Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Fusaroside, a unique glycolipid from *Fusarium* sp., an endophytic fungus isolated from *Melia azedarach*

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Supporting Information

Table S1

Table 1. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR Data of compound **1** and trehalose (C_5D_5N)[a].

	1				trehalose
pos.	δ_H (mult., J in Hz)	δ_C	HMBC (H→C)	COSY	δ_C
1		173.7 (C=O)			
2		55.1 (C)			
3		196.6 (C=O)			
4	6.78 (dt, 15.0, 1.8, 1H)	126.1 (CH)	C-2, 3, 6	H-5	
5	7.15 (dt, 15.0, 7.2, 1H)	148.8 (CH)	C-3, 7	H-4, 6	
6	1.91 (m, 2H)	32.4 (CH_2)	C-4, 5, 8	H-5, 7	
7	1.35 (m, 2H)	27.8 (CH_2)	C-5, 8, 9	H-6, 8	
8	1.27 (m, 2H)	29.4 (CH_2)	C-6, 9, 10	H-7, 9	
9	1.92 (m, 2H) [b]	32.5 (CH_2) [b]	C-7, 11		
10	2.09 (m, 2H) [b]	33.0 (CH_2) [b]	C-8, 11, 12		
11	5.49 (m, 1H) [c]	130.4 (CH) [c]	C-9, 13		
12	5.40 (m, 1H) [c]	130.3 (CH) [c]	C-10, 14		
13	5.40 (m, 1H) [c]	130.4 (CH) [c]	C-11, 15		
14	5.49 (m, 1H) [c]	130.6 (CH) [c]	C-12, 16		
15	2.09 (m, 2H) [b]	32.9 (CH_2) [b]	C-13, 14, 17		
16	1.92 (m, 2H) [b]	32.9(CH_2) [b]	C-14, 18		
17	2.09 (m, 2H) [b]	33.0 (CH_2) [b]	C-15, 19		
18	5.42 (dt, 15.0, 8.0, 1H)	131.3 (CH)	C-16, 20	H-17, 19	
19	5.44 (m, 1H)	125.2 (CH)	C-17, 20	H-18, 20	
20	1.61 (d, 4.8, 3H)	18.0 (CH_3)	C-18, 19	H-19	
21	1.51 (s, 3H)	22.2 (CH_3)	C-1, 2, 3, 22		
22	1.55 (s, 3H)	22.3 (CH_3)	C-1, 2, 3, 21		
1′	5.87 (d, 3.6, 1H)	95.4 (CH)	C-1″, 3′, 5′	H-2′	95.3
2′	4.21 (dd, 9.8, 3.6, 1H)	73.4 (CH)	C1′, 4′	H-1′, 3′	73.3
3′	4.69 (m, 1H)	72.5 (CH)	C-1′, 4′, 5′	H-2′, 4′	74.7
4′	5.77 (m, 1H)	73.5 (CH)	C-1, 2′, 3′, 6′	H-3′, 5′	72.1
5′	4.91 (m, 1H)	71.9 (CH)	C-1′, 3′, 6′	H-4′, 6′	74.1
6′	4.09 (dd, 12.0, 4.8, 1H)	62.0 (CH_2)	C-4′, 5′	H-5′	62.6
	4.19 (m, 1H)				
1″	5.85 (d, 4.2, 1H)	95.9 (CH)	C-1′, 3″, 5″	H-2″	95.3
2″	4.19 (dd, 9.8, 3.8, 1H)	73.7 (CH)	C1″, 4″	H-1″, 3″	73.3
3″	4.72 (m, 1H)	74.9 (CH)	C-1″, 4″, 5″	H-2″, 4″	74.7
4″	4.25 (m, 1H)	72.3 (CH)	C-2″, 3″, 6″	H-3″, 5″	72.1
5″	4.89 (m, 1H)	74.4 (CH)	C-1″, 3″, 6″	H-4″, 6″	74.1
6″	4.36 (dd, 11.4, 4.8, 1H)	62.8 (CH_2)	C-4″, 5″	H-5″	62.6
	4.44 (dd, 12.0, 3.0, 1H)				

[a] Assigned by DEPT, COSY, HSQC, and HMBC experiments.

[b] Assignments may be interchanged. Carbon resonances (δ) for the aliphatic chain: 32.51, 32.96, 32.99, 33.01, 33.04 (multiple overlapping). Broad proton resonance at 1.92-2.09 ppm integrated for 10 H.

[c] Assignments may be interchanged. Carbon resonances (δ) for the conjugated double bond: 130.32, 130.41(×2),

130.57(multiple overlapping). Broad proton resonance at 5.40-5.49 ppm integrated for 4 H.

