Electronic Supplementary Material (ESI) for RSC Advances.

Rapid differentiation of microbial cultures based on the analysis of headspace volatiles by atmospheric pressure chemical ionization mass spectrometry

Supplementary Information

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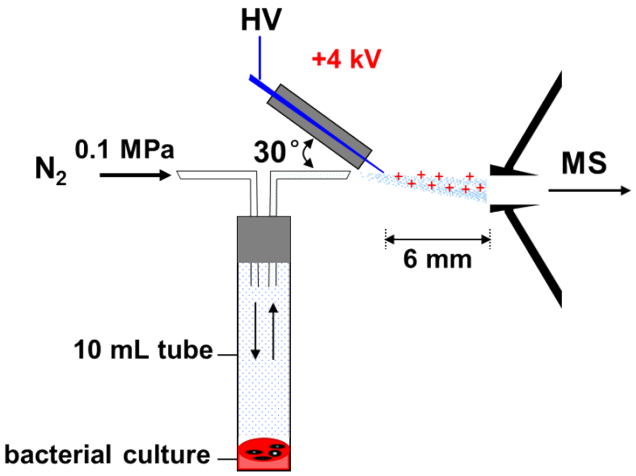

Figure S1: Headspace VOC analysis of microbial cultures by APCI-MS: VOCs from the headspace of a microbial culture in a 10 mL sealing cap round bottom centrifuge tube (Solarbio, Beijing, China) were continuously transferred for APCI with nitrogen carrier gas (0.1 MPa) via plastic tubing (ID 1.0 mm; OD 1.6 mm). To prepare sampling interface, the cap of a blank centrifuge tube was detached from the rest of the tube, and the inlet and the outlet gas lines were sealed onto the top of the cap. The assembly was firmly fixed in front of the LTQ. For APCI-MS analysis, open centrifuge tube with a microbial culture was connected to the mounted cap. To change sample simply required disconnecting the tube and connecting a tube with the next sample to the same cap. This operational workflow allowed the high throughput and reproducibility of analysis. Corona discharge source was built in-house and was used in our earlier studies for the analysis of surface chemicals by surface desorption atmospheric pressure chemical ionization (SDAPCI-MS). Discharge needle was normally maintained at +4 kV in positive (APCI+) ion detection mode and at -3.5 kV in negative (APCI-) ion detection mode. The angle between the needle and the outlet tubing was 30°. The distance from the tip of the needle to the end of the outlet tubing was 2 mm. The distance from the tip of the needle to the inlet of the LTQ capillary was 6 mm. Experiments were done on three different days. In total, each microbial strain was analyzed in ten biological replicates grown independently. APCI fingerprint of each replicate was averaged from the first 20 scans collected in the *m/z* range 60-200. The headspace of pure growth medium without microbes was analyzed for background

correction.

Table S1. Summary of VOC signals observed in this study specific to one or more of the microbial strains: AB = *Acinetobacter baumannii* in MH medium, EC = *Escherichia coli* in MH medium, SA = *Staphylococcus aureus* in MH medium, PA = *Pseudomonas aeruginosa* in MH medium, CA = *Candida albicans* in MH medium, CT = *Candida tropicalis* in MH medium, CP = *Candida parapsilosis* in MH medium, KP = *Klebsiella pneumonia* in MH medium, KP* = *Klebsiella pneumonia* in CBA medium; "+" = LTQ intensity < 10^3; "++" = LTQ intensity between 10^3-10^4; "+++" = LTQ intensity between 10^4-10^5; "++++" = LTQ intensity > 10^5. Tentative chemical assignment is done based on the earlier MS reports of volatile bacterial pathogens summarized in L. D. J. Bos, P. J. Sterk and M. J. Schultz, *PLoS Pathog.*, 2013, 9, e1003311.

APCI+										Tentative chemical assignment
m/z	AB	EC	SA	PA	CT	CP	CA	KP	KP*	
60	++			++					++	trimethylamine
63	++++		++++					++++	+++	1,2-Ethanediol
64		+++		++				++	+++	
70			++	+++						
71				+					++	
83									+++	
84				+					+	
91	+++	+++	+++	+++	++	++	++	+++	+	
100	+	+	+	+				+		
106	+	+	+	+	+	+	+	+	+++	
140					++	++	+++			
APCI-										Tentative chemical assignment
m/z	AB	EC	SA	PA	CT	CP	CA	KP	KP*	
73		+++	+++					+++	++	propionic acid
87			+++		+++		+			ethyl acetate
90	++	++	++	++				++	+++	
92									++++	
101			++++		++	++	++			isovaleric acid
102			++							benzonitrile
103			++							
104		++	++					++		
105			++							
106		++	++					++	++	
115			++							ethyl butanoate
116		++								indole
117			++							
118			++		++	++	++			
119			++						++	
120			++		++					
121			++	++					+++	
132			+++		++	++	++			
134			++							

135		++	++							
148		++	++							
163			++		+	+	+			