ChromSword

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We Enable Science

NEW

# ChromSwordAuto 5

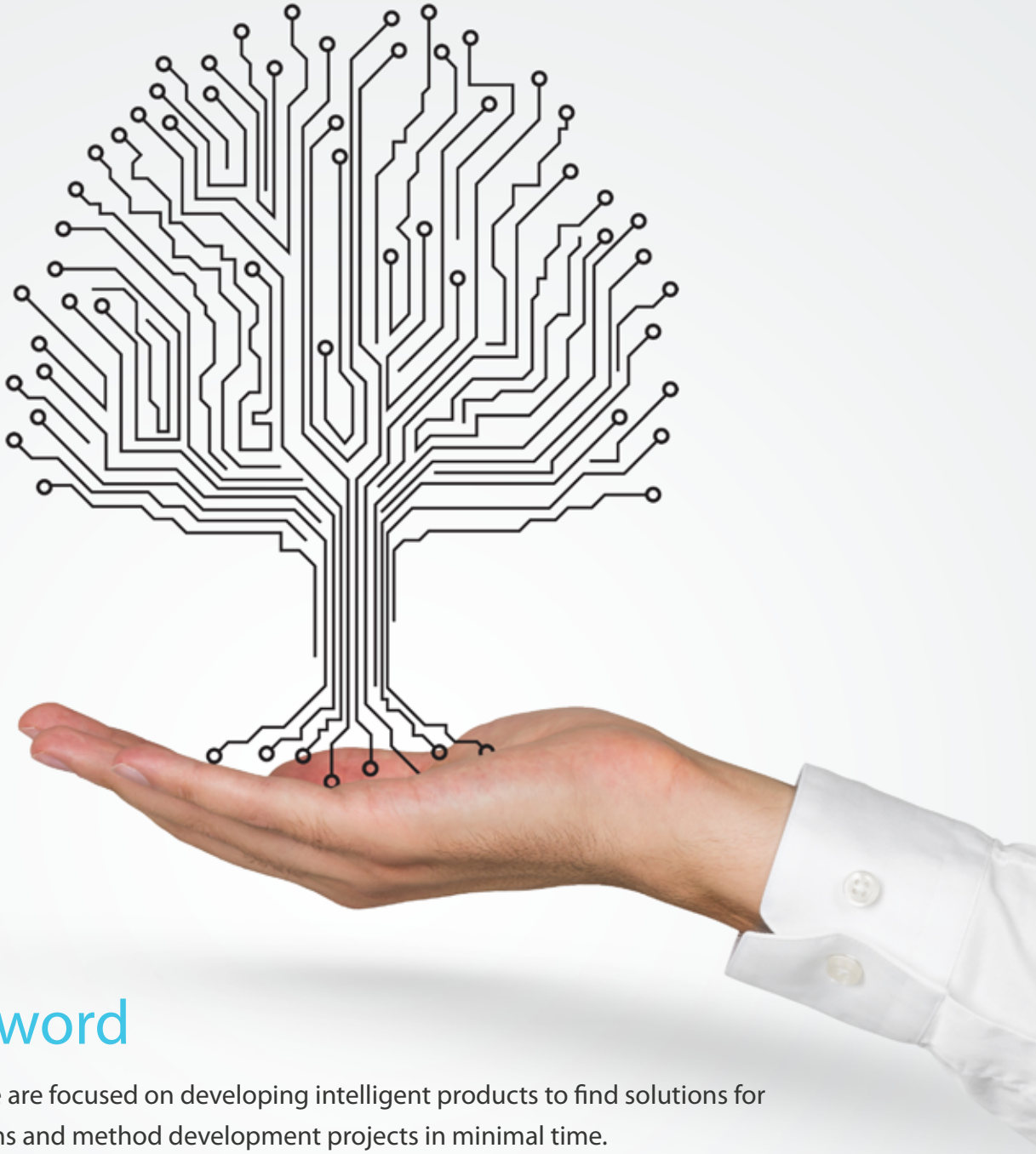
## Solutions for automated HPLC method development in accordance with QbD principles

Looking for better,
more effective way to
develop new HPLC methods?


ChromSword provides the best
solutions

# 20+ Years

For more than twenty years,
we been have developing innovative
software products to support
method development in liquid
chromatography



# ChromSword

At ChromSword we are focused on developing intelligent products to find solutions for separation problems and method development projects in minimal time.

ChromSword currently holds the leading position in automating HPLC method development. Our intelligent software products are  used in different analytical laboratories worldwide.

The ChromSword team is a group of highly skilled separation scientists, analytical chemists and IT specialists who  transfer their knowledge into powerful method development and validation software.

# Support and new developments

Our fully equipped HPLC method development laboratories allow us to support our customers and carry out new developments.

ChromSword also offers outsourced method development and validation services at very competitive prices

# ChromSwordAuto

## Automated HPLC method development

1st ever

## ChromSwordAuto is the first-ever chromatography method development data system.

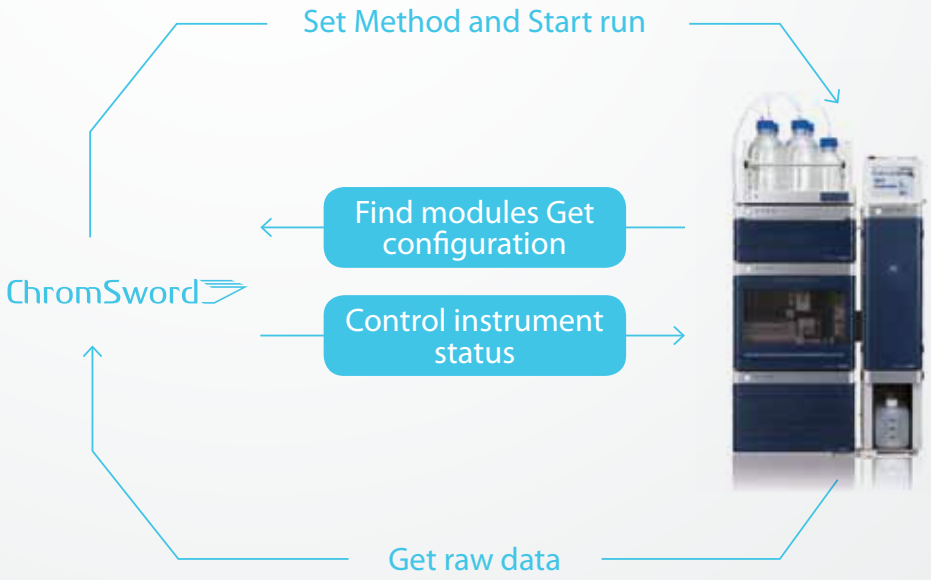
Computer-assisted method development is effective but also proves difficult to understand for many people. There has to be a better way to build method development software. We focus on a special chromatography method development data system — the software that manages and runs the LC instrument and also serves to bridge the gap between the LC instrument and a method development program, such as ChromSword. ChromSwordAuto is the foundation on which HPLC method development instrument can run. Other chromatography data systems might be used with the instrument but they are not necessary when ChromSwordAuto is installed on your PC."

