Supplementary Materials

Content

1. Scheme S1	· S 1
2. Figure S1 ·····	··S1
3. Table S1	·S2
4. Copies of ¹³ C-NMR spectra of all compounds ······	··S3–S4

Scheme S1. Synthesis of 18β -GAMG, 18α -GAMG and 18α -GAMG.

Figure S1. The isomerization reaction was monitored by ¹³C-NMR spectroscopy.

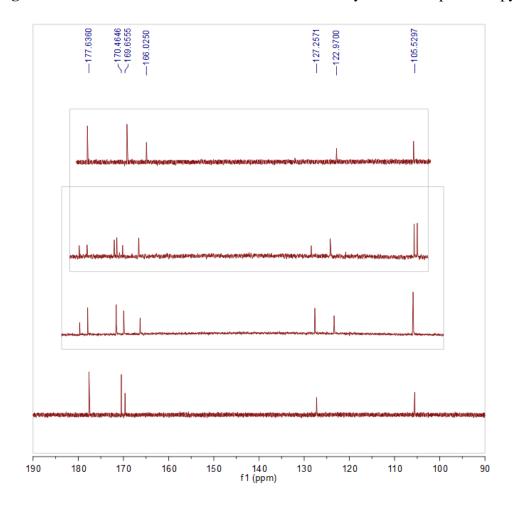


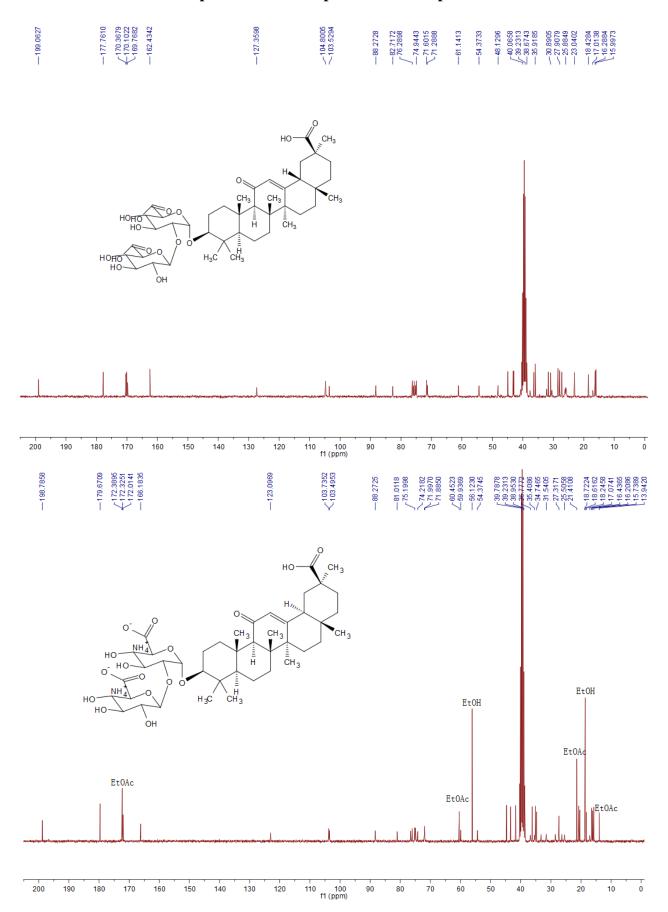
Table S1. ¹³C-NMR data for 18α-GA, 18α-GAMA, 18β-GA and 18β-GAMG in DMSO- d_6 (δ , ppm, J in Hz).

Position	18α-GA	18α-GAMG	18β-GA	18β-GAM
1	38.6	38.3	38.7	38.4
2	25.5	25.7	25.8	25.6
3	88.3	87.9	88.3	87.7
4	39.0	39.1	39.1 ^a	39.1 ^a
5	54.4	54.3	54.4	54.1
6	17.1	17.1	17.0	16.9
7	33.2	33.2	32.2	32.1
8	43.4	43.4	44.9	44.9
9	59.9	59.9	61.1	61.0
10	36.2	36.2	36.4	36.3
11	198.8	198.7	199.1	198.9
12 *	123.1	123.1	127.4	127.3
13 *	166.2	166.1	169.8	169.7
14	44.7	44.7	43.0	42.9
15	26.3	26.3	26.1	26.1
16*	36.8	36.7	25.9	25.8
17 *	35.4	35.3	31.6	31.5
18*	39.6 ^a	39.8 ^a	48.1	48.0
19 *	31.5	31.4	40.7	40.6
20 *	41.7	41.6	43.2	43.1
21 *	28.5	28.4	30.4	30.4
22	35.2	35.1	37.6	37.5
23	27.3	27.5	27.2	27.4
24	16.2	16.45	16.0	16.2
25	16.4	16.49	16.3	16.4
26	18.2	18.2	18.4	18.3
27 *	20.4	20.4	23.0	23.0
28 *	15.7	15.7	28.5	28.4
29 *	20.7	20.6	27.9	27.8
30	179.7	179.5	177.8	177.6
1'	103.5	105.6	104.8	105.5
2'	81.0	75.6	82.7	76.1
3'	74.2	73.7	76.3	75.6
4'	72.0 or 71.9	71.6	71.6 or 71.3	71.5
5'	76.6	76.1	74.9	73.7
6'	172.4	170.6	172.4	170.5
1"	103.7		103.5	
2"	75.0		75.7	
3"	75.2		75.9	
4"	72.0 or 71.9		71.6 or 71.3	
5"	76.0		75.2	
6"	172.0		172.0	

^{*} Carbon atoms of chemical shifts with significant difference; ^a Overlapped with solvent.

Molecules **2014**, *19*

Copies of ¹³C-NMR spectra of all compounds



Molecules **2014**, *19*