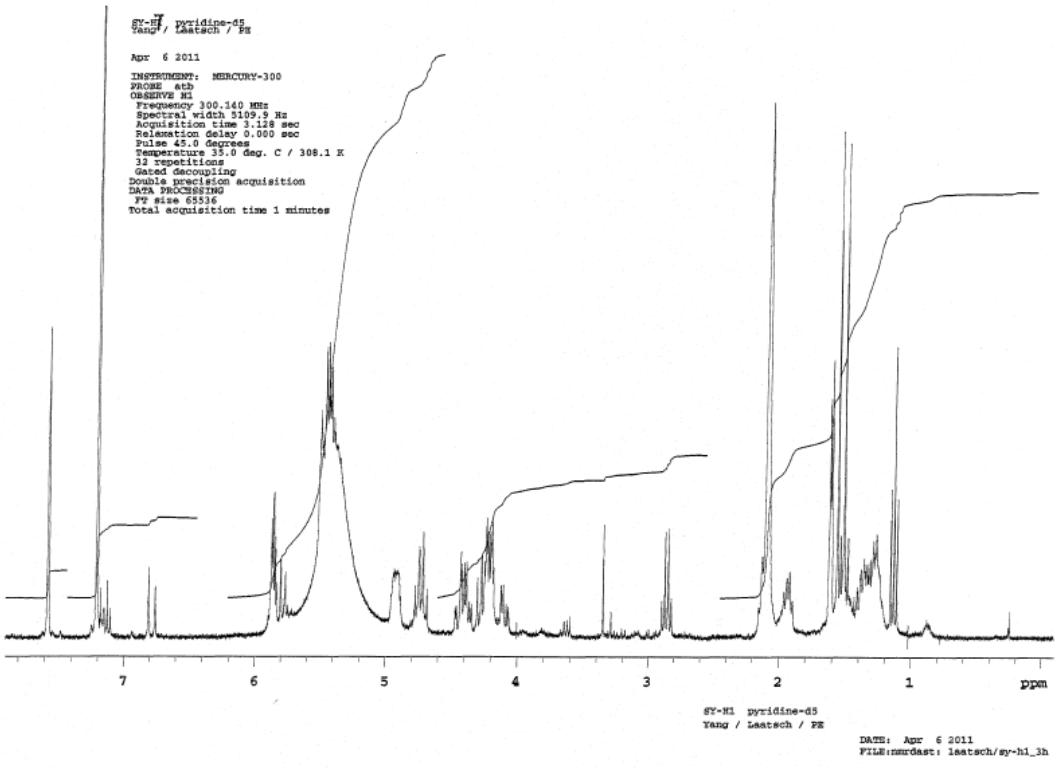


Figure **S1**: 1H-NMR spectrum of compound **1**.

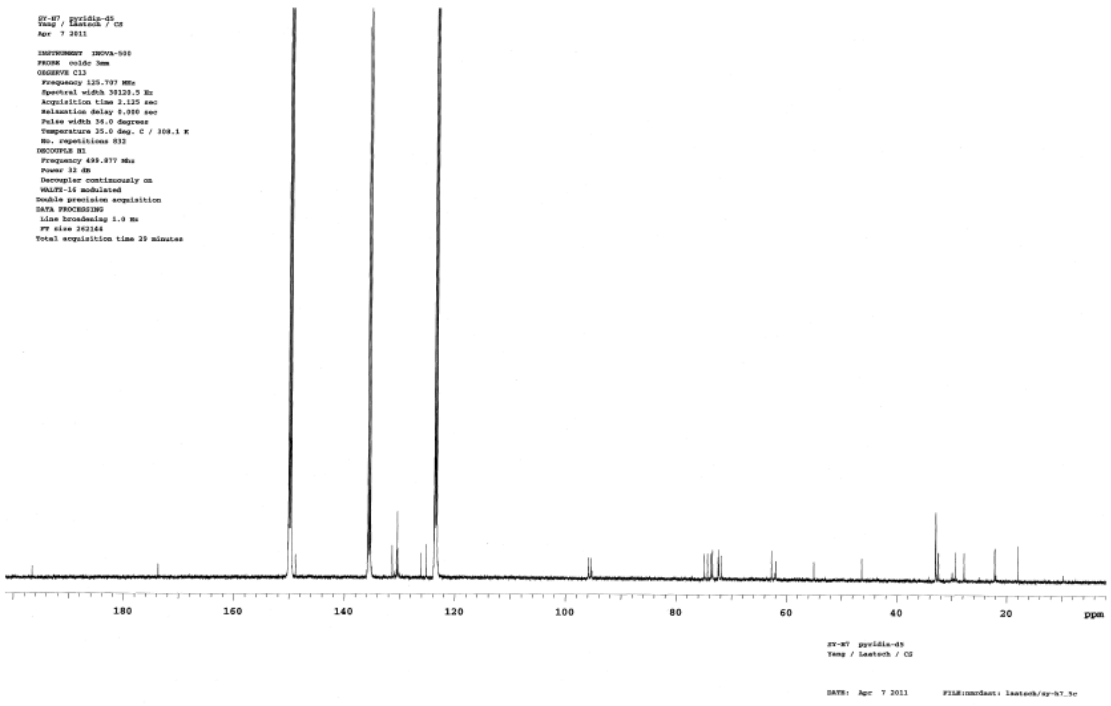


Figure **S2**: 13C-NMR spectrum of compound **1**.