## ChromSword simulates actions and decisions of a human method developer

ChromSword Auto is powerful, method development software capable of developing new methods or improving existing methods fully automatically.

## How does it work ?

ChromSwordAuto(CSA) is based on theory of liquid chromatography, newest computing technologies and more than 20 years of practical experience in HPLC method development. In ChromSwordAuto we have combined automated instrument control and data exchange with mathematical optimization procedures and artificial intelligence methods for making decisions after each run. This extremely powerful combination enables the software to search for optimal separation conditions fully automatically.




1 CSA sends tasks to a Chromatography Data System (CDS) which creates and executes methods to run HPLC instrument.

2 All methods and run data are collected and stored in the CDS.

3 ChromSword receives data, process and estimates them, learns from experiments, makes intelligent decisions for the next run and sends new request to the CDS for execution.

4 After completion of method development task ChromSword generates reports with experiment conditions and results.

# Quality by Design

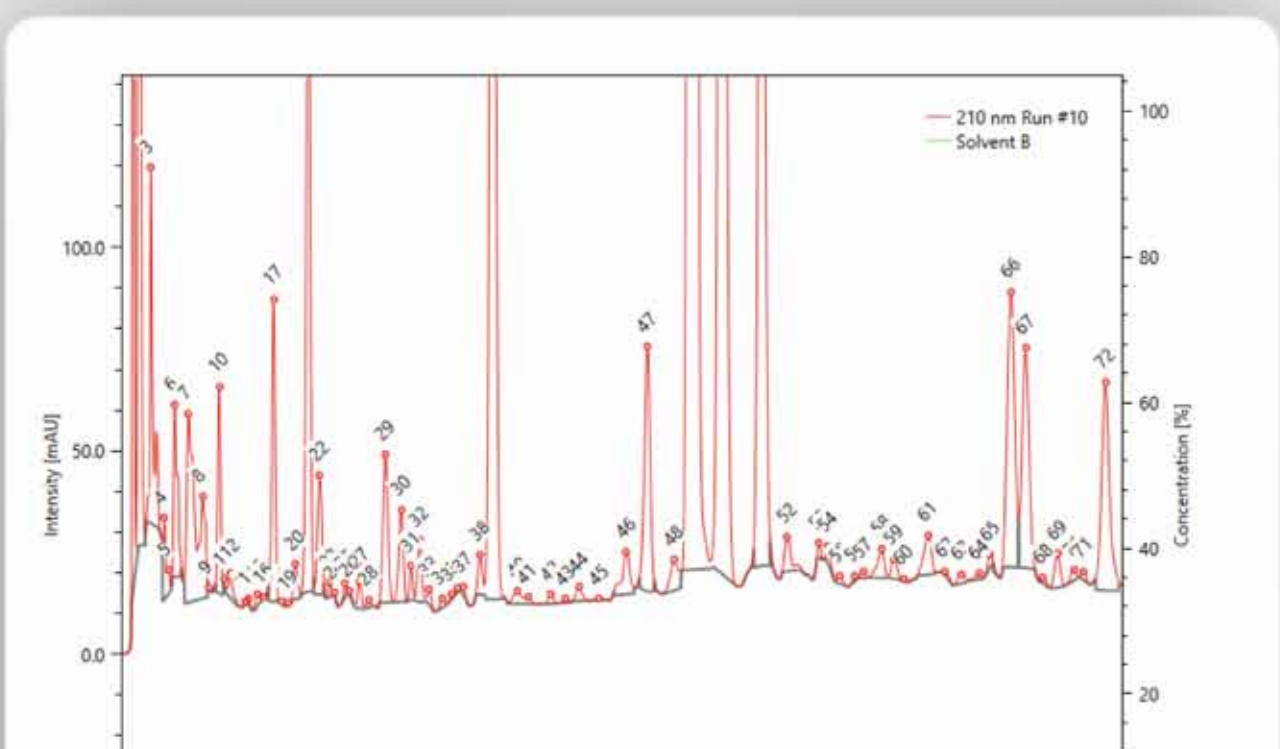
All procedures and steps of method development are structured, documented and available for future review according regulatory requirements. ChromSword AutoRobust module provides automation of method robustness tests to study effects of method variables on resolution and integration results according the QbD approach.


# Peak tracking

ChromSword Auto is equipped with "Intelligent Peak Tracking" function, which ensures reliable peak assignment even in compound mixtures containing impurities. This is achieved without even the need for DAD spectra. By recording and tracking the peaks that emerge under different chromatographic conditions, the system ensures that all peaks are clearly isolated and optimized, regardless of how many compounds are present in the mixture.

This is ideal for developing and optimizing new or existing methods in pharmaceutical and chemical quality control analysis, as well as for process analysis with samples containing impurities or unknown compounds.

impurities less than 0.01%



# Supports Method Development Projects

ChromSwordAuto is your assistant for all project stages from impurities profiling to development of QC methods. Working with all samples, from simple to difficult, ChromSword works effectively with peak areas of less than 0.01% of the total area.

