

DATA ANALYSIS SCAN PROTOCOL

A target list was developed from previous experience. Selectivity and sensitivity was enhanced by employing target ion verification analysis (TIVA) developed by OSB Lab which permits integration of target ion reconstructed chromatograms with downloading of ion areas to the EXCEL spreadsheet.

TIVA requires that ion areas be multiplied by a suitable constant (MF) to generate equivalent total ion counts (TIC) as integrated areas. The MF was obtained experimentally for each target chemical using calibration gas standard TIC areas divided by selected ion areas. This is possible because ion ratios for each chemical remain intrinsically constant. TIVA is a similar but limited substitute for SIM mode. TIVA has a significant advantage at the detection limit (NDL) where coelution or background interferences mask the recovery of any target compound run in SCAN mode.

The method detection limit (MDL) is a statistically defined decision point such that measured results falling at or above this point are interpreted to indicate the presence of analyte in the sample with a specified probability, and assumes that there are no known sources of error in identification or biases in measurement.

Organic chemicals exhibit different sensitivity (response) to the mass selective detector. This is primarily due to the formation of a unique mass fragment distribution for each compound. The sensitivity or response is concentration dependent but not a simple linear relationship throughout a broad concentration range. Response may not be continuous or predictable between zero and the MDL test value (5-10 times the estimated MDL). Many chemicals exhibit high detection thresholds due to poor fragmentation or artifact formation.

MDLs are deliberately determined at a stable response-to-concentration level to provide reliable interlaboratory comparable benchmarks. The NDLs, which do not have a set quantifiable instrument response, are determined at the detection threshold level (presence/absence) to demonstrate statistically the absence of an analyte in SCAN mode.

NDLs fluctuate with daily instrument sensitivity and sample conditions. NDLs are reported for calibration standard response areas ranging from trace to 1.5 million counts (TIC). Sample concentrations have been calculated for target list chemicals as low as 0.1 million counts (TIC). Concentrations less than this minimal value have been usually reported as <(TR). The following convention has been adopted at OSB Lab:

- Blank = Below integration threshold but presence or absence was not verified by manual search
- < = Manual search for compound verified as below MDL/NDL or less than blank
- <(TRACE) = Characteristic ions present but too low to be quantified
- <(ND) = Characteristic ions are not present therefore Not Detected