



## Confirmation of Mass Information for Synthetic Compound

Chromaster 5610 MS detector is a new mass detector, designed for LC users, and it is different from conventional mass spectrometers. By using this detector with syringe pump, a sample solution is introduced directly to 5610 MS Detector and the mass information can be obtained easily. The system allows the confirmation of the mass information of synthetic compounds or simple monitoring for the compound identification when the synthetic conditions are being studied. This time, the system was used for the confirmation of the mass information on the synthetic intermediates in the following synthesis scheme, and the analysis example is introduced here.



5610 MS Detector

### Infusion measurement of synthetic compounds intermediates (1)

#### Analytical Conditions

Table 1 MS Detector Setting Conditions

Ionization method	ESI
Ionization mode	Positive
Ionization voltage	2200 V
Measurement mode	Scan
Gas flow rate	0.5 L/min
IS/AIF temperature	70 °C / 120 °C
Pump flow rate	2 μL/min

#### Sample Preparation

Concentration : 10 μg/mL each  
Solvent : CH<sub>3</sub>OH

#### Measurement Method

By connecting the syringe pump and MS Detector, the sample solution is directly delivered.



#### Synthesis Scheme 1 (Synthesis of Diol)

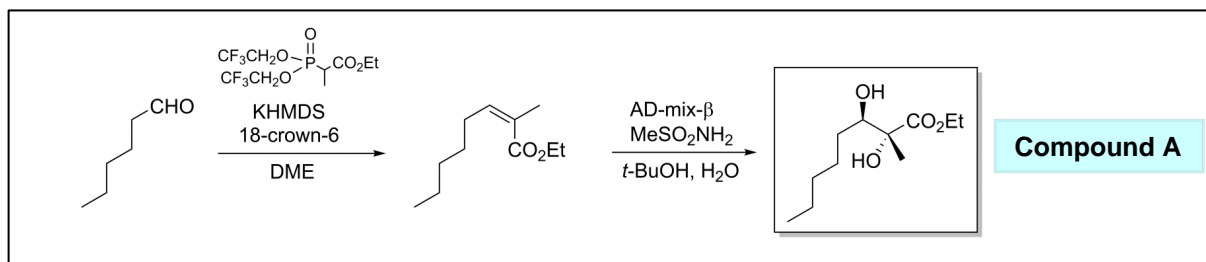
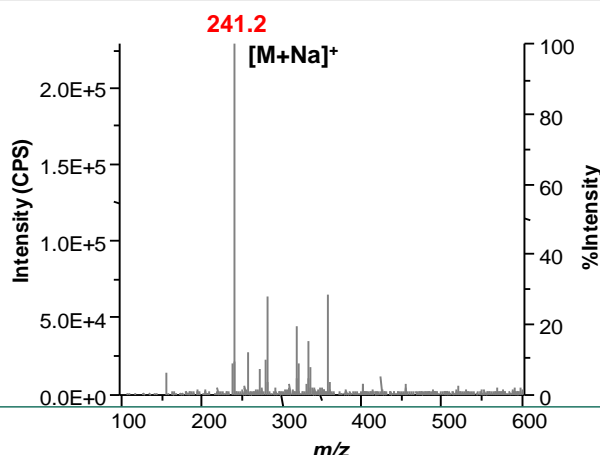
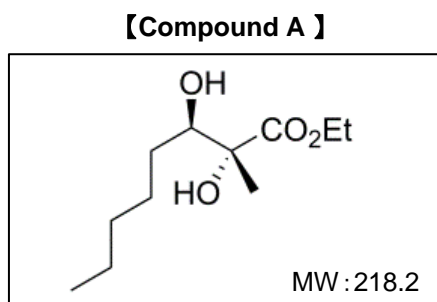


Fig. 1 Synthesis Scheme 1

#### Structural formula and MS Spectrum of Synthetic compound

Sodium adduct molecular ion was observed by direct introduction of the diluted Compound A (10ug/ml) to MS Detector.





