Figure S1. HPLC chromatograms and absorption spectra of the purified MAAs. (a) The crude water-soluble extract of *N. commune* (genotype D) was separated by an HPLC system equipped with a preparative column (IRICA C18, 20 × 250 mm) as shown in Figure 1. The mobile phase changed in a stepwise fashion from distilled water for the initial 40 min, to 0.1% acetic acid 10% methanol for the next 20 min and to 100% methanol for the final 20 min. The flow rate was constant at 4 mL·min⁻¹, and the A₃₃₀ was monitored. The purified 508-Da MAA (b), 450-Da MAA (c) and 612-Da MAA (d) were analyzed by HPLC with an analytical reverse-phase column (Inertsil ODS-3, 4.6 mm × 250 mm; GL Sciences Inc., Tokyo, Japan) using 0.2% acetic acid at a flow rate of 1 mL·min⁻¹ as the mobile phase and were detected by the A₃₃₀. The purified 508-Da MAA (e), 450-Da MAA (f) and 612-Da MAA (g) showed absorption maximum at 334 nm, 322 nm and 322 nm, respectively.
1. NMR Spectra for the Determination of Chemical Structures of the 508-Da MAA (Figures S2–S7) and the 612-Da MAA (Figures S8–S15)

1.1. NMR Data for the 508-Da MAA

**Figure S2.** $^1$H NMR spectra of the 508-Da MAA in D$_2$O.
**Figure S2. Cont.**

![Diagram](image)
**Figure S3.** $^{13}$C NMR spectrum of the 508-Da MAA in D$_2$O.

**Figure S4.** DEPT spectra of the 508-Da MAA in D$_2$O (DEPT135: upper, DEPT90: middle, 13C lower).
Figure S4. Cont.

Figure S5. COSY spectra of the 508-Da MAA in D₂O.
Figure S5. Cont.

Figure S6. HMQC spectra of the 508-Da MAA in D$_2$O.

X: parts per Million : 1H

Y: parts per Million : 13C

Abundance

0 1.0 2.0 3.0

(thousandths)

0 10.0

abundance

0 1.0 2.0 3.0
Figure S6. Cont.

Figure S7. HMBC spectra of the 508-Da MAA in D$_2$O.
Figure S7. Cont.
2.2. NMR Data for the 612-Da MAA

Figure S8. $^1$H NMR spectra of the 612-Da MAA in D$_2$O.
Figure S9. 13C NMR spectra of the 612-Da MAA in D2O.
Figure S9. Cont.

Figure S10. High resolution $^{13}$C NMR spectrum of the 612-Da MAA in D$_2$O at around 160 ppm. Focusing on the narrow X-range at around 160 ppm, $^{13}$C NMR spectrum was recorded with a high resolution to separate the two signals from C1 and C3. Because these chemical shift values were not adjusted by referring internal standard at 0 ppm, the chemical shift values recorded here were different from those in the $^{13}$C NMR spectrum shown in Figure S9.
Figure S11. DEPT90 (upper) and $^{13}$C (lower) NMR spectra of the 612-Da MAA in D$_2$O.
Figure S12. DEPT135 (upper) and $^{13}$C (lower) NMR spectra of the 612-Da MAA in D$_2$O.
**Figure S13.** COSY spectra of the 612-Da MAA in D₂O.
Figure S13. Cont.

Figure S14. HMQC spectra of the 612-Da MAA in D$_2$O.
Figure S15. HMBC spectra of the 612-Da MAA in D$_2$O.
Figure S15. Cont.

File name: peak3_pfg-2011-2.jdf
Author: ai
Date: 2011
Sample_id: S703297
Spectrometer: 7-T NMR
Dimensions: X Y
Data format: 2D REAL REAL
Comment: in D2O

Field_strength: 9.4 Tesla (400 MHz)

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Grad_1_amp = 0.18 [T/m]
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Y_acq_time = 10.17856 [ms]
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Tri_domain = 1H
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Y_resolution = 98.24572435 [Hz]
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Recvr_gain = 84
Long_range_j = 8 [Hz]
Recvr_gain = 84
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Field_strength = 9.4 Tesla (400 MHz)
Figure S15. Cont.

![Figure S15](image-url)