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Rapid Identification of Double Bond Positions of Lipids in Butter by using Probe ESI Q-TOF LCMS-9050 and OAD-MS/MS

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Overview

- Probe Electro Spray Ionization(PESI) is one of the direct ionization techniques. Fig. 1 shows the scheme of PESI system.
- Oxygen Attachment Dissociation(OAD) is one of the unique fragmentation technologies. It is known to cleave specifically at the double-bond position, making it possible to estimate the double-bond position in compounds.
- By combining PESI and OAD techniques, unique MS/MS fragment ions can be rapidly detected with only a very simple pre-treatment. This technique was applied to estimate the double-bond position of Triglycerides(TG) in butter.

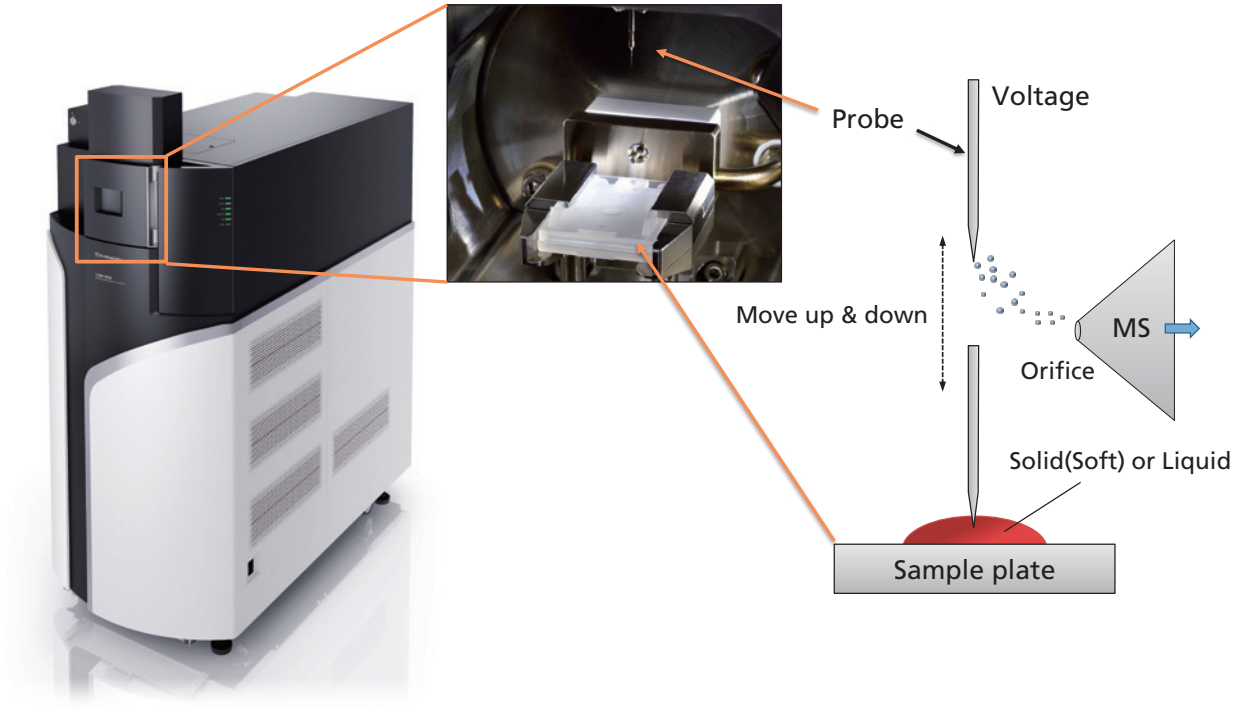

Fig. 1 Scheme of the DPiMS™ QT system

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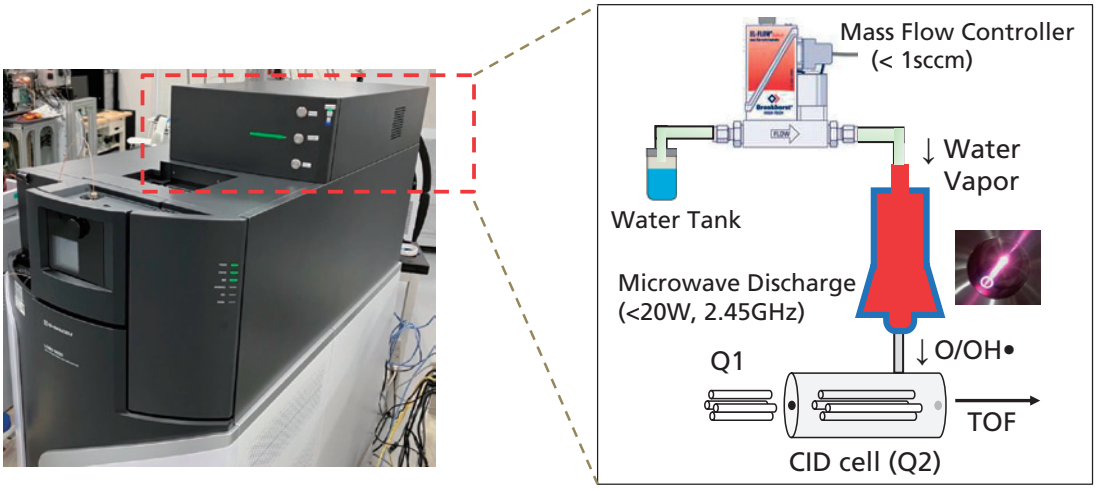

