PeakMaster 5.3 Manual

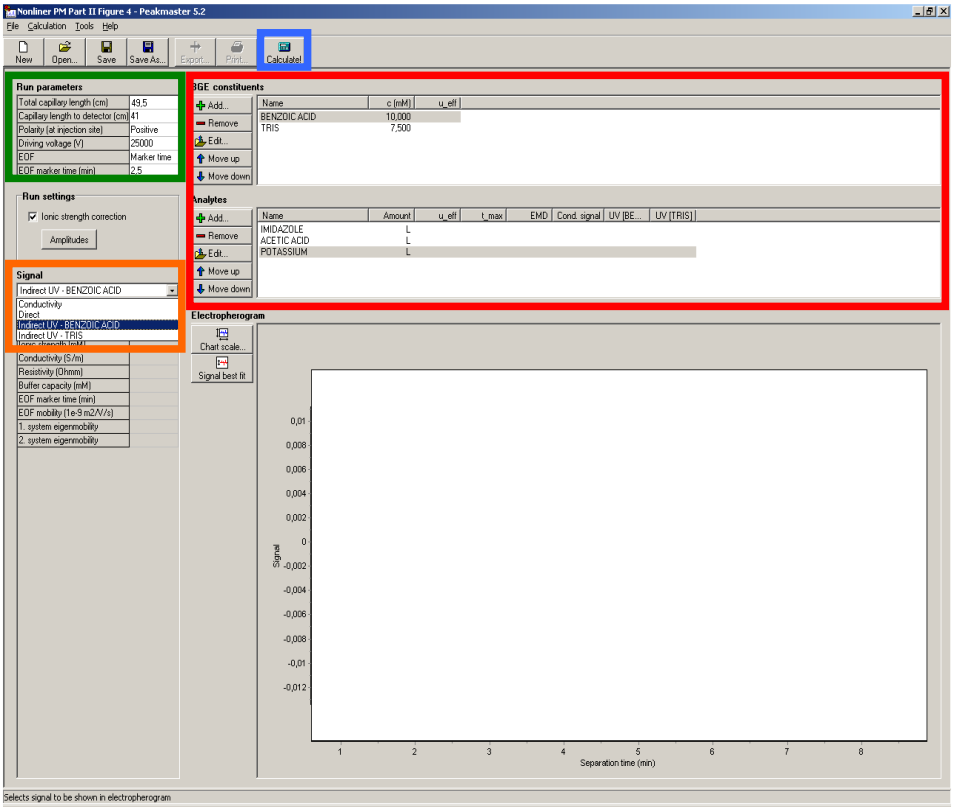
PeakMaster 5.3 keeps all features and abilities known from previous versions of PeakMaster. In addition, PeakMaster 5.3 enables to calculate and predict the shapes of the system peaks. General setup of calculations is the same as in the previous versions and is described in "Help" in PeakMaster. The new feature of PeakMaster 5.3 is attainable in the "Amplitudes and Shapes" window.

Basic calculations and predictions:

Necessary input parameters for analysis of the electrophoretic system in new PeakMaster are the same as in the version:

- limiting ionic mobilities and dissociation constants for all BGE constituents and analytes (*PeakMaster contains a database of pKa and limiting mobilities, based on Takeshi Hirokawa's tables, with the data of many ions – compounds can be easily selected from the database*)
- concentration of all compounds in BGE
- run parameters (total length of capillary, capillary length to detector, driving voltage and mobility of EOF or position of EOF marker)

Input of these data if in the main window.



