

Supplementary Materials

Microbial Transformation of Prenylquercetins by *Mucor hiemalis*

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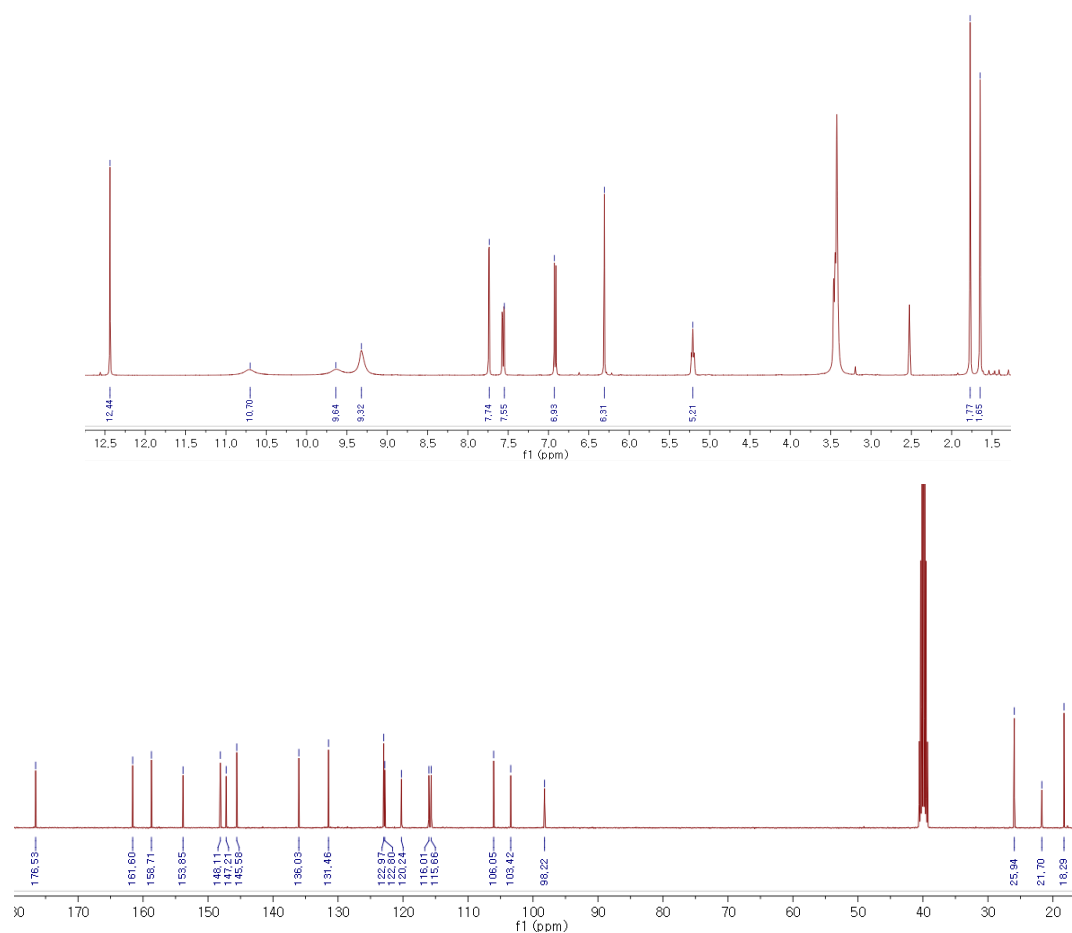


Figure S1. ¹H and ¹³C NMR spectra of 8-prenylquercetin (**1**) (DMSO-*d*₆)

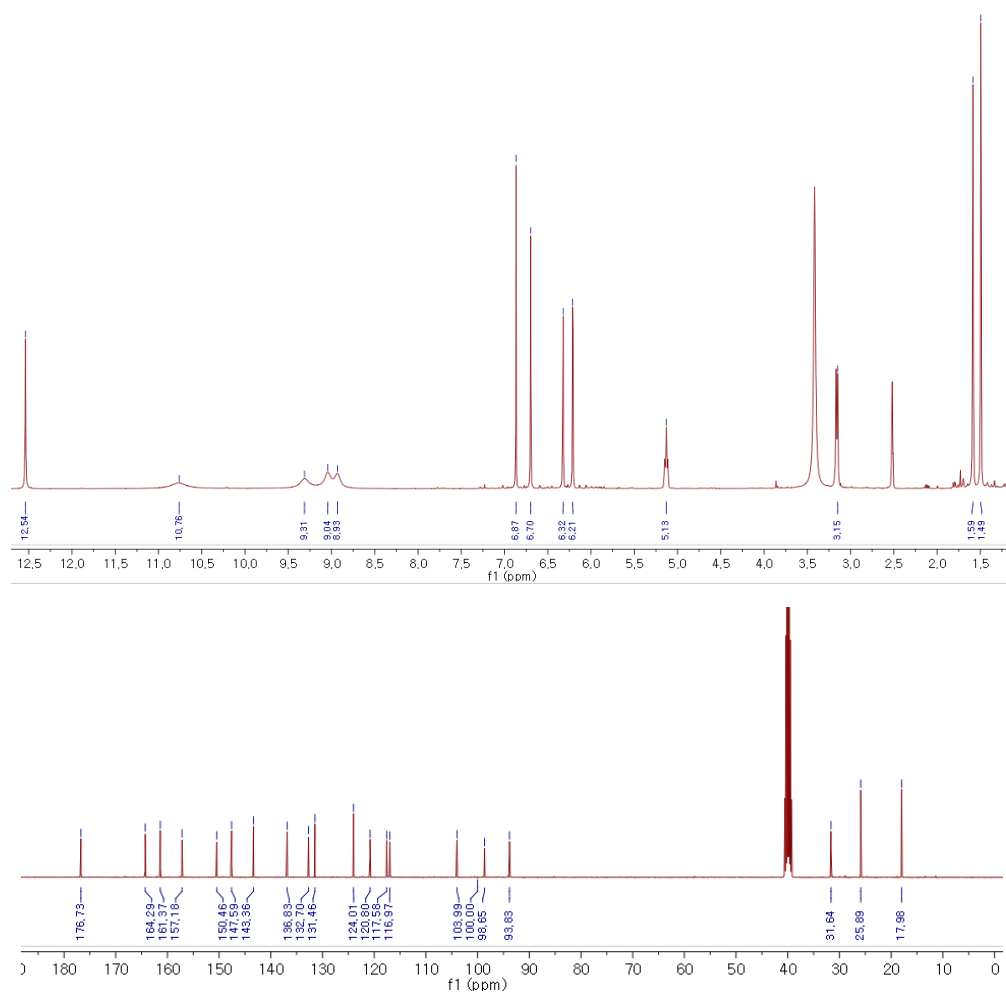


Figure S2. ¹H and ¹³C NMR spectra of 6'-prenylquercetin (**2**) (DMSO-*d*₆)

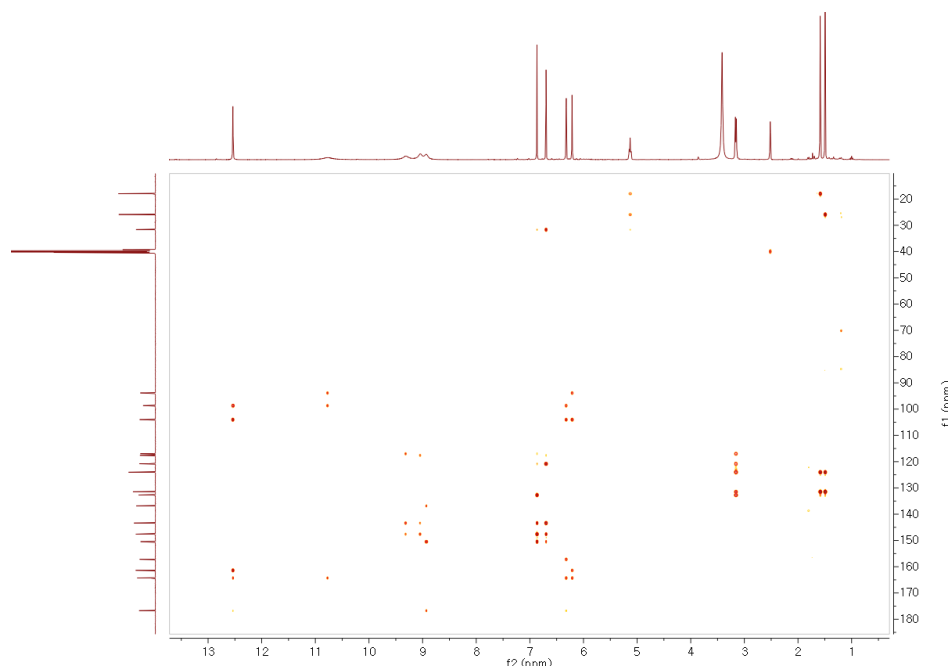


Figure S3. HMBC spectrum of 6'-prenylquercetin (**2**) (DMSO-*d*₆)

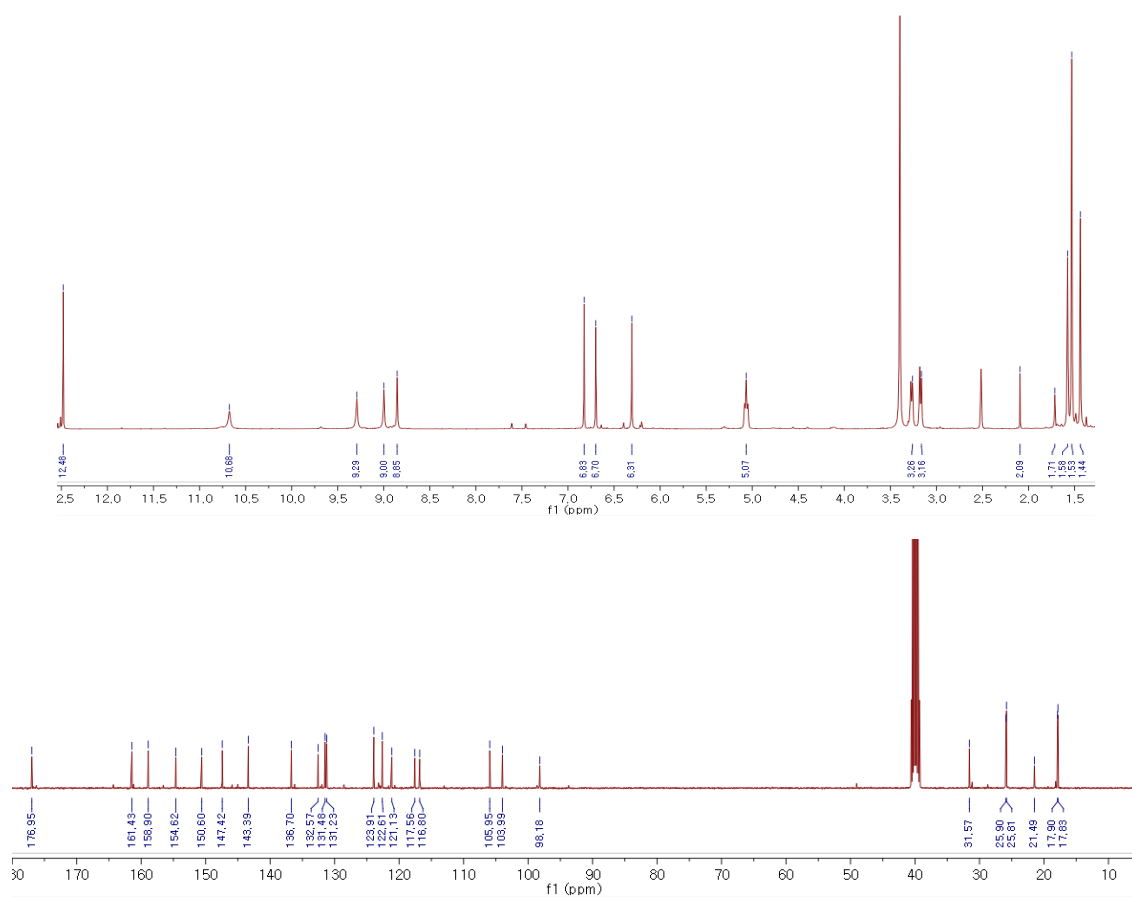


Figure S4. ^1H and ^{13}C NMR spectra of 8,6'-diprenylquercetin (**3**) ($\text{DMSO-}d_6$)