Fig. 2 Shimadzu LCMS-9050 and OAD system

Methods

All experiments were performed using a PESI Q-TOF, DPiMS™ QT and LCMS-9050 (Shimadzu, Kyoto, Japan). Collision Induced Dissociation (CID) and OAD fragmentation were used for determination of the chemical structure. Shimadzu DPiMS QT connected OAD system was used for direct ionization of the butter extract. The sample was pre-treated within 5 minutes by the following procedure shown in Fig. 3.

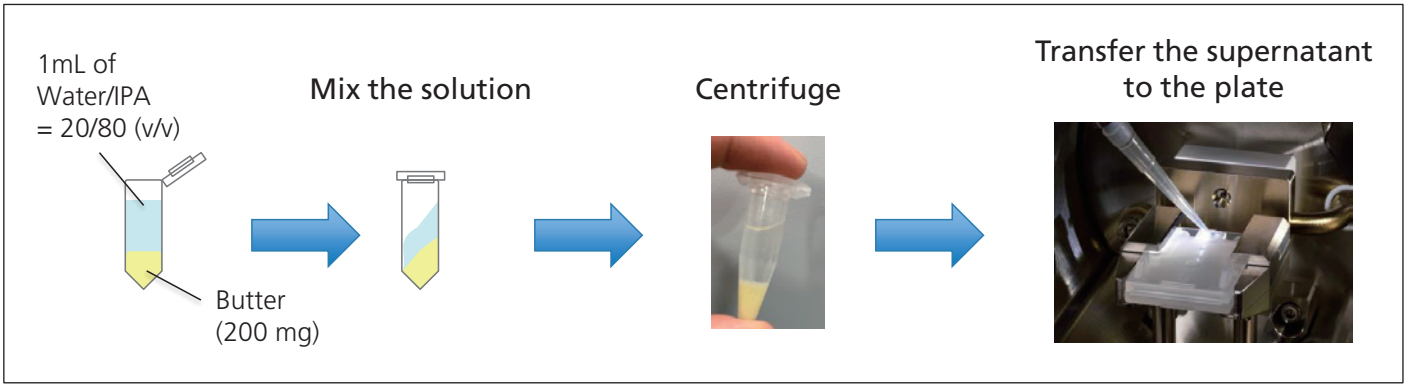

Fig. 3 Scheme of sample pretreatment for analysis

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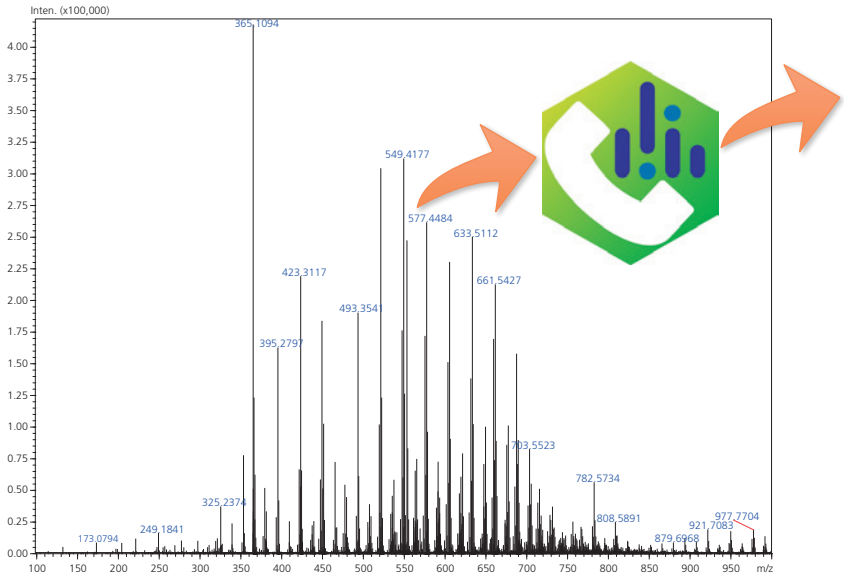
Results

Selection of Lipids in Butter for Identification

Samples of butter extracts were subjected to analysis with DPiMS QT and MS scans were performed. MS-DIAL was used to extract the m/z list of inferred lipids in the samples. From the list, selected TG 38: 1 and TG 38: 2 as candidates to identify their chemical structures.



