SUPPLEMENT INFORMATION

Identification and characterization of α -glucosidase inhibition flavonol glycosides from jack bean (*Canavalia ensiformis* (L.) DC.

Anita M. Sutedja^{1,2,3}, Emiko Yanase^{1,*}, Irmanida Batubara^{4,5}, Dedi Fardiaz² and Hanifah N. Lioe²

- ¹ Faculty of Applied Biological Sciences, Graduate School of Applied Biological Sciences, Gifu University, 1-1 Yanagido, Gifu City, Gifu 501-1193, Japan; <u>e-vanase@gifu-u.ac.jp</u>
- ² Department of Food Science and Technology, Faculty of Agricultural Engineering and Technology, IPB University, Kampus IPB Dramaga, Bogor 16680, West Java, Indonesia; hanifahlioe@apps.ipb.ac.id; <a href="https://dedi.gov/dedi.g
- ³ Department of Food Technology, Faculty of Agricultural Technology, Widya Mandala Catholic University Surabaya, Jalan Dinoyo 42-44, Surabaya 60265, East Java, Indonesia; maya@ukwms.ac.id
- ⁴ Department of Chemistry, Faculty of Mathematics and Natural Science, IPB University, Kampus IPB Dramaga, Bogor 16680, West Java, Indonesia; imebatubara@gmail.com
- ⁵ Tropical Biopharmaca Research Center IPB University, Kampus IPB Taman Kencana No 3, Bogor 16128, West Java, Indonesia
- * Correspondence: e-yanase@gifu-u.ac.jp; Tel.: +81-58 293 2914

Table of Content

Figure S1. ¹ H NMR spectrum of compound 1 (CD ₃ OD, 800 MHz)	4
Figure S2. ¹³ C NMR spectrum of compound 1 (CD ₃ OD, 800 MHz)	5
Figure S3. ¹ H- ¹ H COSY of compound 1 (CD ₃ OD, 800 MHz)	6
Figure S4. HMQC of compound 1 (CD₃OD, 800 MHz)	7
Figure S5. HMBC of compound 1 (CD3OD, 800 MHz)	8
Figure S6. ¹ H NMR spectrum of compound 2 (CD ₃ OD, 800 MHz)	9
Figure S7. ¹³ C NMR spectrum of compound 2 (CD ₃ OD, 800 MHz)	10
Figure S8. ¹ H- ¹ H COSY of compound 2 (CD ₃ OD, 800 MHz)	11
Figure S9. HMQC of compound 2 (CD₃OD, 800 MHz)	12
Figure S10. HMBC of compound 2 (CD ₃ OD, 800 MHz)	13
Figure S11. ¹ H NMR spectrum of compound 3 (CD ₃ OD, 800 MHz)	14
Figure S12. ¹³ C NMR spectrum of compound 3 (CD ₃ OD, 800 MHz)	15
Figure S13. ¹ H- ¹ H COSY of compound 3 (CD ₃ OD, 800 MHz)	16
Figure S14. HMQC of compound 3 (CD3OD, 800 MHz)	17
Figure S15. HMBC of compound 3 (CD ₃ OD, 800 MHz)	18
Figure S16. ¹ H NMR spectrum of compound 4 (CD ₃ OD, 600 MHz)	19
Figure S17. ¹³ C NMR spectrum of compound 4 (CD ₃ OD, 600 MHz)	20
Figure S18. ¹ H- ¹ H COSY of compound 4 (CD ₃ OD, 600 MHz)	21
Figure S19. HMQC of compound 4 (CD3OD, 600 MHz)	22
Figure S20. HMBC of compound 4 (CD ₃ OD, 600 MHz)	23
Figure S21. LC/ESI/MS/MS data of compound 1	24
Figure S22. LC/ESI/MS/MS data of compound 2	25
Figure S23. LC/ESI/MS/MS data of compound 3	26
Figure S24. LC/ESI/MS/MS data of compound 4	27
Figure S25. LC/ESI/MS/MS data of compound 5	28
Figure S26. LC/ESI/MS/MS data of compound 6	29
Figure S27. LC/ESI/MS/MS data of compound 7	30
Figure S28. LC/ESI/MS/MS data of compound 8	31
Figure S29. LC/ESI/MS/MS data of compound 9	32
Figure S30. LC/ESI/MS/MS data of compound 10	33
Figure S31. LC/ESI/MS/MS data of compound 11	34
Figure S32. LC/ESI/MS/MS data of compound 12	35
Figure S33. LC/ESI/MS/MS data of compound 13	36
Figure S34. LC/ESI/MS/MS data of compound 14	37
Figure S35. GC-MS total ion chromatogram and extracted ion chromatogram of trimethylsilyl (TMS) derivatives of galactose	38

Figure S36.	GC-MS total ion chromatogram and extracted ion chromatogram of trimethylsilyl (TMS) derivatives of glucose	39
Figure S37.	GC-MS total ion chromatogram and extracted ion chromatogram of trimethylsilyl (TMS) derivatives of rhamnose	40
Figure S38.	GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound 1	41
Figure S39.	GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound 2	42
Figure S40.	GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound 3	43
Figure S41.	GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound 4	44
Figure S42.	Chromatogram of compounds 1 (a) and 2 (b)	45
Figure S43.	Chromatogram of compounds 3 (a) and 4 (b)	46

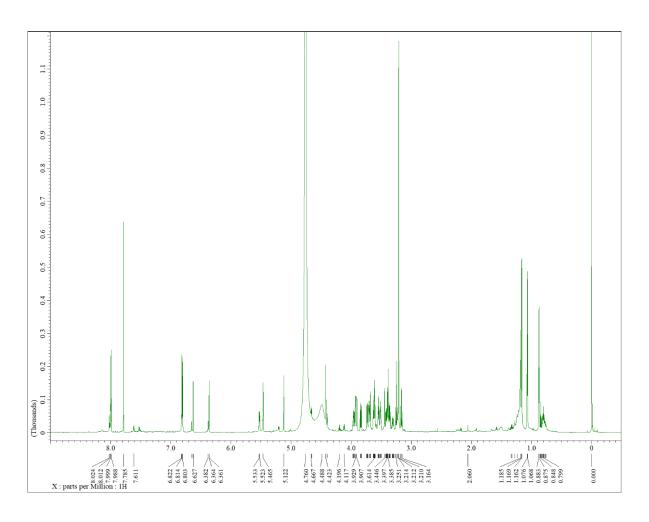


Figure S1. ¹H NMR spectrum of compound 1 (CD₃OD, 800 MHz)

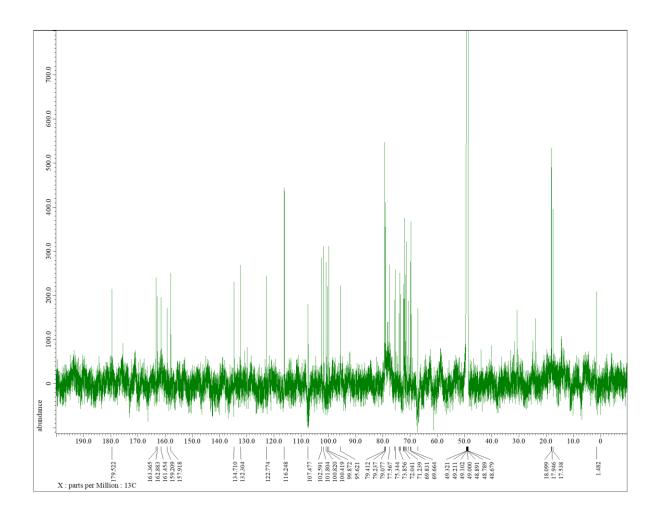
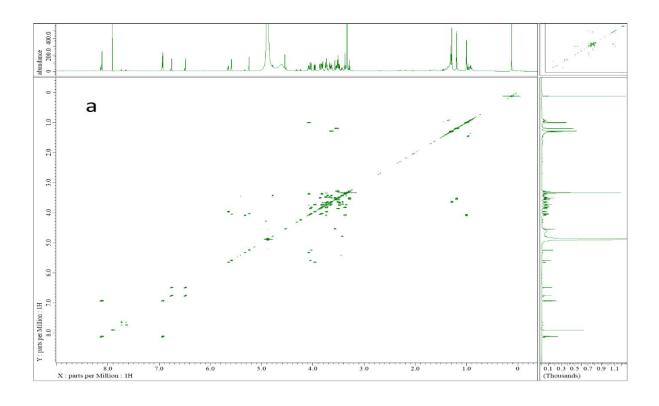