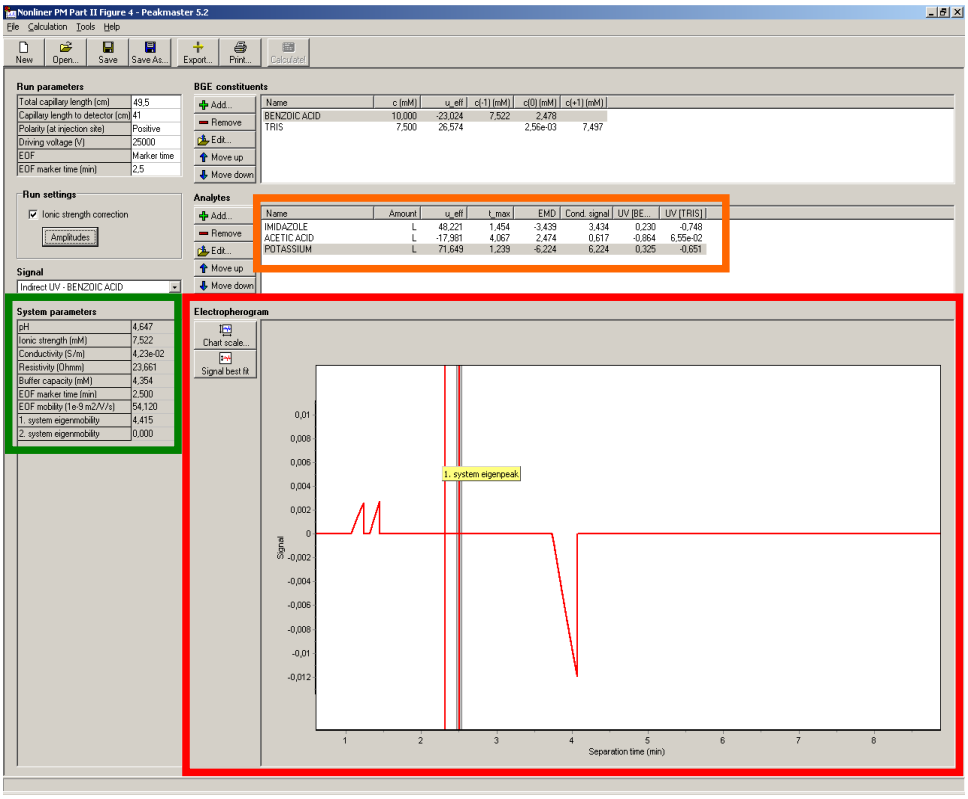
The detection mode can be selected.
When the system peaks shapes are calculated, only indirect UV or conductivity detection modes are meaningful.

When clicking "Calculate!" button, the basic outputs of the analysis, are:

- characteristics of BGE (pH, ionic strength, buffering capacity and conductivity)

- system eigenmobilities
- effective mobilities of analytes
- transfer ratios for prediction of the signal in indirect photometric detection
- molar conductivity detection response for prediction of the signal in conductivity detection
- relative velocity slope which is a measure of the tendency of the analyte to undergo electromigration dispersion
- simulated record shown in “Electropherogram” subwindow