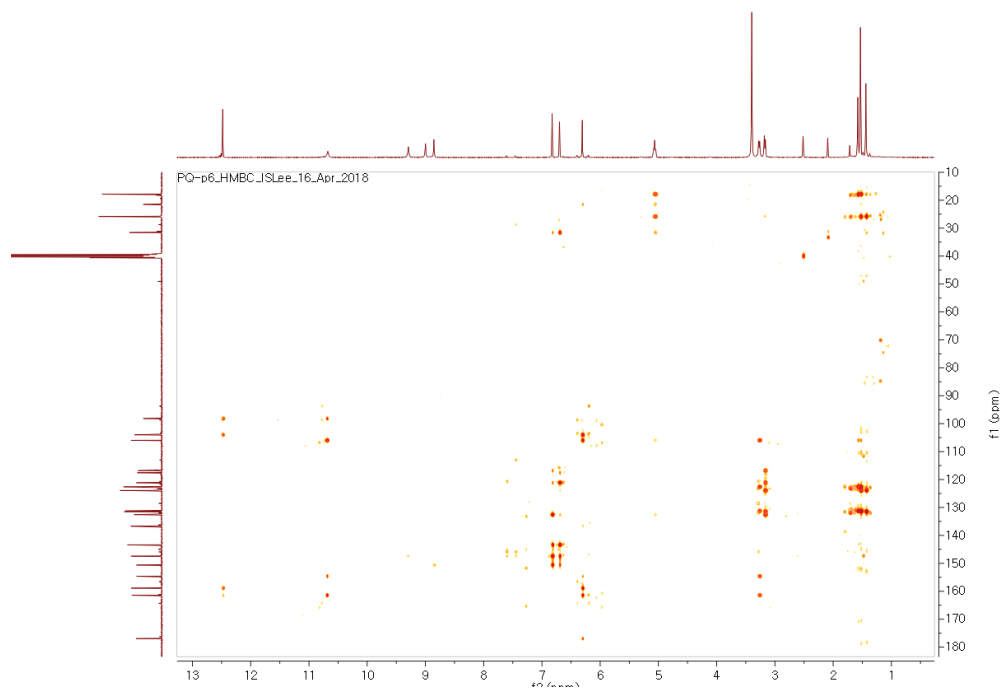


Figure S5. HMBC spectrum of 8,6'-diprenylquercetin (**3**) ($\text{DMSO-}d_6$)

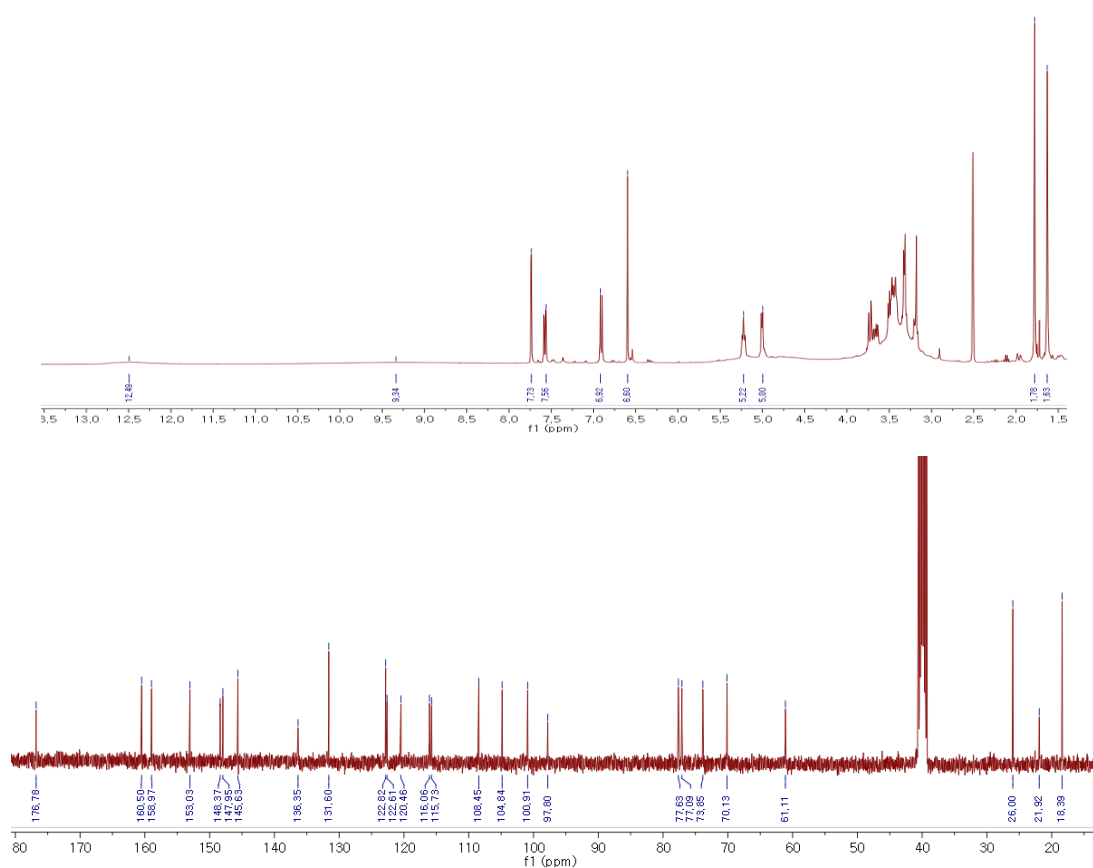


Figure S6. ^1H and ^{13}C NMR spectra of metabolite 4 (DMSO- d_6)

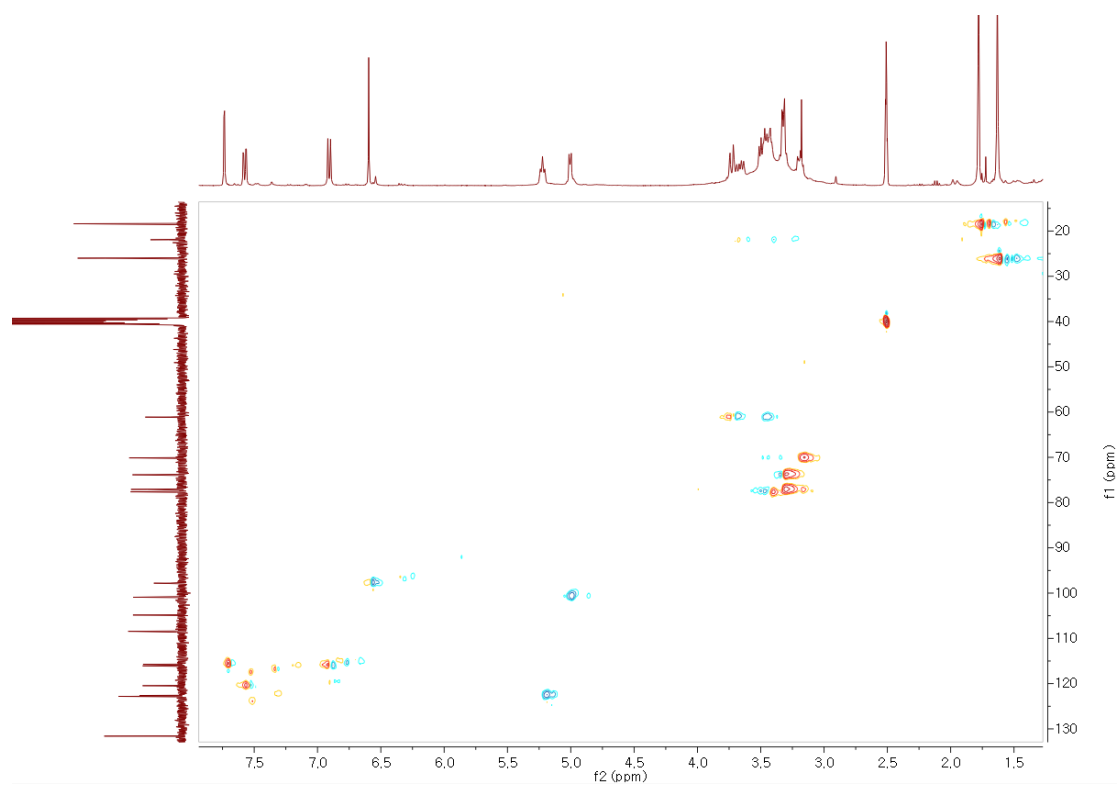


Figure S7. HSQC spectrum of metabolite 4 (DMSO- d_6)

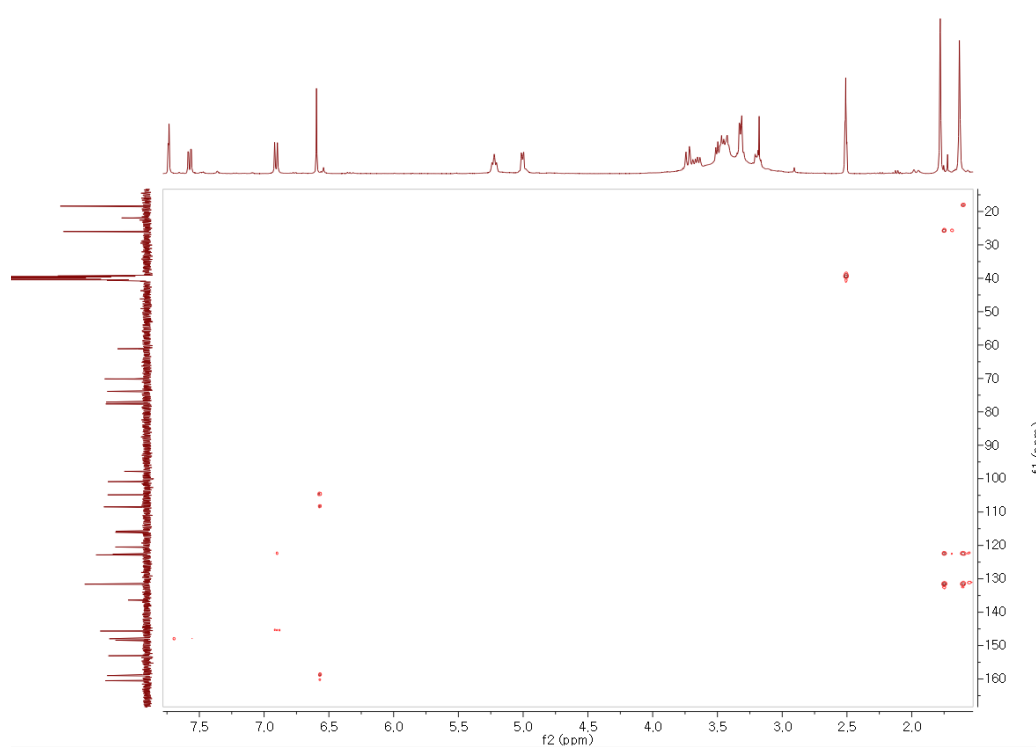


Figure S8. HMBC spectrum of metabolite **4** (DMSO- d_6)