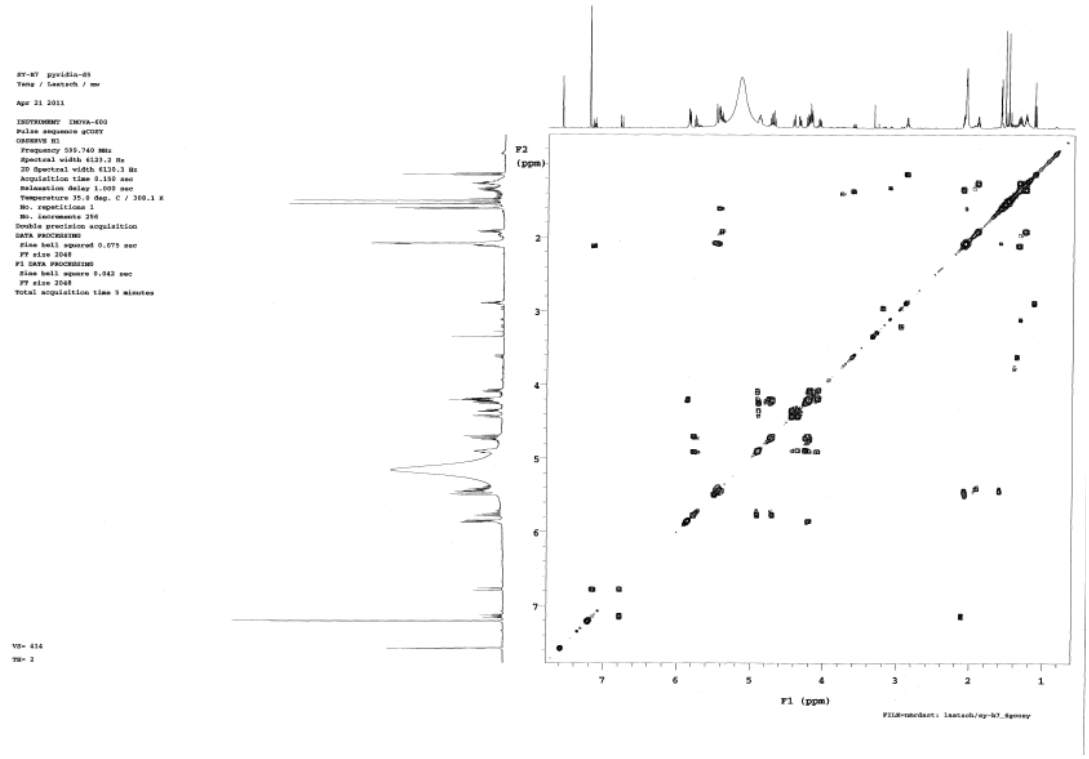


Figure **S3**: H-H COSY spectrum of compound **1**.

