

## MS ANALYSIS OF ISOTOPICALLY ENRICHED GASES USING SIMPLEX

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Simplex method is one of the search algorithms used extensively for optimization of chromatographic parameters, NMR shimming, and nonlinear parameter fitting. In case of parameter fitting, simplex method starts with sets of initial values. During the iterative fitting process, the simplex "grows", "flips" and "shrinks", discarding the poorly fitted value sets and creating better fitted value sets, finally leading to a set of best fitted values satisfying a preset goal.

Simplex method has been adapted to our mass spectral data analysis for isotopic enrichment determination. Due to the nominal mass resolution of quad MS detection, it is common to observe the overlap of isotopic peaks, resulting in difficulty in determination of individual isotopic enrichment percentage. A simple case is NO analysis, where M/Z 31 could be  $^{15}\text{N}-^{16}\text{O}$ , or  $^{14}\text{N}-^{17}\text{O}$ , and M/Z 32 could be  $^{15}\text{N}-^{17}\text{O}$  or  $^{14}\text{N}-^{18}\text{O}$ . In reality, this seemingly simple problem is difficult to solve if one is limited to a pencil and paper. With simplex, however, we can obtain more reliable results ensured by the minimized sum of square error (SSE) value.

Both uniformly-weighted least square method and weighted least square methods are used in our analysis. The effect of the weighing factors, system randomization, and the effect of initial values to the final result will be presented. The limitation of the method and possible error sources will be discussed using examples of MS analysis for isotopically enriched gases.