MS1 (m/z)	Adduct	Predicted Structure
493.3504	[M+Na]+	TG 24:0
521.3825	[M+Na]+	TG 26:0
535.3969	[M+Na]+	TG 27:0
549.4146	[M+Na]+	TG 28:0
563.4274	[M+Na]+	TG 29:0
575.4286	[M+Na]+	TG 30:1
577.4457	[M+Na]+	TG 30:0
591.4584	[M+Na]+	TG 31:0
603.4599	[M+Na]+	TG 32:1
605.4765	[M+Na]+	TG 32:0
631.4913	[M+Na]+	TG 34:1
633.5084	[M+Na]+	TG 34:0
657.507	[M+Na]+	TG 36:2
659.5223	[M+Na]+	TG 36:1
661.5384	[M+Na]+	TG 36:0
673.5362	[M+Na]+	TG 37:1
685.5381	[M+Na]+	TG 38:2
687.5538	[M+Na]+	TG 38:1
689.5681	[M+Na]+	TG 38:0
713.5682	[M+Na]+	TG 40:2
715.5845	[M+Na]+	TG 40:1

Fig. 4 Spectra acquired by DPiMS QT and TG lists generated by MS-DIAL

The length of respective carbon chains bonded to glycerol in TG (38:1) and TG (38:2) were estimated by MS/MS spectra based on CID as shown in Fig. 5 and 7. The double-bond positions were determined by spectra based on OAD, as shown in Fig. 6 and 8.

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Identification of Chemical Structure (TG(38:1))