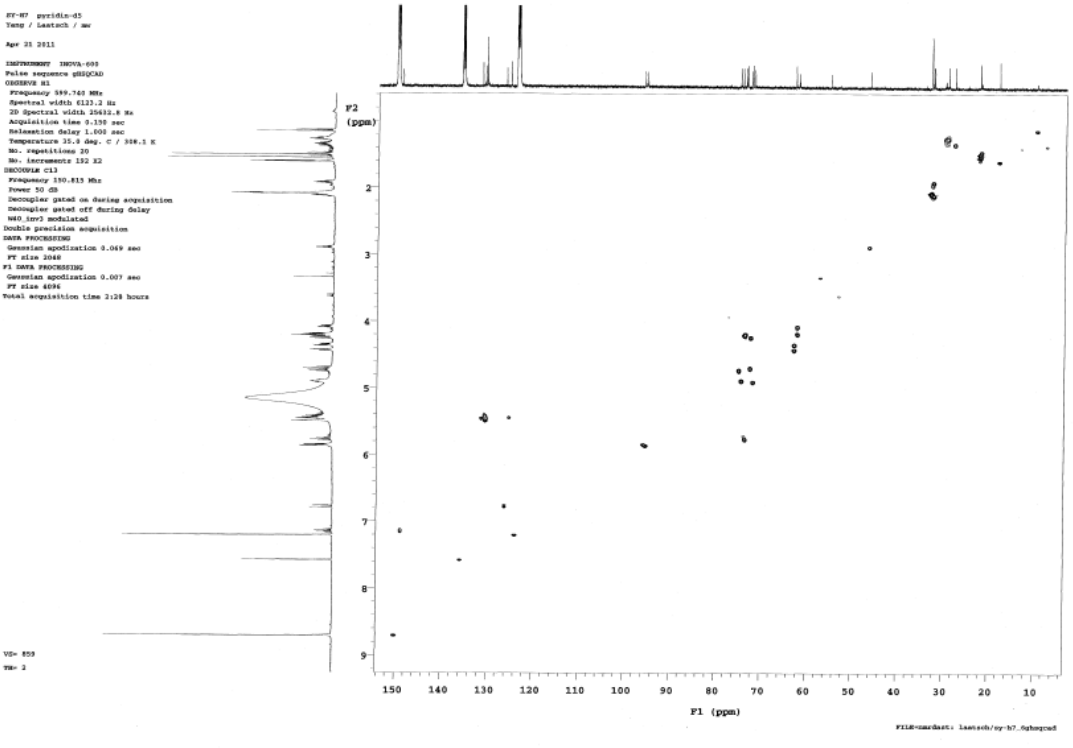


Figure **S4**: HSQC spectrum of compound **1**.

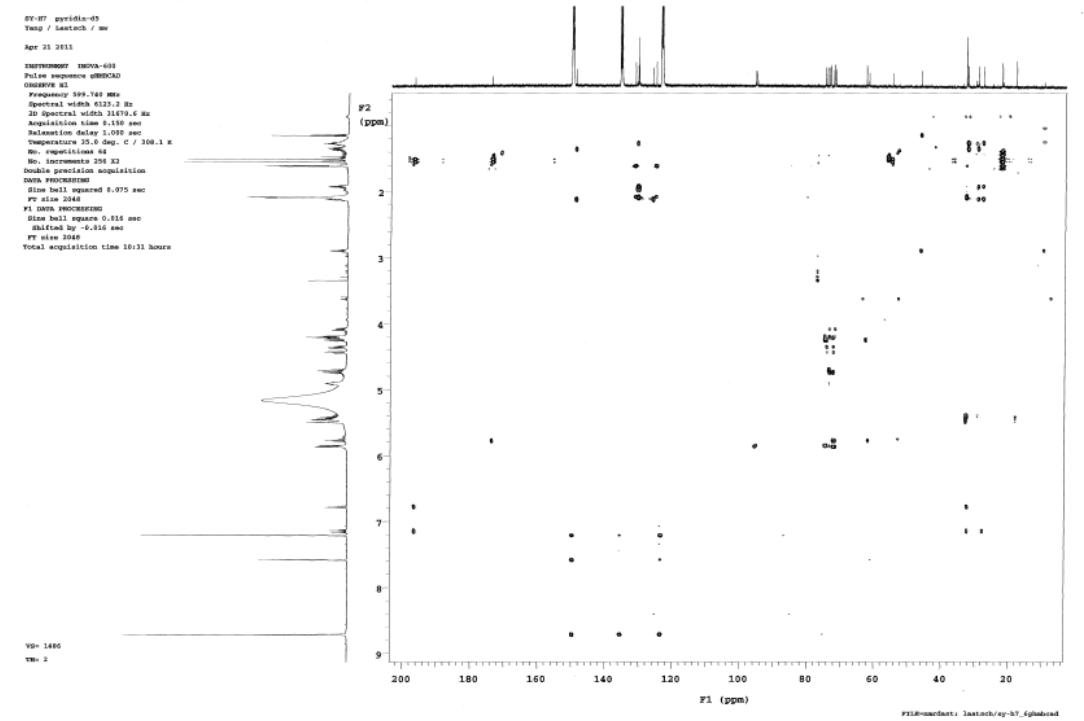


Figure **S5**: HMBC spectrum of compound **1**.