Figure S2. ¹³C NMR spectrum of compound 1 (CD₃OD, 800 MHz)



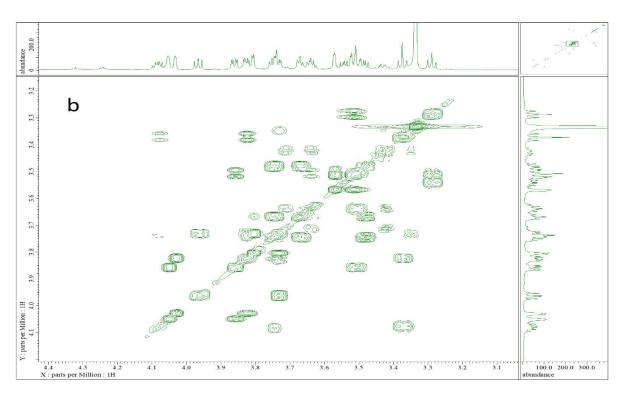
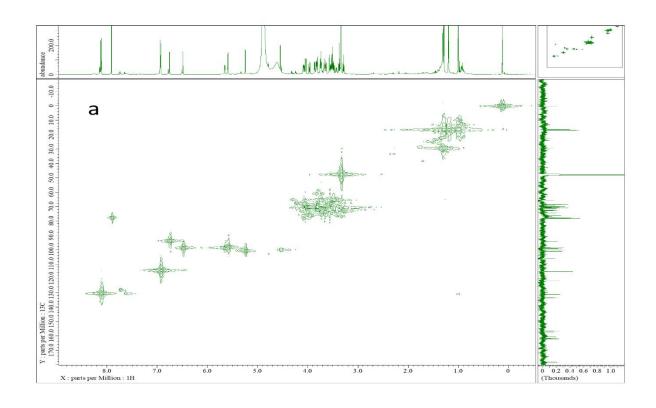


Figure S3. ¹H-¹H COSY of compound 1 (CD₃OD, 800 MHz)



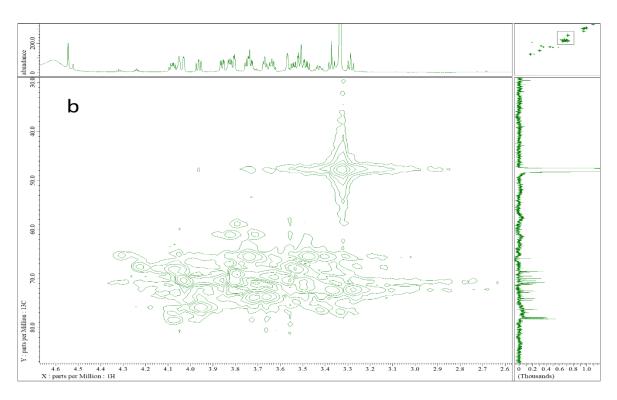
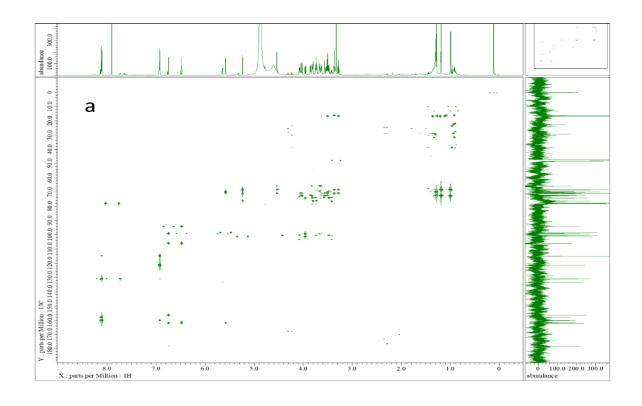


Figure S4. HMQC of compound 1 (CD₃OD, 800 MHz)



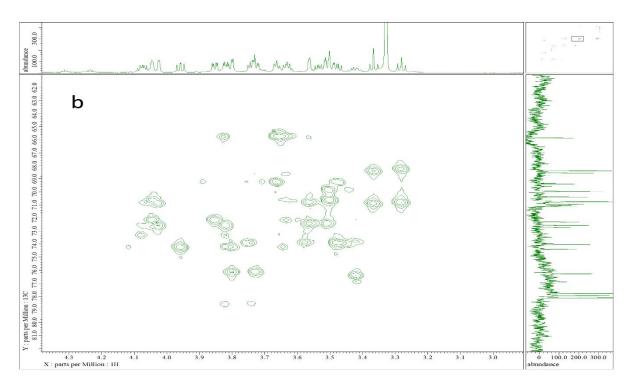


Figure S5. HMBC of compound 1 (CD₃OD, 800 MHz)

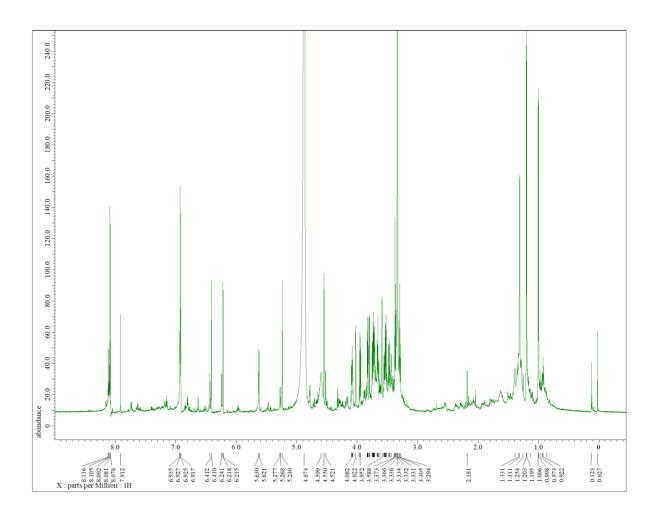


Figure S6. ¹H NMR spectrum of compound **2** (CD₃OD, 800 MHz)

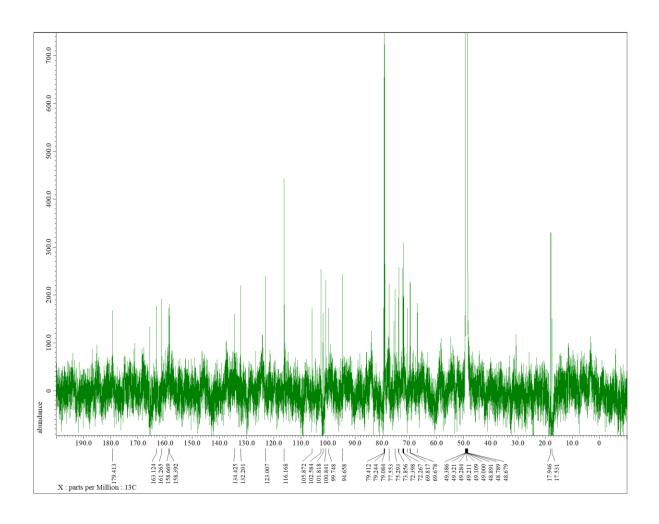
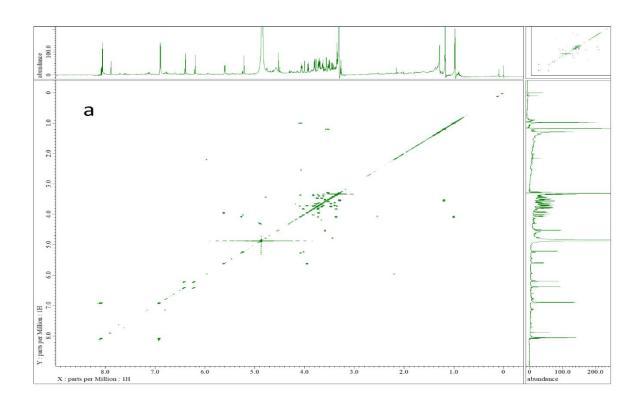


Figure S7. ¹³C NMR spectrum of compound **2** (CD₃OD, 800 MHz)