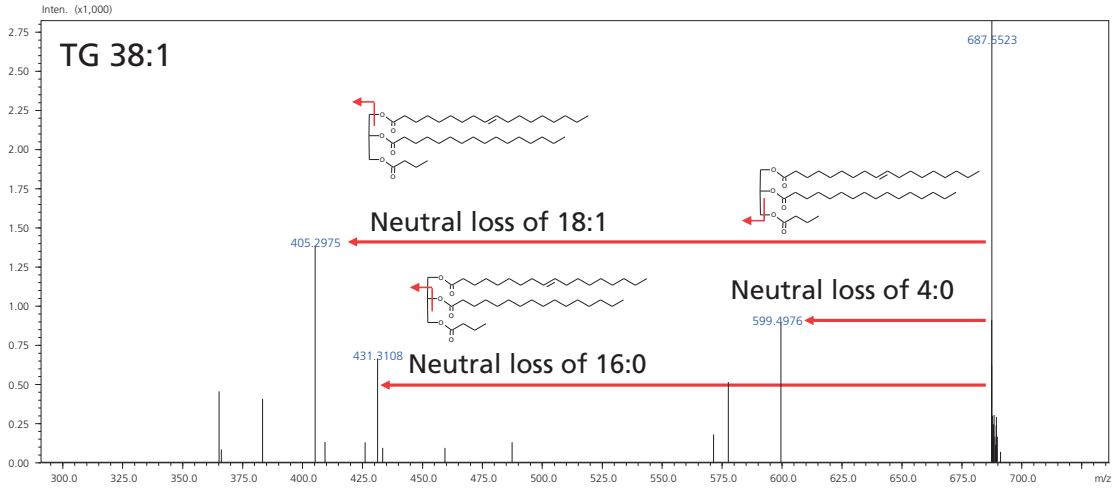

Fig. 5 MS/MS spectra of TG 38:1 acquired by CID mode

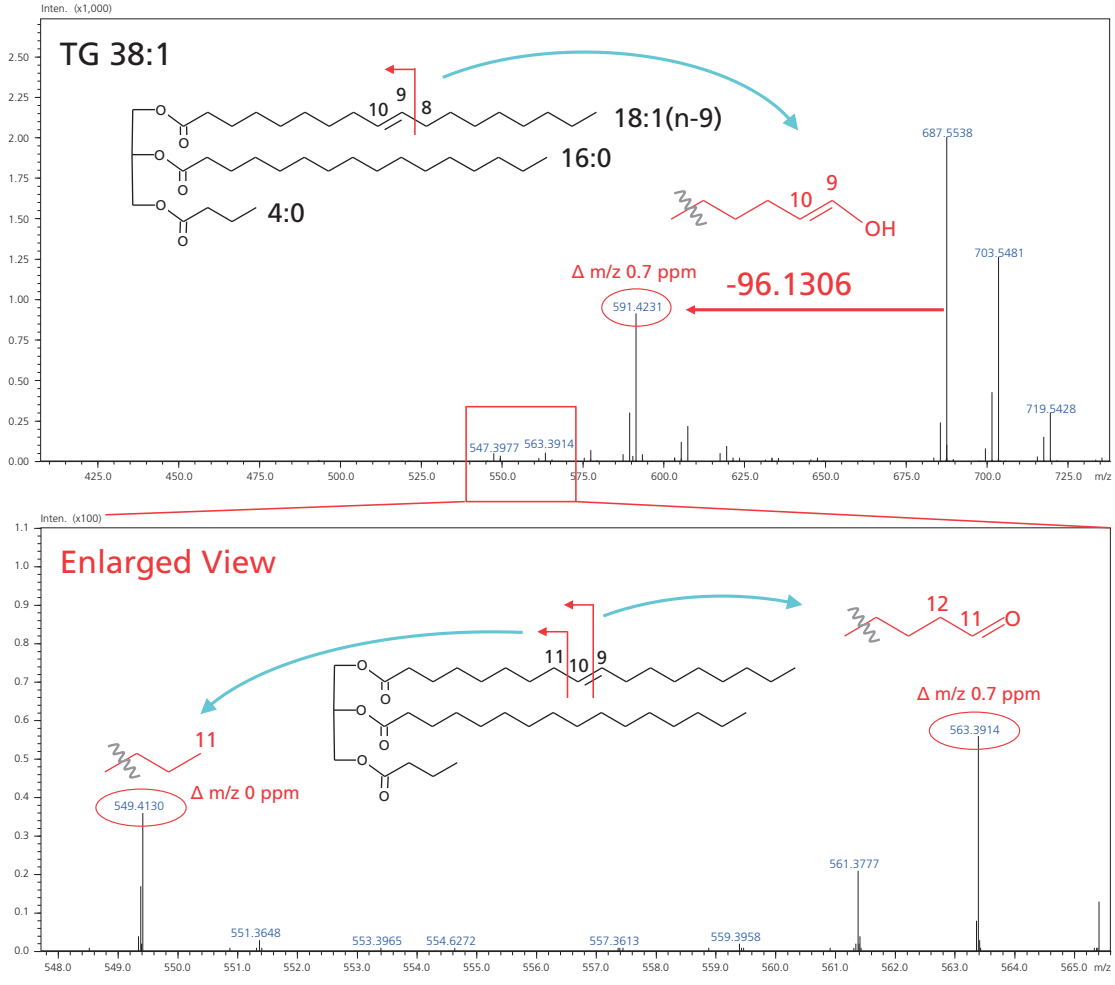

Fig. 6 Upper) MS/MS spectra of TG 38:1 acquired by OAD mode
Lower) Enlarged View of upper spectra

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Identification of Chemical Structure (TG(38:2))

