Characterization of gaseous and particulate phase polycyclic aromatic hydrocarbons emitted during pre-harvest burning of sugar cane in different regions of Kwa-Zulu Natal, South Africa
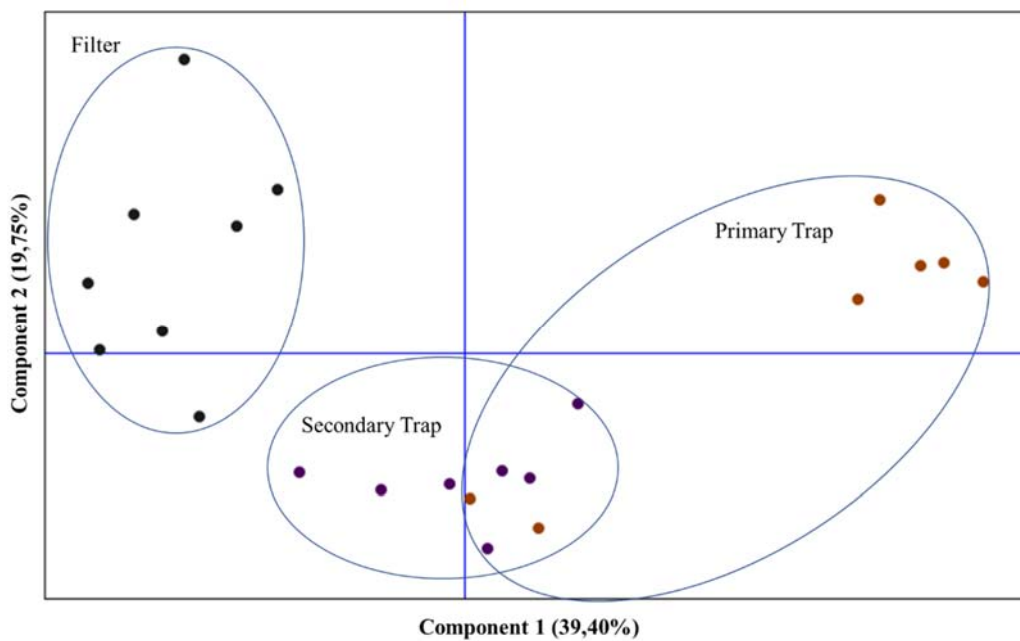
Supporting Information

Table S1 Quantified PAHs (µg m^{-3}) as the sum of the primary trap (PT), filter (F) and secondary trap (ST) for each burn event.

	Field Blank Nap	Field Blank Nap 1M
FB PT	0.27	0.38
FB F	0.78	
FB ST	1.25	

	Upwind Nap	Upwind Nap 1M	Downwind Nap	Nap 1M	Acy	Ace	Flu	Phe	Ant	FluAn	Pyr	Total
Burn 1 PT	<LOQ	<LOQ	0.86	0.40	0.32	<LOQ	<LOQ	0.04	0.09	<LOQ	<LOQ	**1.71**
Burn 2 PT	<LOQ	<LOQ	7.19	<LOQ	1.80	0.20	0.08	0.20	0.60	<LOQ	0.16	**10.23**
Burn 3 PT	<LOQ	<LOQ					Loss					
Burn 4 PT	<LOQ	<LOQ	<LOQ	<LOQ	0.06	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.06**
Burn 5 PT	<LOQ	<LOQ	3.09	0.05	1.29	0.19	0.03	0.56	<LOQ	0.22	0.18	**5.58**
Burn 1 F	Loss	Loss	<LOQ	0.05	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.05**
Burn 2 F	<LOQ	0.06	0.18	0.23	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.46**
Burn 3 F	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	0.18	**0.18**
Burn 4 F	<LOQ	<LOQ	<LOQ	0.09	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.09**
Burn 5 F	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**<LOQ**
Burn 1 ST	Loss	Loss	<LOQ	0.11	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.11**
Burn 2 ST	<LOQ	0.10	<LOQ	0.30	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.40**
Burn 3 ST	<LOQ	<LOQ	<LOQ	0.23	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.23**
Burn 4 ST	<LOQ	0.08	<LOQ	0.10	<LOQ	<LOQ	<LOQ	0.04	<LOQ	0.24	<LOQ	**0.47**
Burn 5 ST	<LOQ	0.08	<LOQ	0.07	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	**0.15**

Table S2: Data processing parameters for ChromaTOF Tile (Version v1.01.00.0, Leco, USA)