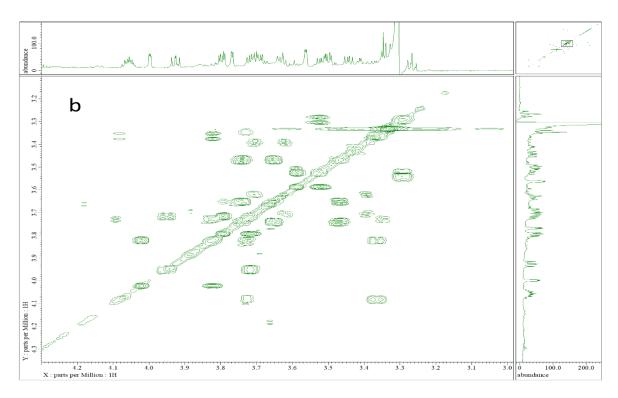
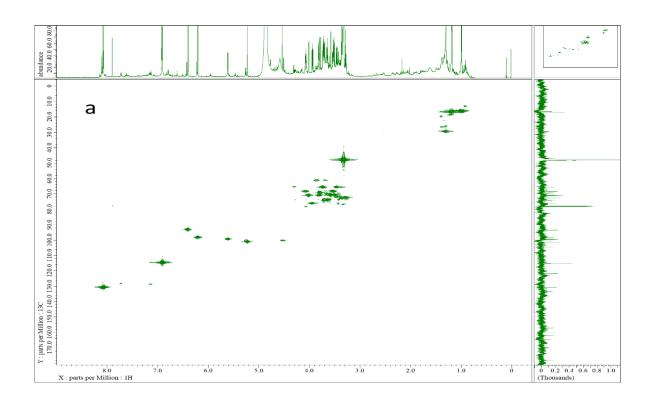


Figure S8. ¹H-¹H COSY of compound 2 (CD₃OD, 800 MHz)



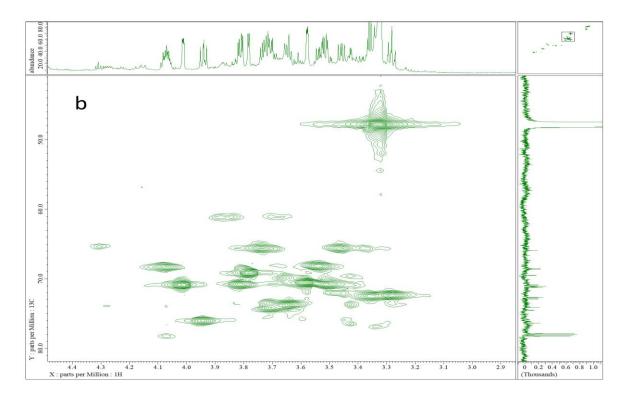
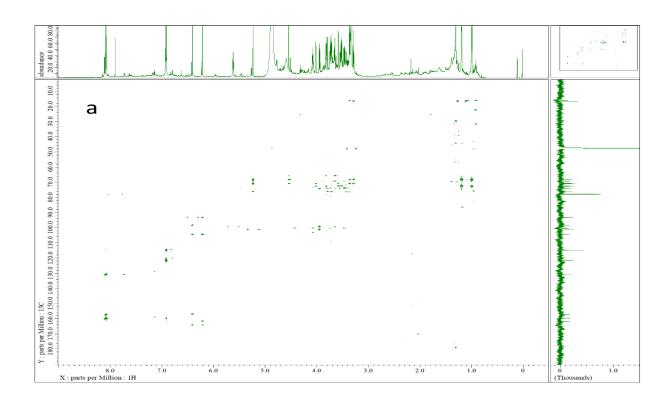


Figure S9. HMQC of compound 2 (CD₃OD, 800 MHz)



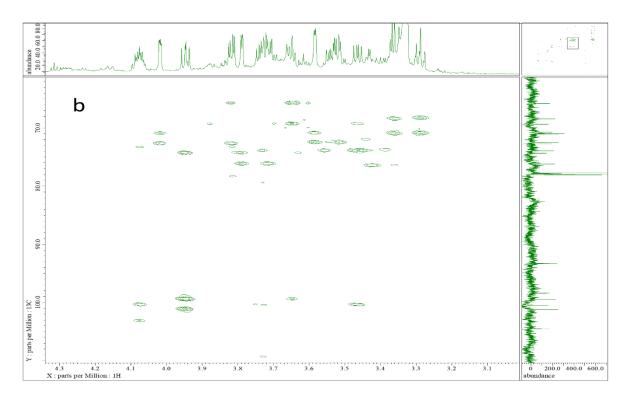


Figure S10. HMBC of compound 2 (CD₃OD, 800 MHz)

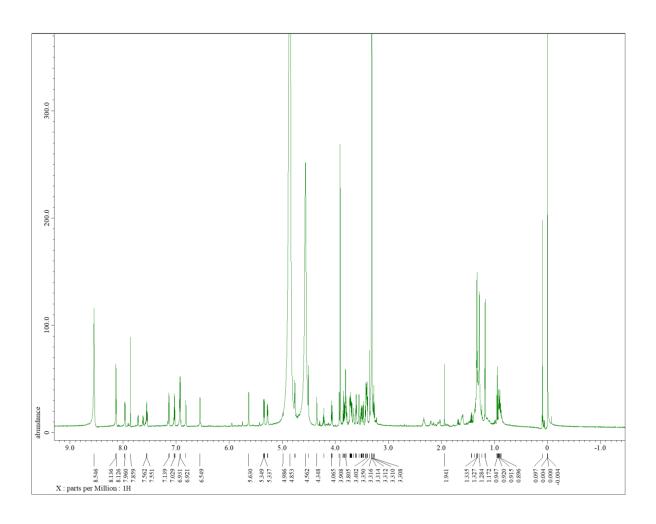


Figure S11. ¹H NMR spectrum of compound 3 (CD₃OD, 800 MHz)

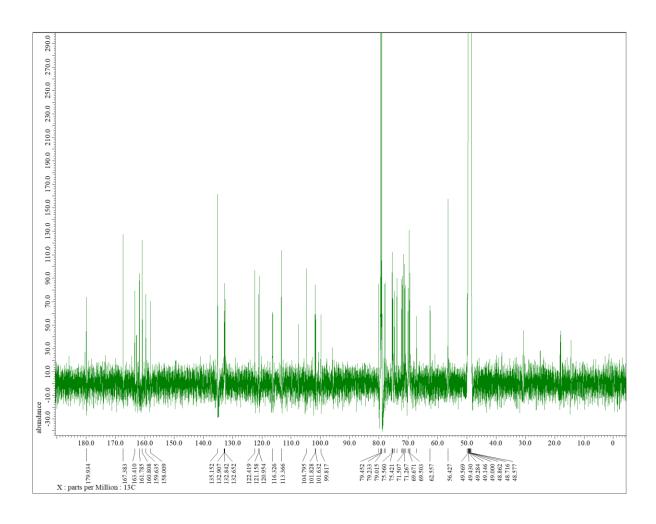
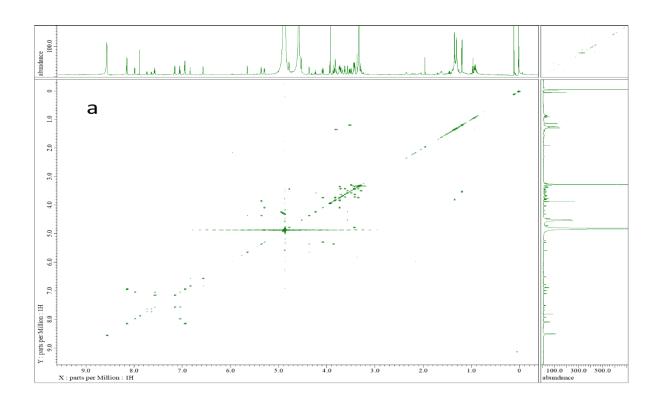


Figure S12. ¹³C NMR spectrum of compound 3 (CD₃OD, 800 MHz)