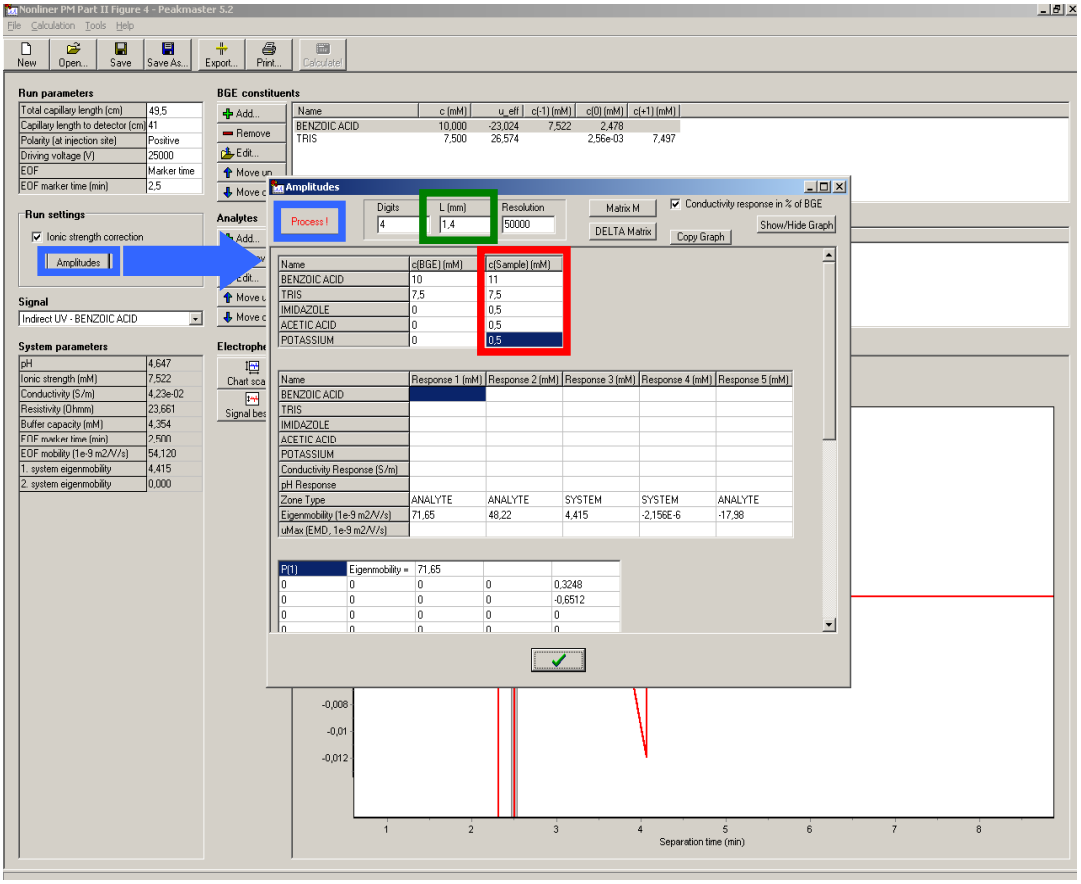
In the basic mode, system peaks are depicted in the simulated record only as a vertical line line.



All these results can be obtained also in previous version of PeakMaster.

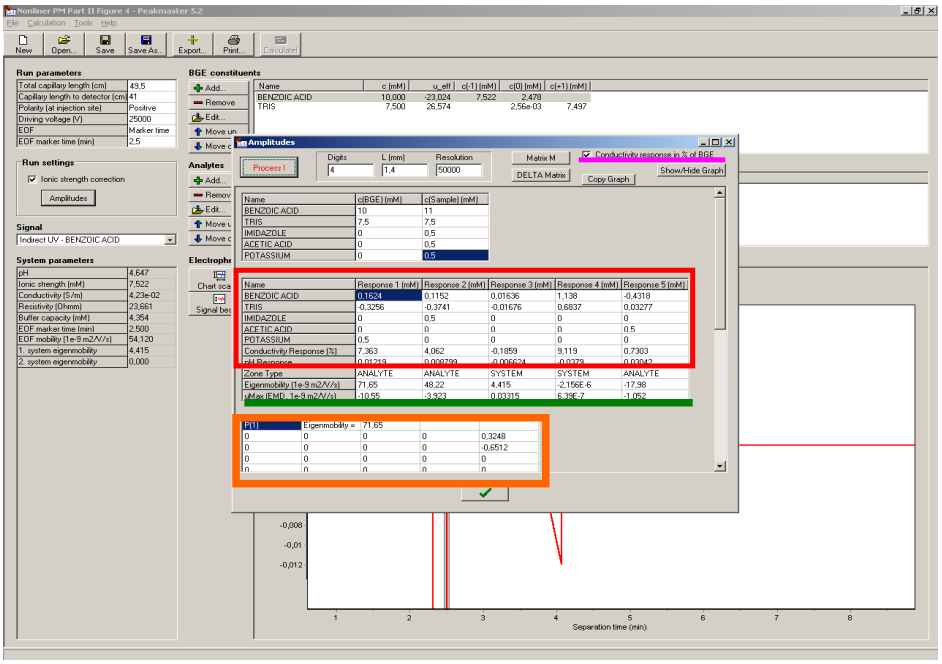
New feature of PeakMaster 5.3: Shapes of system peaks:

- by clicking on "Amplitudes and Shapes" button in the main window, the new window is opened
- the composition of sample zone ("c(Sample)") has to be inserted for prediction of system peak shapes; composition of BGE is copied automatically from main window
- length of the sample zone has to be inserted *(For hydrodynamic injection the length of the zone can be easily calculated from injection and capillary parameters by Hagen - Poiseuille equation)*

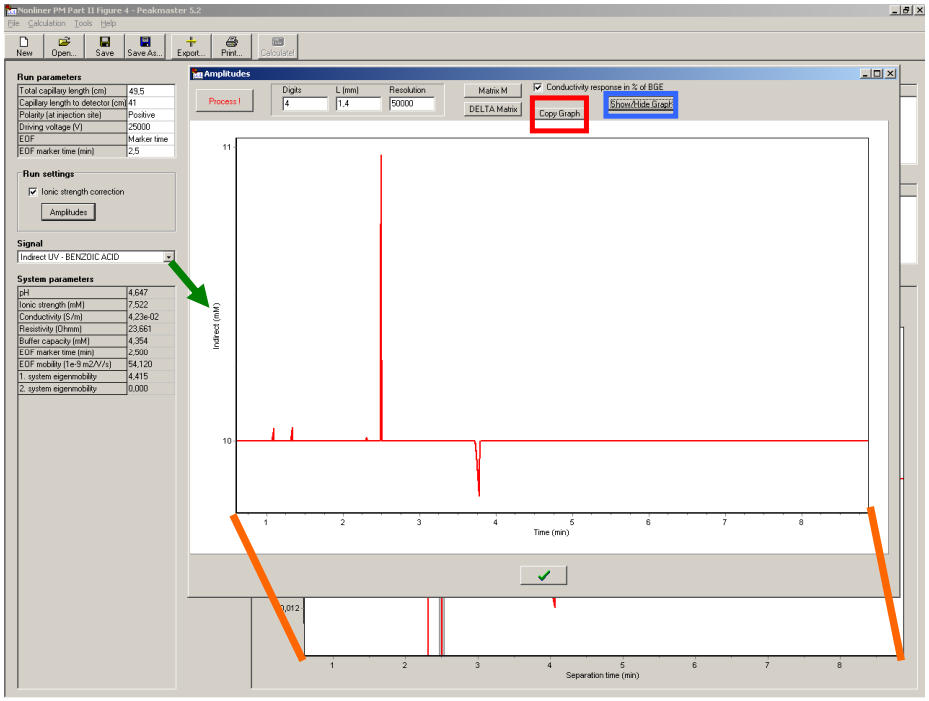


By clicking "Process!" button, many advanced parameters of the system are calculated:

- matrices of amplitudes **P**
- responses in concentration, conductivity and pH (*In case of conductivity response, the user can select between two ways of representation of conductivity response – [S/m] or [% of BGE conductivity]*)
- uMax (EMD) – electromigration mobility of all peaks



Depiction of the peak shapes of all peaks (analyte and system peaks) is done by clicking "Show/Hide Graph" button. Clicking this button again toggles between the graph and the calculated results.



- the simulated signal is depicted in detection mode chosen in the main window
- the range of the time axes is the same as in the electropherogram in the main window *(When the electropherogram is zoomed in the main window, only the zoomed part will be depicted in the "Amplitudes and Shapes" window)*
- By clicking on "Copy Graph" button, the graph is copied to the clipboard and can be inserted into spreadsheet (Excel, Origin,....)
- "Amplitudes and Shapes" window can be closed by  button