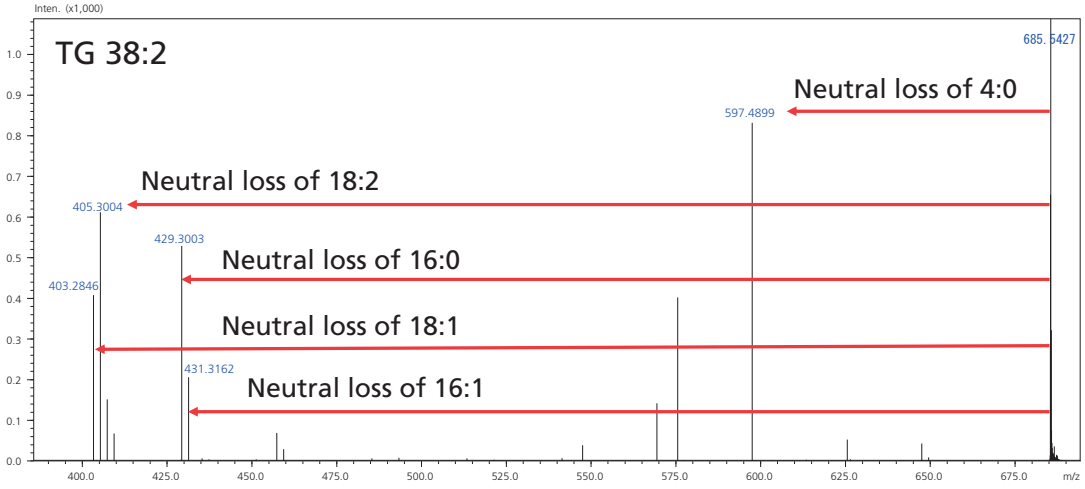

Fig. 7 MS/MS spectra of TG 38:2 acquired by CID mode

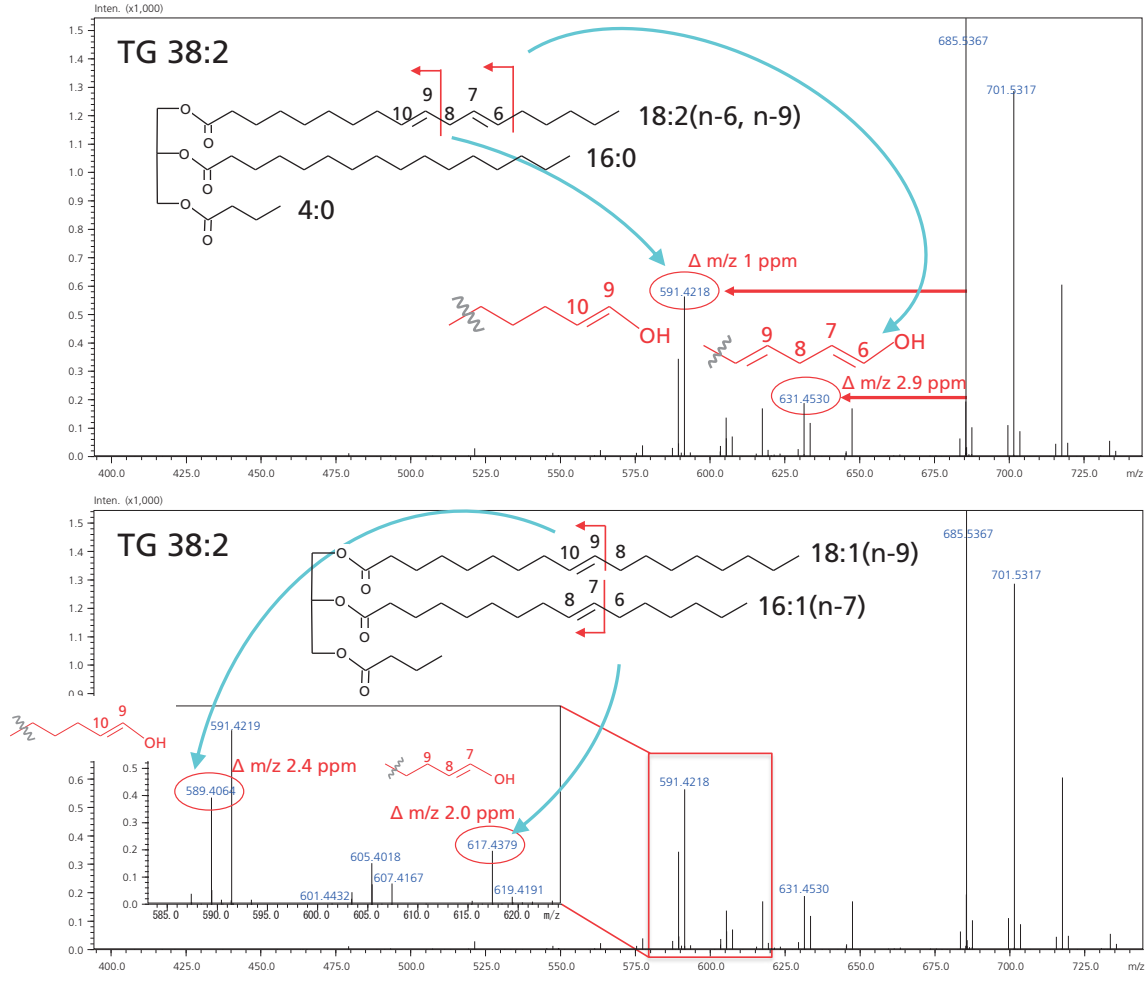

Fig. 8 MS/MS spectra of TG 38:2 acquired by OAD mode

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Conclusion

- It was confirmed that the double-bond position could be easily and quickly identified by combining PESI and OAD.
- The carbon chain length and double-bond position of fatty acids in TG were able to be identified by combining CID and OAD

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