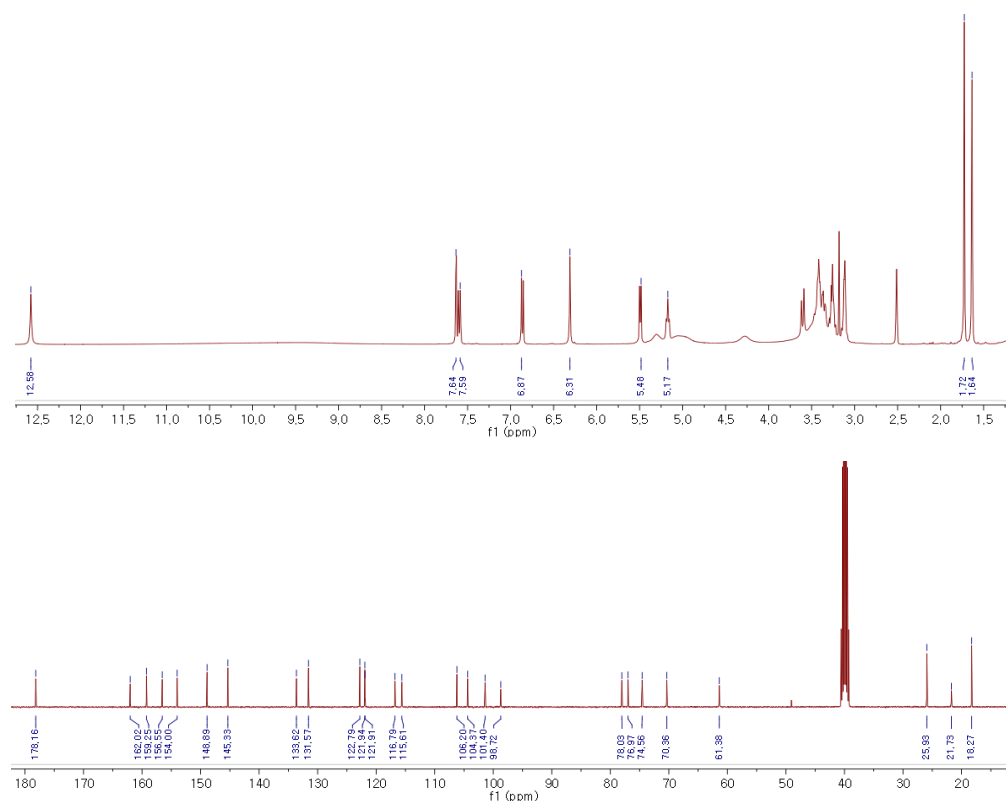


Figure S9. ^1H and ^{13}C NMR spectra of metabolite **5** (DMSO- d_6)

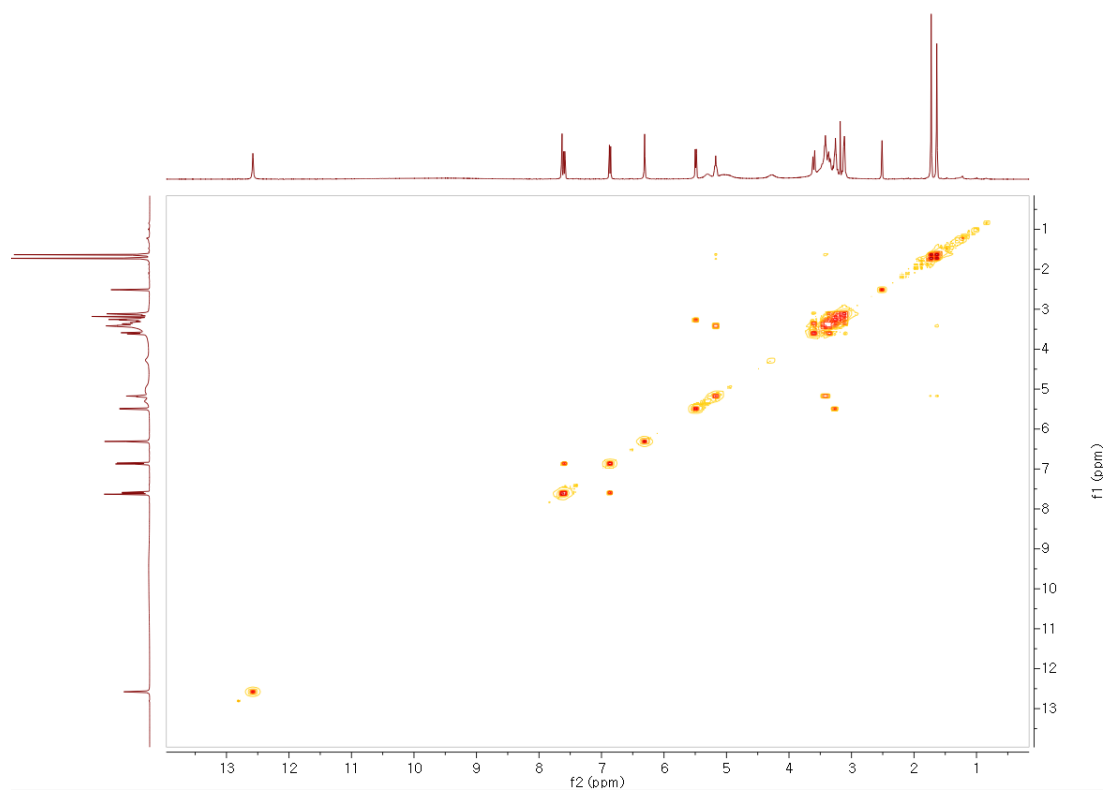


Figure S10. COSY spectrum of metabolite **5** (DMSO-*d*₆)

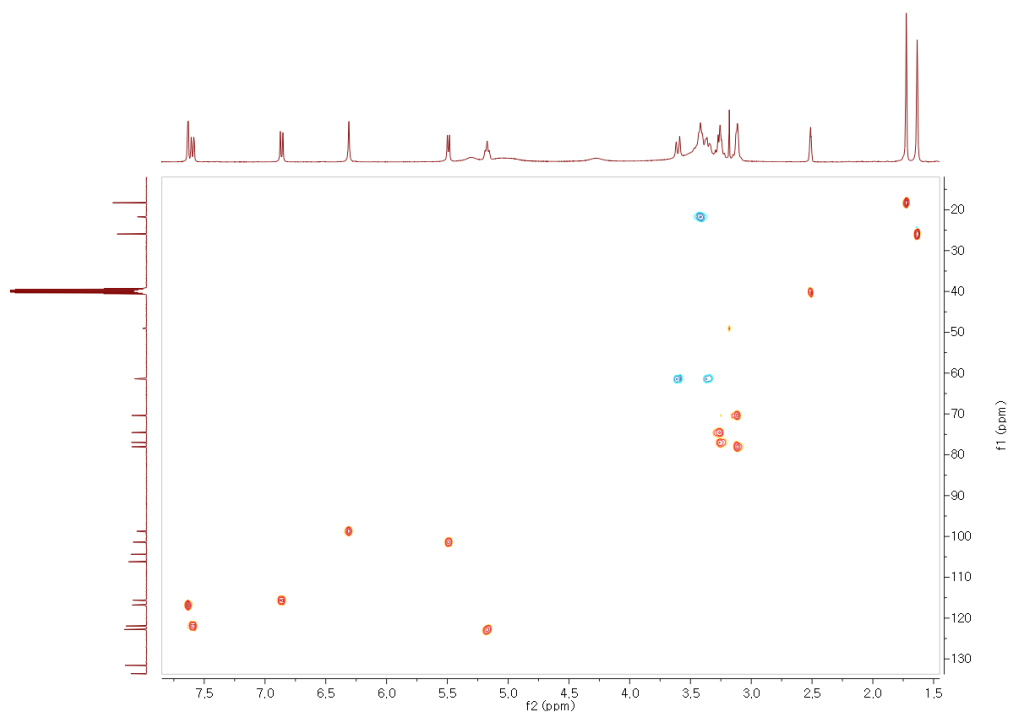


Figure S11. HSQC spectrum of metabolite **5** (DMSO-*d*₆)

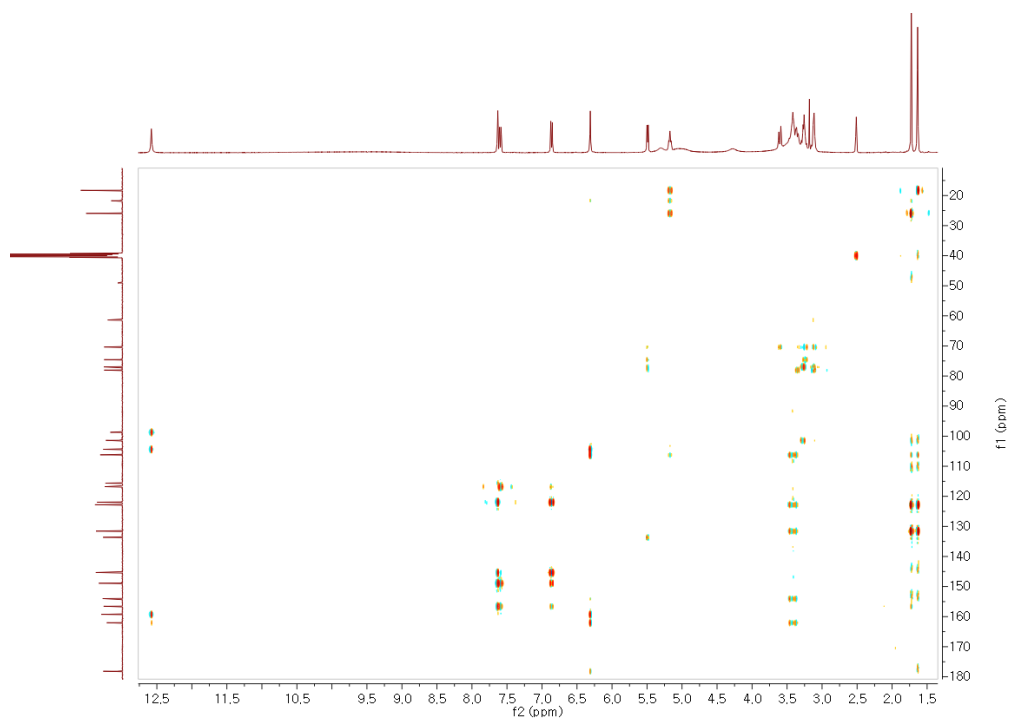


Figure S12. HMBC spectrum of metabolite **5** (DMSO- d_6)

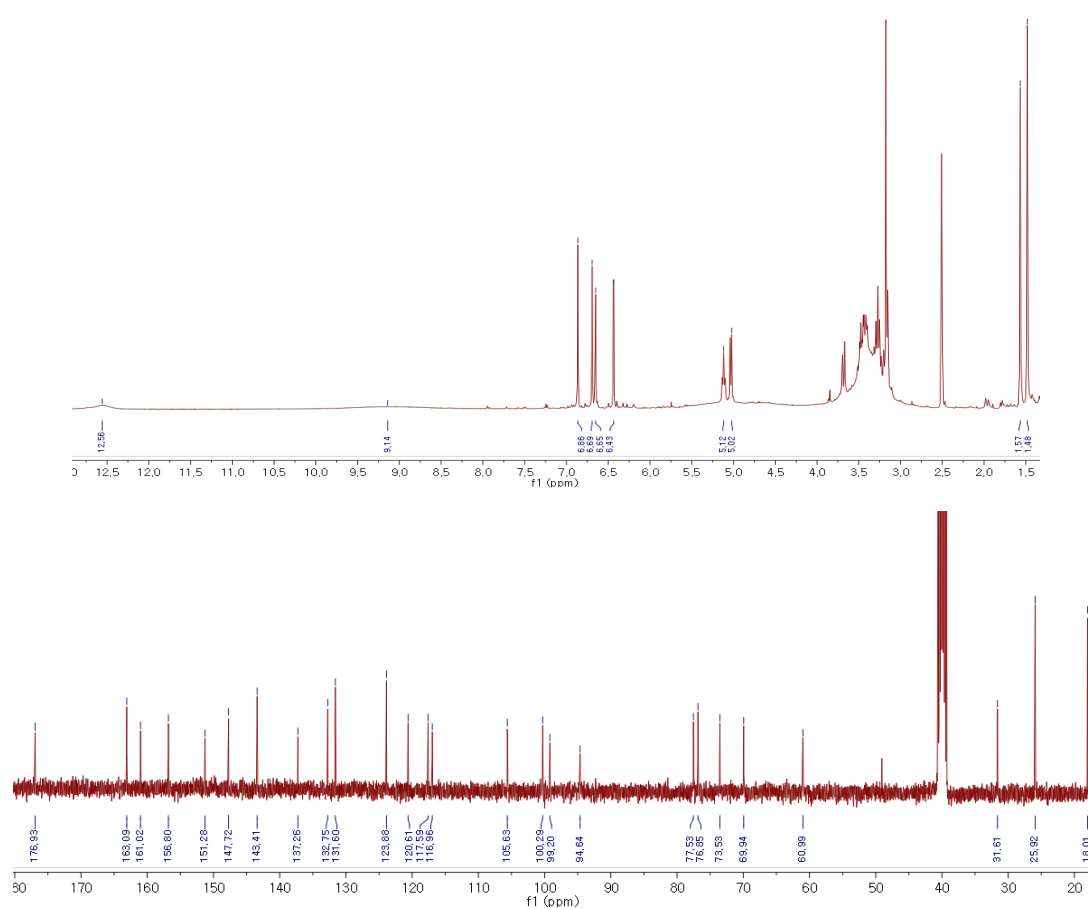


Figure S13. ^1H and ^{13}C NMR spectra of metabolite **6** (DMSO- d_6)

