Electronic Supplementary Information

Development of an adaptable headspace sampling method for metabolic profiling of the fungal volatome

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Table S1. *A List of QC compounds and external standards with retention times*

VOC standards mix	Average retention time (min)	External standards	Average retention time (min)
Acetone	1.83 (co-elutes)	α-pinene	6.83
Isoprene	1.83	Camphene	7.25
Benzene	2.48	Longifolene	18.40
3-pentanone	2.71	α-bergamotene	19.31
1,4-dioxane	2.84	Humulene	19.77
Toluene	3.54	Valencene	20.58
Octane	4.00		
Butyl acetate	4.22		
p-xylene	5.36		
Nonane	5.95		
Benzaldehyde	7.55		
1-heptanol	7.62		
Decane	8.39		
3-carene	8.63		
Limonene	9.22		
Undecane	10.99		
Nonanal	11.21		
Tetralin	12.65		
Dodecane	13.56		
Methyl indole	15.30		
Tridecane	16.04		
Tetradecane	18.40		
Pentadecane	20.63		

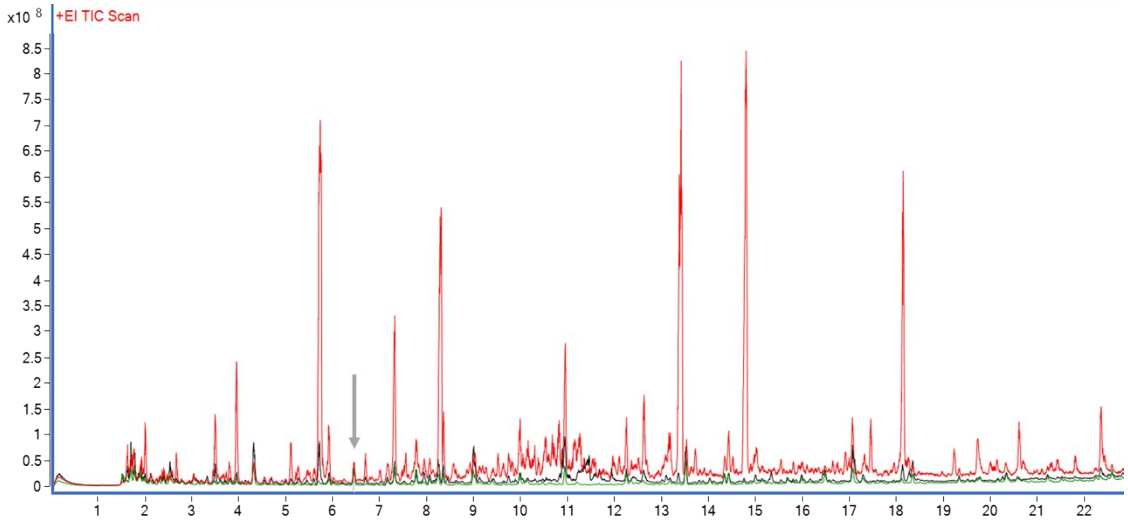

Figure S1. Typical headspace chamber material chromatgrams showing glass chamber (black), plastic chamber (red), sorbent only (green), and the internal standard highlighted (grey arrow)