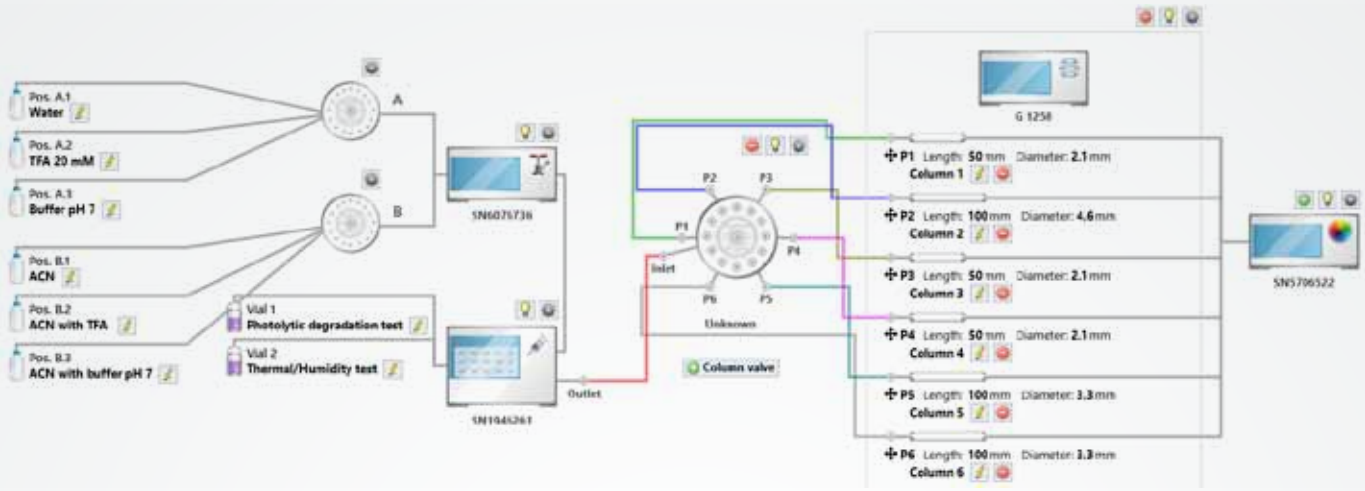
## Typical method development projects:

- Impurities profiling for process developments
- Degradation products profiling for stability tests
- Development of stability Indicating methods
- Development and optimisation of quality control methods
- Separation of bio samples

# Typical Samples for Automatic Method Development:

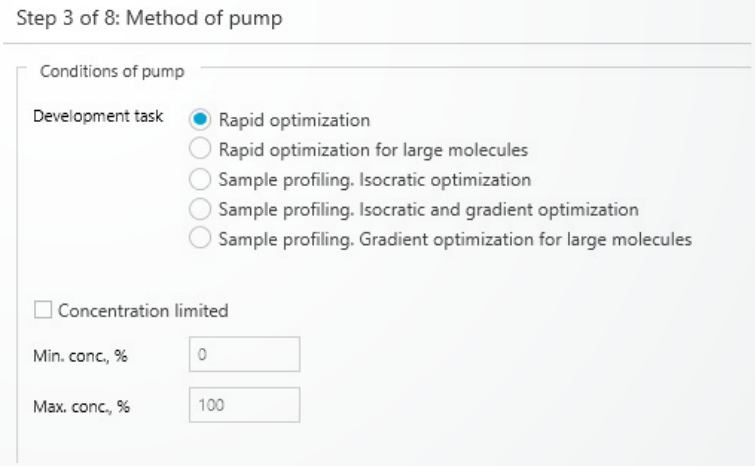
- Drug substances and new compounds
- Drug products
- Stress mixtures
- Reaction mixtures
- Natural samples
- Separation of bio samples

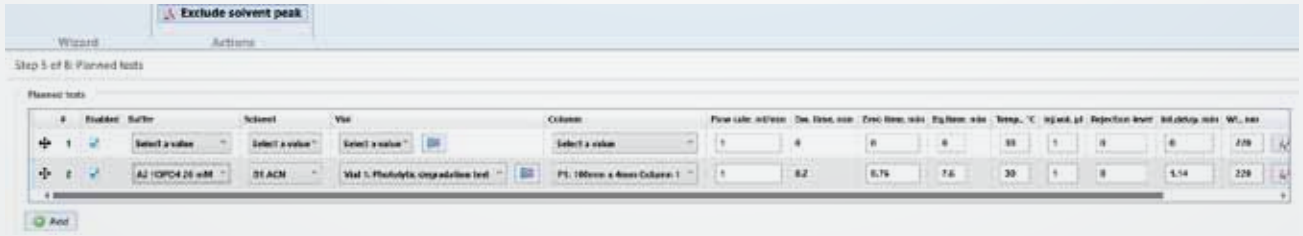
# How to start working with ChromSwordAuto




It is very easy to start method development with ChromSwordAuto.

1. Prepare your instrument
2. Choose one of CSA procedures described below depending on your task
3. Define initial conditions as flow rate, infection volume, etc.
4. Press **GO** and start optimization



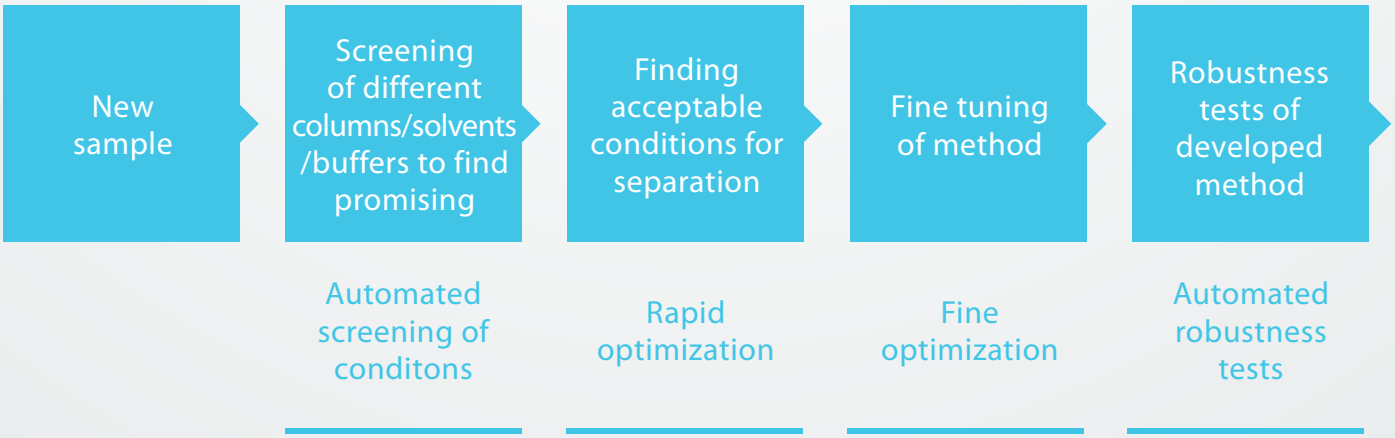

After finishing automatic work browse  results and generate a report if necessary

# ChromSwordAuto main features

- ☑ Automatic optimization of isocratic conditions, linear and multi-step gradients
- ☑ Automated methods screening with different column/solvent/buffer/temperature combinations
- ☑ Works with 1-10 different columns, 1-3 organic solvents, 1-16 buffers, different temperature and flow rates
- ☑ Automatic search for impurities (>= 0.01 Area% )
- ☑ Automatic search for maximal number of peaks
- ☑ Automatic optimization of separation of only target compounds
- ☑ Automatic optimization of separation of only the main ingredient from other compounds
- ☑ Automated peak tracking using UV, DAD or MS data
- ☑ Automated reporting results

# Method development procedure

ChromSword provides a complete portfolio of fully automated procedures and tools to cover all steps of a typical method development process as described in the picture below.