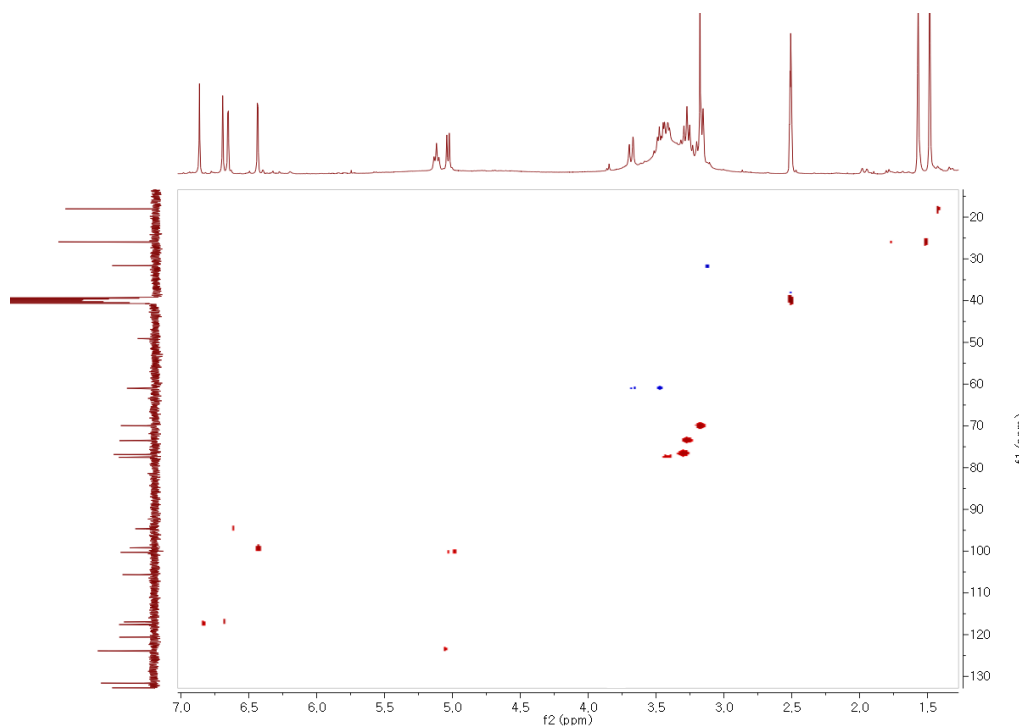


Figure S14. HSQC spectrum of metabolite **6** (DMSO- d_6)

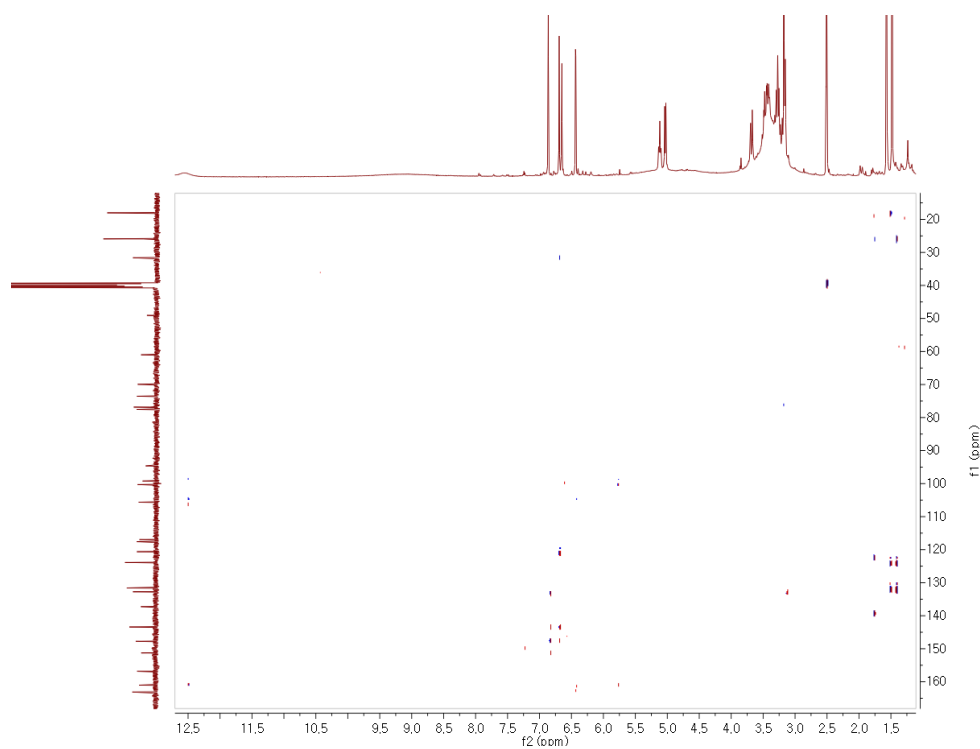


Figure S15. HMBC spectrum of metabolite **6** (DMSO- d_6)

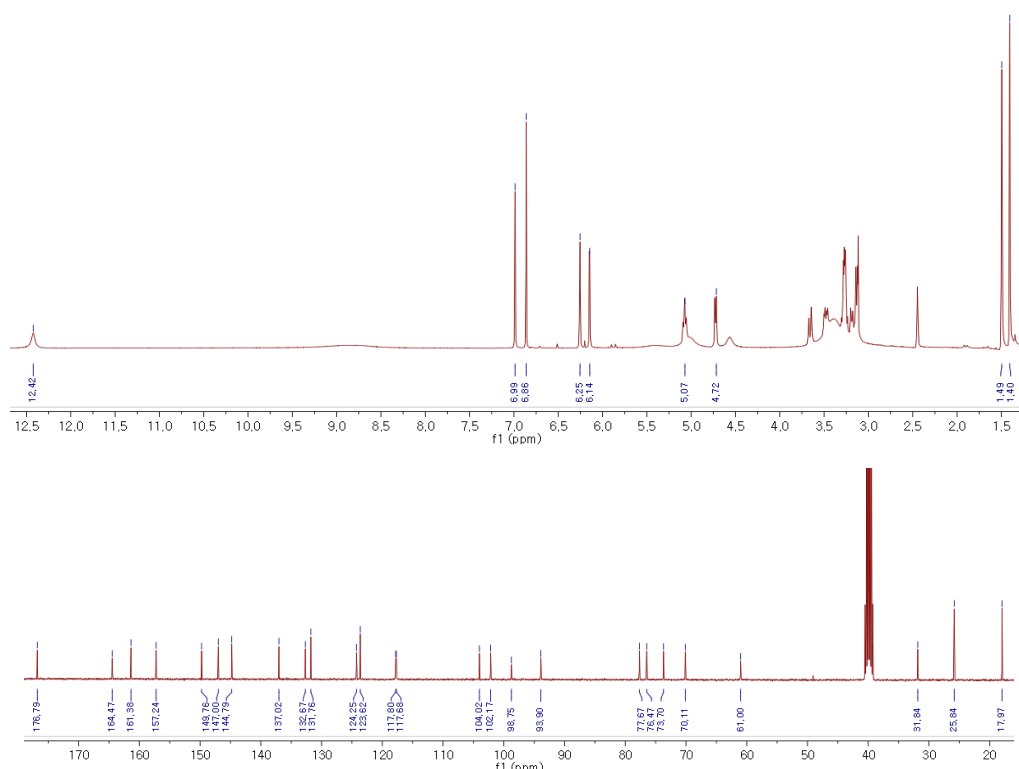


Figure S16. ^1H and ^{13}C NMR spectra of metabolite 7 (DMSO- d_6)

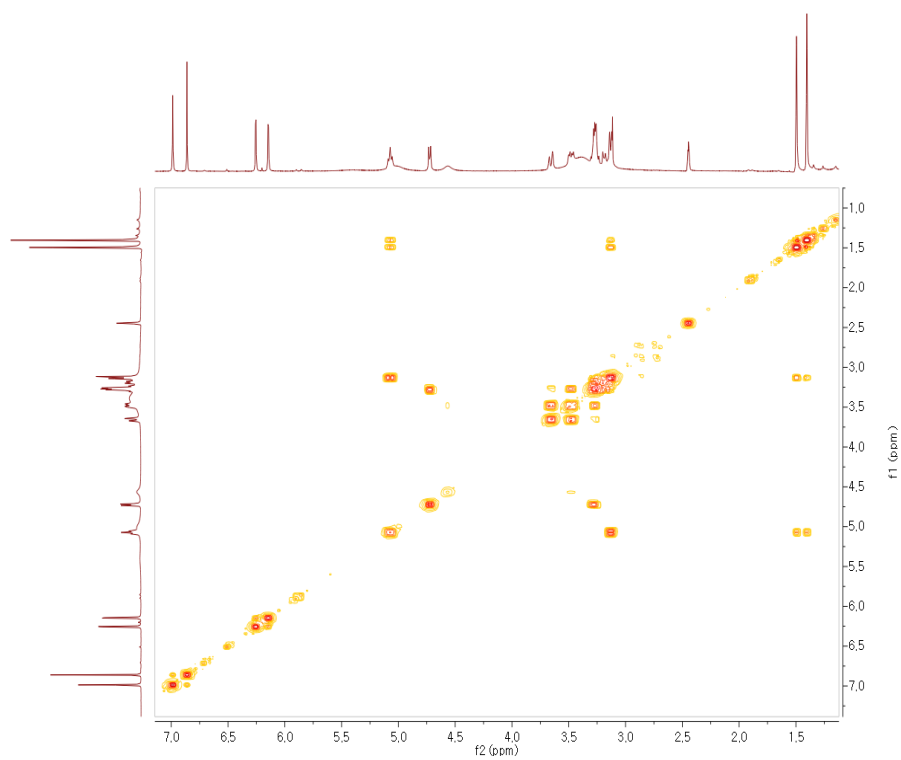


Figure S17. COSY spectrum of metabolite 7 (DMSO- d_6)

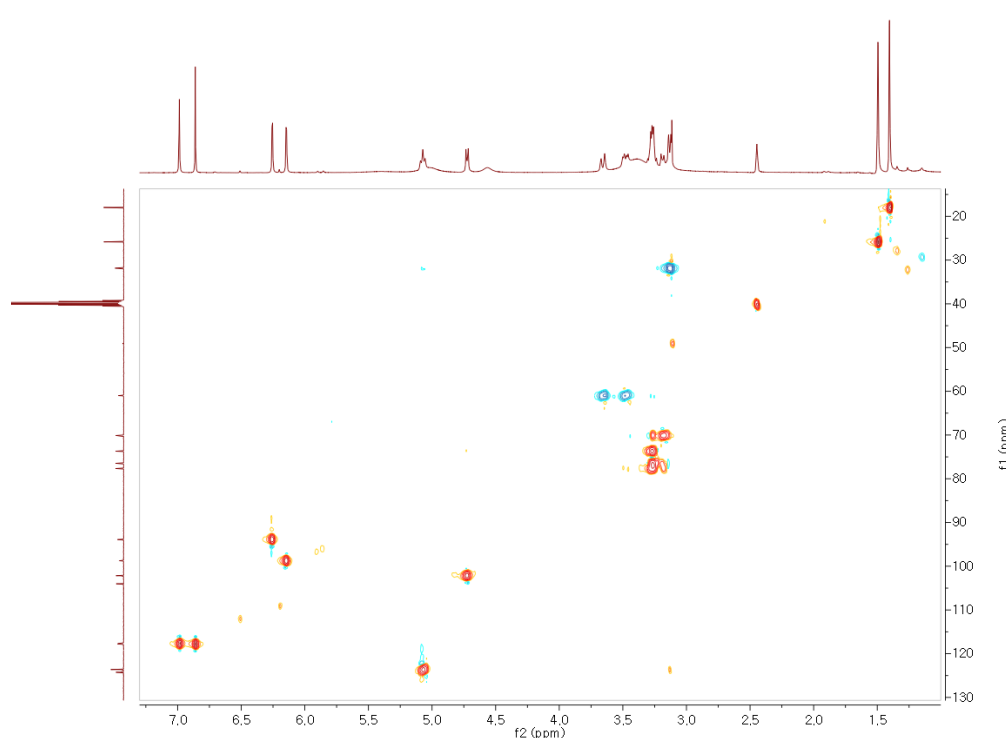


Figure S18. HSQC spectrum of metabolite **7** (DMSO- d_6)