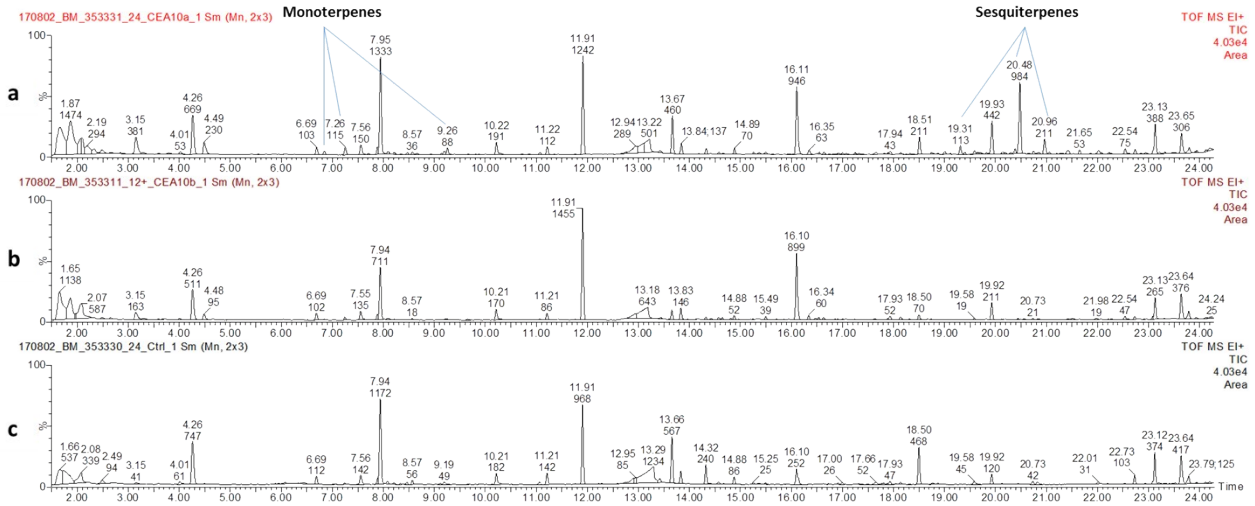

Figure S2. *Examples of TIC chromatograms of A. fumigatus CEA10, showing a) actively sampled headspace, b) passively sampled headspace from 12 to 24 h, and c) media-only control. Each peak is annotated with the retention time and integrated peak area. Monoterpenes and sesquiterpene compound peaks are annotated with blue lines.*

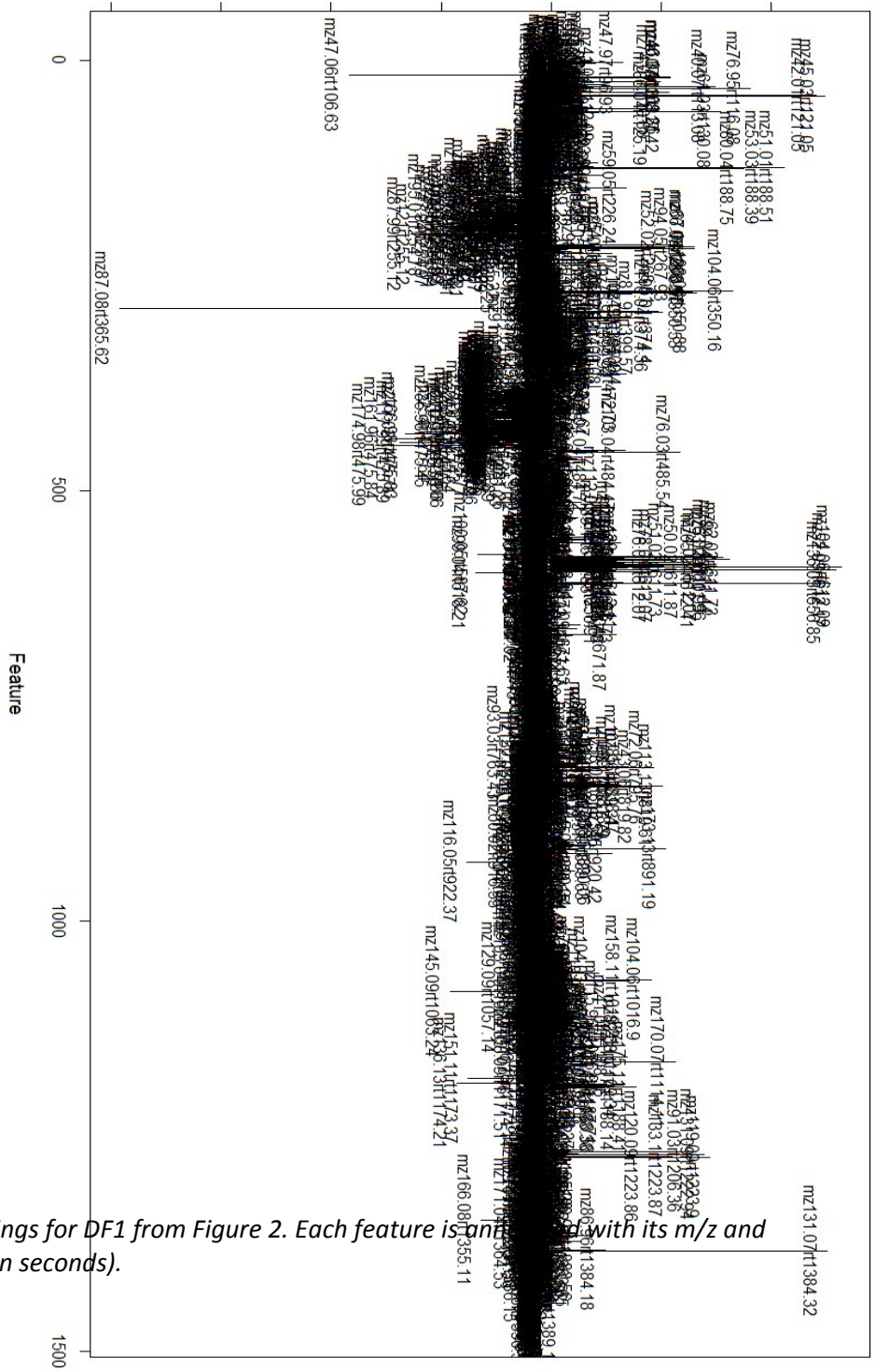

Figure S3. *PC-DFA loadings for DF1 from Figure 2. Each feature is annotated with its m/z and retention time (in seconds).*