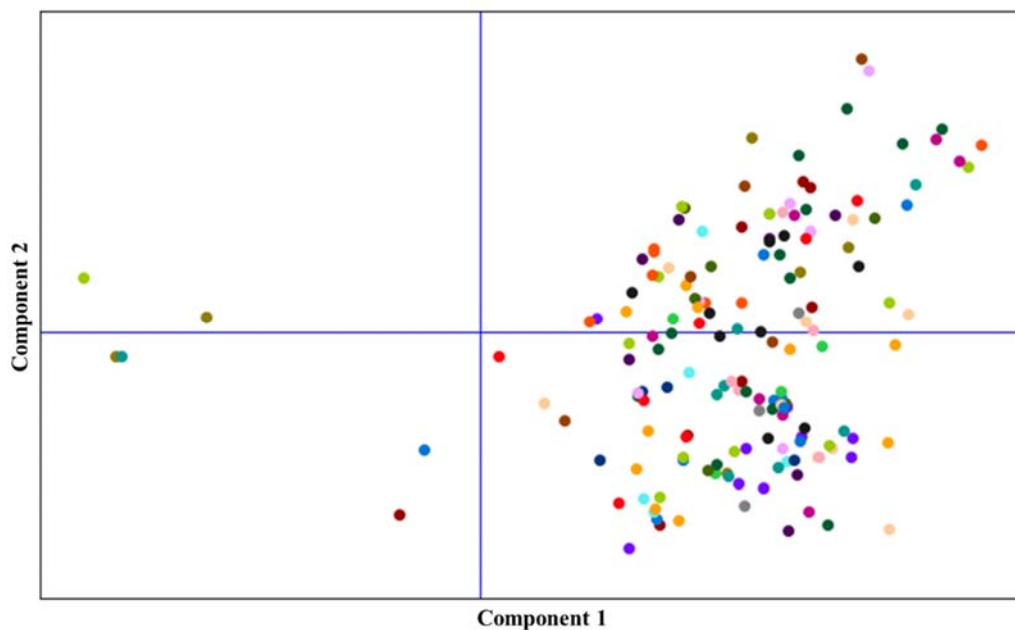| Parameter	Detail
Tile size D1 (modulations)	5
Tile size D2 (spectra)	12
S/N threshold	200
Samples that must exceed S/N threshold	3
Mass F-ratios to average	1
Threshold type to apply	p-value
p-value threshold	0.05
Minimum masses per tile	3
Minimum mass	29
Maximum mass	650

Figure S1 ChromaTOF Tile scores (top) and loading (bottom) plot for sampling and meteorological variables relating to individual burn events.

Figure S1. shows the PCA scores (top) and loading (bottom) plot for the primary trap, filter and secondary traps that take all other chemical compounds responsible for variance into account. The chemical compounds that had the highest loading are represented in **Table S2**.

Table S3: Chemical components with highest loadings towards the three classes of samples namely the primary trap, filter and secondary trap. Identification and similarity calculations were based on NIST library hits with a similarity >700.

Name	Similarity	Probability	CAS	Quant mass
1,2,3-Trimethoxybenzene	719	6947	634-36-6	168
1,3-Dioxolane	825	8841	646-06-0	66
1,3-Dioxolane, 2-heptyl-	836	6247	4359-57-3	114
2H-Inden-2-one, 1,3-dihydro-	767	7528	615-13-4	132
Azulene	886	6103	275-51-4	129
Benzaldehyde	863	8329	100-52-7	77
Benzene, 1,2,4-trimethyl-	895	3217	95-63-6	106
Benzene, 1,3-dimethyl-	947	5238	108-38-3	63
Benzene, 1-ethyl-4-methyl-	761	2144	622-96-8	134
Benzene, 1-methyl-2-(1-methylethyl)-	844	4520	527-84-4	114
Benzonitrile	825	5939	100-47-0	76
Benzonitrile, 2-methyl-	784	3751	529-19-1	116

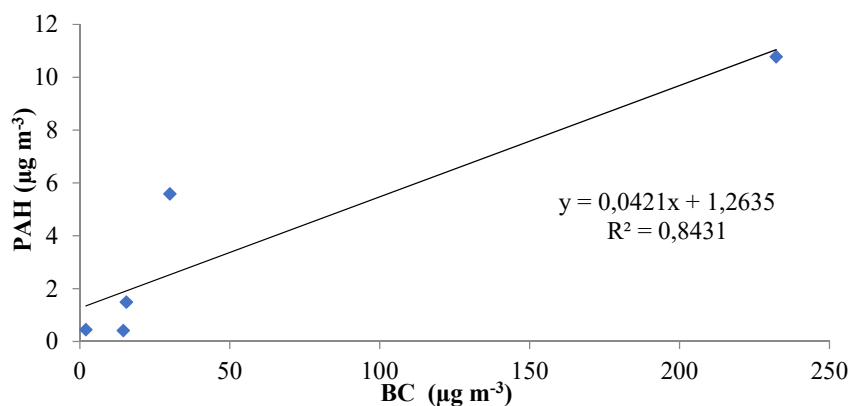| Biphenyl	738	7498	92-52-4	152
Biphenylene	871	7015	259-79-0	150
Decane	805	3229	124-18-5	85
Dibenzofuran	831	9440	132-64-9	168
Ethylbenzene	952	8429	100-41-4	75
Furfural	960	8174	1998-01-01	97
Heptane, 2,2,4,6,6-pentamethyl-	862	4877	13475-82-6	99
Indene	871	5686	95-13-6	116
Indole	821	6331	120-72-9	90
Naphthalene, 1-methyl-	889	5371	90-12-0	115
Nonane	912	7584	111-84-2	128
o-Xylene	957	4282	95-47-6	62
Phenol, 2-(1,1-dimethylethyl)-	764	3771	88-18-6	90
Phenol, 2-methoxy-	883	6643	1990-05-01	124
Phenol, 2-methoxy-4-(1-propenyl)-	883	6663	97-54-1	78
Phenol, 2-methoxy-4-methyl-	875	5034	93-51-6	63
Phenol, 2-methoxy-4-propyl-	710	7113	2785-87-7	137
Phenol, 3-methyl-	869	4984	108-39-4	90
Phenol, 4-ethyl-	897	6718	123-07-9	122
Phenol, p-tert-butyl-	766	5015	98-54-4	107
Phthalan	764	6456	496-14-0	92
Phthalic anhydride	905	6771	85-44-9	50
Styrene	927	6075	100-42-5	104
Tridecane	862	3512	629-50-5	99

Figure S2. Correlation between total PAH and black carbon (BC) emissions at each of the five burn events.