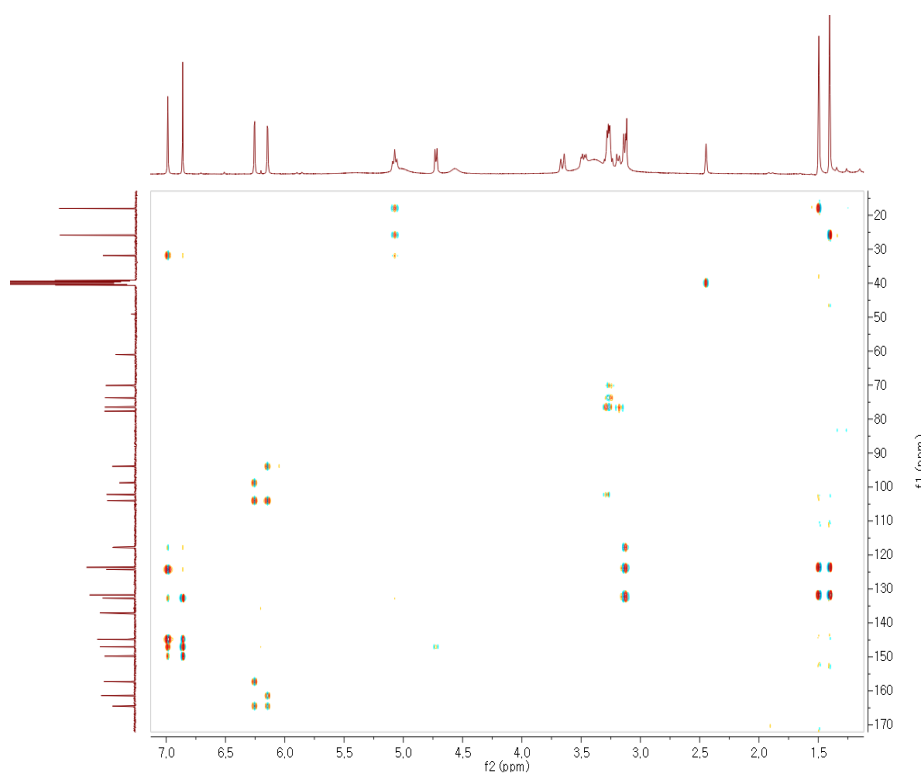


Figure S19. HMBC spectrum of metabolite **7** (DMSO- d_6)

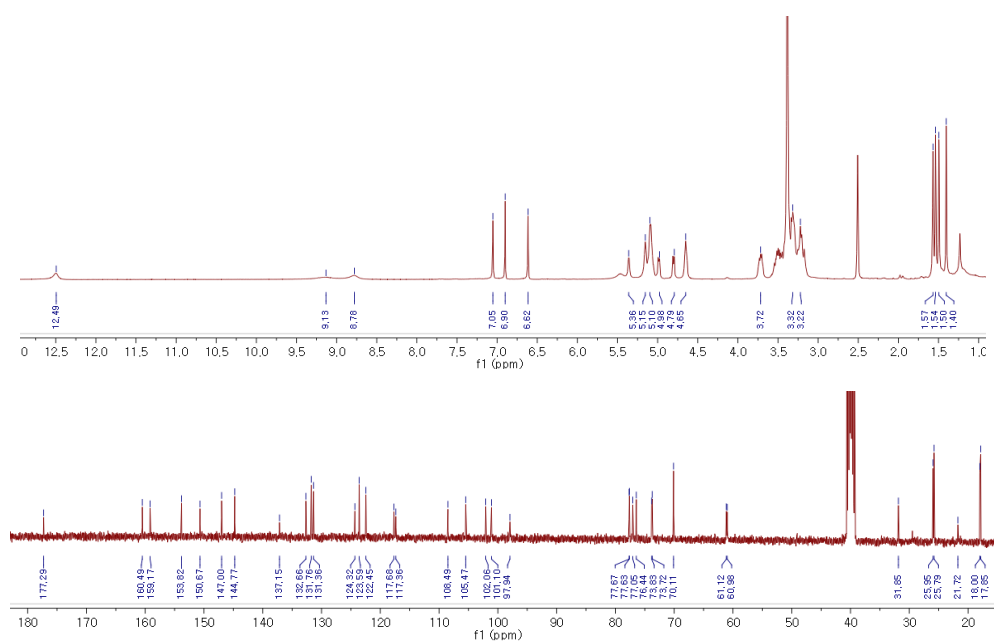


Figure S20. ^1H and ^{13}C NMR spectra of metabolite **8** ($\text{DMSO}-d_6$)

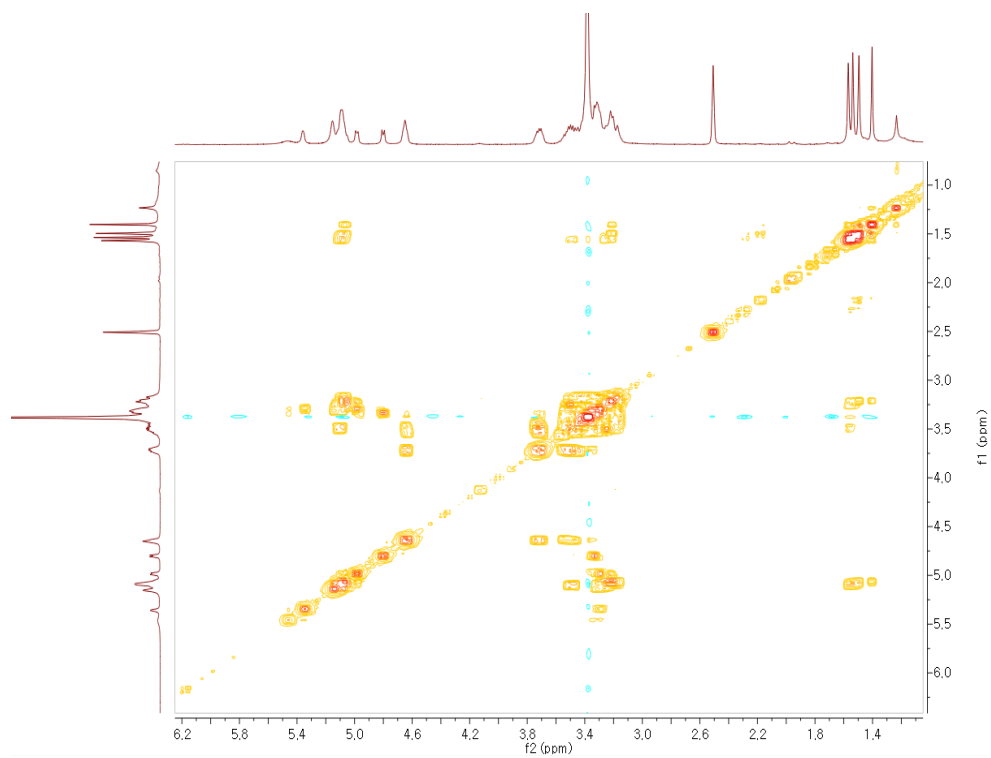


Figure S21. COSY spectrum of metabolite **8** ($\text{DMSO}-d_6$)

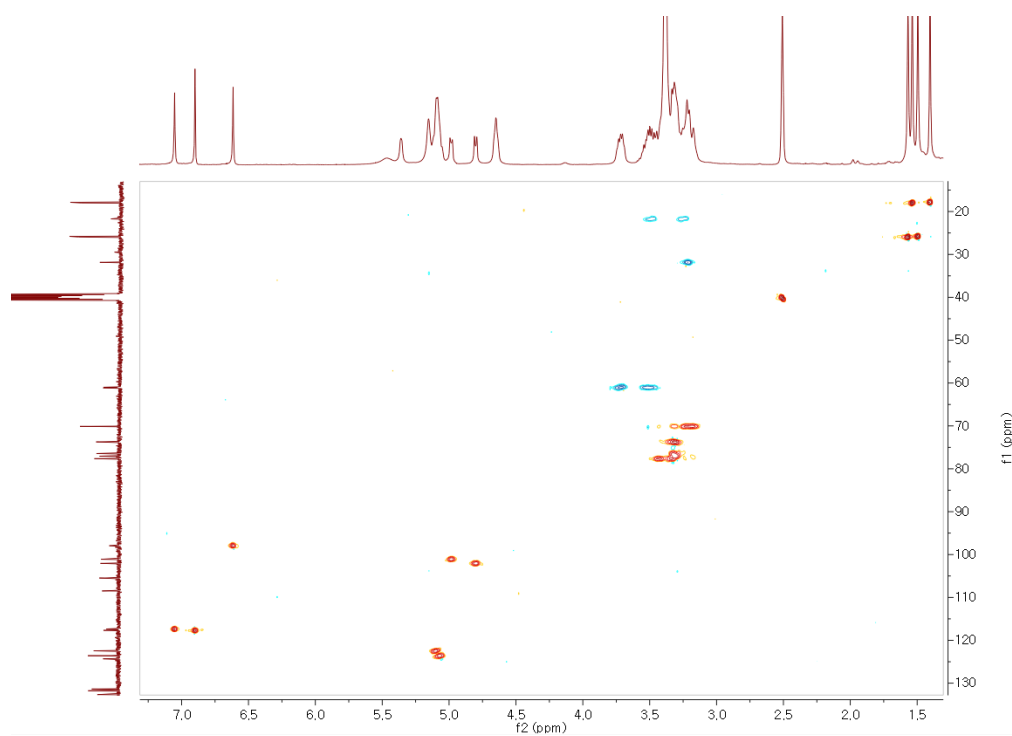


Figure S22. HSQC spectrum of metabolite **8** (DMSO- d_6)

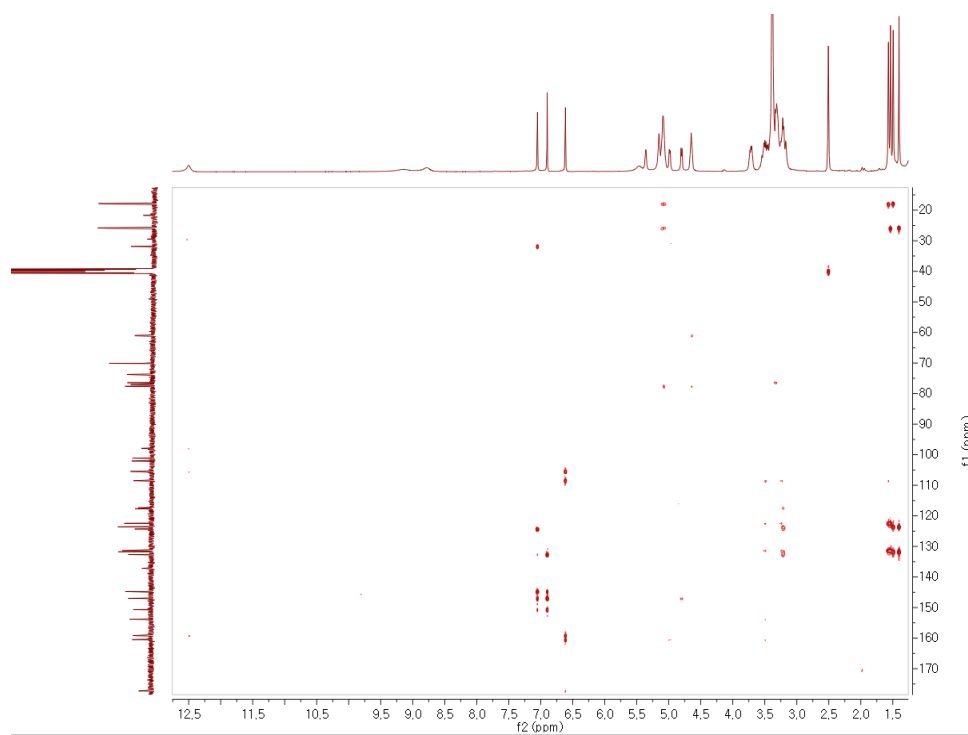


Figure S23. HMBC spectrum of metabolite **8** (DMSO- d_6)