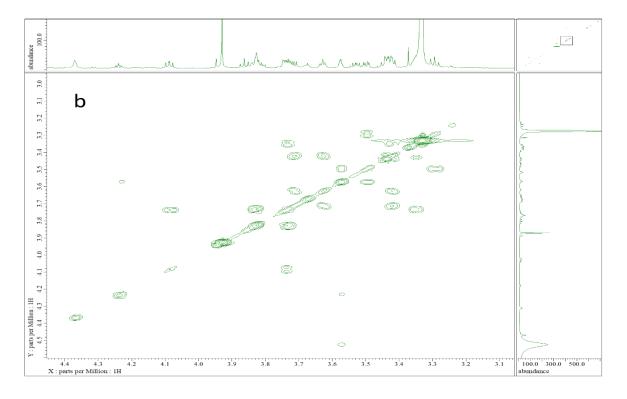
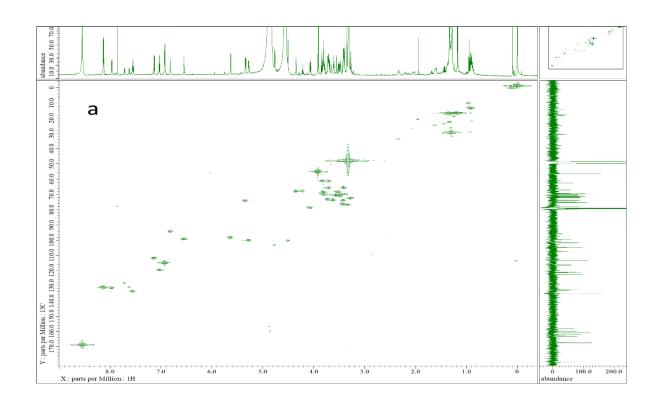


Figure S13. ¹H-¹H COSY of compound 3 (CD₃OD, 800 MHz)



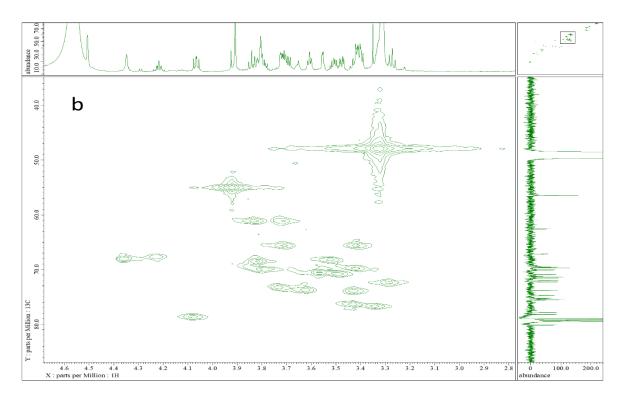
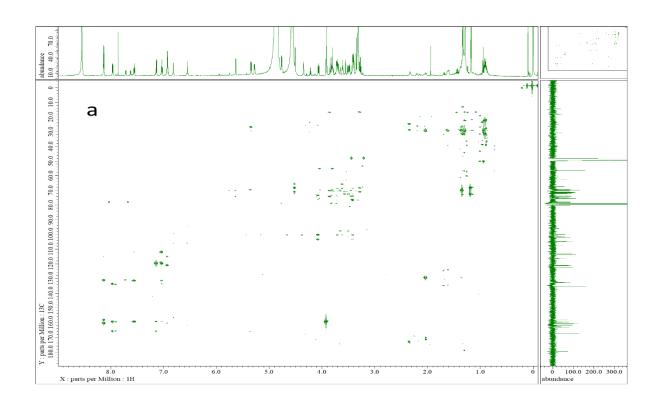


Figure S14. HMQC of compound 3 (CD₃OD, 800 MHz)



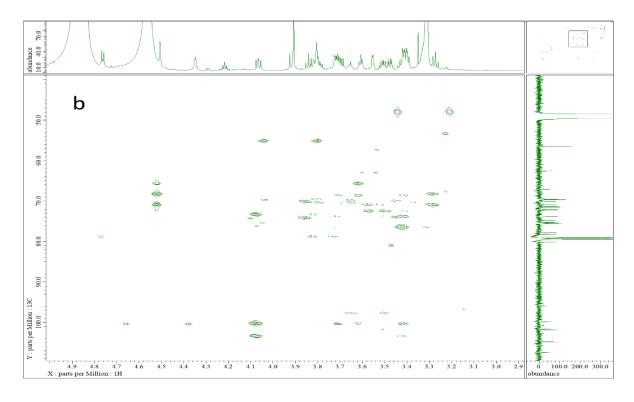


Figure S15. HMBC of compound 3 (CD₃OD, 800 MHz)

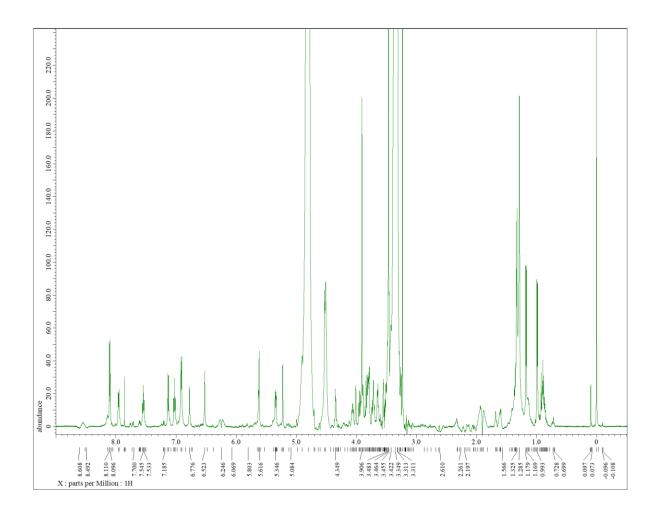


Figure S16. ¹H NMR spectrum of compound 4 (CD₃OD, 600 MHz)

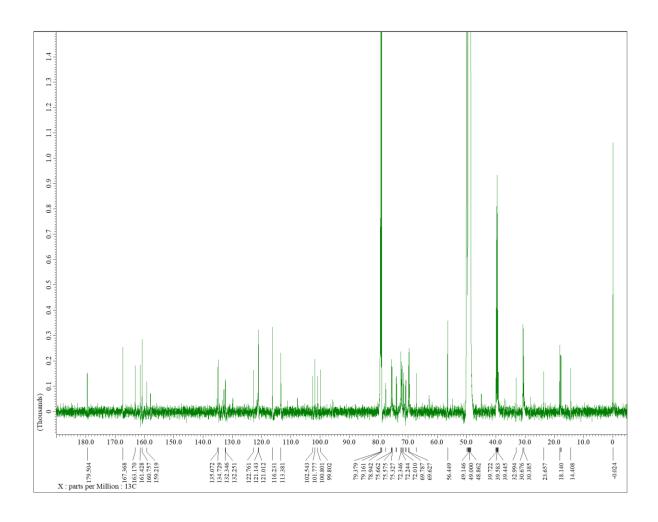
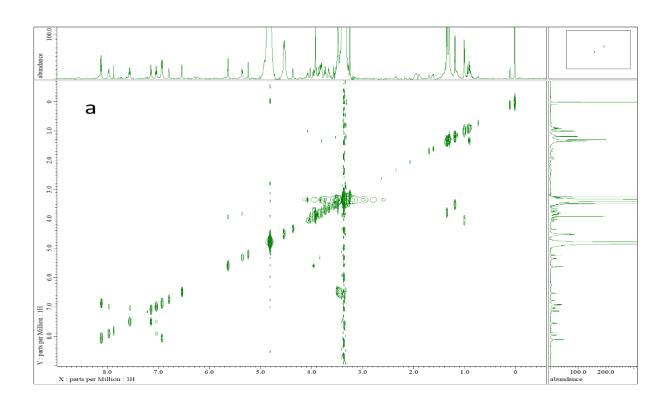


Figure S17. ¹³C NMR spectrum of compound **4** (CD₃OD, 600 MHz)