# ChromSwordAuto Screening

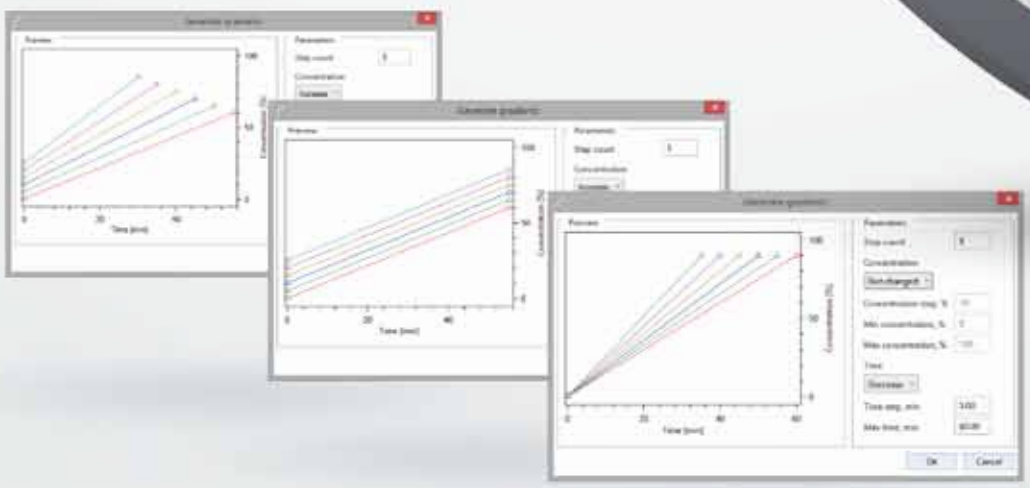
- Quick screening of different columns / solvents / buffers
- Determine best columns / solvent / buffers combination – Sample profiling

CSA Screening is a procedure that allows you to create and modify complicated screening procedures just in minutes.

For example, consider plan of a screening of a new sample with the following combinations:

2 gradients x 5 columns
x 2 solvents x 3 buffers
x 2 different temperatures
**= 120 combinations.**

We also should take into account that running all these combinations with only two standard gradients will not provide us with consistent results to find a best column.

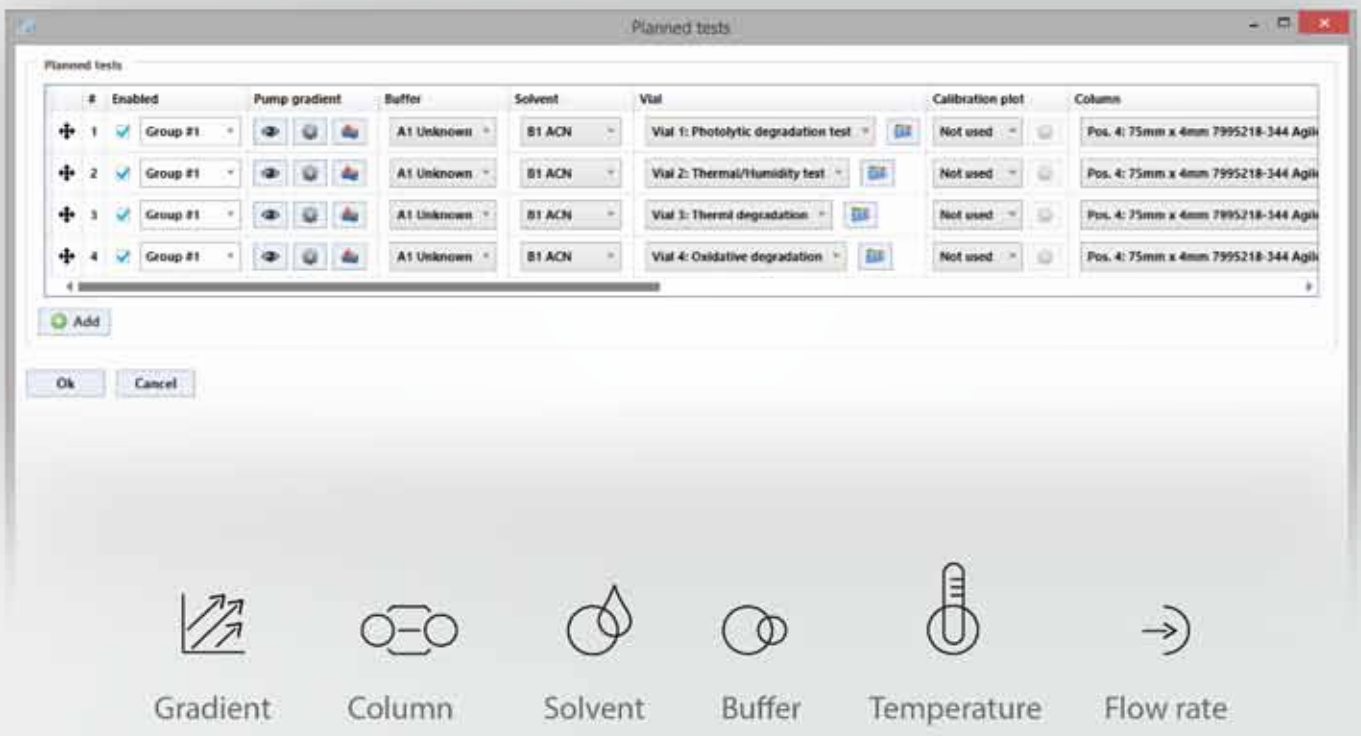


More objective solution would be to run multiple gradients because sometimes an excellent column exhibits bad resolution just due to a non-optimal method.

Preparing screening procedures we should also program additional steps between changing columns, solvents or buffers like washing out, bypassing, equilibrating and it takes much time.

When you use ChromSwordAuto to plan and run screening you can avoid many steps which are build in ChromSwordAuto procedures.

## It takes only few minutes for preparing any complex multistep screening plan with ChromSwordAuto !!!




## One consolidated report

In the end of automated session all results are included in one report. The results, tables and chromatograms can be exported in the html or doc file reports.

