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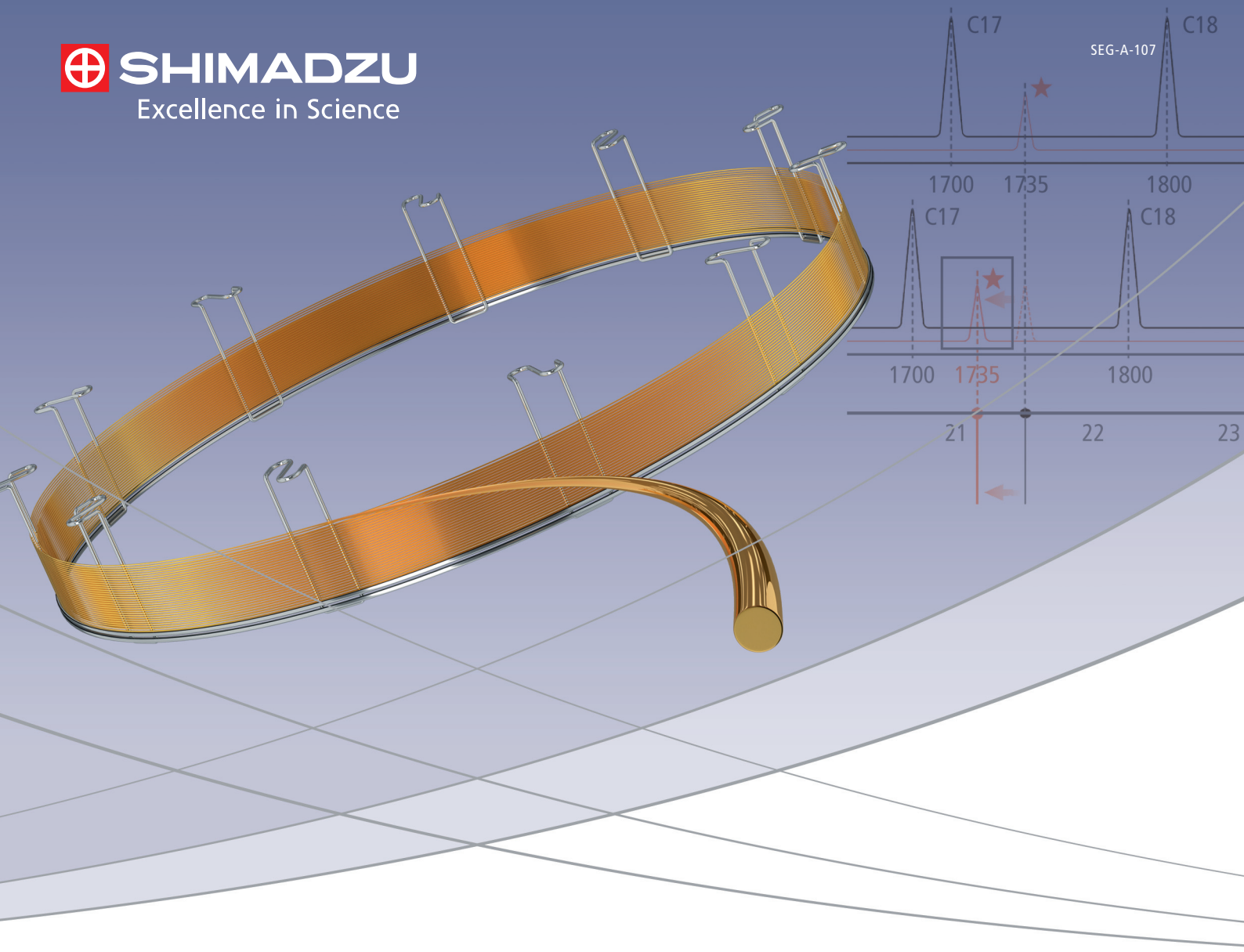
Excellence in Science



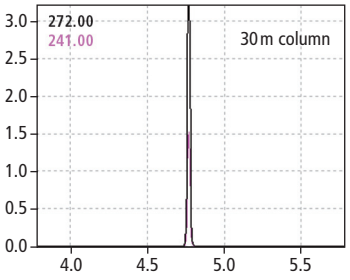
Automatic Adjustment of Retention Time (AART)

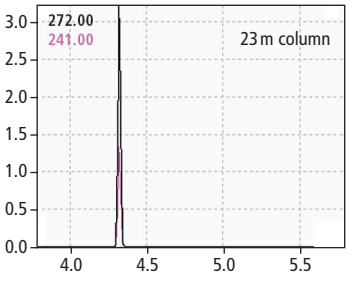
Annoyed of changing retention time manually?