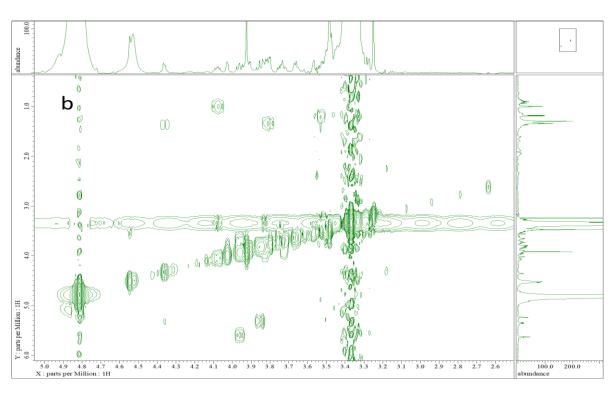
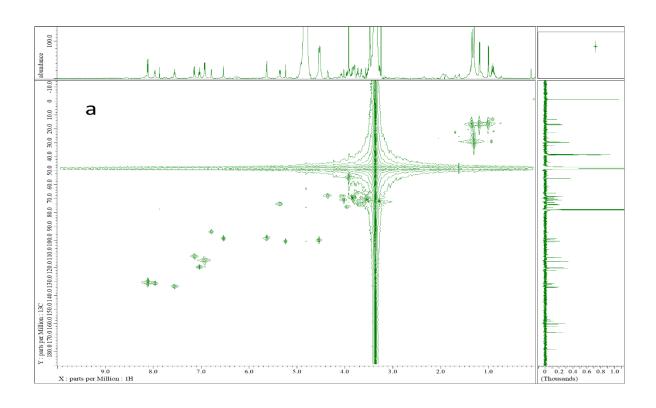


Figure S18. ¹H-¹H COSY of compound 4 (CD₃OD, 600 MHz)



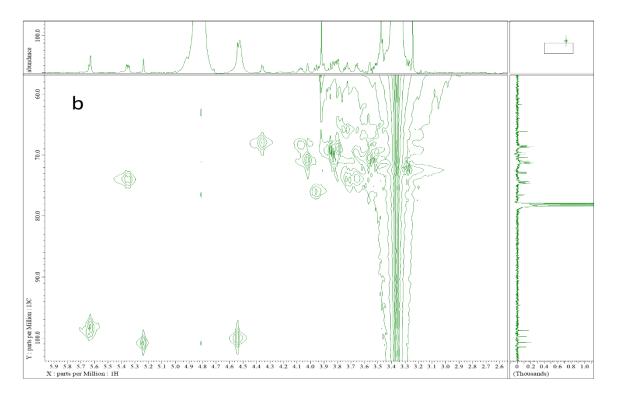
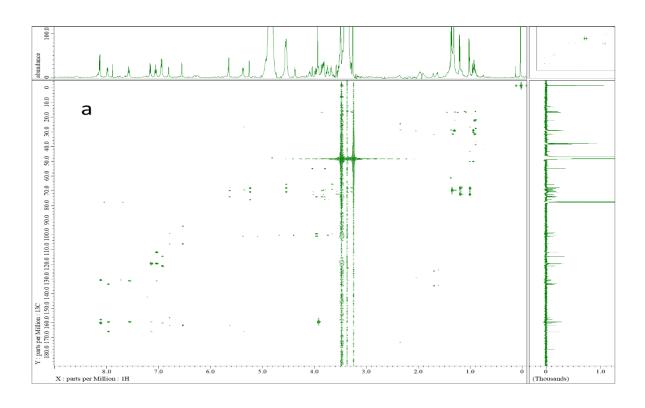


Figure S19. HMQC of compound 4 (CD₃OD, 600 MHz)



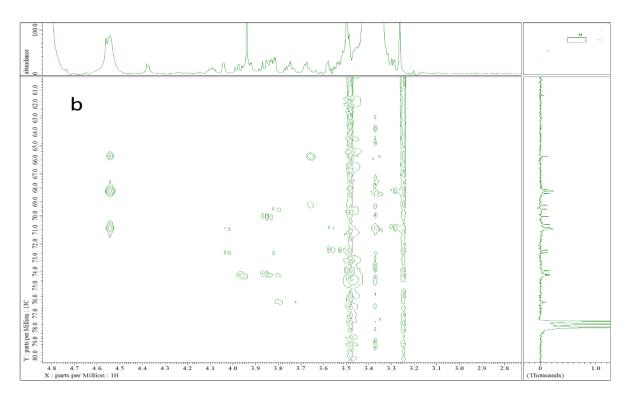


Figure S20. HMBC of compound 4 (CD₃OD, 600 MHz)