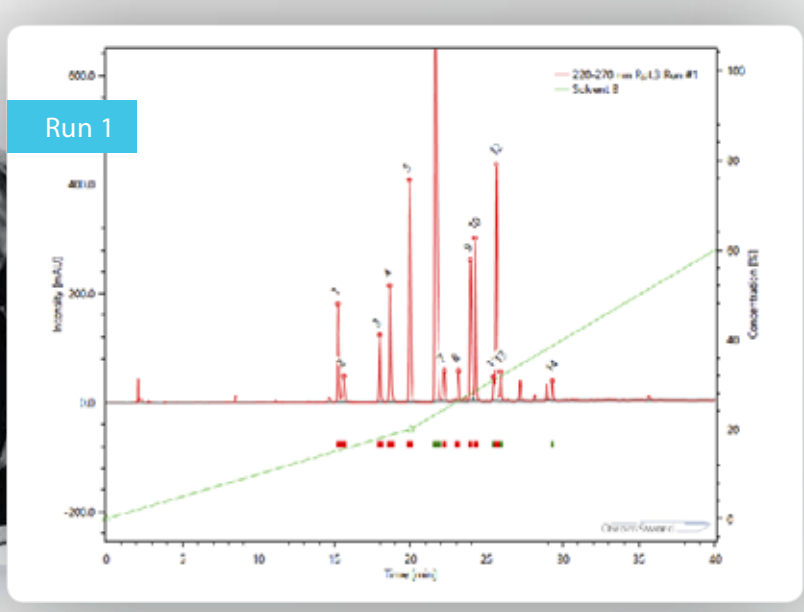
Depending on system availability and number of experiments ChromSword can work in unattended mode days and overnights and delivers not only good methods however also detailed and easy to review reports. It is easily for an analyst with ChromSwordAuto to review data and make decisions regarding next method development or robustness study steps.

# ChromSwordAuto
# Rapid Optimization

## The goal of ChromSword rapid optimization are:

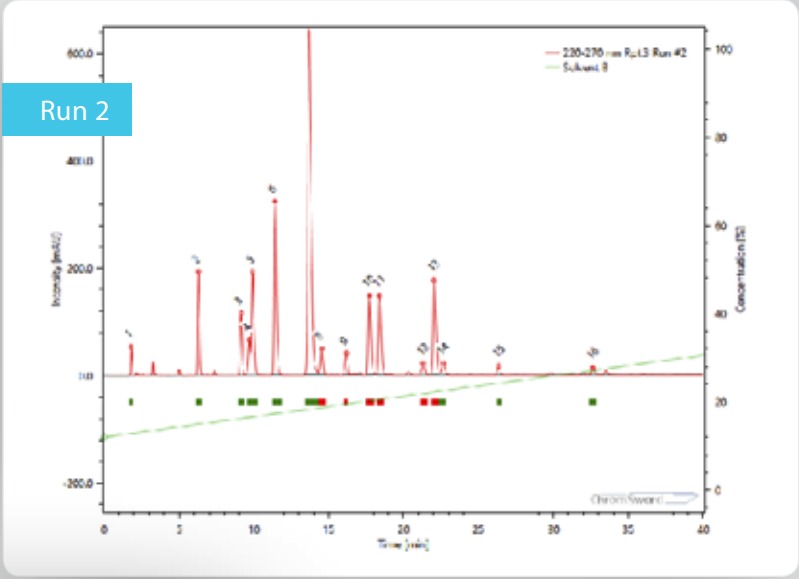
- to obtain practically reasonable methods for early method development projects as soon as possible.
- to find the best column/ solvent/buffer combination to be used in the following fine optimization

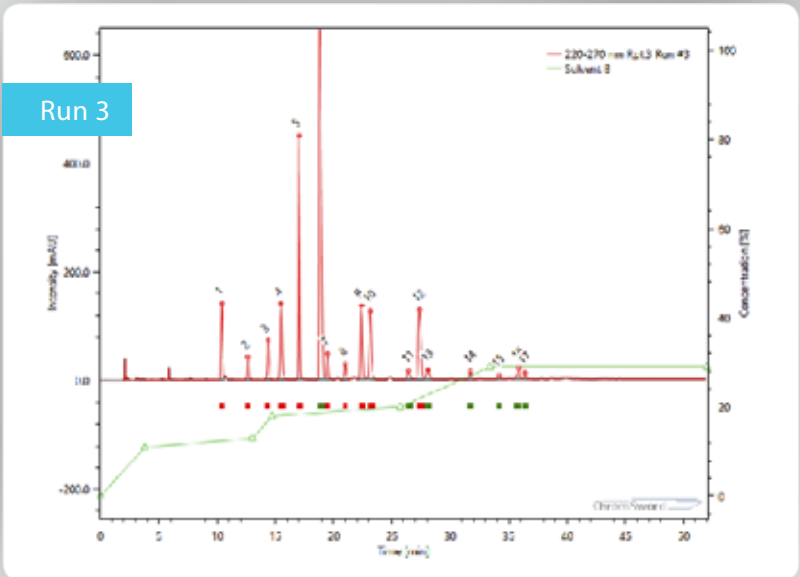
The ChromSwordAuto Rapid Optimization algorithm is an unique and extremely powerful solution for fast method development. The Rapid Optimization algorithm finds good conditions making only few runs.



The first gradient run from low to high concentration of an organic modifier is aimed at understanding a sample and a column properties. The purpose of this run is to determine area and conditions when compounds of the sample are eluted. The time of experiment depends on column length and flow rate.

The second run is a linear gradient and is based on results of the 1st run. ChromSword makes decision on starting and end concentration of organic modifier and run time depending on results in 1st run.




After processing data from 2 runs ChromSword automatically creates retention models, simulates chromatograms at different conditions and makes decisions for 3rd run trying to separate all peaks with a target resolution.

