

# IdentifyIR™

CUSTOMIZED FOR SYNTHETIC ORGANIC CHEMISTRY APPLICATIONS



#### Rapid Results for Optimizing Organic Chemistry

- Reaction spot-checking and end-point analysis
- Solid form screening
- Reaction profiling
- Compound identification and verification
- And much more....

IdentifyIR is a rugged, miniaturized FT-IR (Fourier Transform Infrared) analysis system that is fast, easy-to-use, and accurate. Designed specifically for tasks performed by organic chemists and chemical engineers, its ChemAssist software takes the mystery out of IR analysis – it is like having a team of IR experts by your side.

IdentifyIR's small footprint (only 7"x14"), sturdy all-metal construction, and sealed housing make it ideal for use in the hood or on the bench.

IdentifyIR uses a diamond attenuated total reflection (DATR) sampling interface, which means it can rapidly analyze any solid or liquid sample, including caustic and corrosive materials. The integrated 100x video microscope facilitates both spectral and visual characterization of solid forms. Video images and infrared spectra are linked for rapid screening of polymorphs and solvates.

IdentifyIR and ChemAssist™ together provide rapid results for faster decision making.

#### Product Highlights

- Easy to use - no spectroscopy expertise required
- Little to no sample prep
- Results in seconds - not minutes or hours
- Works where you work: in the hood or on the bench

## Diamond ATR (DATR)

DATR sampling interface offers several advantages:

- Rugged: diamond is impervious to organics, acids, bases, reducing and oxidizing agents, and solids pressed against it to ensure proper contact cannot scratch it.
- Versatile: can handle powders, solids, liquids, gels, and pastes in both organic and aqueous solvents.
- Easy cleaning: sampling surface cleans up in seconds by wiping with ordinary solvents, making it ready to analyze the next sample with virtually no delay.
- Optical performance: provides state-of-the-art accuracy and precision.
- Pathlength selection: pathlength (*i.e.*, the number of reflections through the diamond crystal) can be selected to match the application requirements.

## ChemAssist Software

ChemAssist instrument control and data analysis software eliminates the need for IR spectroscopy expertise to obtain accurate and valuable information about the user's materials and reactions.

This easy-to-learn and easy-to-operate software includes organic chemistry-specific task modules for tracking chemical changes, characterizing solid forms, and identifying and verifying materials.

Each task module features customizable, one-click report generation.

The heart of ChemAssist is a proprietary database of molecular functional groups and their characteristic IR absorption frequencies. Specialized algorithms within ChemAssist

use this database, along with molecular structures entered by the user, to automatically create an optimized set of IR absorption bands that can be used, for example, to measure chemical changes. In addition, ChemAssist can identify the presence of functional groups based on a sample's IR spectrum – whether the user is tracking a reaction in progress or analyzing an unknown. ChemAssist makes IR correlation tables a thing of the past for the practicing chemist.

ChemAssist can also search on-board spectral libraries to verify the identity of materials and identify unknowns. These libraries can be customized for the user's own proprietary compounds.

## Technical Data

### General Specifications

Input Power	100-240 VAC, 2.0 Amps max, 50-60 Hz
Weight	22 lbs. (10kg)
Size	7" x 15" x 14" (18 cm x 39 cm x 36 cm)
Range	4000 to 650 cm <sup>-1</sup>
Sample Size	As small as 5 µL or 100 µm
Sample Interface	DATR
ChemAssist User Interface	Easy-to-use interface with Wizard-guided method set-up
Operating System	Customized for organic chemistry tasks
Computer Interface	Windows XP
Integrated Video Microscopy System	USB 2.0
Options	100x Magnification Solids & Liquids Configuration Liquids-only Configuration 1, 3, and 9 reflection DATR disks Inert atmosphere sampling cell Aldrich/Smiths Detection ATR Spectral Libraries IChem STJapan ATR Spectral Library Smiths Detection ATR Libraries

### USA

Smiths Detection Inc.  
14 Commerce Drive  
Danbury, CT 06810  
T: +1 203 207 9700  
F: +1 203 207 9780  
[danbury@smithsdetection.com](mailto:danbury@smithsdetection.com)

### INTERNATIONAL

Smiths Detection Ltd.  
Genesis Centre  
Science Park South  
Birchwood  
Warrington WA3 7BH  
T: +44 (0) 19 2583 8494  
F: +44 (0) 19 2583 8463  
[sddinternational@smithsdetection.com](mailto:sddinternational@smithsdetection.com)