## Infusion measurement of synthetic compounds intermediates (2)

### ■ Synthesis Scheme 2 (Synthesis of Dihydropyran Derivative)

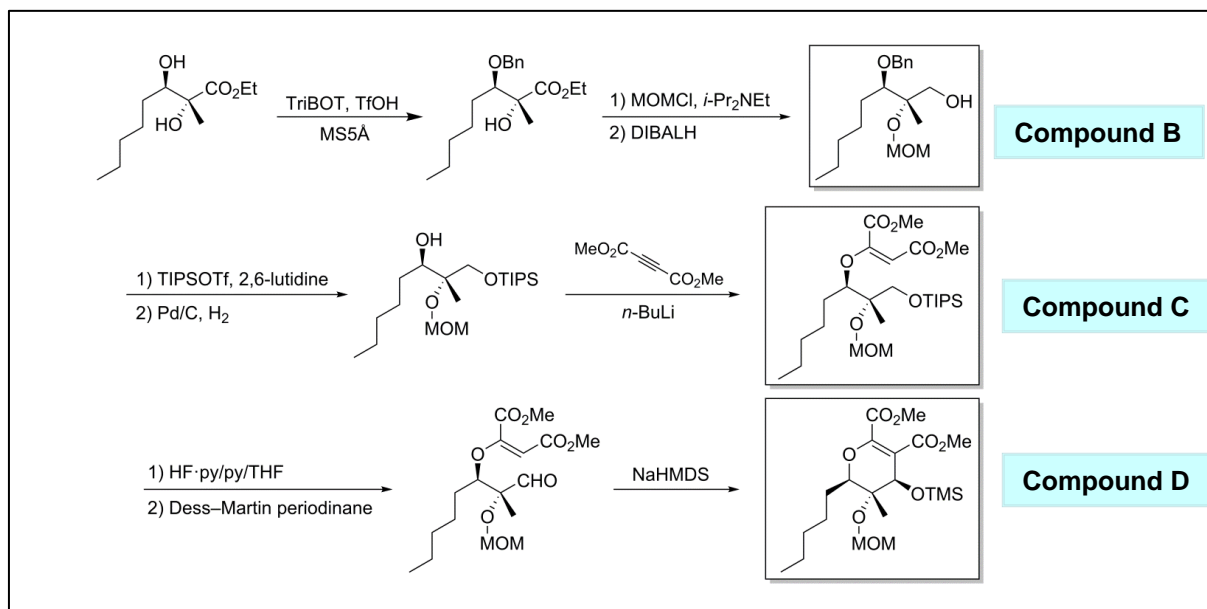
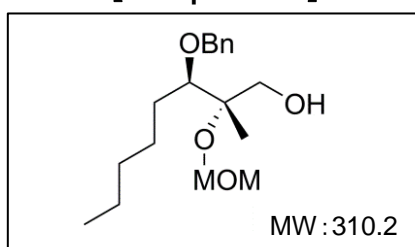


Fig.3 Synthesis Scheme 2

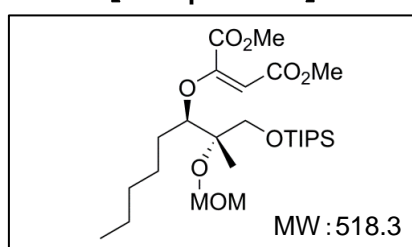
### ■ Structural formula and MS Spectrum of Synthetic compound

Compounds B, C, and D were diluted to 10 ppm with methanol and directly analyzed by the mass detector. As a result, a sodium adduct molecular ion, [M+Na]<sup>+</sup>, was observed.

【 Compound B 】



【 Compound C 】



【 Compound D 】

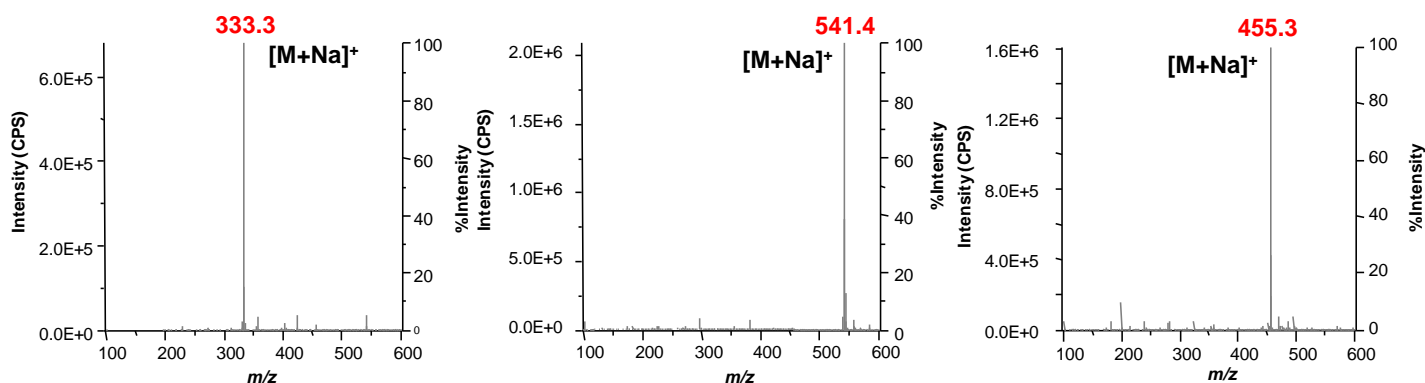
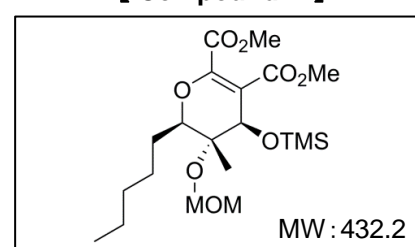


Fig.4 Structural formula and MS Spectrum of Compound B, C and D

\* The sample analyzed this time was provided by Pharmaceutical Molecular Design Class, Department of Life and Pharmaceutical

Main system configuration: Chromaster 5610 MS Detector, Syringe pump

NOTE: These data are an example of measurement; the individual values cannot be guaranteed.