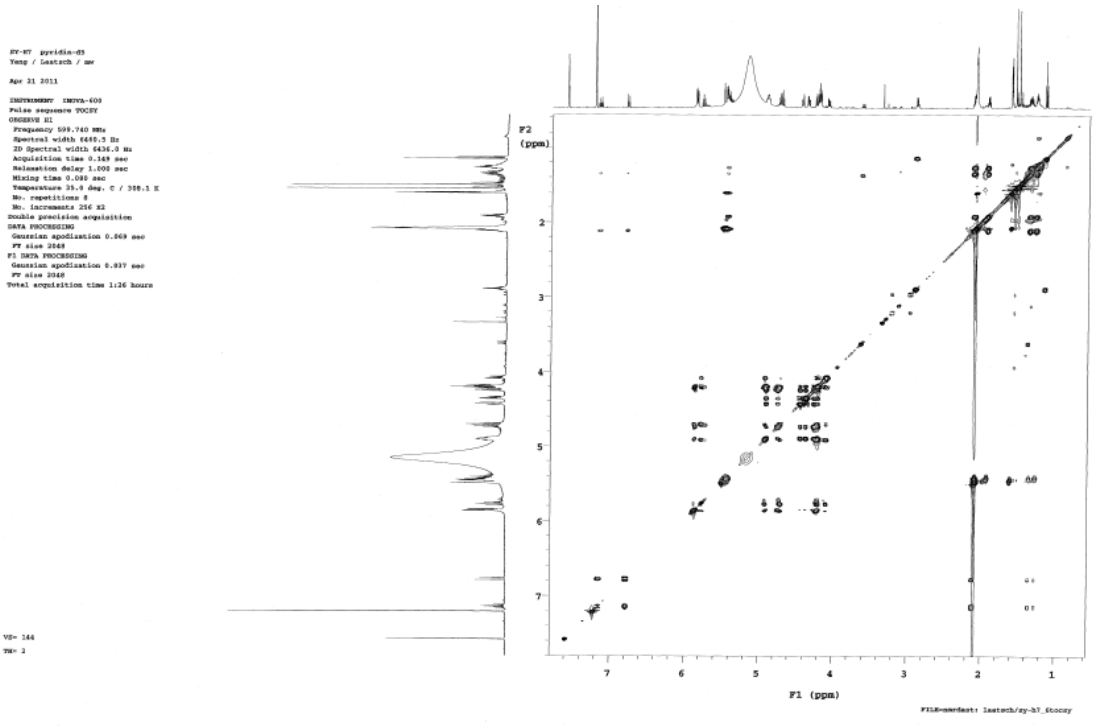


Figure **S6**: TOCSY spectrum of compound **1**.

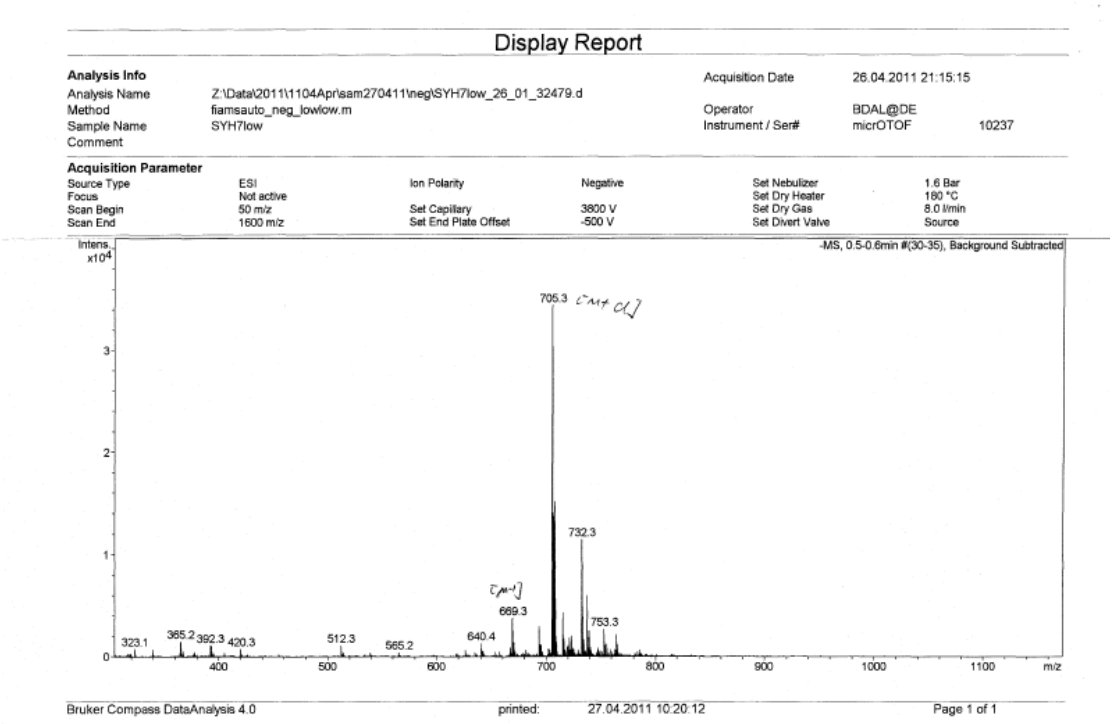


Figure **S7**: ESI-MS(-) spectrum of compound **1**.

