InfoMetrix®

LineUp™ version 2.03
Product Description and Specifications

As analyses move toward a more routine quality control or process environment, maintenance of retention time reproducibility in chromatography becomes a challenge. Recent changes to chromatographic hardware alleviate the problem to some extent, but many situations remain where a software approach is mandated. Some software alignment methods try to solve the problem by using specified marker peaks to adjust the retention time of intervening peaks. This "rubber band" approach works well if ubiquitous native peaks or internal standards are present. Lack of qualified marker peaks or changes in peak shape due to overloading can reduce the reliability of this approach.
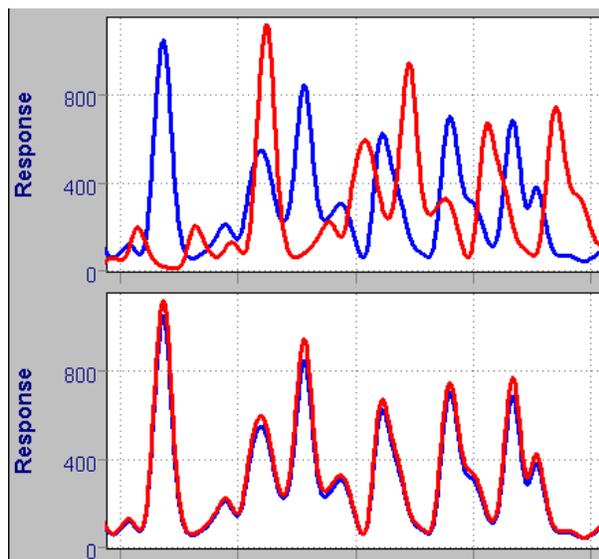
Our LineUp software is a tool for adjusting retention times that does not require markers nor any other prior information. Using a multivariate correlation method, LineUp will adjust a chromatogram's retention axis to more closely resemble that of a target chromatogram. Thus, variation in column loading, column aging and changes in flow are accommodated in the aligned profile.

LineUp can be run manually, but is also designed to run invisibly. The user needs only to specify the alignment standard and place the call to LineUp in the chromatographic software. When LineUp has finished, it writes a new, aligned file, in the same format of the input data.

In the example at left are two chromatograms, before and after alignment. The blue profile is the target, and the red is a sample where peak retention had shifted; LineUp has brought them into alignment.

Alignment can be made against more than one target chromatogram. A correlation coefficient that specifies the fit quality is computed for each, the alignment with the highest correlation is accepted, and the corresponding aligned chromatogram is written to file. LineUp works with Agilent GCs spanning the 5890, 6850 and 6890 models; ChemStation macros to facilitate the processing are included in the package. LineUp can also process AIA files exported from any single-channel chromatography system. Extra tools are provided for automated processing of data from the EZChrom Elite™ platform. Files in the Thermo GRAMS *.SPC format can be handled by LineUp as well, benefitting Raman and NMR users.

With LineUp, automated alignment can be incorporated into any company site without requiring specialized training of the technician. Chromatograms from different sites can be aligned without requiring that instruments be set up in any particular way ahead of time, as is required by pressure modulation systems.

LineUp™ Specifications

Windows 2000, XP – 256 MB+ RAM

DATA FILES
Read/Write
Agilent 5890, 6850, 6890 (*.CH) ChemStation format
American Instrument Association (AIA; *.CDF) format
Thermo GRAMS (*.SPC) spectral data format

AUTOMATION TOOLS REQUIREMENTS
ChemStation System Version A.06 or later, 16- and 32-bit
EZChrom Elite™ System Version 3.1.4 or later

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