separations

Supplementary Materials

Table S1. Decomposition standard compounds analyzed and their retention times using the current optimized stage 2 method and instrumentation. Note: over the course of the study, the major peaks of all the standards appeared within ± 5 s in 1D and ± 0.1 s in 2D from the retention values listed below.

Standard mix	Name	1st Dimension retention time (s)	2nd Dimension retention time (s)
Standard mix 8	Formaldehyde	89.9981	0.481
	Butanal, 3-methyl-	409.978	0.594
	Pentanal	499.972	0.622
	Hexanal	764.955	0.653
	Heptanal	1049.94	0.668
	Octanal	1329.92	0.684
	2-Octenal, (E)-	1514.91	0.763
	Nonanal	1594.9	0.699
	Decanal	1844.89	0.718
Standard mix 2	Furan, 2-methyl-	279.986	0.569
	2-Butanol	324.983	0.723
	1-Butanol	459.974	0.862
	3-Pentanol	529.97	0.743
	Disulfide, dimethyl	589.966	0.682
	1-Pentanol	714.958	0.881
	Dimethyl trisulfide	1219.93	0.817
	Furan, 2-pentyl-	1229.93	0.653
	Indole	2229.86	2.371
Standard mix 1	Acetic acid, methyl ester	199.991	0.56
	Acetic acid ethyl ester	309.984	0.577
	2-Butanone, 3-methyl-	419.977	0.593
	2-Pentanone	484.973	0.617
	Methyl Isobutyl Ketone	609.965	0.615
	2-Heptanone	1024.94	0.664
	Butyrolactone	1254.92	1.342

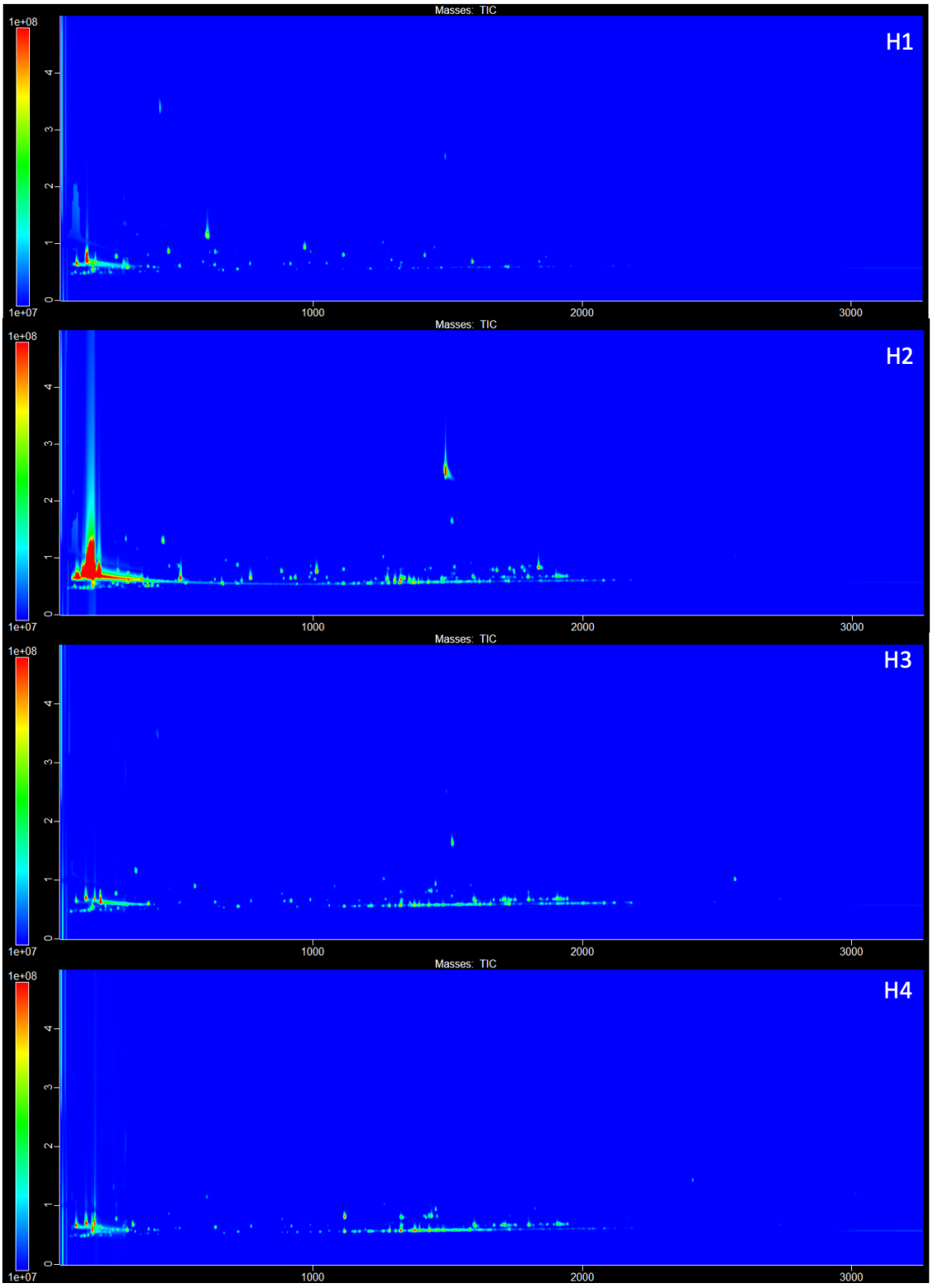

Figure S1. GC×GC-TOFMS total ion current (TIC) contour plots of headspace VOC samples collected from donors H1, H2, H3 and H4.

