

Application Data Sheet

No.141

GC-MS

Gas Chromatograph Mass Spectrometer

Analysis of Nootropics Using GC-MS(/MS) - Part 1

Nootropics is the general term for substances intended to improve cognitive function or abilities, such as certain drugs and supplements used to improve concentration or memory. Such nootropics are sometimes sold via the Internet without proper licensing, and there is concern that they could be harmful if used without the prescription of a physician because nootropics also include therapeutic drugs intended for epilepsy, attention-deficit hyperactivity disorder (ADHD), or depression.

Due to the relative newness of such substances, there are cases in which they are not registered in NIST, Wiley, or other mass spectral libraries commonly used for GC/MS analysis.

This Application Data Sheet describes an example of measuring 19 nootropics measurable by GC/MS.

Experimental

Standards of each component were dissolved in methanol to prepare a 10 µg/mL standard mixture solution. For components that cannot be measured without derivatization, 500 µL of the 10 µg/mL standard mixture solution was obtained, dried under a stream of nitrogen gas, and dissolved in 500 µL of BSTFA. Then the solutions were heated for 30 minutes at 60 °C for TMS derivatization.

Target compounds are listed in Table 1 and analytical conditions in Table 2.

Table 1: Target Compounds

Compound Name	Compound Name
Adrafinil	Vinpocetine
Atomoxetine	Pramiracetam
Aniracetam	Pregnenolone
Oxiracetam	Levetiracetam
Dihydroergotoxine	Etiracetam
Dehydroepiandrosterone (DHEA)	Atenolol
Nicergoline	Nadolol
Nimodipine	Idebenone
Nefiracetam	Furosemide
Piracetam	Tianeptine

Table 2: Analytical Conditions

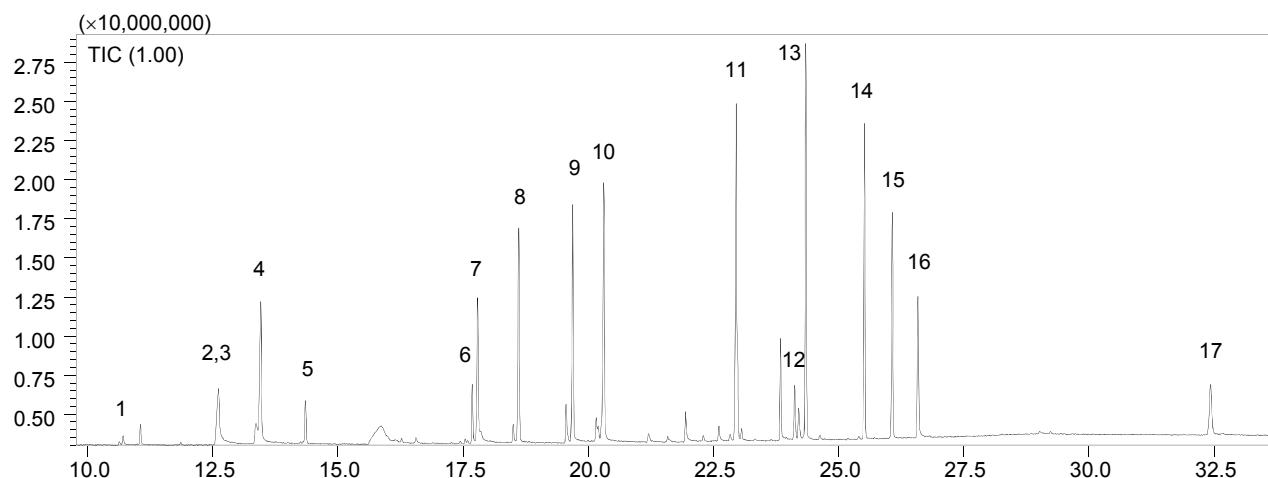
GC-MS: GCMS-QP2020
 Column: SH-RxiTM-5Sil MS (30 m long, 0.25 mm I.D., df = 0.25 µm) (Shimadzu, P/N: 221-75940-30)
 Glass Liner: Deactivated splitless liner with wool (PN:221-48876-03)

GC
 Injection Temp.: 260 °C
 Column Oven Temp.: 60 °C (2 min) → (10 °C/min) → 320 °C (15 min)
 Carrier Gas: Helium
 Flow Control: Linear velocity (45.6 cm/sec)
 Injection Mode: Splitless
 High Pressure Injection: 250 kPa (1.5 min)