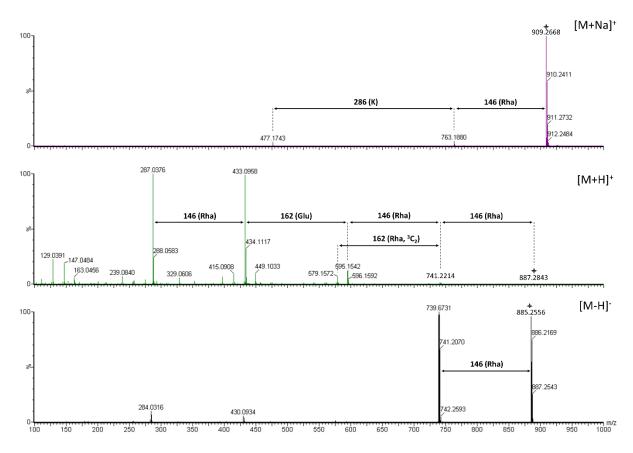


Figure S21. LC/ESI/MS/MS data of compound 1

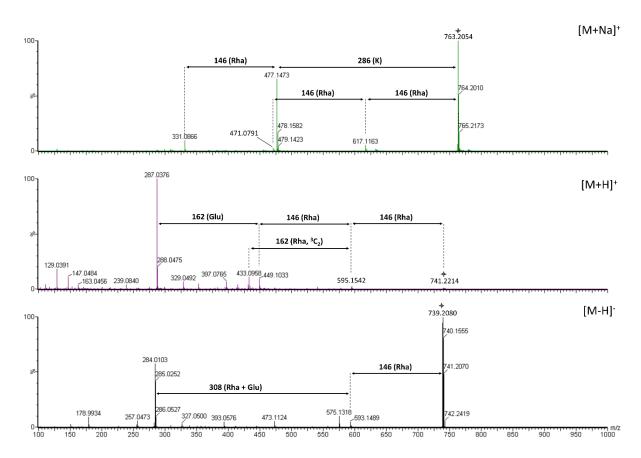


Figure S22. LC/ESI/MS/MS data of compound 2

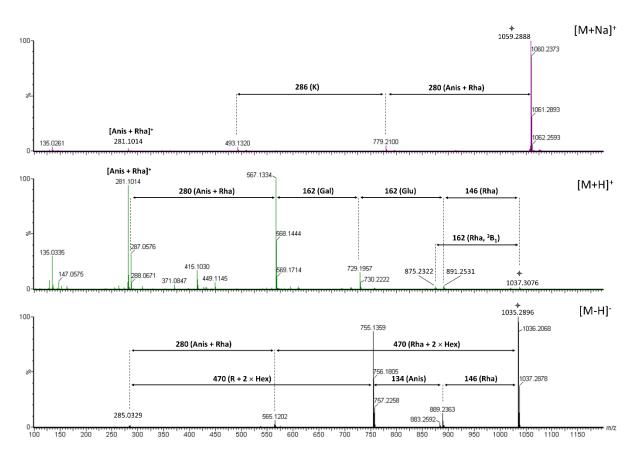


Figure S23. LC/ESI/MS/MS data of compound 3

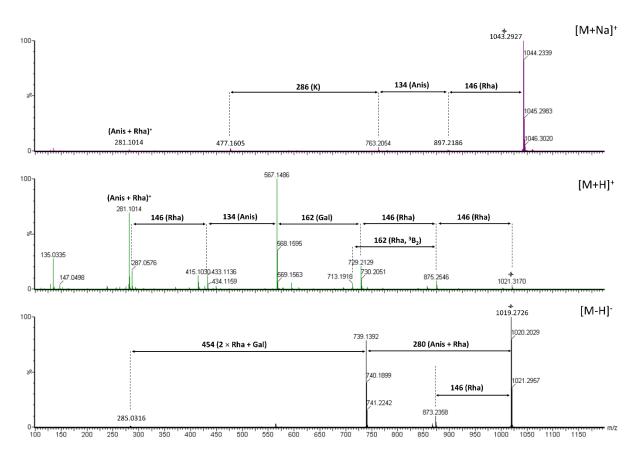


Figure S24. LC/ESI/MS/MS data of compound 4

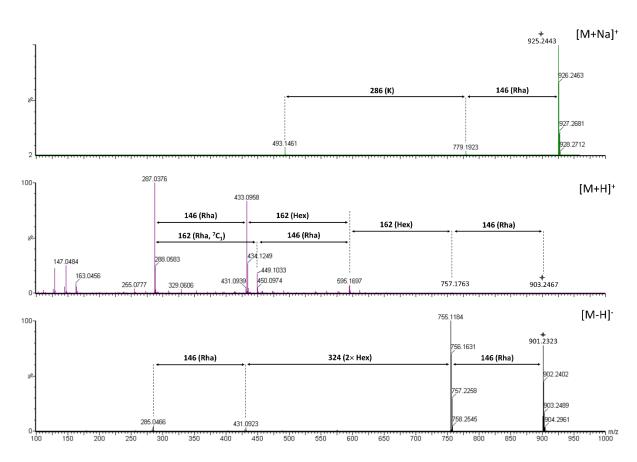


Figure S25. LC/ESI/MS/MS data of compound 5

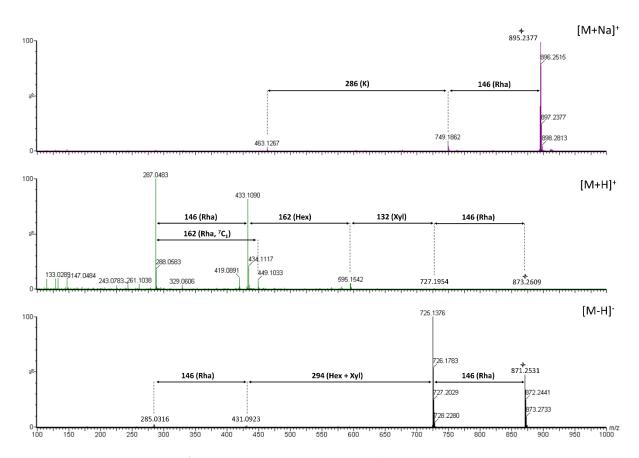


Figure S26. LC/ESI/MS/MS data of compound 6

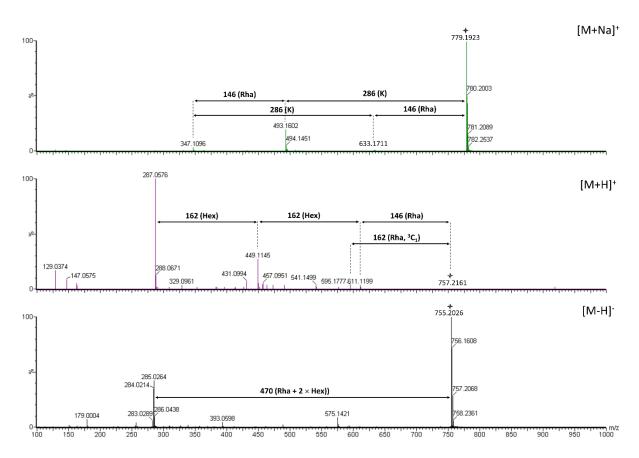


Figure S27. LC/ESI/MS/MS data of compound 7

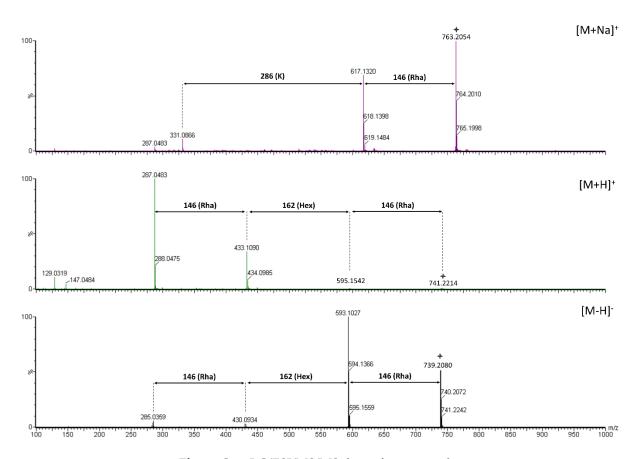


Figure S28. LC/ESI/MS/MS data of compound 8

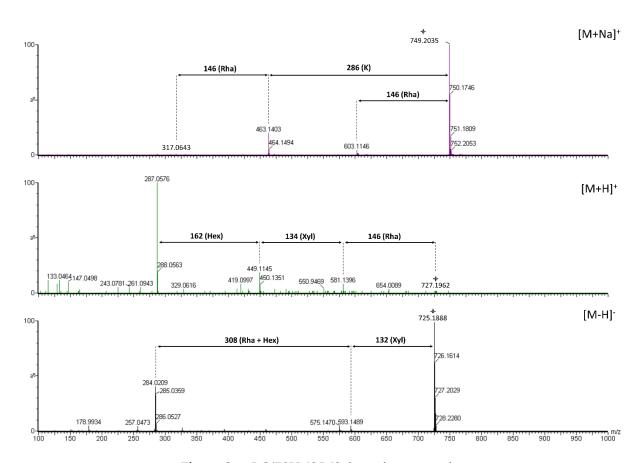


Figure S29. LC/ESI/MS/MS data of compound 9

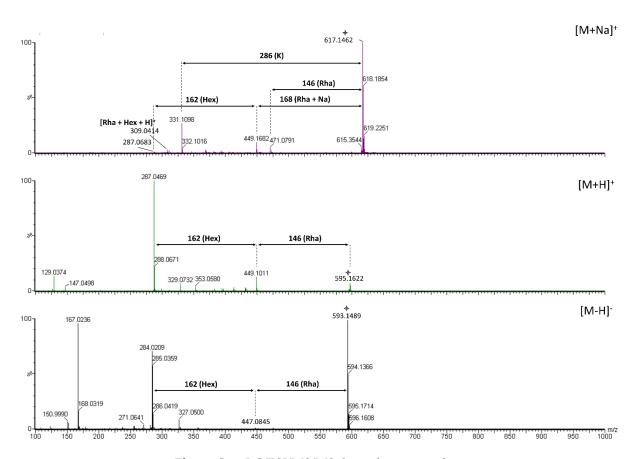


Figure S30. LC/ESI/MS/MS data of compound 10

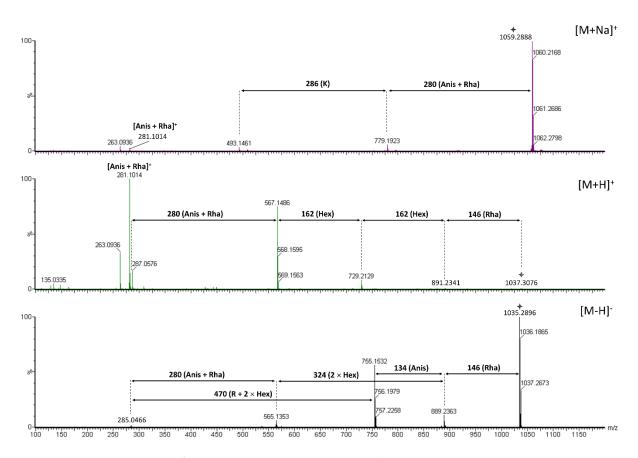


Figure S31. LC/ESI/MS/MS data of compound 11