**Only 3 runs for a short period of time**

## The main value of the Rapid Optimization is that it is a very fast reachable milestone for the analyst, before making future decisions as:

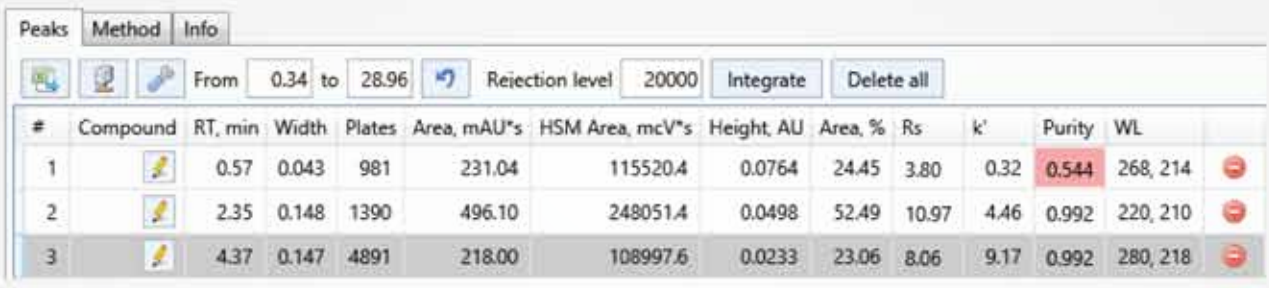
- Change a combination of column/ solvent/ buffer if results are no good
- Proceed to the Fine Optimization if results are good but could be improved and sample should be checked for some unknown or not separated impurities
- Proceed to robustness tests if a method is acceptable.

ChromSwordAuto

# Fine Optimization

You can perform detailed (fine) method optimization based on results of the rapid optimization or screening. The Fine Optimization is an ideal, powerful and fully automated procedure for impurity profiling of new products, and batch-to-batch reproducibility of 3rd party supplies

## ChromSwordAuto Fine Optimization is the most powerful solution for detailed analysis of samples with full impurity profiling, and development of best isocratic and gradient conditions for full separation of sample components.

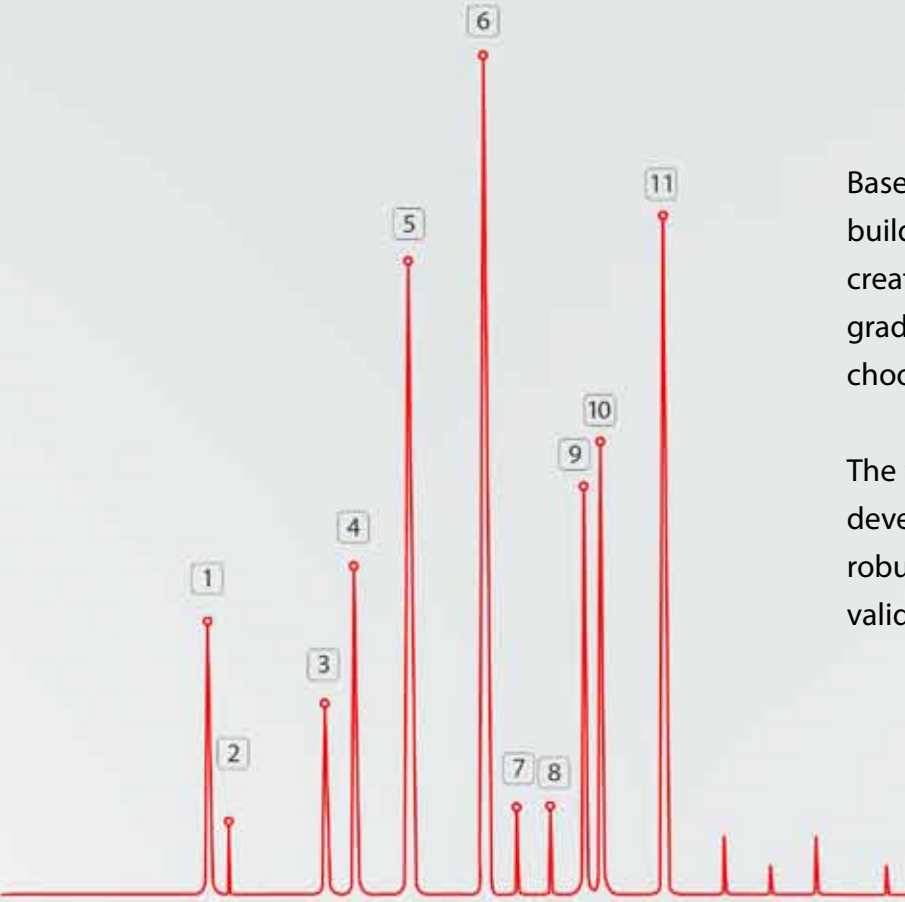



| # | Compound | RT, min | Width | Plates | Area, mAU*s | HSM Area, mcV*s | Height, AU | Area, % | Rs | k' | Purity | WL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | 0.57 | 0.043 | 981 | 231.04 | 115520.4 | 0.0764 | 24.45 | 3.80 | 0.32 | 0.544 | 268, 214 |
| 2 | | 2.35 | 0.148 | 1390 | 496.10 | 248051.4 | 0.0498 | 52.49 | 10.97 | 4.46 | 0.992 | 220, 210 |
| 3 | | 4.37 | 0.147 | 4891 | 218.00 | 108997.6 | 0.0233 | 23.06 | 8.06 | 9.17 | 0.992 | 280, 218 |

Before starting the Fine Optimization procedure the analyst already knows results of the screening or the Rapid Optimization and selected a promising column/ solvent/ buffer combination for separation of the sample. The only additional thing the analyst should define is a starting concentration of an organic modifier that is enough high to elute all components.

During the Fine Optimisation process ChromSwordAuto performs both isocratic and gradient runs to study a sample in details.

Studying a sample ChromSwordAuto performs different numbers of isocratic runs depending on sample complexity which gives unique peak tracking and impurity profiling capability. After each run ChromSword will change concentration of an organic modifier step by step depending on results of previous experiments to make full peak tracking and elution modelling. In the end of isocratic runs ChromSword offers best conditions for isocratic separation.

