BIO-RAD

Spectral **Databases**

ATR-IR - Flavors & Fragrances - Bio-Rad Sadtler

Product Code - This database is available only as part of the KnowItAll® IR Spectral Library Spectra - 600

Bio-Rad Laboratories is the leading producer of IR and Raman spectral databases with their Sadtler™ Spectral Databases, known for their high-quality.

Description

This ATR-IR spectral database provides scientists with a representative collection of 600 spectra of compounds used in the manufacture of flavors and fragrances, natural product oils, synthesized fragrance compounds, etc. It includes compounds approved by the Flavor and Extracts Manufacturers' Association of the United States (FEMA) and the FEMA number is listed when available.

Additional Information

The following information is supplied for each record when available: name, synonyms, CAS Registry Number, catalog number, lot number, source of spectrum, source of sample, instrument name, technique, melting point, boiling point, flash point, density, sample type, physical state, purity, storage requirements, molecular weight, and molecular formula. Molecular structures are also available with the database.

Technique

Every effort is made to maintain the highest standard of accuracy for spectra placed in the Sadtler collections. Each compound was prepared under standard conditions at Bio-Rad Laboratories, Informatics Division Laboratories. All spectra were run using a Bruker Tensor 27 FT-IR spectrometer with a DuraSamplIR II accessory which is an in-compartment, single reflection, diamond ATR accessory. Three different techniques were employed: ATR Neat, ATR Film, and ATR Suspension.

- The ATR Neat technique was used for liquids, pastes, oils, and materials with melting points < 120°C. The ATR Neat technique is also used for solids or crystalline materials with melting points >120°C.
- The ATR Film technique is only used for compounds that are too strong with the ATR Neat technique. The solvent used is usually acetone unless noted otherwise.
- The ATR Suspension technique is only used for samples that display the Christiansen effect and do not readily dissolve.

Samples were checked to ensure that non-linearity was avoided to maximize reproducibility and provide for the best subtraction of reference spectra. Any spectra with evidence of decomposition, impurities, or reaction with sampling apparatus were rejected.

Each spectrum was then reviewed independently before inclusion in the database. These quality control procedures provide the best sample purity and structural formula confirmation available for the broad range of compounds in the collection.

This collection has been subject to the Sadtler Data Review Protocol™ to provide you with the highest standard in spectral data today. These rigorous qualifying procedures start at data acquisition and continue throughout the database development process.