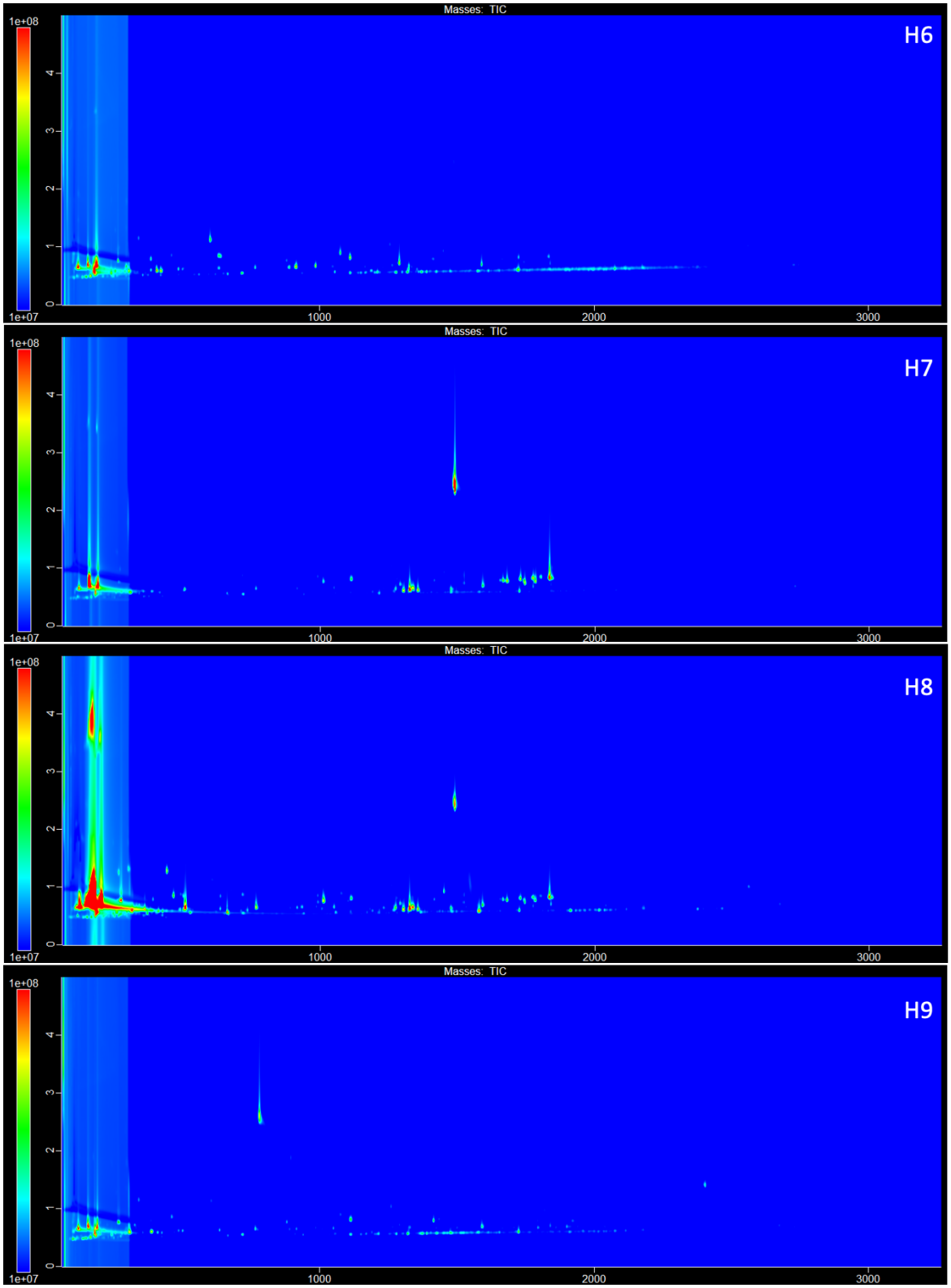

Figure S2. GC×GC-TOFMS total ion current (TIC) contour plots of headspace VOC samples collected from donors H6, H7, H8 and H9.

Table S2. List of compounds related to decomposition identified in lower PMI donors causing their separation and clustering in the scores plot made with seven donors. These compounds were located closest to the outer ellipses on the correlations loadings plot indicating a strong association and correlation with the donors causing variance in the VOC profiles.

Donor	Compound	Frequency of detection	Previously reported in decomposition literature
H8	Heptane,2-4 dimethyl	3	[27]
H8	Thiocyanic acid, methyl ester	3	[42]
H8	1H-indene-dihydro-4-methyl	3	Not detected
H8	Butanal, 3-methyl	5	[27]
H2 and H7	Terpineol	3	[32]
H6 and H9	Acetic acid butyl ester	5	[43]
H6 and H9	2-Propenoic acid, butyl ester	3	[43]
H6 and H9	Butanenitrile	3	[8,44]
H6 and H9	Butanenitrile 3-methyl	3	[44]
H6 and H9	2-pentanol	4	[43]