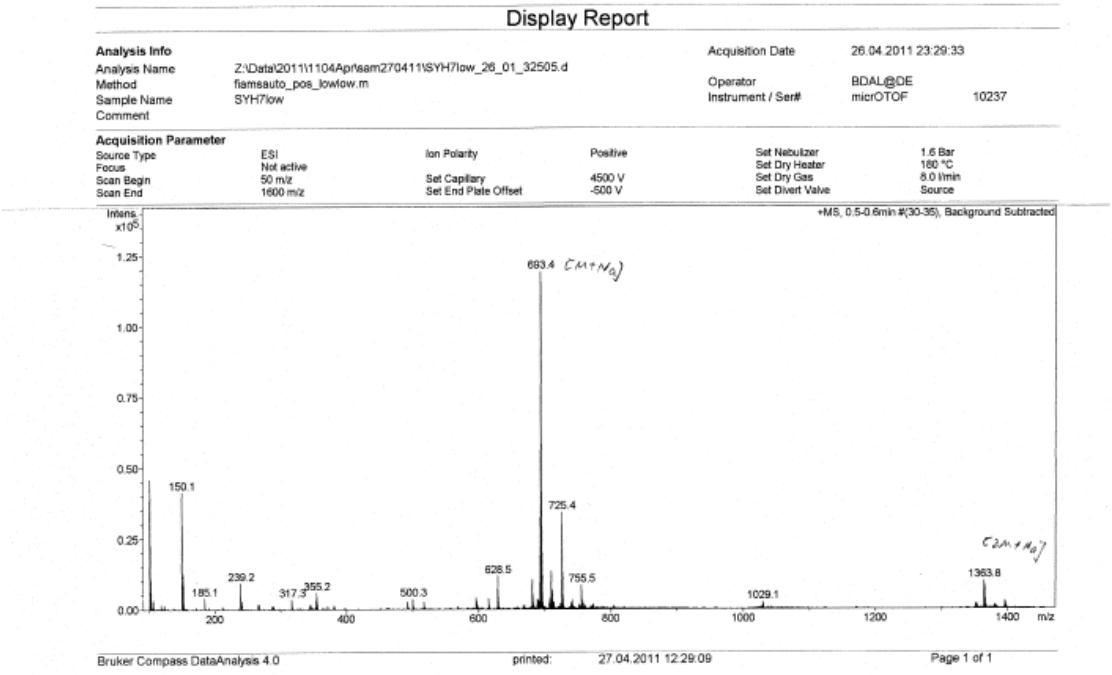


Figure **S7**: ESI-MS(+) spectrum of compound **1**.

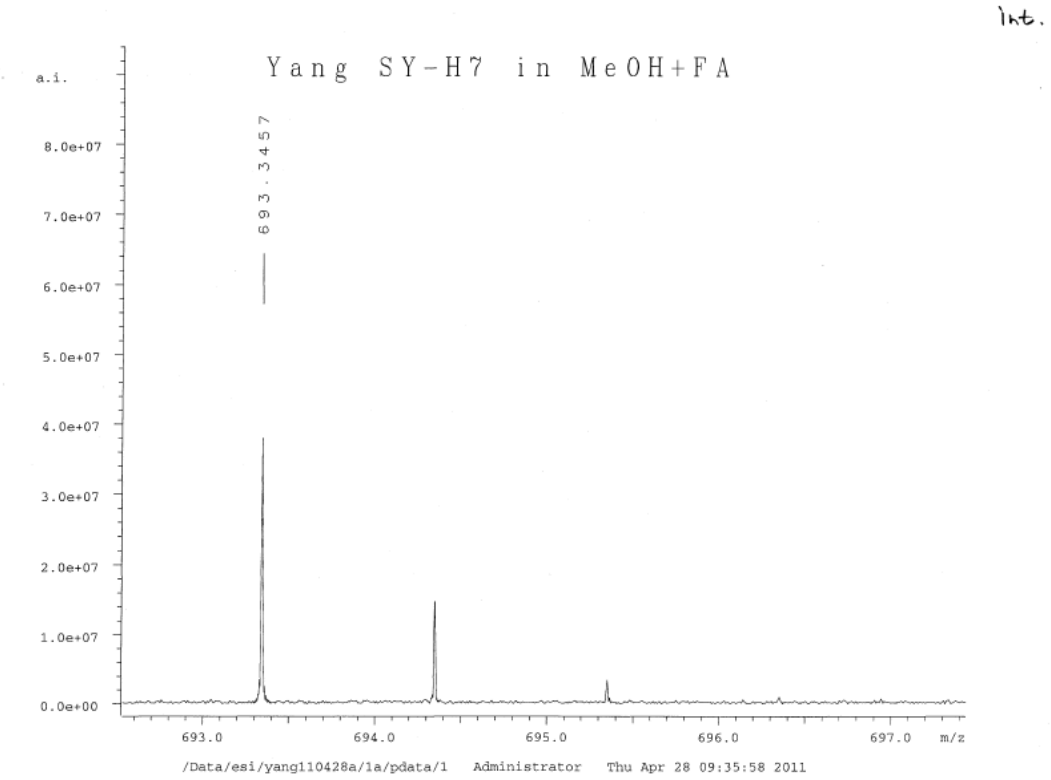
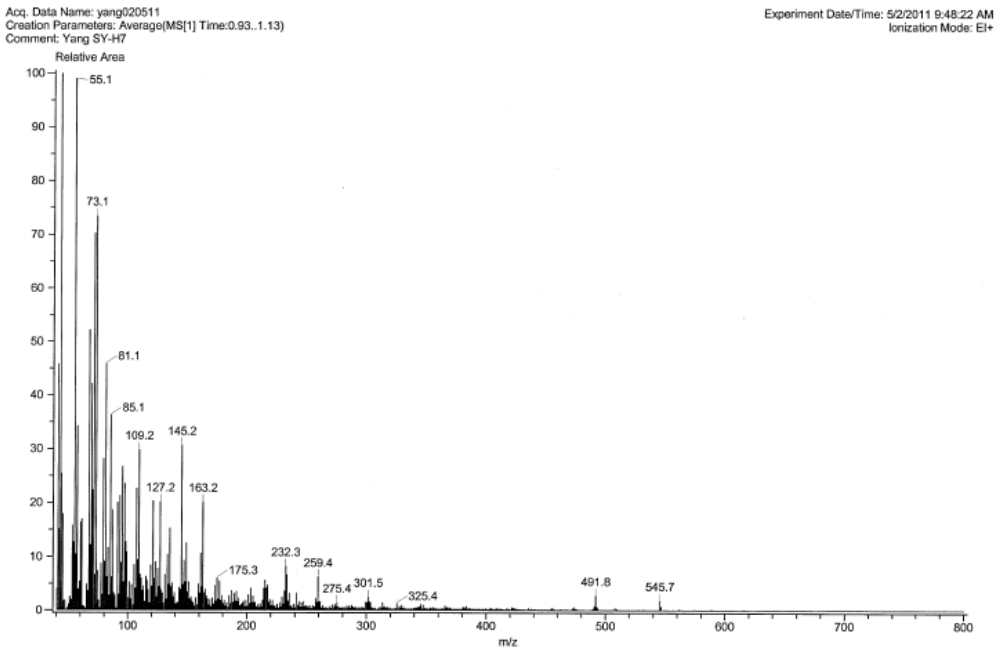


