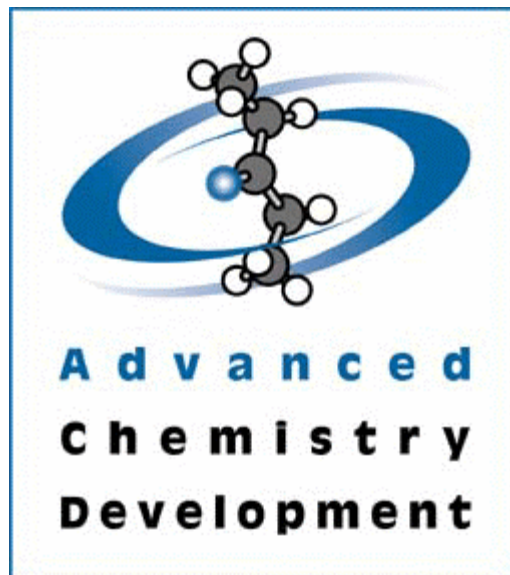


ACD/GC Simulator

Version 5.0 for Windows

Technical Note

**GC separation of C-substituted aromatics
Predicting retention times for new compounds with
ACD/GC Simulator**



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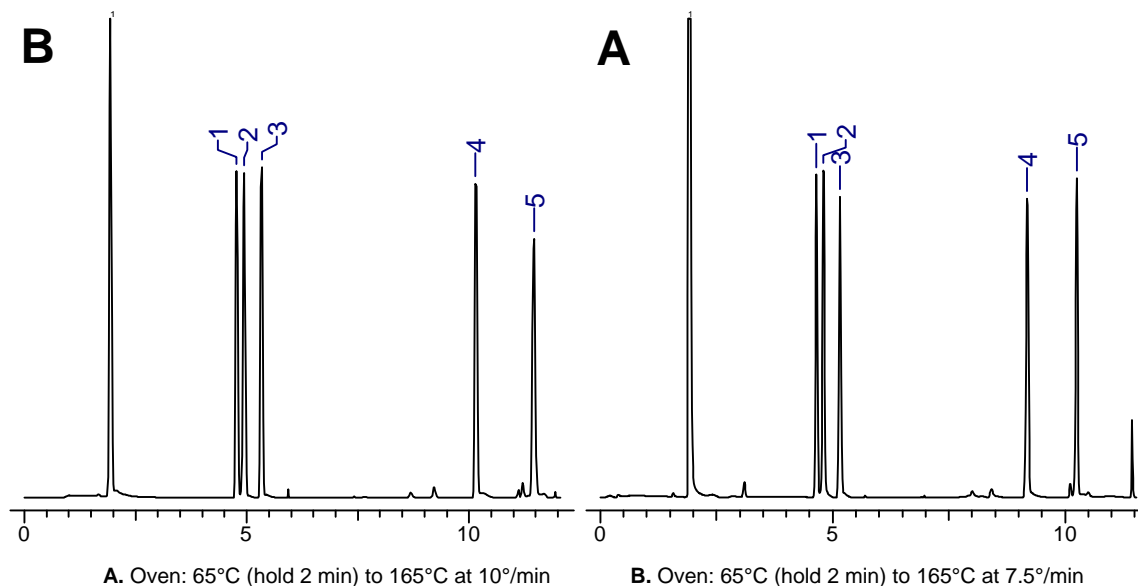
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Introduction

This document will familiarize you with gradient program optimization for a set of **C-substituted aromatics** and retention time predictions for new compounds in new conditions.

