# Why is TDT Air Scan® different from the library search that other laboratories provide?

*Prism's clients must be able to rely on the accuracy and validity of the data they receive because they are staking their professional reputation on it. That is why professionals choose TDT Air Scan® and place their trust in Prism Analytical Technologies*

## Library Search

Prism does not offer library searches to its clients because they are unreliable. Any laboratory with a computerized GC-MS can do a library search on all of the peaks in a chromatogram. Any operator, no matter what educational or experience level, can perform the library search operation after only a few minutes training. This appears to be a wonderful application of modern technology; however, the library identification is frequently incorrect. Incorrect identification of compounds causes several problems, especially when a particularly hazardous compound is identified. This type of misidentification can mandate unnecessary and expensive follow-up testing, can cause grave concern when it is unwarranted, and can embarrass the submitter in front of his client. Misidentification arises primarily because every library search routine will select one compound as the best match. Oftentimes the second best match, which is a completely different compound, is only minutely lower in its search quality. Also, different search criteria will result in the selection of different compounds as having the best match. In some cases, the computer will select an outlandish compound which is totally inconsistent with the retention time. This uncertainty is seldom, if ever, transmitted to the submitter as part of the analytical report. As a result, the submitter has no idea whatsoever of the validity of the results. An example of these problems is shown in the following table:

| Library Search Misidentification | Correct Identification | Comments |
|---|---|---|
| Propionaldehyde (80% quality) | Acetone | If high levels of a compound are present, chemical ionization may occur which will alter the mass spectrum. This will cause the library search to misidentify the compound. |
| Isobutanol | Isopropanol | Library searches do not consider retention time and, therefore, cannot take into account the fact that the compound eluded before tert-butanol. It is not possible for the compound to be a C4 saturated alcohol. |
| Propane | Formaldehyde | The library search was not able to take advantage of supporting infrared data available to an Air Scan analyst. |
| 2-methylcyclopentanone | α-pinene and cyclohexanone | The library search did not recognize that the peak is actually two overlapping peaks. |
| Tridecane | Tetradecane | Especially on higher molecular weight compounds, the library search frequently misidentifies compounds. That is why it is important to have available an in-house library that contains hundreds of reference compounds with exact retention times and reference mass spectra. |

# TDT Air Scan® Analysis

An TDT Air Scan® analysis is performed by an analyst with a minimum of a BS degree in chemistry and at least one year of closely supervised training in mass spectral interpretation. In addition to having a large, in-house library of compounds listing reference mass spectra as well as retention times, an Air Scan analyst has several other tools available. To determine the validity of the compound identification, the analyst will use various computerized search algorithms, his knowledge and skill in mass spectral interpretation, his supportive data from the Fourier Transform Infrared, and his experience in the details and quirks of GC-MS analysis. The operator must be at least 95% confident in the validity of an identification before it will be listed specifically by

name under "Compound" in a TDT Air Scan® analysis. Where there is uncertainty in the validity of the identity of a compound, that level of uncertainty is written in standardized format and is provided to the submitter as part of the analytical report. This is shown in the following table:

| **Level of Certainty** | **This is an example of what is reported in the TDT Air Scan® report** | | | |
|---|---|---|---|---|
| | **Compound** | **Calculated(1)** | **Actual(2)** | **Comments** |
| Quantitative (Calibrated) | 1,1,1-Trichloroethane | | 56 | 1,1,1-TCA PPB 10 MW 132 CAS 71-55-6 |
| Semiquantitative (95% Confident) | Ethylene glycol | 67 | 33-140 | 1,2-Ethanediol PPB 26 MW 62 CAS 107-21-1 |
| Semiquantitative (75% to 95% Confident) | C5-C7 Hydrocarbon | 32 | 16-64 | 22.7 min; Oxygen-containing; probably hexanal |
| Semiquantitative (50% to 75% Confident) | C5-C7 Hydrocarbon | 80 | 40-160 | 26.0 min; Oxygen-containing; possibly 2-butoxyethanol |
| Semiquantitative (Less Than 50% Confident) | C5-C7 Hydrocarbon | 17 | 8-34 | 31.1 min; Oxygen-containing |

*Notes:*

1. *For compounds for which we do not maintain calibration curves, an estimated concentration is calculated based on the ion abundance relative to an internal standard. The calculated result is listed on the report primarily for serving as a basis for comparison between samples. Since the fragmentation pattern and efficiency are always the same for a specific compound, the calculated results can be quantitatively compared between samples. However, it is estimated that the actual result will fall between the limits listed. These limits are typically 50% to 200% of the calculated result.*
2. *For compounds for which we maintain calibration curves, the actual result is presented as a number (two significant figures). This is a quantitative determination*

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