Figure **S8**: HR-ESI-MS spectrum of compound **1**.



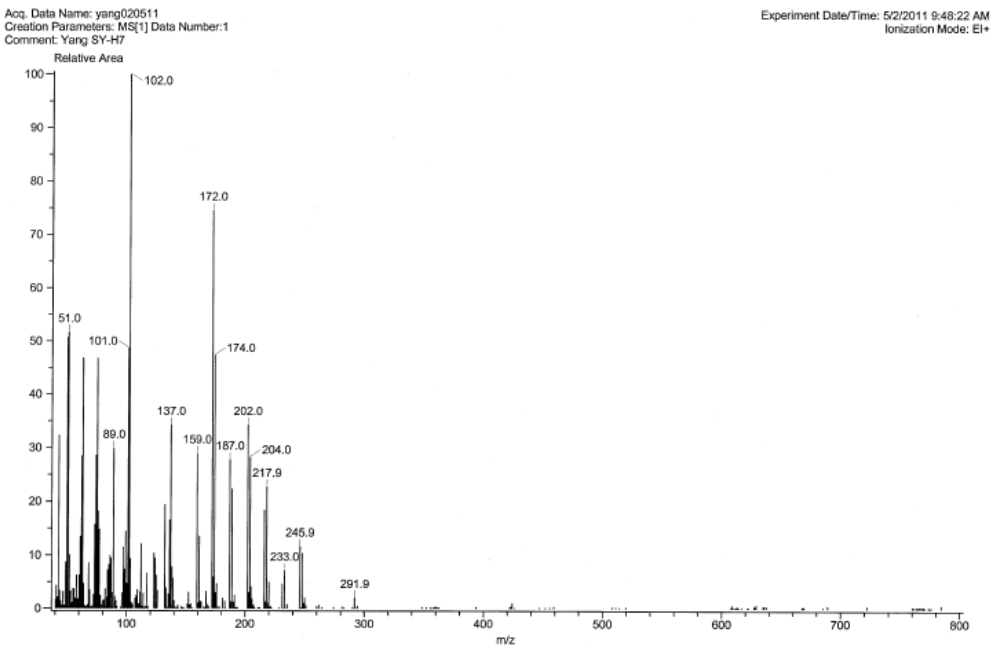


Figure **S9**: EI-MS spectra of compound **1**.

