i>n</i> -heptane	7.5%	3
	4	cyclohexane	7.5%	55
	5	<i>n</i> -octane	7.5%	0.66
branch	6	isopentane	7.5%	48
	7	2-methylpentane	7.5%	14
	8	3-methylpentane	7.5%	17.9
	9	isooctane	7.5%	2
	10	methylcyclopentane	7.5%	42
aromatic	11	1,2,4-trimethylbenzene	7.5%	57
	12	1-methyl-3-ethylbenzene	0.8%	39.99
	13	1,3,5-trimethylbenzene	7.5%	20
	14	1-methyl-4-ethylbenzene	0.8%	74.5
	15	1,2,3-trimethylbenzene	7.5%	75.2
olefin	16	1-hexene	1.0%	50

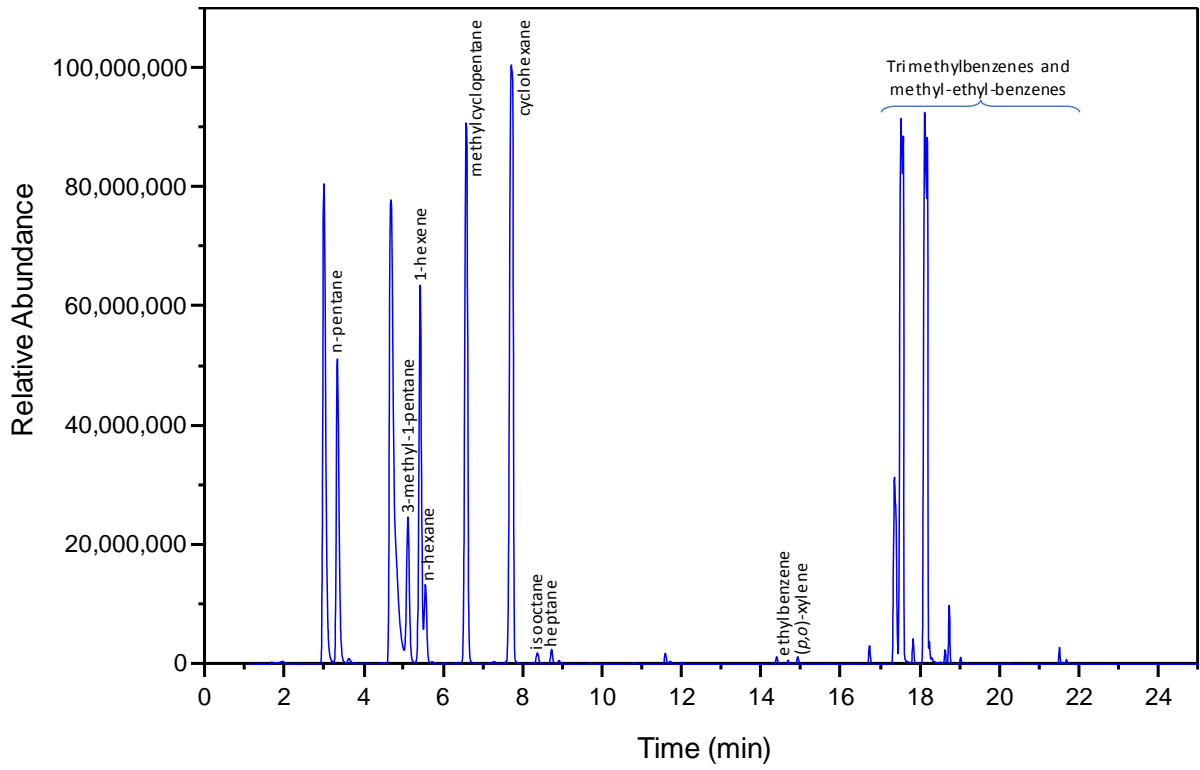


Figure S-1, GC-MS Spectra of water soluble fraction of the synthetic gasoline mixture

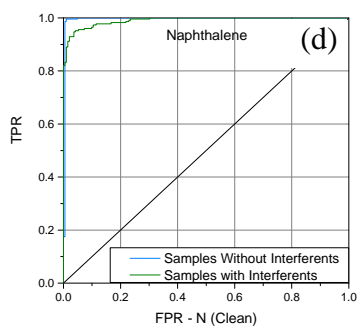
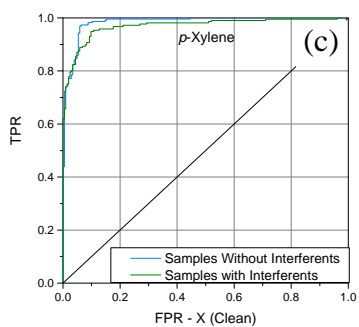
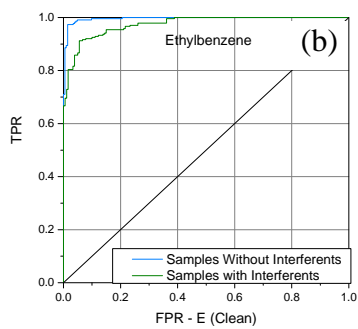
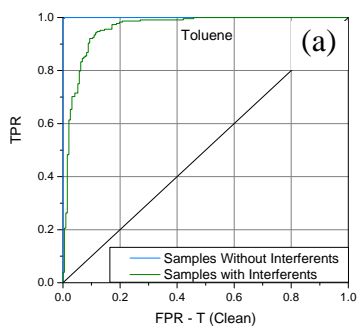


Figure S-2 ROC Curves for (a) toluene, (b) ethylbenzene, (c) *p*-xylene, (d) Naphthalene