Supporting Information

for

The volatiles of pathogenic and nonpathogenic mycobacteria and related bacteria

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Identification of compounds

The following compounds were identified by comparison with mass spectra and retention indices of authentic samples: 4-hydroxy-4-methylpentan-2-one (**14**), 4-pentanolide (**10**), methyl 2-furoate (**15**), 4-methylanisol (**5**), methyl benzoate (**8**), 2-phenylethanol, methyl nicotinate (**3**), ethyl benzoate (**9**), methyl phenylacetate (**1**), methyl salicylate (**6**), benzothiazole, methyl 2-aminobenzoate (**7**), methyl *p*-anisate (**2**), ethyl *p*-anisate (**18**), 2-phenylanisol (**4**), dimethyl disulfide (**11**), dimethyl trisulfide (**12**), 6-methylhept-5-en-2-one, dimethyl tetrasulfide (**13**), ethyl salicylate, 1-hexanol (**20**), phenol (**21**), camphor (**22**), 2-methylbutanol, methyl isovalerate, isobutyl isobutyrate, indole, 2-aminoacetophenone, 2-hydroxypentan-3-one, linalool. These compounds were available in our in-house compound library, originating from suppliers such as Aldrich, Acros, Fluka or, were synthesized previously.

The lactones 3-methyl-4-pentanolide (**16**) and 4-methyl-5-hexanolide (**17**) show characteristic mass spectra and occur as two closely eluting peaks: the two possible diastereomers. Aciphyllene (**19**) shows an identical mass spectrum and retention index to those reported in a critically evaluated data compilation [S1].

The compounds methyl methylsalicylate, methyl dimethylbenzoate (**24**), and methylbutenolide exhibited mass spectra similar to those in mass-spectral libraries, but no information of the retention indices of all possible isomers was available. Therefore, a full characterization was not possible. The mass spectrum of trimethyloxazole was identical to those in the databases, but again no retention-index information was found.

Table S1: Details of microorganisms used for the analysis of volatile compounds.

No.	Species	Strain	Source
1	*Mtb*	H37Rv	Lab. strain
2	*Mtb*	H37Ra	Lab. strain
3	*Mtb*	Beijing 2	Human-Netherlands
4	*Mtb*	Beijing 5	Human-South Africa
5	*Mtb*	Beijing 6	Human-Mongolia
6	*M. smegmatis*	MC^2155	n/a
7	*M. avium* subspecies avium	n/a	n/a
8	*M. scrofulaceum*	n/a	n/a
9	*M. vaccae*	n/a	n/a
10	*M. aichiense*	LMG 19259	Soil
11	*M. aurum*	LMG 19255	Soil
12	*M. neoaurum*	LMG 19258	Soil
16	*Nocardia asteroides*	LMG 4062	n/a
17	*N. africana*	DSM 44499	Human-Sudan

Media composition

Middlebrook 7H9 Broth

Approximate formula per liter of purified water: monopotassium phosphate 2.0 g, disodium phosphate 1.5 g, monosodium glutamate 0.5 g, sodium citrate 0.1 g, ammonium sulfate 0.5 g, pyridoxine 0.001 g, zinc sulfate 0.001 g, copper sulfate 0.001 g, biotin 0.5 mg, calcium chloride 0.5 mg ferric ammonium citrate 0.04 g, magnesium sulfate 0.05 g,
ADC enrichment: sodium chloride 0.85 g, bovine albumin (fraction v) 5.0 g, dextrose 2.0 g, catalase 4.0 mg, sodium pyruvate 1.0 g

Difco™ Mycobacteria 7H11 Agar

Approximate formula per 900 mL purified water:
Pancreatic digest of casein 1.0 g, L-glutamic acid 0.5 g, sodium citrate 0.4 g, pyridoxine 1.0 mg, biotin 0.5 mg, ferric ammonium citrate 0.04 g, ammonium sulfate 0.5 g, disodium phosphate 1.5 g, monopotassium phosphate 1.5 g, magnesium
sulfate 0.05 g, agar 15.0 g, malachite green 1.0 mg
OADC enrichment: Approximate formula per liter purified water:
bovine albumin 50.0 g, dextrose 20.0 g, catalase 0.03 g, oleic acid 0.6 g

References

[S1] Joulain, D.; König, W. A. *The Atlas of Spectral Data of Sesquiterpene Hydrocarbons*; E.-B. Verlag: Hamburg, 1998.