Hydrocarbon Expert™
Detailed Hydrocarbon Analysis Made Easy
Hydrocarbon Expert™ software was the very first to exploit the power of on-screen computer graphics and comprehensive time mapping algorithms to make it very easy for GC operators to reliably identify individual components in ‘light’ hydrocarbon streams/feedstocks (ex. naphtha, reformate, gasoline, jet fuel, alkylate) without a high level of skill and experience. Since its introduction, it’s become recognized worldwide as the gold standard when it comes to detailed hydrocarbon analysis (DHA).

Hydrocarbon Expert™ is compatible with all popular GC Chromatography Data Handling Software systems including: Agilent GC Chemstation, Agilent OpenLab, Agilent EZChrom, Thermo/Dionex Chromeleon, Thermo Atlas, PerkinElmer TotalChrom, Justice Innovation ChromPerfect, Data Apex Clarity, Scion Compass and others.

The software includes hydrocarbon component templates and a calibration standard containing nearly 400 individually identified peaks (using MS) to adjust the template to your GC/conditions to establish and build your own hydrocarbon component database(s).

Now with the available Hydrocarbon Expert/MS™ module analysts are able to identify individual peaks not contained in the component database and/or co-eluting species by simultaneously using a mass spectrometry detector (ex. MSD) to produce high quality spectra that can be automatically compared to spectral databases.

This diagram represents a small section of a DHA chromatogram showing identified components and ‘undefined’. Hydrocarbon Expert™ dramatically simplifies the identification of undefined components using reference component database templates.
Comprehensive pattern recognition (Sure-ID™). The original algorithm was modified to be more accurate and forgiving to subtle pattern variations. It is now applied to the whole signal, not just ‘marker’ peaks. All the components are identified with a single click of the mouse. The algorithm is built into the software. Therefore it is available to all GC data acquisition systems. Pattern recognition is carried out on the original unadulterated signal, not on a time shifted chromatogram.

Tangent peaks can be drawn in the built-in graphic integrator.

HCDX file format consolidates HCD and HCX into a single container.
  - Reduces the complexity of keeping track of identification databases and templates
  - The identification template is automatically displayed with the corresponding signal
  - Backward compatibility is maintained with HCD and HCX files.

Molecular weight and specific gravity are available in most of the available reports.

Summary by carbon in a tabular format has been added to the list of calculated reports.

Instantaneous highlighting of conflicting peak identification. Duplicated components are highlighted in red while components out of elution order are highlighted in yellow.

On-click continuous alignment. When this option is activated, the reference signal is automatically aligned with the sample signal every time when a component is transferred.

Two points signal stretching. This feature facilitates setting the same time scale between the sample and reference signals. Tandem stretching is achieved by selecting two points in the sample signal and two corresponding points in the reference signal.

System templates are stored in a protected database to ensure integrity. A template can be restored by specifying the part number of the calibration standard, the chromatographic method and the carrier gas used.

Signal template information dialog. Reveals the signal file and the identification template used to create the reference template.

% Oxygen was added to the “Additional Properties” report. This is particularly useful information for ASTM-D5501.

Redesigned user interfaces
  - Load sample signal dialog:
    - Templates can be loaded from multiple locations in the software
    - % Water and % Recovery can be overwritten. % Water correction is useful for ASTM D5501.
    - Signal processing order can be altered by clicking and dragging files
  - Configuration dialog
    - Groups are displayed in a tree-hierarchy structure
    - Groups can be disabled so components belonging to the disabled group will not be automatically identified.
    - More options to set RF, MW and Specific Gravity for unknown components.
  - Component selection dialog
    - Can be configured to display unassigned components only
    - Co-elution ratios can be set without going to the component table
    - Additional information such as group type, carbon number and time offset is also displayed.
    - Shows the area percent of the selected peak
  - Peak label dialog
    - Groups displayed in a tree-hierarchy structures
    - ‘Select’ and ‘Unselect All’ buttons were added
Most Probable ID for Unknown Peaks is Selected

Components

51.992 min  0.2358%

Group: Naphtheno-Olefins
Carbon: 8  Offset: 2.320

3,5-Dimethyl-3-heptene
Group: iso-Olefins
Carbon: 9  Offset: 2.732

2,5-Dimethylheptane
Group: iso-Paraffins
Carbon: 9  Offset: 3.098

m-Xylene  p-Xylene

52.50  54.00  55.50  57.00  58.50  60.00

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Two Point Signal Stretching

Misaligned

Aligned

www.separationsystems.com
Compare unlimited number of signals and reports. Comparison can be carried out at any level. From summary by group to custom formulas.
Eliminates the need to jump from the Hydrocarbon Expert™ to the GC Data System and Back to Reprocess Signals. And with Tangent Skimming, it is the perfect tool to carry out ASTM D5501.

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Groups & subgroups can be configured

Many configurable preferences

Extend calculations via the built-in Formula Editor

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This capability is useful when differences between the reference signal and sample signal are not easily discerned. In this mode the superimposition of the signals can be adjusted by a single pixel to make sure they are clearly aligned.
Additional Software Highlights

- Compatible with Windows XP and above
- Complies with ASTM D-6729 and ASTM D-6730. Can also be customized to any other method.
- On-screen peak identification. This feature allows to visually verify and correct the identification carried out by the built-in algorithms. The sample chromatogram is displayed on the screen with components' name on the apex of each identified peak. No typing is required to make corrections.
- Built-in peak integration. The signal can be re-integrated within the analysis environment.
- Allows class sub-grouping.
- Improved octane number calculations.
- Can use Mass Spectrometry data to improve peak identification accuracy. It requires the NIST database, an MS acquisition system (i.e. Thermo Xcalibur, Agilent MassHunter, etc.) and the Separation Systems MS Module.
- Allows the creation of reference chromatograms. This is a very powerful tool when used in conjunction with On-screen Peak Identification. It can help reduce uncertainty by visually identifying elution patterns.
- All the reports can be reviewed on-screen.
- Any component can be designated as reference. Instead of using the traditional KOVATS indices approach, which limits the references to normal paraffin, Hydrocarbon Expert uses a set of polynomial equations. These equations predict the retention time of a particular peak based on the time shift of any other two components. This approach also eliminates the need to carry out a primary and secondary calibration.
- Customizable reports. Chromatogram and calculations can be combined into a multi-page printed report.
- Reports can be saved into an ASCII delimited file and Microsoft Excel.
- Users and access levels can be defined for security purpose.
- Multiple stored reports can be compared, both on screen and on paper, against the sample being analyzed.
- Several reference chromatograms can be overlaid during the analysis.
- Customizable groups. Group names can be added, removed or changed. Each group can also be included or excluded from the normalization.
- Co-elution. Two or more components can be assigned to the same integrated peak. The co-elution ratio can also be specified.
- Grouping. Several integrated peaks can be reported as a single component.
- Automatic pattern recognition of reference peaks. When activated, this feature improves the reproducibility by identifying the reference peaks based on elution pattern instead of time windows.
- Quick check of possible names for unidentified components. Only the available labels will be displayed based on the identified components that precede and succeed the unknown peak.
- Zoom in through clicking and dragging.
- User-defined correlation points can be added and optimized.
- Customizable report header.
- Formula editor.
- Multi-language: English, Spanish
- Available for Client/Server configurations

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- Tightly integrated and streamlined FID and MS workflow. No need to switch between different data software systems.
- Verify and extend FID identification by spectral review and NIST/Wiley MS databases searches.
- Unlimited individual extracted ion signals.
- Spectrum clean-up tool to remove individual masses to simplify identification
- Create your own proprietary component database.
For additional information please contact us:

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