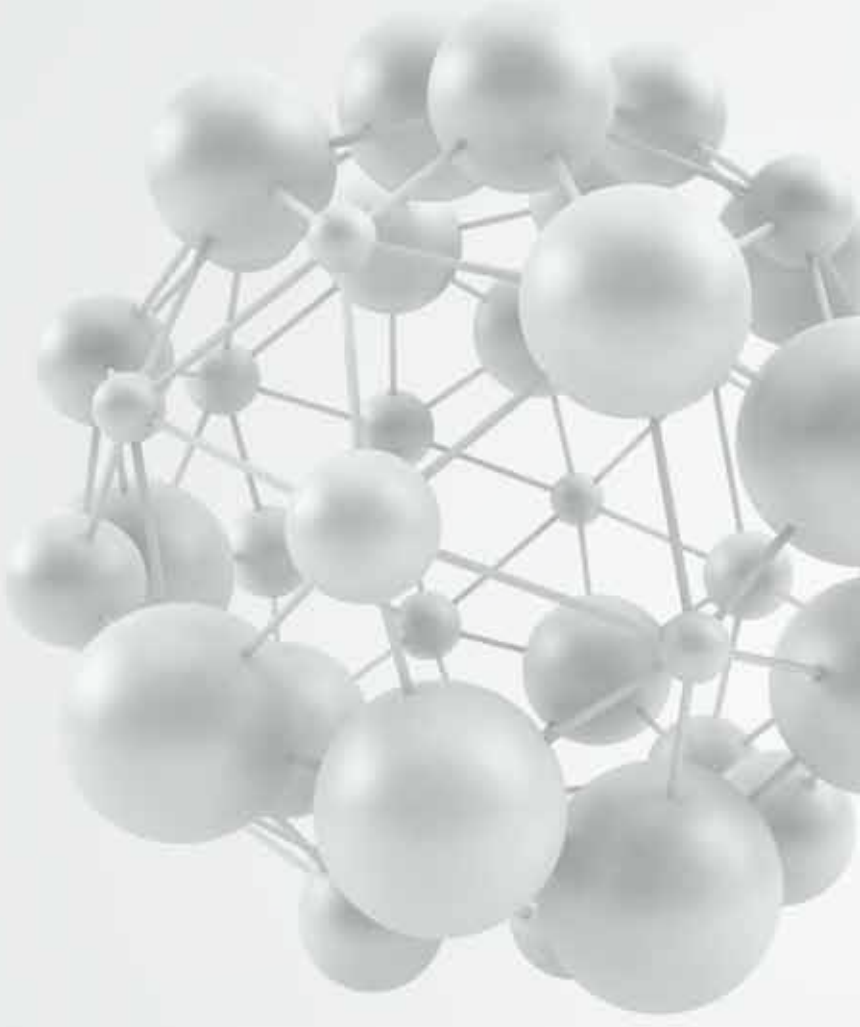



Based on results of study of a sample and building retention models ChromSword creates and performs multiple linear and step gradient runs for analyst to compare and choose best methods depending on his target.

The result of the Fine Optimization is a fully developed method that should be tested for robustness or transferred to QC for future validation.

## ChromSwordAuto Optimization procedures for large molecules

The ChromSwordAuto contains unique algorithms for optimization of separation of large molecules. ChromSwordAuto is a real companion and assistant for projects when homogeneity characterization of oligonucleotides, polypeptides, proteins and synthetic polymers is necessary.



# ChromSwordAuto
# AutoRobust

- Easy and fast way to plan your robustness tests experiments
- All tests are performed according QBD principles
- One or multiple parameter change according design of experiments (DeO)
- Full report with export options

After finishing method development with ChromSword, you can start AutoRobust with all method parameters specified automatically. It Is only necessary to specify variables to be tested, range of a level and a procedure to test one parameter at a time or several and choose a design of experiments method

With AutoRobust you can choose the following parameters to be tested:

**Temperature**
e.g. +/- 1°C

**Flow Rate**
e.g. +/- 0.1 ml/min

**Concentration**
e.g. +/- 1% org. modifier e.g.

**Gradient profile variations**
e.g. steps +/- 0.1 min

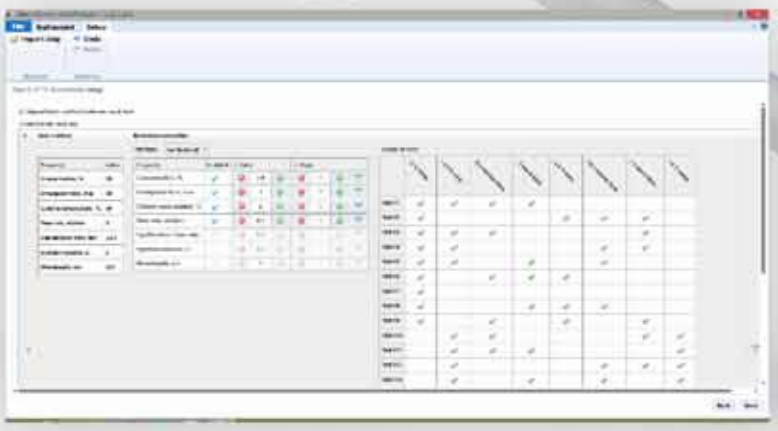
**Buffer concentration / pH**
e.g. +/- 0.1 pH values

**Injection Volume**
e.g. +/- 1 µl

**Equilibration Time**
e.g. +/- 1 min

**Wavelength**
e.g. +/- 1 nm

**Column Batch**
e.g. 3 different batches
using a column switching valve

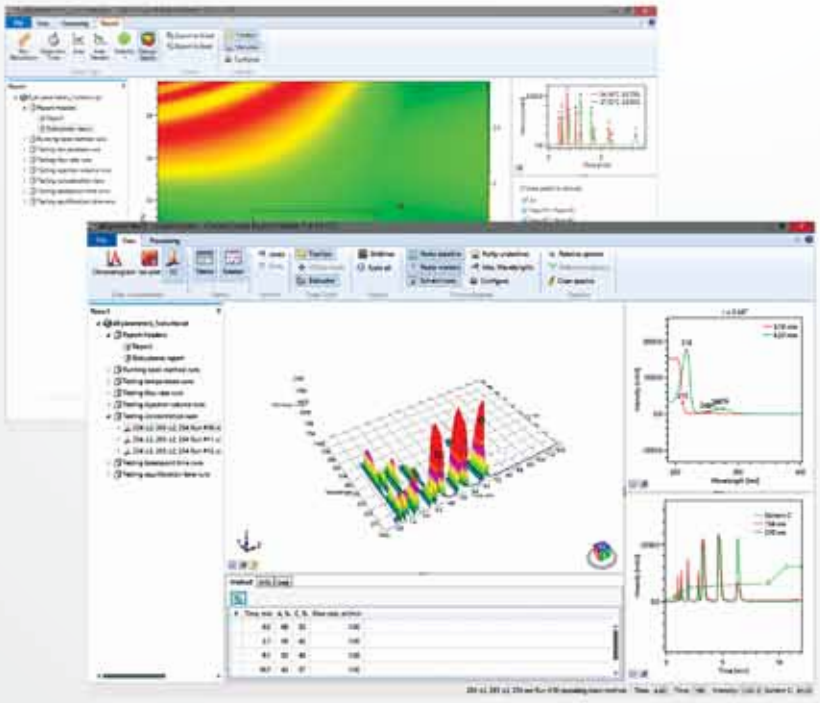


After runs AutoRobust prepares a report that includes all chromatograms and data including resolution, retention time, area, area % and standard deviations of these values. All tables can be exported into Microsoft Word, WordPad and Excel to prepare charts, tables and graphs.