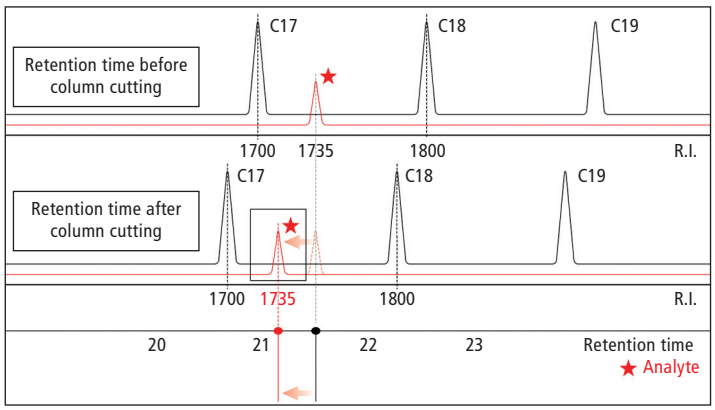
The development of highly selective GCMS techniques like GC-MS/MS and GC-HRMS have given routine analysts the chance to reduce their sample preparation costs (e.g. QuEChERS). This cost down is bought dearly with dirty samples showing higher tendency to contaminate the chromatographic system. Maintenance of these contaminated systems normally contains cutting of the contaminated part of the column.

In times, where only few compounds were analyzed in one run, it was no problem to do retention time changes manually. Since the introduction of highly selective GC-MS/MS, the simultaneous analysis of hundreds of compounds in one run has become state of the art. Therefore, manual retention time adjustment is nowadays a very time consuming, annoying and expensive work.

Shimadzu provides a very stable, robust, and reliable method for the automatic adjustment of retention time (AART). The approach is based on the well-known linear retention indices (LRI). Instead of spending several hours in manual adjustment, only one injection of an alkane standard is needed to predict with very high precision the new retention time of all compounds.







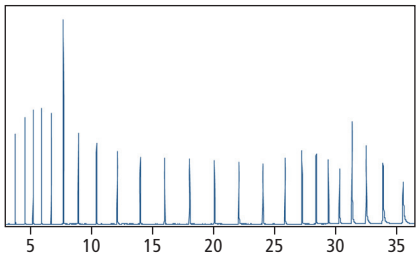
Using linear retention indices (LRI) for AART, every compound gets a virtual carbon number depending on its position between two adjacent alkane peaks.

When a column is cut, reducing absolute retention times, the relative positions remain unchanged. Adjusting retention times based on the alkane injection, no physical method changes are needed, but a single software calculation is performed.

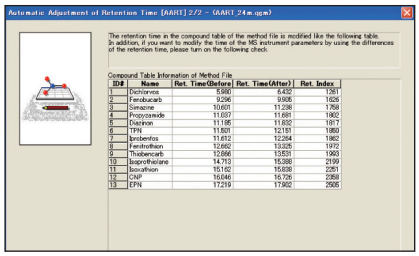
In addition to the retention times, all SIM or MRM windows are adjusted according to the new retention times simultaneously.

Workflow:

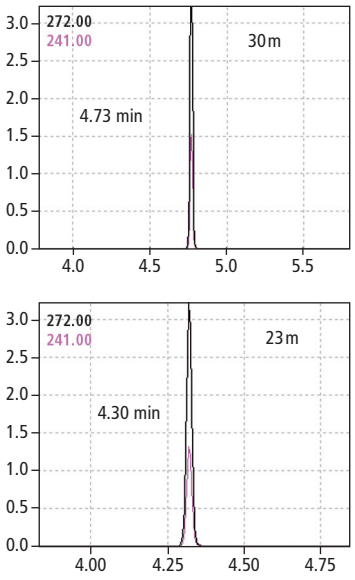
1.: n-alkane injection



2.: AART execution



3.: Changed retention time



The comparison of pesticide retention times predicted on a former 30 m column cut to a new length of 23 m with real measured retention times on this column reveals the high precision predictive power:

Even for such an extreme case, the differences are found to be below 2.5 sec.

Pesticide	23 m column			Pesticide	23 m column		
	RT measured	RT predicted	ART		RT measured	RT predicted	ART
Dichlorvos	5.653	5.652	0.001	Pirimiphos-methyl	13.453	13.452	0.001
Butylate	7.384	7.394	-0.010	Malathion	13.628	13.627	0.001
Isoprocarb	8.559	8.571	-0.012	Cyfluthrin-1	20.363	20.356	0.007
Ethoprophos	9.560	9.577	-0.017	Cyfluthrin-2	20.446	20.443	0.003
Bendiocarb	9.986	10.001	-0.015	Cyfluthrin-3,4	20.562	20.555	0.007
alpha-HCH	10.320	10.353	-0.033	Halfenprox	20.718	20.708	0.012
beta-HCH	10.871	10.906	-0.035	Silafluofen	21.095	21.086	0.009
Terbufos	11.058	11.079	-0.021	Fenvalerate-1	21.597	21.584	0.013
Tefluthrin	11.500	11.501	-0.001	Fenvalerate-2	21.802	21.788	0.014
delta-HCH	11.469	11.505	-0.036	Difenoconazole-1	22.054	22.039	0.015
Ethiofencarb	11.843	11.867	-0.024	Difenoconazole-2	22.126	22.111	0.015
Tolclofos-methyl	12.331	12.360	-0.029	Imibenconazole	23.516	23.503	0.013

SHIMADZU

Shimadzu Europa GmbH
Albert-Hahn-Str. 6-10 · D-47269 Duisburg
Tel.: +49 - (0)203 - 76 87-0
Fax: +49 - (0)203 - 76 66 25
shimadzu@shimadzu.eu
www.shimadzu.eu

For more details