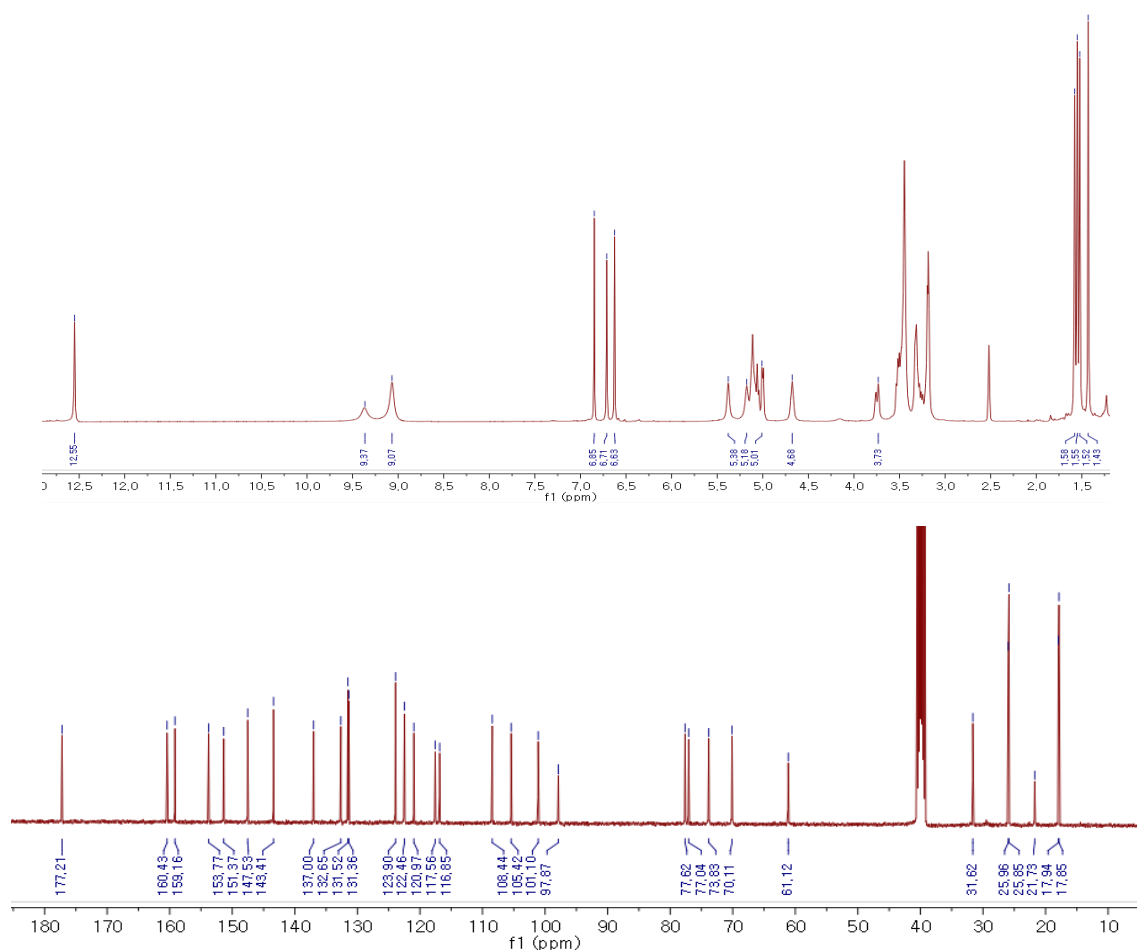


Figure S24. ¹H and ¹³C NMR spectra of metabolite **9** (DMSO-*d*₆)

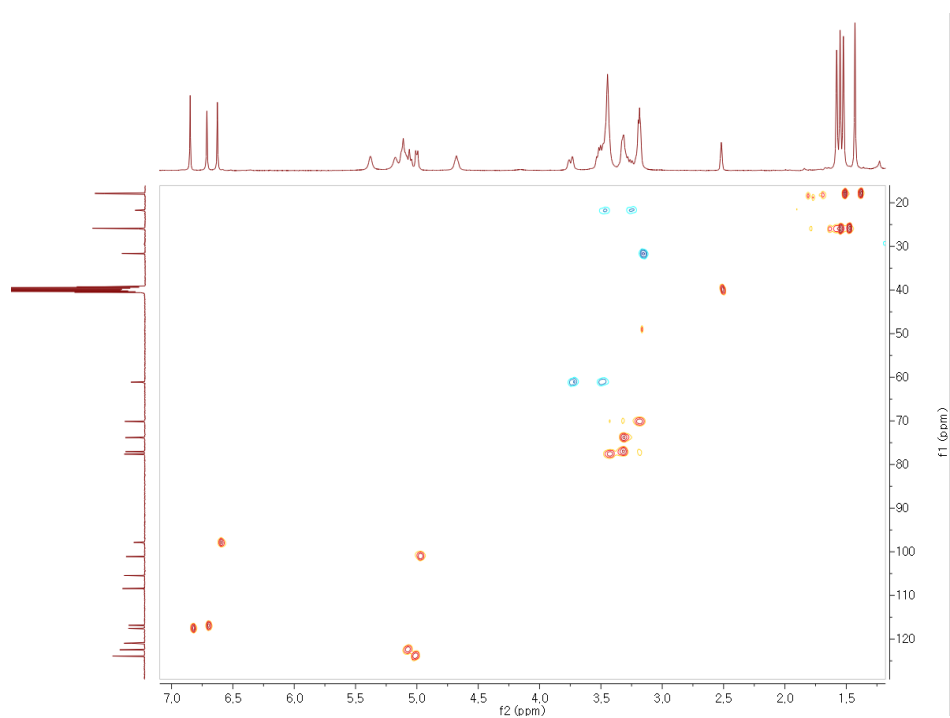


Figure S25. HSQC spectrum of metabolite **9** (DMSO-*d*₆)

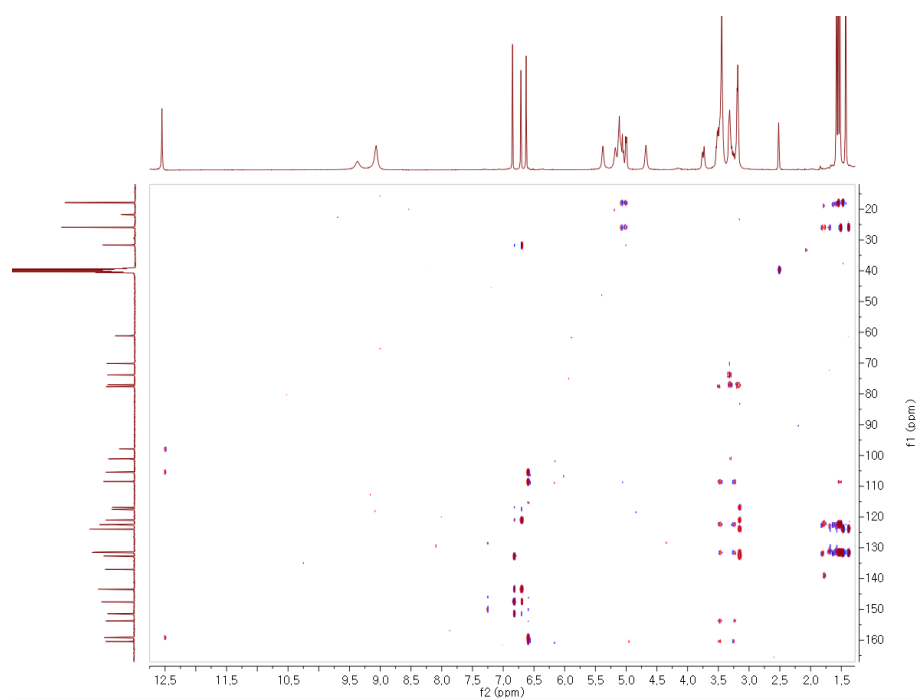
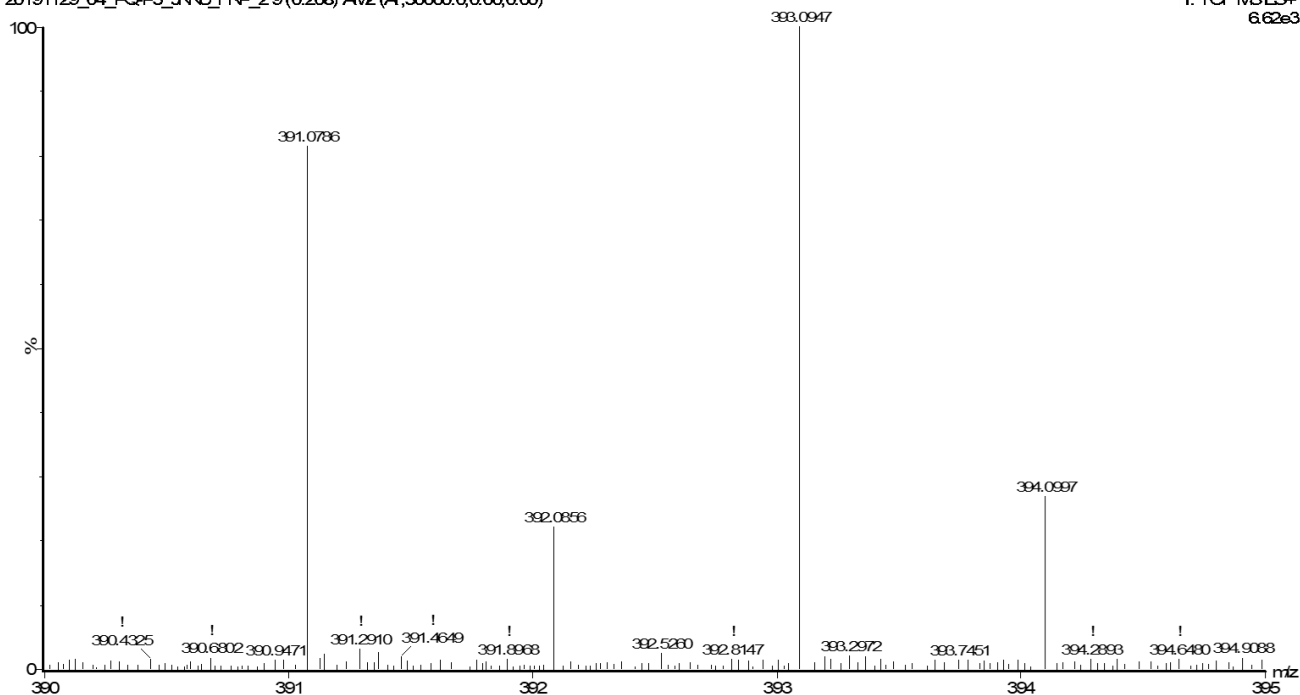


Figure S26. HMBC spectrum of metabolite **9** (DMSO- d_6)

20191129_04_PQ-P3_JNU_HRP_2.9 (0.208) AM2 (Ar,30000.0,0.00,0.00)

1: TOF MS ES+
6.62e3



Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

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Monoisotopic Mass, Even Electron Ions

132 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 1-40 H: 1-50 O: 1-20 Na: 0-1

Minimum: -1.5

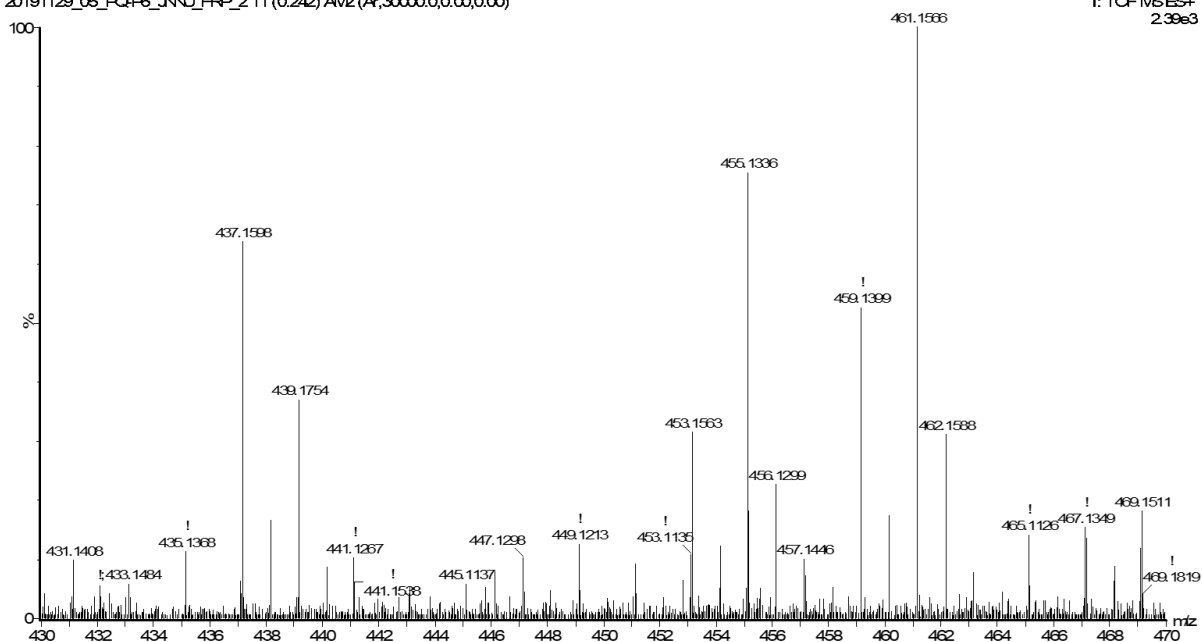
Maximum: 100.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
393.0947	393.0950	-0.3	-0.8	11.5	590.6	n/a	n/a	C20 H18 O7 Na