The Process

1. The following pictures display experimental GC chromatograms for 5 compounds. The corresponding separation conditions are stipulated below each chromatogram:



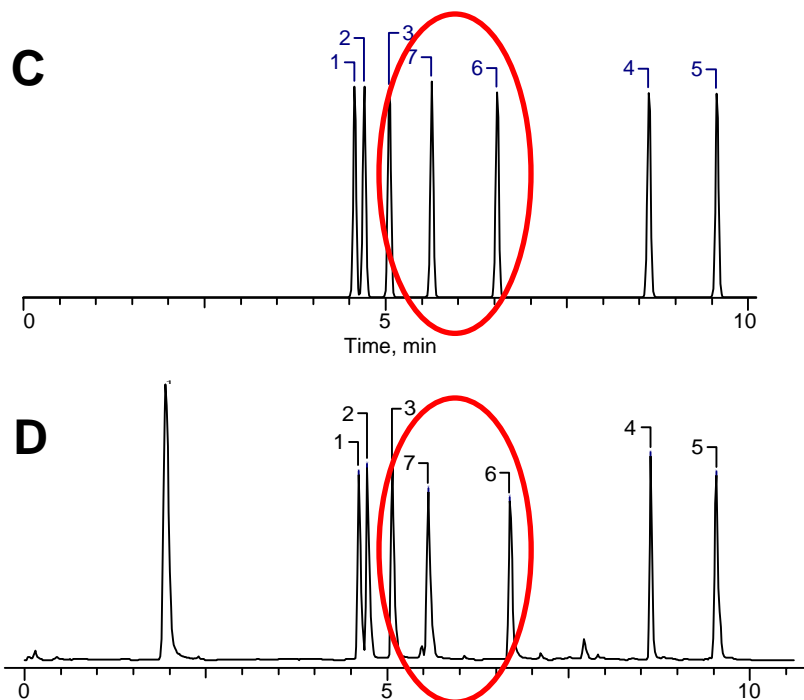
The following table shows retention times for every compound in experiments A and B:

No.	Compound	t_R for exp. A	t_R for exp. B
1	ethylbenzene	4.65	4.77
2	p-xylene	4.80	4.94
3	o-xylene	5.16	5.34
4	1,2,4,5-tetramethylbenzene	9.19	10.14
5	naphthalene	10.26	11.46

2. These experimental GC chromatograms along with the conditions in which the separations were performed were transferred to ACD/GC Simulator¹. The program calculated the correlation equation based on physicochemical properties (boiling point and $\log P$) of these compounds in the specified conditions.
3. On the basis of these correlations, retention times were predicted for two new compounds—structural isomers: **1,2,4-trimethylbenzene** and **isopropylbenzene**.

¹ Retention times and GC parameters may be transferred directly from ChromManager 5.0

4. A new temperature gradient was then emulated [65°C (hold 2 min) to 165°C at 12°/min]. The calculated (C) and experimental (D) chromatograms in these conditions can be compared on the pictures shown below



The following table indicates calculated and experimental retention times for every compound used for the chromatogram simulation. Note that the ***new compounds*** (for which retention times were predicted on the basis of the two experiments) are emphasized in bold italics.

No.	Compound	t_R (calc) in new conditions	t_R (exp) in new conditions
1	ethylbenzene	4.57	4.60
2	p-xylene	4.70	4.72
3	o-xylene	5.05	5.07
4	1,2,4,5-tetramethylbenzene	8.63	8.63
5	naphthalene	9.56	9.54
6	<i>1,2,4-trimethylbenzene</i>	<i>6.54</i>	<i>6.69</i>
7	<i>isopropylbenzene</i>	<i>5.63</i>	<i>5.57</i>

ACD/GC Simulator features that were used for successful simulation of retention times for NEW structures in NEW conditions

1. A temperature optimizing mechanism that allows optimizing temperature gradient using two experimental chromatograms for the same compounds in different conditions. **Chemical structures are not used.**
2. A predicting mechanism that allows to calculate retention times for new compounds on the basis of the correlation equation that is calculated using retention times of related compounds that were separated in certain conditions versus different physicochemical properties which can be calculated with ACD/Labs software (boiling point, log*P*, MW, MV, MR). **Chemical structures are used.**
3. A predicting-optimizing mechanism that is founded on a combination of the temperature optimizing and predicting mechanisms, it allows prediction of retention times for NEW COMPOUNDS in any NEW CONDITIONS.