Agilent CrossLab
From Insight to Outcome

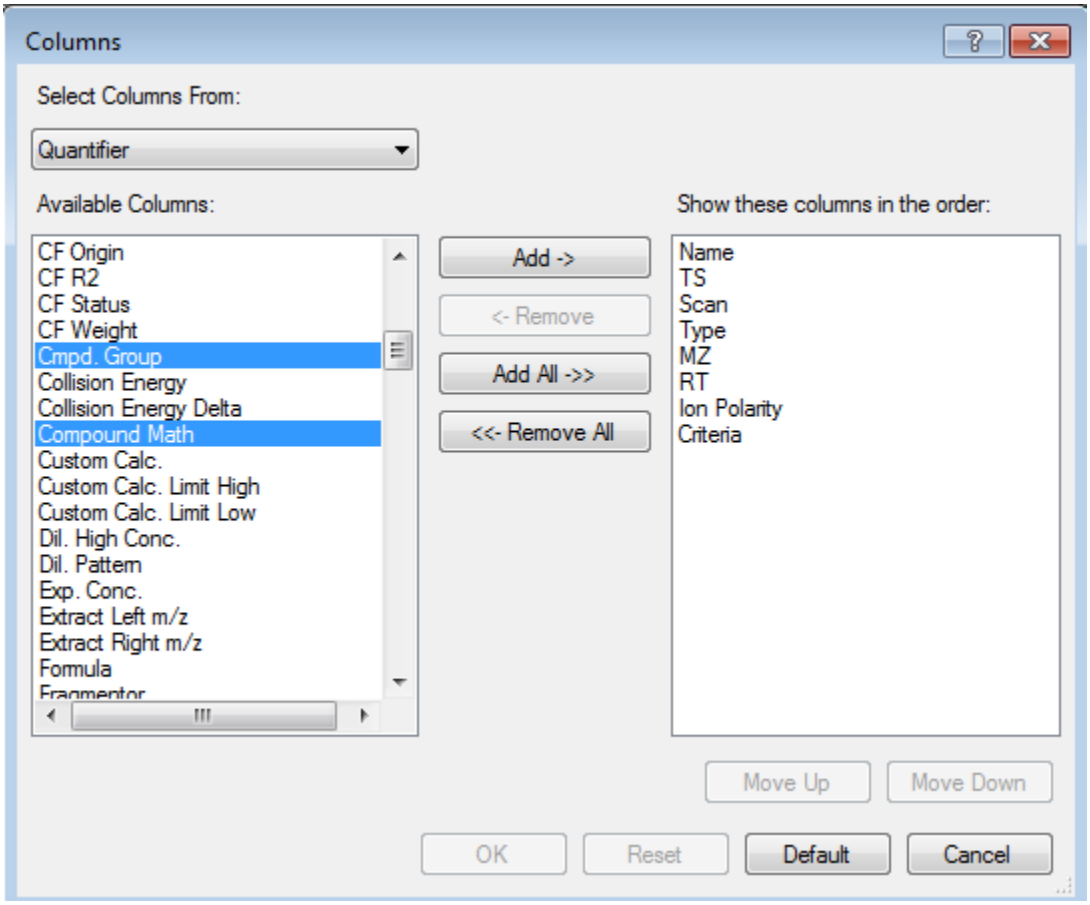
Peak Grouping in MassHunter Quantitative Analysis B.07.01

Peak grouping refers to a concept where several chromatographic peaks or isomers which elute at different retention times are reported as a total value or grouped together. In the MassHunter Quantitative analysis software the specific peak groups are designated by a special parameter in Method Editor entitled Cmpd. Group (Compound Group). The Peak Grouping concept then utilizes another feature in the software called Compound Math. The Compound Math calculations will then combine the individual peaks or isomers into an aggregate compound (the total compound). All of the individual isomers and the aggregate compound are designated as members of a single Compound Group.

One of the typical applications of peak grouping is with Polychlorinated Biphenyls (PCBs) or Aroclors. Generally speaking, compounds groups are easily added to a previously generated quantitative method.

The following hypothetical example utilizes the RI-PEST-MATRIX demo data and combines BHC isomers, BHC alpha isomer, BHC beta isomer and BHC delta isomer into one aggregate compound BHC Isomer Total.

1. Establish a quantitative method where each of the individual isomers are uniquely identified.
2. With a batch table with calibrators loaded and the previously established quantitation method (quant database) loaded, go to Method→Edit.
3. Select either Compound Setup or MRM Compound Setup in the Method Setup Tasks on the left side. Move the mouse into the Method Table and right click to select Add/Remove Columns.
4. In the Columns dialogue box, Add the Cmpd. Group and Compound Math columns.



5. For this exercise, clear any existing entries in the Cmpd. Group column.
6. Under Manual Setup Tasks→New Compound add the BHC Total compound. Be sure to assign a bogus mass and retention time to the BHC Total compound in order to pass validation of the quantitation method.
7. Assign the 3 BHC isomers and BHC Total to the group BHC. In the Compound Math column select Concentration Sum for only the BHC Total compound.

Quantifier

Name	TS	Scan	Type	MZ	RT	Ion Polarity	Criteria	Cmpd. Group	Compound Math
4,4'-Dibromooct...	1	Scan	ISTD	456.0	12.808	Positive	Close RT		
Aldrin	1	Scan	Target	263.0	19.671	Positive	Close RT		
Azinphos-ethyl	1	Scan	Target	132.0	31.018	Positive	Close RT		
Azinphos-methyl	1	Scan	Target	160.0	30.082	Positive	Close RT		
BHC alpha isom...	1	Scan	Target	181.0	13.185	Positive	Close RT	BHC	
BHC beta isomer	1	Scan	Target	219.0	14.327	Positive	Close RT	BHC	
BHC delta isomer	1	Scan	Target	181.0	15.693	Positive	Close RT	BHC	
BHC Total	1	Scan	Target	100.0	15.000	Positive	Close RT	BHC	Concentration Sum
Carbophenothion	1	Scan	Target	157.0	27.267	Positive	Close RT		
Chlorpyrifos	1	Scan	Target	197.0	20.355	Positive	Close RT		

8. Validate the Method, Exit and Analyze the batch.

For an excellent explanation see the video entitled Method Editor - Compound Math aggregate - Advanced.mp4.