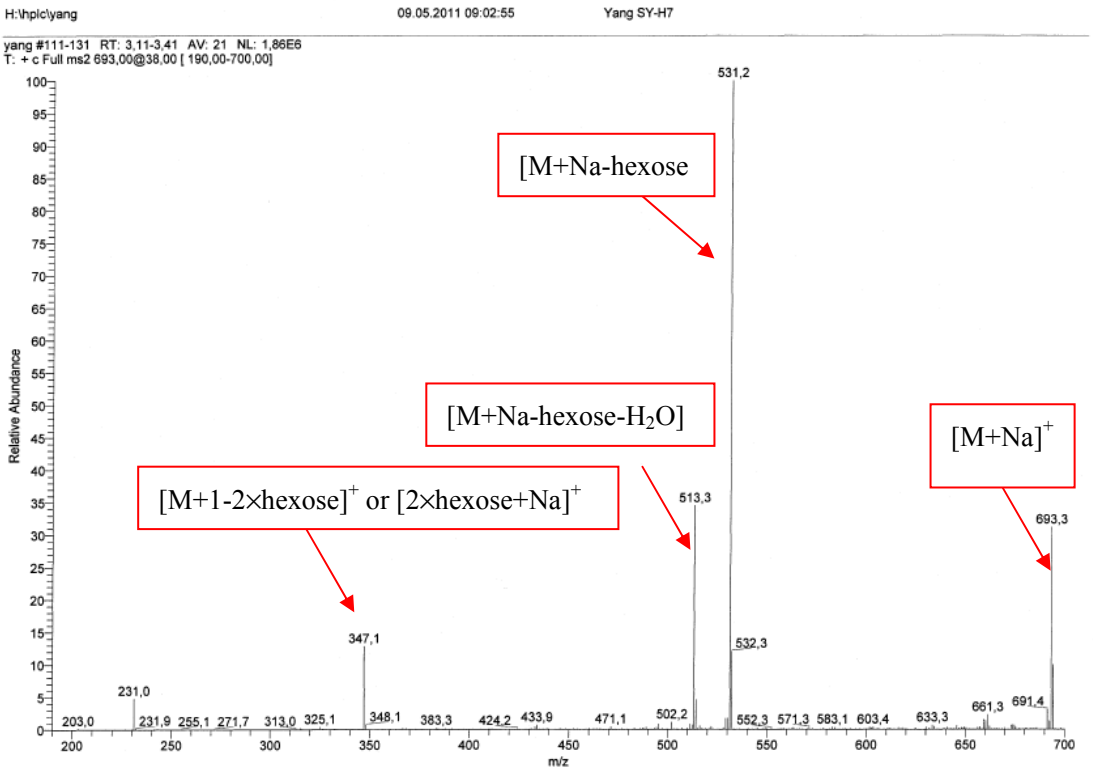


Figure **S10**: MS-MS spectrum of compound **1**.

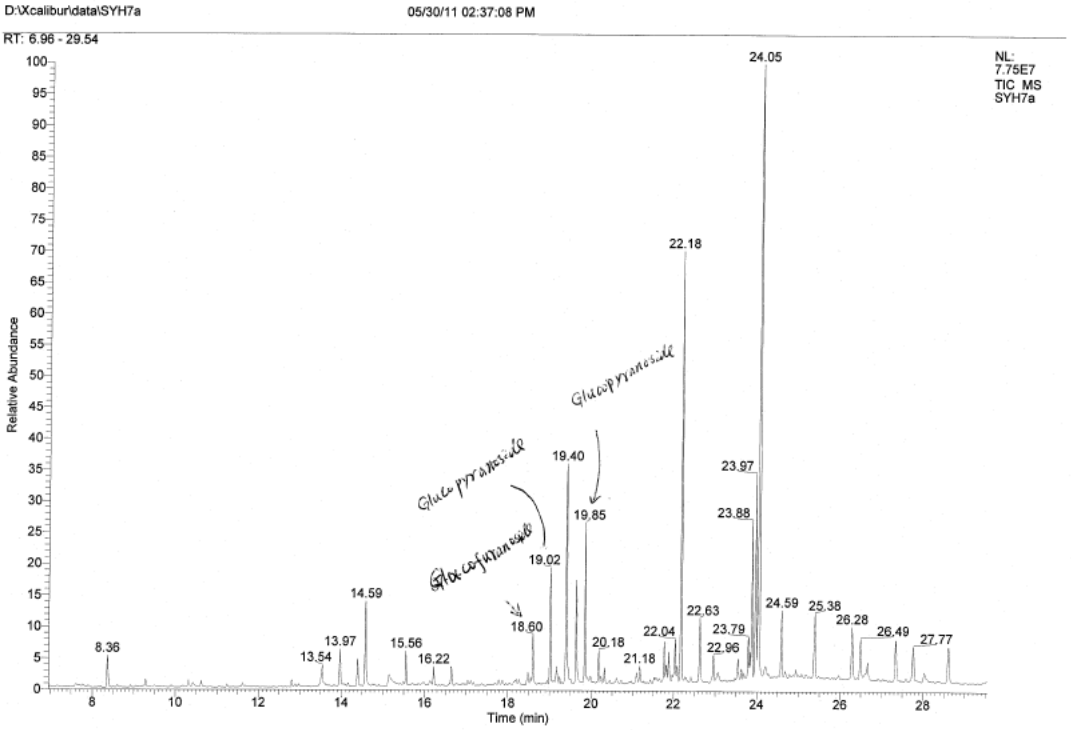


Figure **S11**: Total ion current (TIC) chromatograms of silylated sugar.