MS
 Interface Temp.: 280 °C
 Ion Source Temp.: 200 °C
 Solvent Cut Time: 2 min
 Acquisition Time: 6 to 43 min
 Acquisition Mode: Scan
 Mass Range: *m/z* 40 to 600
 Event Time: 0.3 sec

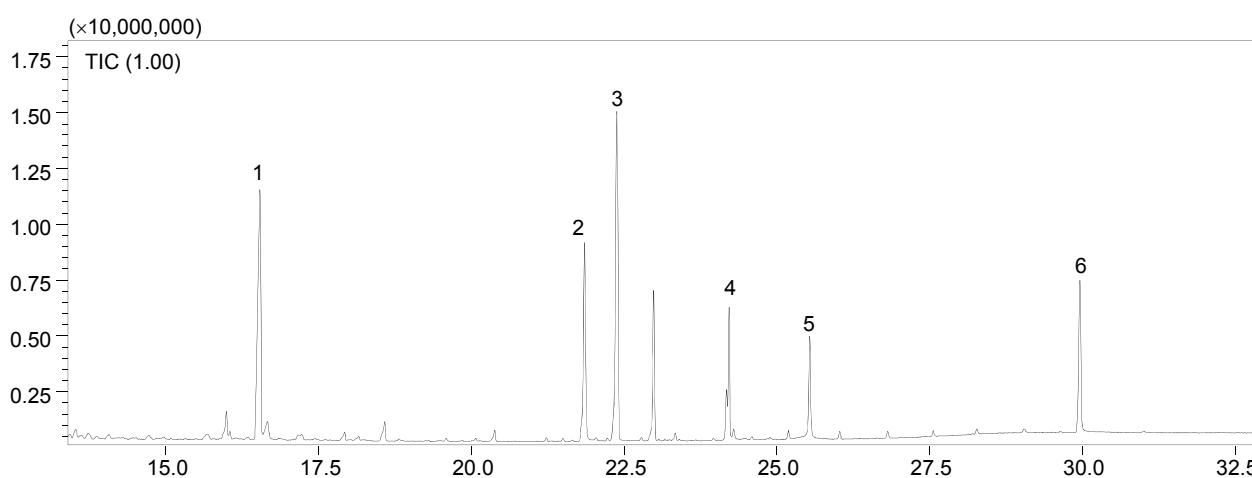
Analytical Results

The total ion current chromatogram (TIC) obtained by measuring the underderivatized 10 µg/mL standard mixture solution is shown in Fig. 1 and the TIC obtained by measuring the TMS derivatized 10 µg/mL standard mixture solution is shown in Fig. 2. Decomposition products were detected for nicergoline, adrafinil, and dihydroergotoxine. The decomposition products for adrafinil had the same retention time and mass spectral pattern as the decomposition products for modafinil. Because levetiracetam and etiracetam are optical isomers, they were detected at the same retention time and mass spectral pattern.



ID	Compound Name	Retention Time	Retention Index	ID	Compound Name	Retention Time	Retention Index
1	Nicergoline deg.1	10.707	1349	10	Nefiracetam	20.310	2230
2	Oxiracetam	12.603	1493	11	Dehydroepiandrosterone	22.950	2551
3	Piracetam	12.611	1493	12	Nicergoline deg. 2	24.202	2718
4	Levetiracetam/Etiracetam	13.458	1563	13	Pregnenolone	24.344	2738
5	Adrafinil deg. 1	14.348	1638	14	Vinpocetine	25.516	2904
6	Adrafinil deg. 2	17.683	1949	15	Nimodipine	26.074	2988
7	Atomoxetine	17.785	1959	16	Dihydroergotoxine deg.	26.585	3066
8	Aniracetam	18.608	2044	17	Nicergoline	32.430	3813
9	Pramiracetam	19.686	2160				

Fig. 1: Total Ion Current Chromatogram (TIC) of 10 µg/mL Standard Solution (Underderivatized)



ID	Compound Name	Retention Time	Retention Index
1	Oxiracetam-2TMS	16.535	1836
2	Atenolol-2TMS	21.849	2412
3	Nadolol-3TMS	22.380	2478
4	Idebenone-TMS	24.214	2720
5	Furosemide-2TMS	25.539	2908
6	Tianeptine-TMS	29.959	3567

Fig. 2: Total Ion Current Chromatogram (TIC) of 10 µg/mL Standard Solution (TMS Derivatives)

Mass Spectra

The mass spectra for typical nootropics obtained by measuring the underivatized standard mixture are shown in Fig. 3 and the mass spectra obtained by measuring the TMS derivatized standard are shown in Fig. 4.