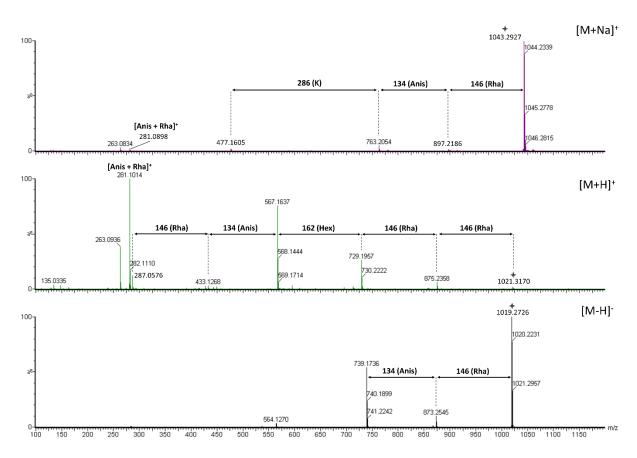


Figure S32. LC/ESI/MS/MS data of compound 12

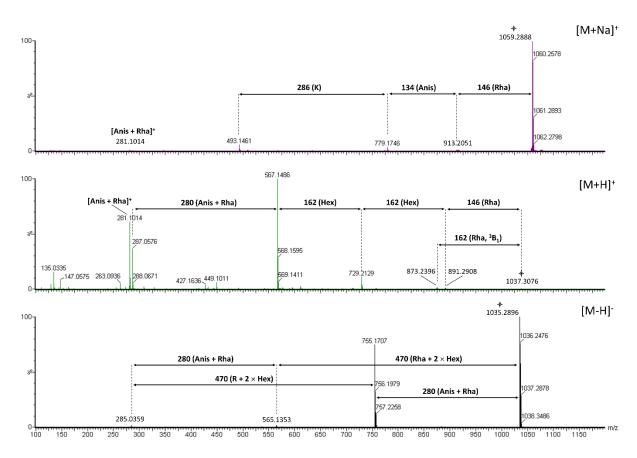


Figure S33. LC/ESI/MS/MS data of compound 13

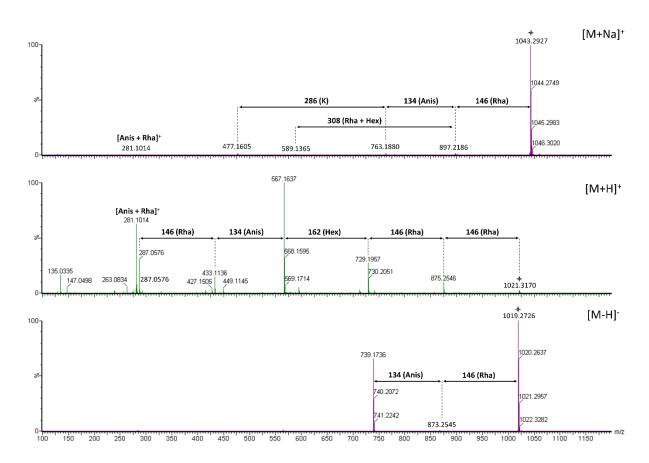


Figure S34. LC/ESI/MS/MS data of compound 14

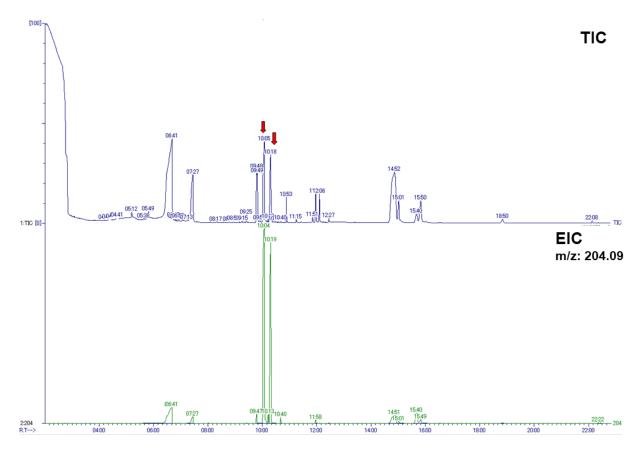


Figure S35. GC-MS total ion chromatogram and extracted ion chromatogram of trimethylsilyl (TMS) derivatives of galactose

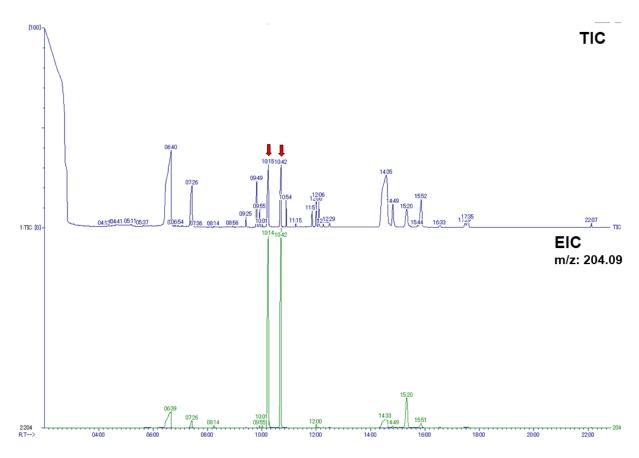


Figure S36. GC-MS total ion chromatogram and extracted ion chromatogram of trimethylsilyl (TMS) derivatives of glucose

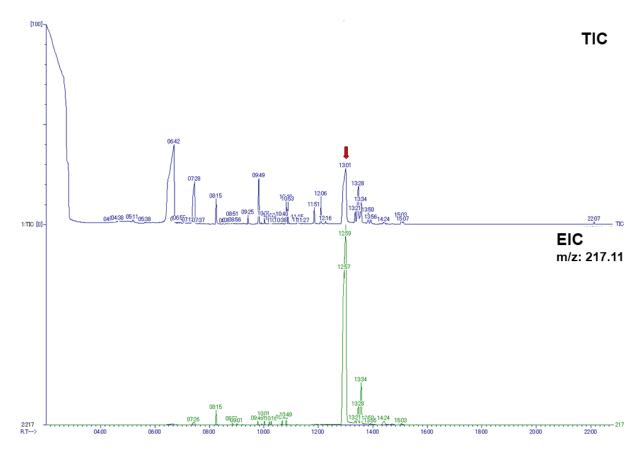


Figure S37. GC-MS total ion chromatogram and extracted ion chromatogram of trimethylsilyl (TMS) derivatives of rhamnose

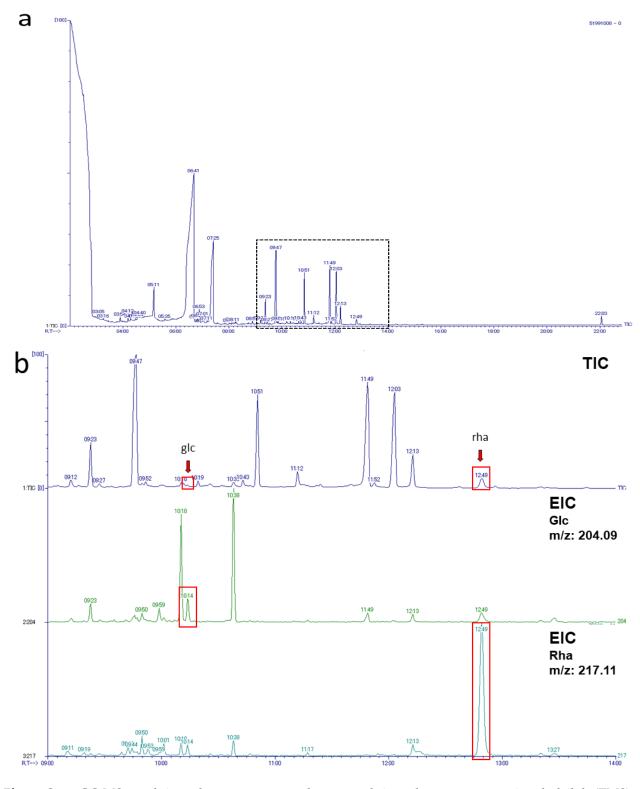


Figure S38. GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound **1**. (a) full retention time chromatogram, (b) expand on retention time chromatogram.