# ChromSwordAuto ReportViewer

- Report Viewer is a navigator of method development and robustness study projects
- Browse data of all project runs in one click
- Compare and overlay chromatograms
- Reprocess chromatograms
- Generate reports in format compatible with Microsoft Word and WordPad.

Report Viewer is a data manager application and also a navigation tool that is included in ChromSwordAuto and AutoRobust. It provides a graphical user interface for accessing chromatograms, spectra, methods and integration results.



## Report Viewer contains many useful features:

1. All data of a method development project are organized in one report
2. Overlay, compare and reprocess chromatograms and spectra
3. Peak tables with comprehensive analysis
4. Methods used to generate results
5. UV and MS spectra data
6. Flexible export and copy options to prepare reports

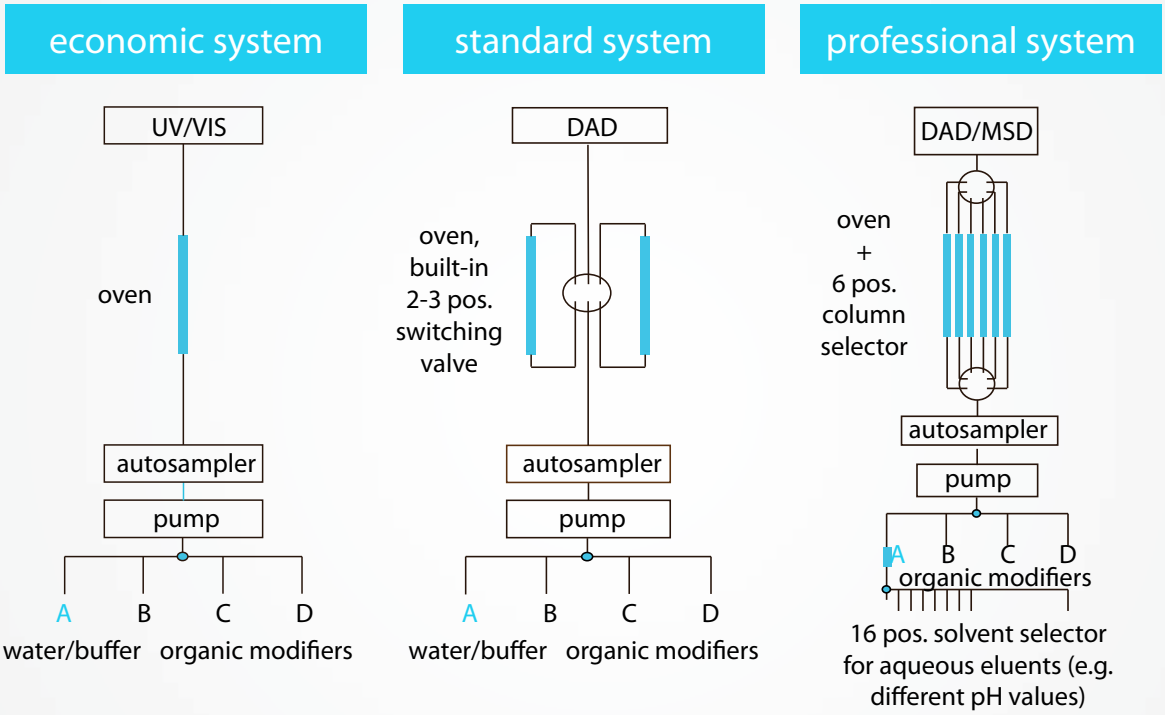

Flexible export and copy options to prepare reports

ChromSwordAuto

# System versatility

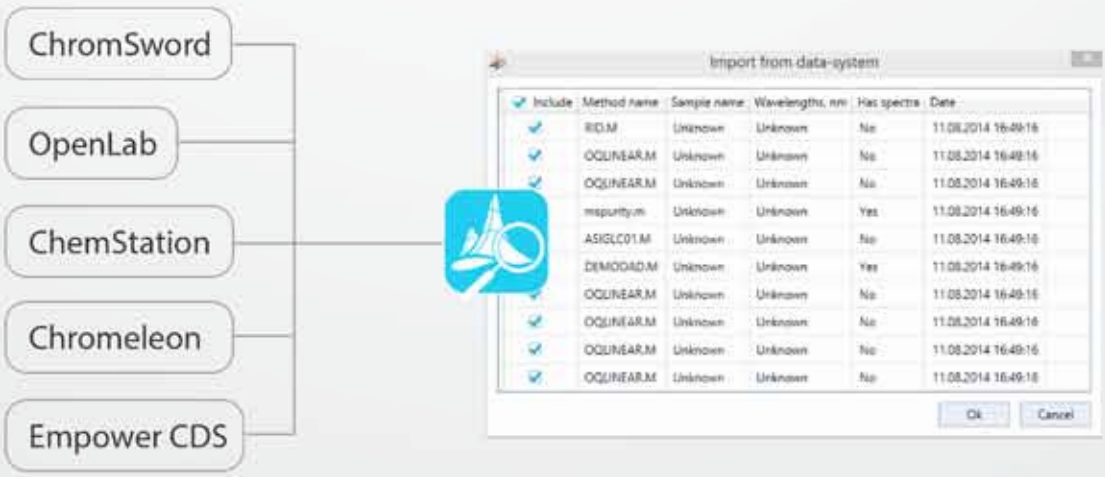
From a simplest instrument up to the most advanced method development solution
Compatible with all major instrument and data systems

ChromSwordAuto supports different system configurations from the simplest HPLC instrument with one column and UV detector up to advanced method development system with column and solvent switching valves and two different detectors from basic UV up to DAD, FLD, MS and other.




## ChromSwordAuto supports instruments from different vendors:

Agilent HITACHI Thermo Waters



# 20+ YEARS

## ChromSword has more than 20 years experience

in working with different instrument and CDS. If you plan to buy a system for automated method development please contact us and we will share our experience.

ChromSwordAuto software package includes ChromSword Off-line were on the basis of few experiments or only structural formulae of compounds, you can computer simulate many chromatographic experiments with different compounds, various columns and eluents and, finally, optimize conditions with a minimum of time for the chromatographic run. Typical method variables for computer optimization are: concentration of an organic modifier, gradient profile, temperature, pH , column coupling and combination of two different variables.

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