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### ACCEPTED MANUSCRIPT

# Molecule confirmation and structure characterization of pentatriacontatrienyl mycolate in *Mycobacterium smegmatis*

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#### HIGHLIGHTS

- Mycolate ester wax found in *Mycobacterium smegmatis* was accurately characterized
- Mycolate ester wax structure corresponds to pentatriacontatrienyl mycolate,
  PTTM 1
- The characterization was based on 1D and 2D NMR analysis
- These results allow the future quick identification by a 1D <sup>1</sup>H NMR experiment

#### **ABSTRACT**

*Mycobacterium smegmatis* is often used to study the different components of mycobacterial cell wall. Mycolic acids are important components of mycobacterial cell wall that have been associated with virulence. Recently, a novel lipid containing mycolic acids has been described in *M. smegmatis*. However, some uncertainties regarding the structure of this molecule named mycolate ester wax have been reported. The objective of this work was to perform an in depth structural study of this molecule for its precise characterization. Using <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy, the molecular structure of mycolate ester wax found in *M. smegmatis* has been elucidated. The

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