Underivatized

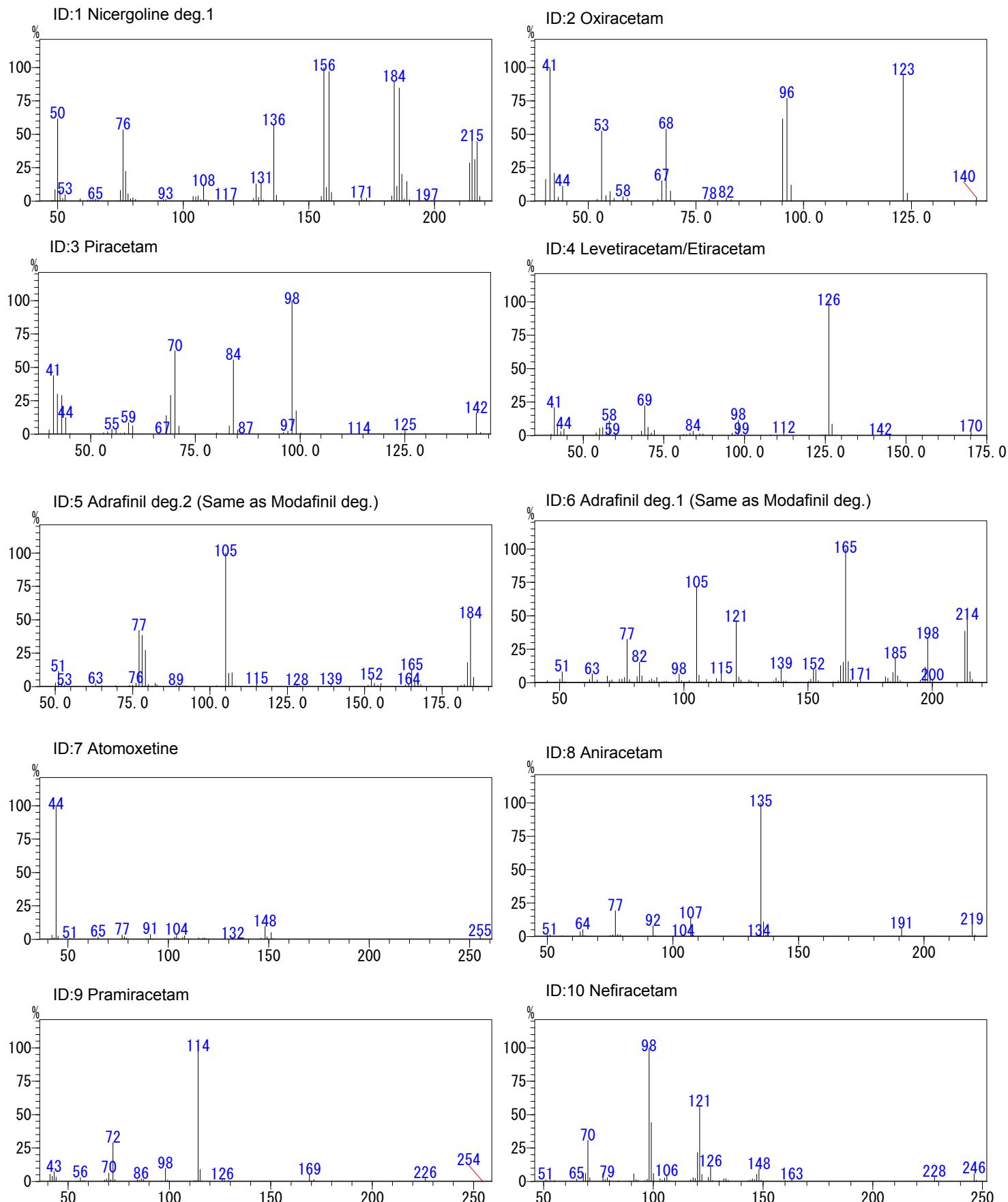


Fig. 3-1: Mass Spectra of Underivatized Typical Nootropics

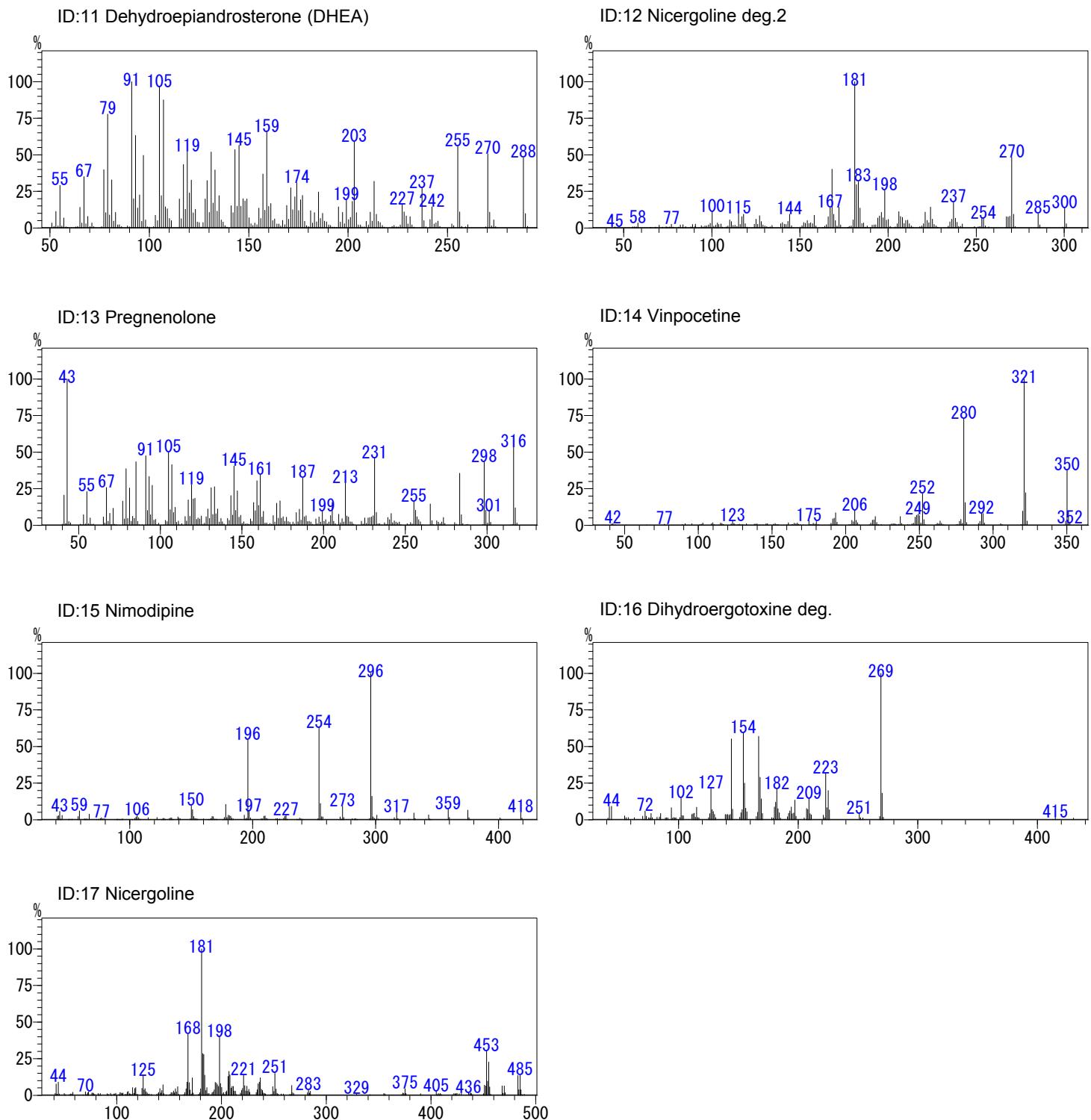


Fig. 3-2: Mass Spectra of Underivatized Typical Nootropics

TMS Derivatives

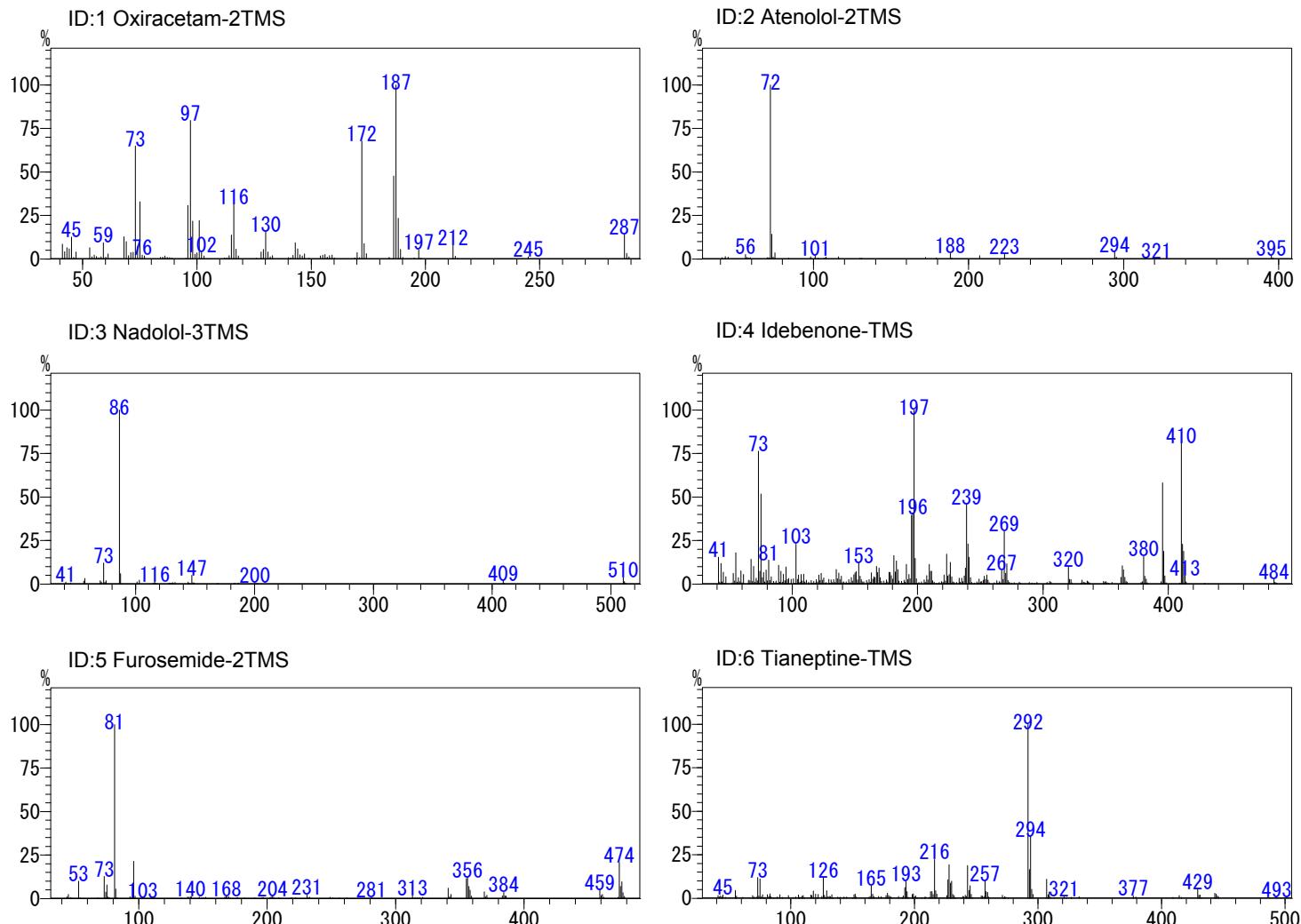


Fig. 4: Mass Spectra of TMS Derivatized Typical Nootropics

GCMS-TQ is trademarks of Shimadzu Corporation.
Rxi is a registered trademark of Restek Corporation.

First Edition: March 2018



For Research Use Only. Not for use in diagnostic procedures.
The content of this publication shall not be reproduced, altered or sold for any commercial purpose without the written approval of Shimadzu. The information contained herein is provided to you "as is" without warranty of any kind including without limitation warranties as to its accuracy or completeness. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication. This publication is based upon the information available to Shimadzu on or before the date of publication, and subject to change without notice.