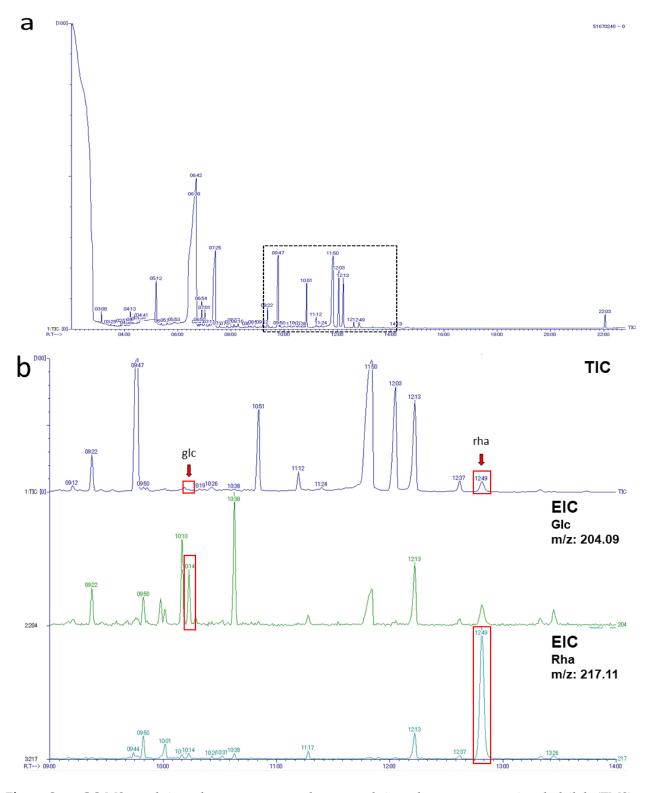


Figure S39. GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound **2**. (a) full retention time chromatogram, (b) expand on retention time chromatogram.

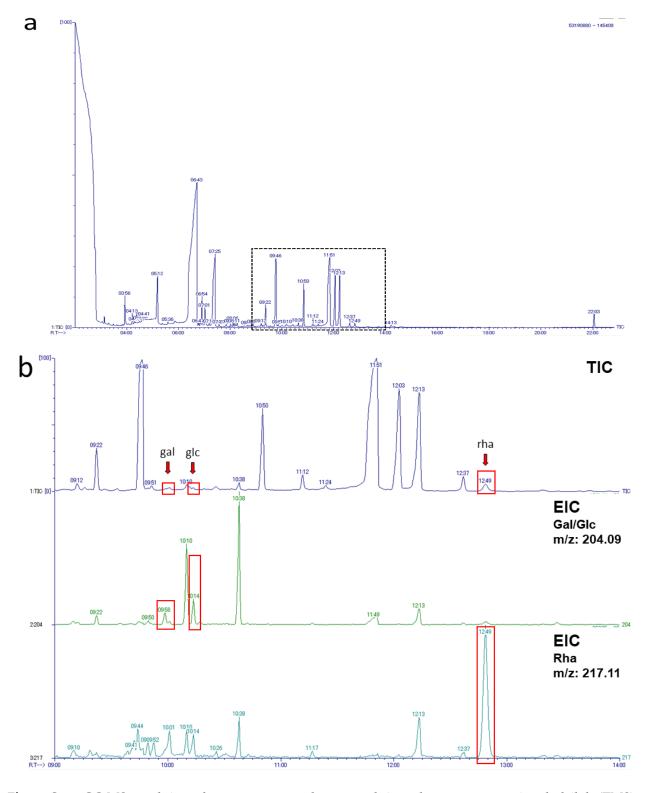


Figure S40. GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound **3**. (a) full retention time chromatogram, (b) expand on retention time chromatogram.

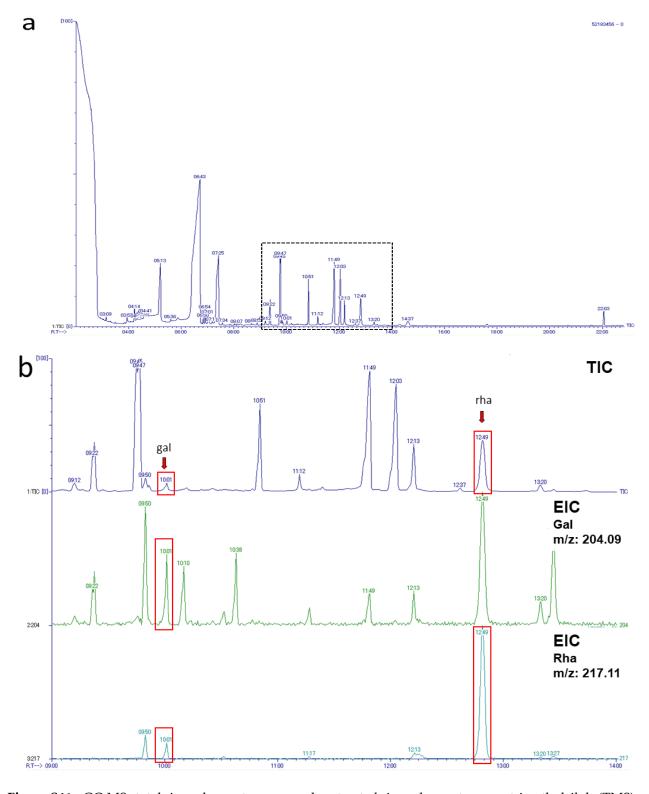


Figure S41. GC-MS total ion chromatogram and extracted ion chromatogram trimethylsilyl (TMS) derivatives of compound **4**. (a) full retention time chromatogram, (b) expand on retention time chromatogram.

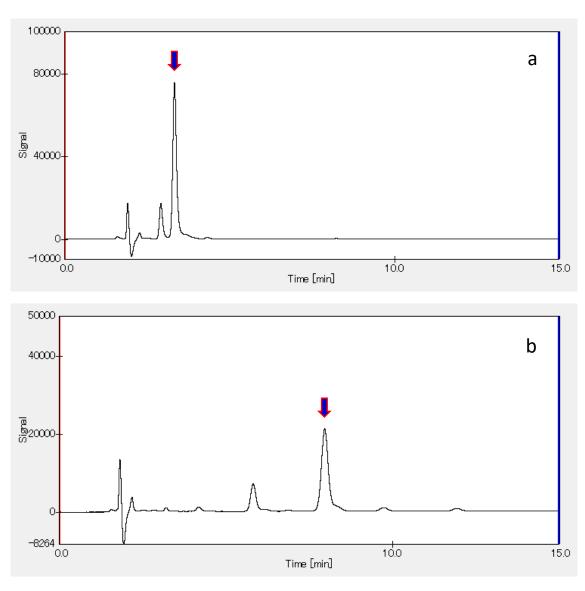


Figure S42. Chromatogram of compounds 1 (a) and 2 (b)

Note:

HPLC was performed using a Jasco PU2089 intelligent pump equipped with a Jasco UV-2075 detector (Tokyo, Japan) and a Shimadzu CTO-10ACVP column oven (Kyoto, Japan). Cosmosil 5C18-MS-II column (4.6 mm I.D. \times 150 mm, particle size of 5 μ m) was used and the temperature was 35 °C. Elution was performed with 15% MeCN and 0.5% HCOOH in water. The flow rate of the eluent was 1.0 mL/min.

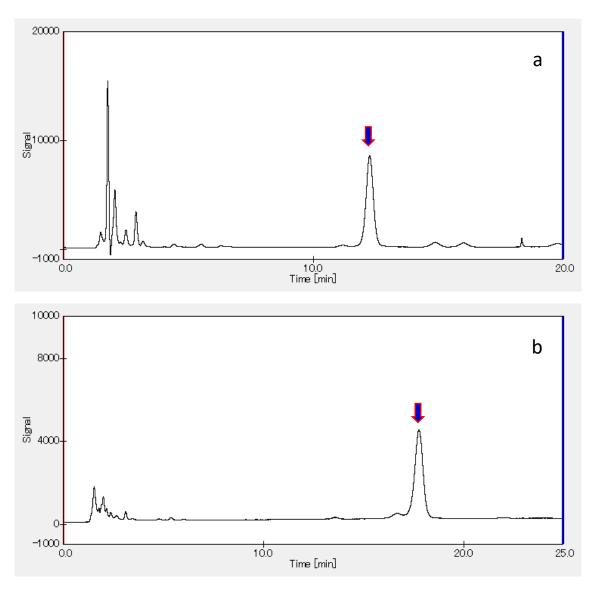


Figure S43. Chromatogram of compounds 3 (a) and 4 (b)

Note:

HPLC was performed using a Jasco PU2089 intelligent pump equipped with a Jasco UV-2075 detector (Tokyo, Japan) and a Shimadzu CTO-10ACVP column oven (Kyoto, Japan). Cosmosil 5C18-MS-II column (4.6 mm I.D. \times 150 mm, particle size of 5 μm) was used and the temperature was 35 °C. Elution was performed with 20 % MeCN and 0.5% HCOOH in water. The flow rate of the eluent was 1.0 mL/min.