Figure S27. HRESIMS spectrum of compound 2

20191129_05_FQ-F6_NNJJ_HRP_2_11 (0.242) AM2 (Ar,30000.0,0.00,0.00)

1: TOF MS ES+
2.39e3



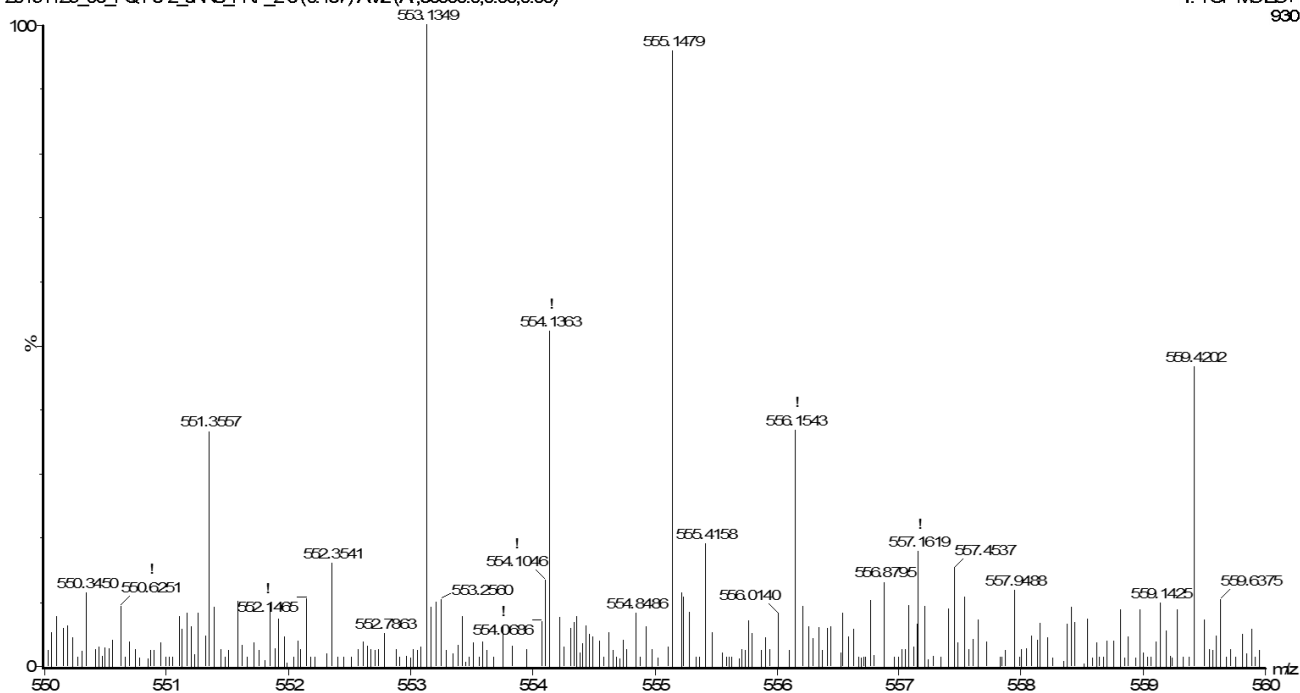
Elemental Composition Report.

Single Mass Analysis.
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.
Element prediction: Off.
Number of isotope peaks used for i-FIT = 3.

Monoisotopic Mass, Even Electron Ions.
Elements Used:

C: 1-40		H: 1-50		O: 1-20		Na: 0-1			
Minimum:								-1.5	
Maximum:								100.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula	
439.1754	439.1757	-0.3	-0.7	12.5	402.9	1.602	20.15	C25 H27 O7	
	439.1733	2.1	4.8	9.5	401.5	0.225	79.85	C23 H28 O7 Na	
461.1566	461.1576	-1.0	-2.2	12.5	444.0	n/a	n/a	C25 H26 O7 Na	

Figure S28. HRESIMS spectrum of compound **3**



Elemental Composition Report.

Single Mass Analysis.
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.
Element prediction: Off
Number of isotope peaks used for i-FIT = 3.

Monoisotopic Mass, Even Electron Ions.
145 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass).
Elements Used:

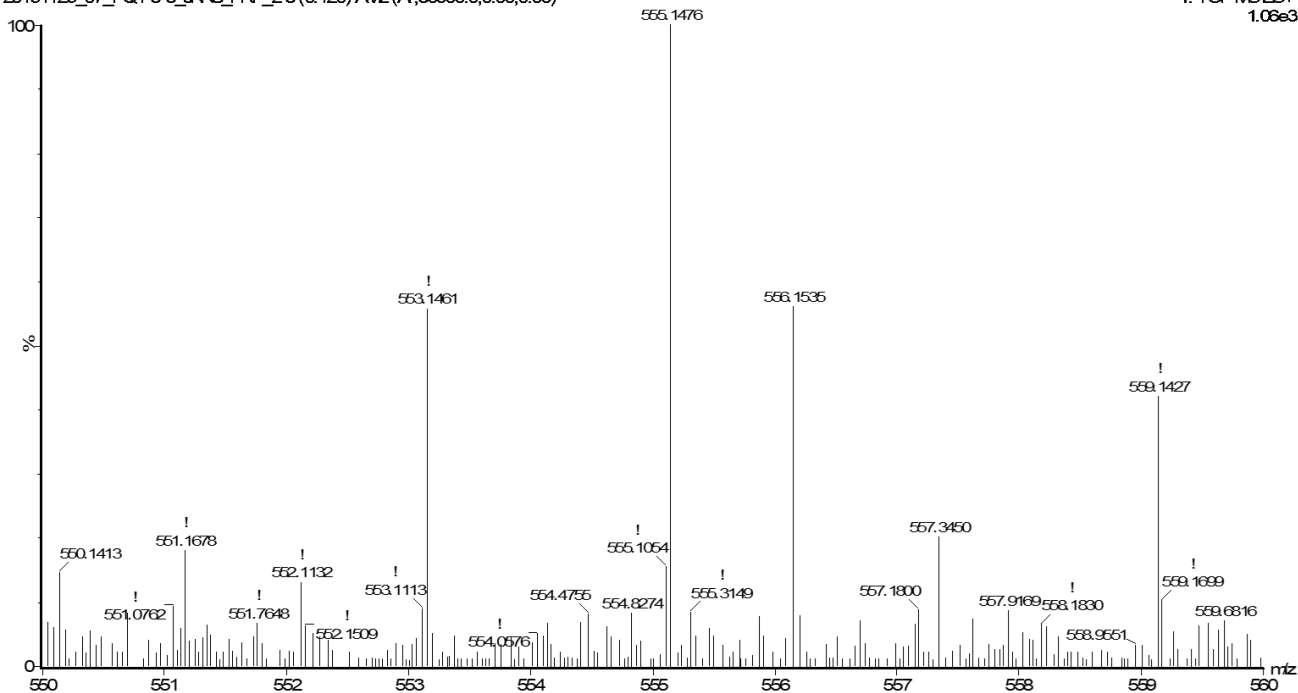
C: 1-40 H: 1-50 O: 1-20 Na: 0-1
Minimum: -1.5
Maximum: 100.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
555.1479	555.1478	0.1	0.2	12.5	409.0	1.109	32.99	C26 H28 O12 Na
	555.1503	-2.4	-4.3	15.5	408.3	0.400	67.01	C28 H27 O12

Figure S29. HRESIMS spectrum of metabolite 4

20191129_07_FQ-P3-3_NNJ_HRP_2.5 (0.120) AM2 (Ar,30000.0,0.00,0.00)

1: TCF MS ES+
1.06e3



Elemental Composition Report.

Single Mass Analysis.

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.

Element prediction: Off

Number of isotope peaks used for i-FIT = 3.

Monoisotopic Mass, Even Electron Ions.

145 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass).

Elements Used:

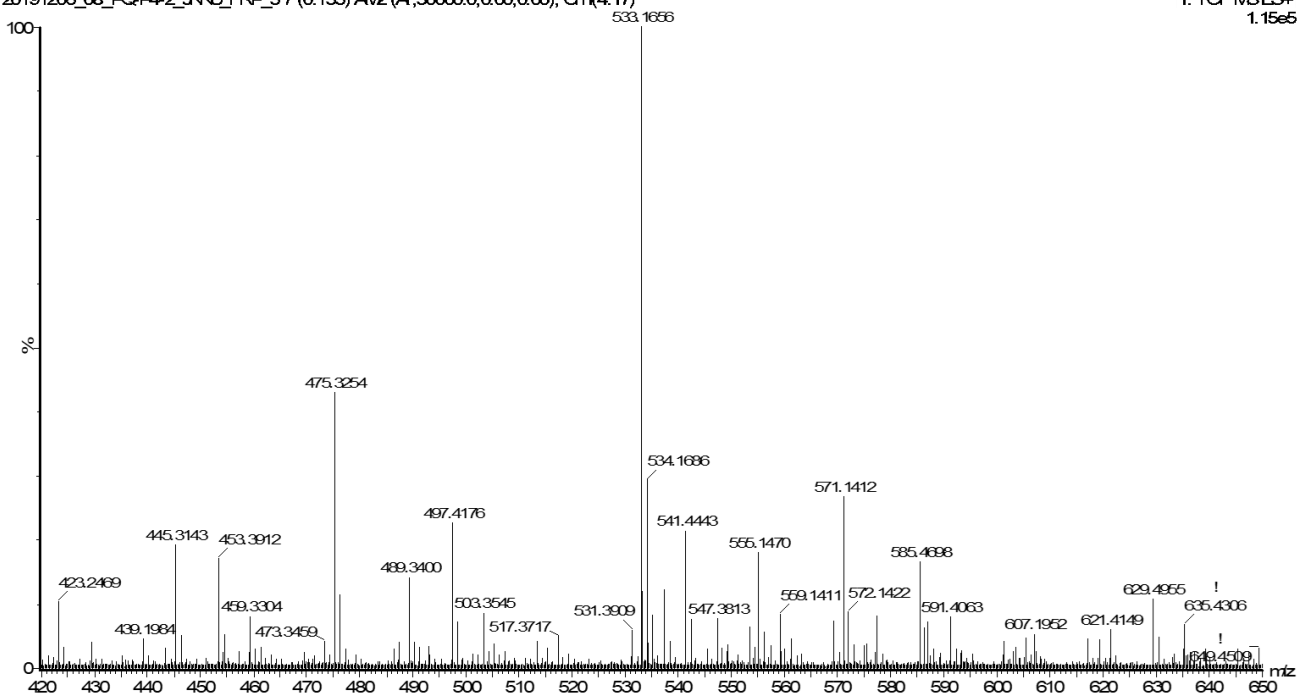
C: 1-40 H: 1-50 O: 1-20 Na: 0-1

Minimum: -1.5

Maximum: 100.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
555.1476	555.1478	-0.2	-0.4	12.5	355.6	0.714	48.97	C26 H28 O12 Na
	555.1503	-2.7	-4.9	15.5	355.6	0.673	51.03	C28 H27 O12

Figure S30. HRESIMS spectrum of metabolite 5



Elemental Composition Report.

Single Mass Analysis.

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.

Element prediction: Off.

Number of isotope peaks used for i-FIT = 3.

