



SOFTWARE

FAMEs Fatty Acid Methyl Esters: Mass Spectral Database

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Software
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Description

Fatty acids are important compounds in food analysis, since they are sample-specific. They can be used as markers or their profile can be used as a fingerprint (e.g., bacteria fatty acids) or to reveal fraud (e.g., seed oil added to olive oil). In GC, fatty acids are analyzed after derivatization to methyl esters (FAMEs). FAME is a library of 240 spectra and structures of **fatty acid methyl esters**, including their Linear Retention Index and calculated Kovats Retention Index.

The database contains linear retention index data, registered using an alkane mixture on an apolar column and using also a FAMEs and a FAEEs (**fatty acid ethyl esters**) mixture on a polar one. The addition of the retention index data enables more reliable compound matching and identification of unknowns.

While other methods, such as LC-MSMS can be used, when using such a highly selective method technicians can only detect what they are looking for, while when performing broader TIC screening using GC/MS, no information is lost. Applications include building FAMEs profiles of target bacteria (e.g., *Pseudomonas aeruginosa*).

- Each record contains the mass spectrum, searchable structure, chemical information, and LRI retention data
- Records indexed by name, molecular weight, and retention time
- Highly controlled: Measured on a single instrument in controlled conditions
- Quality samples sourced from leading suppliers and manufacturers

Available in six manufacturer formats for use with most common mass spectrometry applications: 1) NIST MS Search, 2) Agilent Chemstation, 3) PerkinElmer TurboMass, 4) ThermoFisher Spectral ID, 5) Waters MassLynx, and 6) ACD/Labs MSManager.

A version in the Shimadzu GCMS Solution format is available directly from [Shimadzu](#). Data were acquired on a GCMS QP2010 Plus (Shimadzu), Autosampler AOC-20i (Shimadzu), split/splitless injector inlet, Supelcowax 30 m x 0.25 mm x 0.25 µm (Supelco), Helium in constant linear velocity mode (35cm/s) carrier gas, with an oven temperature of 50°C to 280°C (or 350°C) at 30C/min. Ion source temperature 220°C, interface temperature 250°C, scan range 50-550 u, EI 70 eV.