



## Optional unit for the GCMS-NX SMCI Unit

SMCI stands for Solvent Mediated Chemical Ionization, a soft ionization method for GCMS. The headspace reagent gas from the sample bottle is introduced into the GCMS ionization unit to be ionized, which then causes chemical ionization (CI) of the target molecule via protonation.\* Previous CI methods have required the use of flammable reagent gas cylinders, but SMCI can be carried out with a general organic solvent such as methanol or acetonitrile, together with nitrogen or argon gas. This results in greater safety and lower running costs.



Outside view



Inside view



SMCI unit+GCMS-QP2020 NX

### A safe and simple ionization method

Cylinders of flammable gas such as methane or isobutane are not used in this method, so it is easy and safe to install the equipment.

### Can handle a large number of compounds

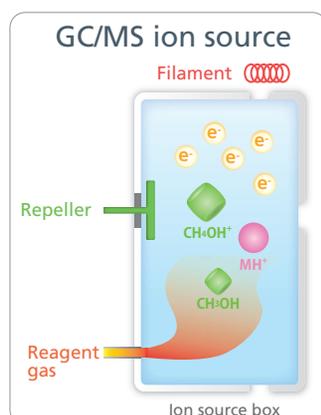
Compared to the CI substitution method, the SMCI method with methanol is less dependent on the compound, but can produce the same results. Because the SMCI method results in less fragmentation, it is very effective for verifying molecular weights for qualitative analysis.

### Provides unique structural information to identify compounds

SMCI can provide structural information in addition to molecular weights. For example, using acetonitrile as the reagent gas with a TQ, it is possible to identify the position of double bonds in unsaturated fatty acids.

### Low running costs

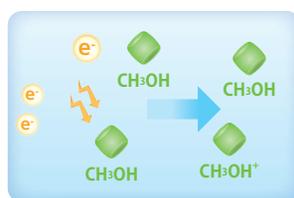
The reagent gas is less expensive than for other CI methods, so running costs can be reduced by over 80%.



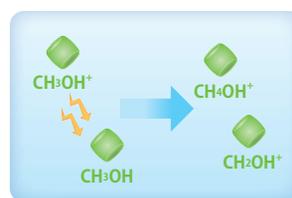
\*Patent pending

### Ionization mechanism

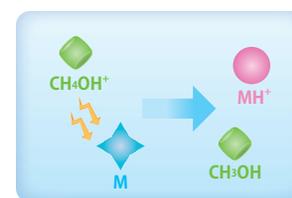
1. Reagent molecule is ionized



2. Reaction ion is created



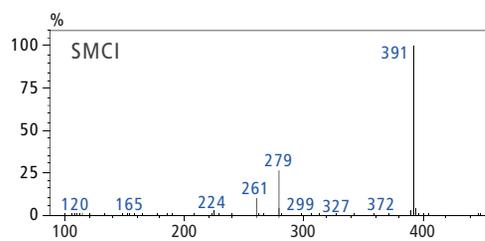
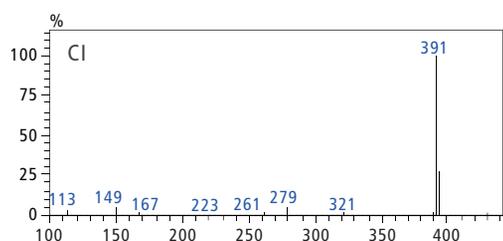
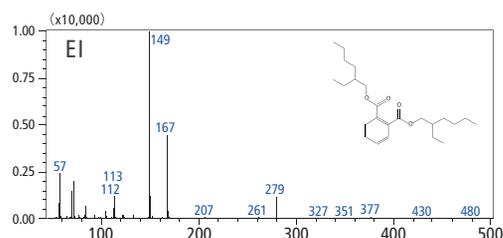
3. Sample molecule is ionized



Principles of SMCI

## A CI method that can deal with various types of compounds

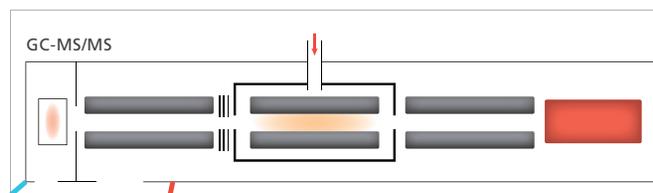
There are many cases where the ionization energy for EI is too high to verify molecular weights, but a soft ionization method such as SMCI is effective. For example, SMCI can be used to verify the molecular weights of bis (2-ethylhexyl) phthalate, whereas EI cannot. SMCI can obtain the same results as previously-existing CI methods, but is less dependent on the compound.



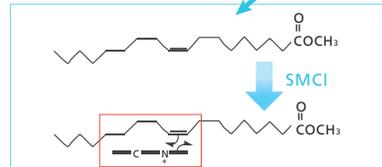
The mass spectrum of bis (2-ethylhexyl) phthalate (MW=390) obtained using different ionization methods

## Identifying the position of double bonds in unsaturated fatty acids

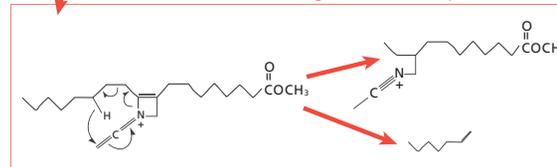
The functionality of unsaturated fatty acids varies greatly depending on branching and the position of double bonds. Using SMCI with acetonitrile as the reagent gas, particular reaction ions selectively attach to the double bonds. If a product ion scan is then carried out, fragmentation will occur at these attachment sites, so the positions of double bonds in the original fatty acid can be identified.



Addition of reaction ion



Fragmentation from product ion scan



### Compatible GCMS models

GCMS-TQ8050 NX, GCMS-TQ8040 NX, GCMS-QP2020 NX

### Recommended consumables

HPLC grade methanol or acetonitrile  
Nitrogen or argon gas (99.99+% purity)



Shimadzu Corporation

[www.shimadzu.com/an/](http://www.shimadzu.com/an/)

**For Research Use Only. Not for use in diagnostic procedure.**

This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.

Company names, product/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation or its affiliates, whether or not they are used with trademark symbol "TM" or "®". Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services. Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.

First edition: September 2019

© Shimadzu Corporation, 2019