Monoisotopic Mass, Even Electron Ions.

48 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass).

Elements Used:

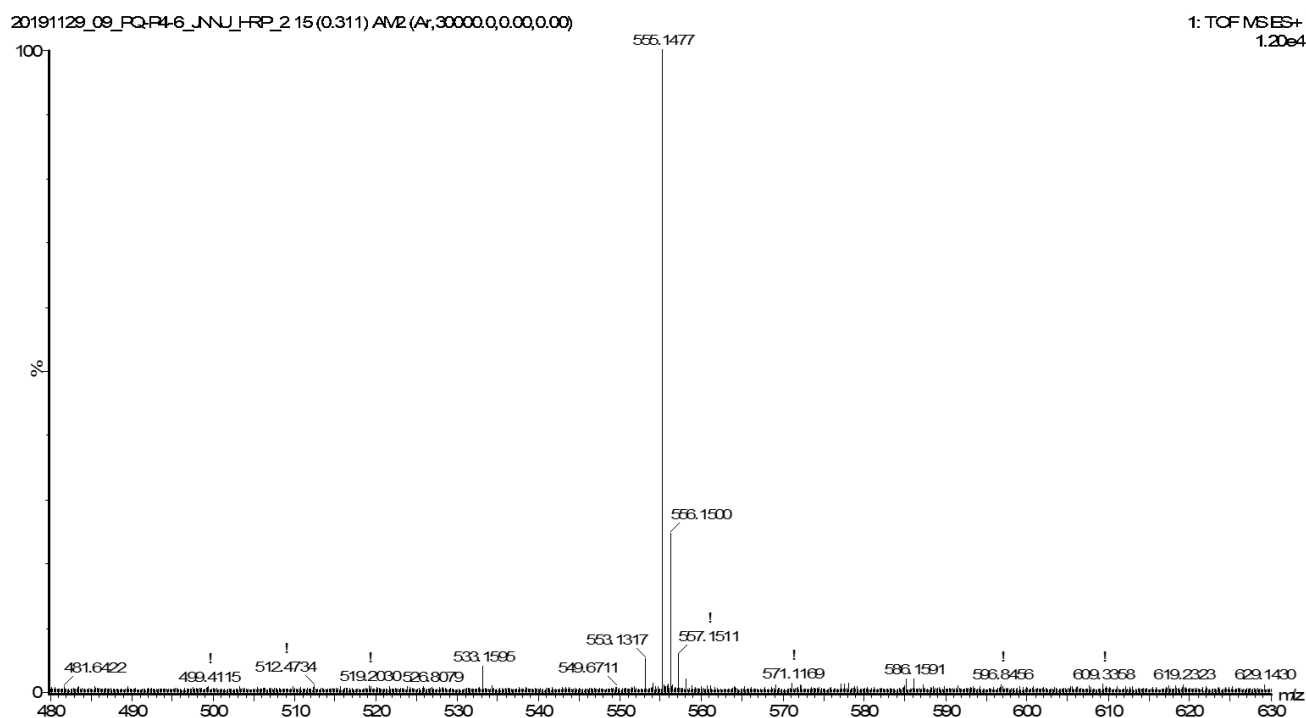
C: 1-30 H: 1-30 O: 0-15 Na: 0-1

Minimum: -1.5

Maximum: 100.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
533.1656	533.1659	-0.3	-0.6	12.5	748.3	0.028	97.24	C ₂₆ H ₂₉ O ₁₂
	533.1635	2.1	3.9	9.5	751.8	3.591	2.76	C ₂₄ H ₃₀ O ₁₂ Na

Figure S31. HRESIMS spectrum of metabolite 6



Elemental Composition Report.

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Single Mass Analysis.

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.

Element prediction: Off ..

Number of isotope peaks used for i-FIT = 3.

..

Monoisotopic Mass, Even Electron Ions.

145 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass).

Elements Used: ..

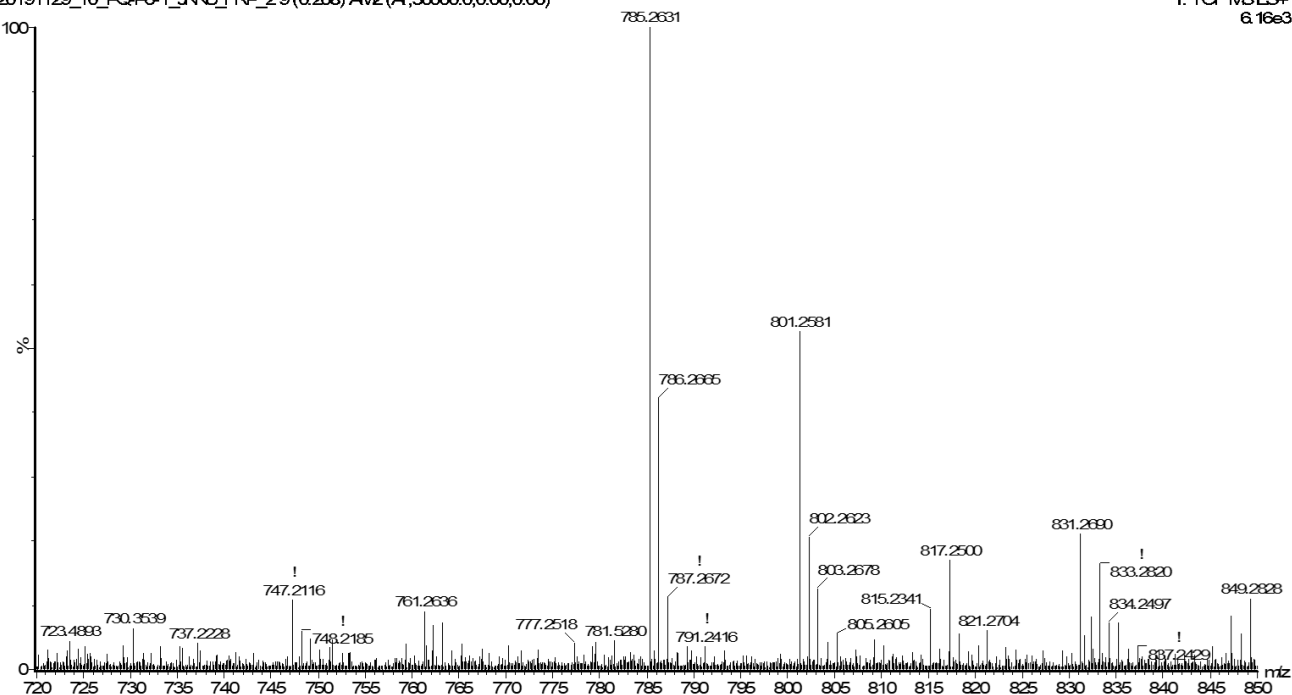
C: 1-40 H: 1-50 O: 1-20 Na: 0-1 ..

Minimum: -1.5 ..

Maximum: 100.0 5.0 100.0 ..

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula..
555.1477	555.1478	-0.1	-0.2	12.5	437.2	0.042	95.87	C26 H28 O12 Na ..
	555.1503	-2.6	-4.7	15.5	440.3	3.187	4.13	C28 H27 O12 ..

Figure S32. HRESIMS spectrum of metabolite 7

**Elemental Composition Report.**

Single Mass Analysis.

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.

Element prediction: Off

Number of isotope peaks used for i-FIT = 3.

Monoisotopic Mass, Even Electron Ions.

60 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass).

Elements Used:

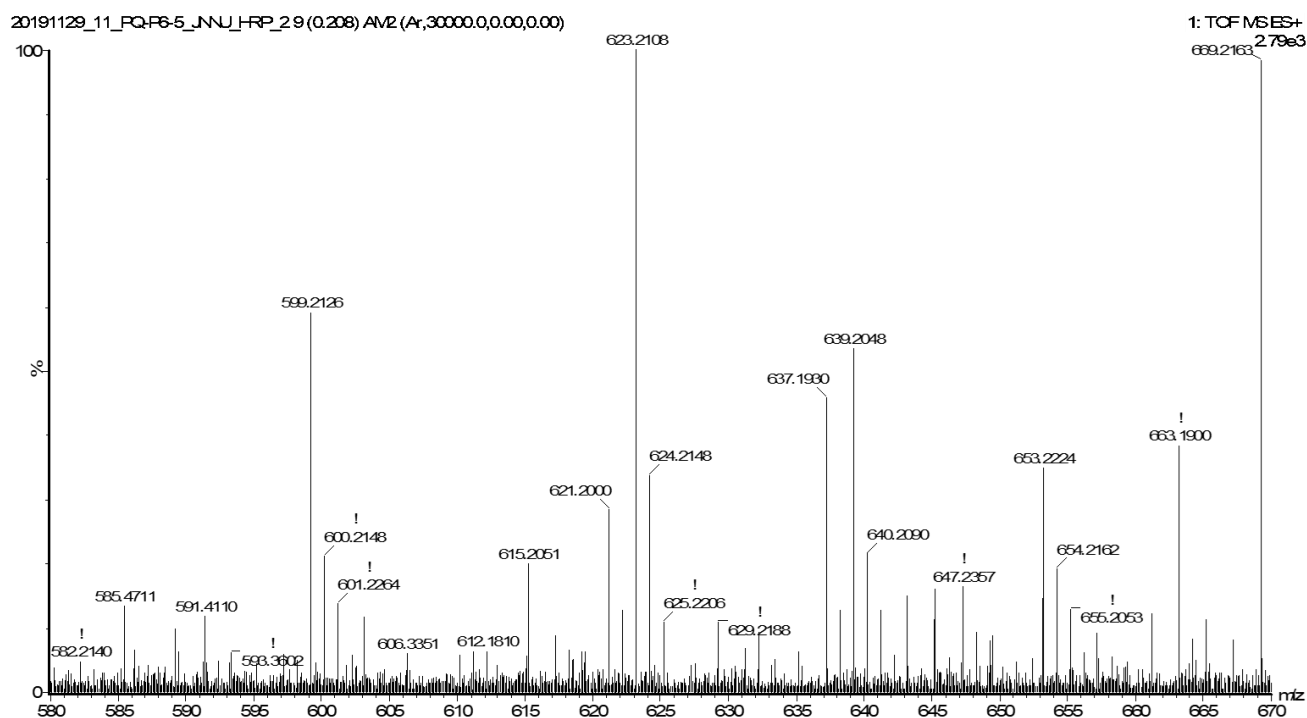
C: 1-40 H: 1-50 O: 1-20 Na: 0-1

Minimum: -1.5

Maximum: 100.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
785.2631	785.2633	-0.2	-0.3	14.5	285.8	0.034	96.68	C37 H46 O17 Na
	785.2657	-2.6	-3.3	17.5	289.1	3.406	3.32	C39 H45 O17

Figure S33. HRESIMS spectrum of metabolite 8



Elemental Composition Report.

Single Mass Analysis.

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0.

Element prediction: Off

Number of isotope peaks used for i-FIT = 3.

Monoisotopic Mass, Even Electron Ions.

118 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass).

Elements Used:

C: 1-40 H: 1-50 O: 1-20 Na: 0-1

Minimum: -1.5

Maximum: 100.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
623.2108	623.2104	0.4	0.6	13.5	376.5	0.925	39.64	C31 H36 O12 Na
	623.2129	-2.1	-3.4	16.5	376.1	0.505	60.36	C33 H35 O12

Figure S34. HRESIMS spectrum of metabolite 9

Table S1. Screening for the microorganisms that transform prenylquercetins

Microorganism name	KCTC number	Transformation capability
<i>A. alternate</i>	6005	-
<i>A. coerulea</i>	6936	+
<i>A. fumigatus</i>	6145	-
<i>C. elegans</i> var. <i>elegans</i>	6992	-
<i>F. merismoides</i>	6153	-
<i>G. deliquescens</i>	6173	+
<i>G. cingulata</i>	6075	-
<i>M. ramanniana</i> var. <i>angulispora</i>	6137	+
<i>M. hiemalis</i>	26779	+++
<i>P. chrysogenum</i>	6933	-
<i>T. koningii</i>	6042	-

Table S2. Water solubility of compounds **1-9**

Compounds	Solubility (mg/mL)	Compounds	Solubility (mg/mL)
1	0.013	6	1.978
2	0.063	7	3.635
3	0.020	8	>4
4	0.501	9	0.613
5	0.385	Quercetin	0.036