Supporting information

New Derivatives of Lupeol and Their Biological Activity

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Abstract: The natural product lupeol (**1**) was isolated from *Bombax ceiba* leaves, which were used as starting material in the semisynthetic approach. Three new derivatives (**2a**, **2b**, and **3**) were synthesized using oxidation and aldolization. Their chemical structures were elucidated by spectroscopic analyses (HRESIMS and NMR). Compounds **3** showed significant α-glucosidase inhibition with an IC_{50} value of 202 μM, whereas **2a** and **2b** were inactive.

Keywords: lupeol derivative; benzylidene derivative; α-glucosidase inhibition; Oxone®

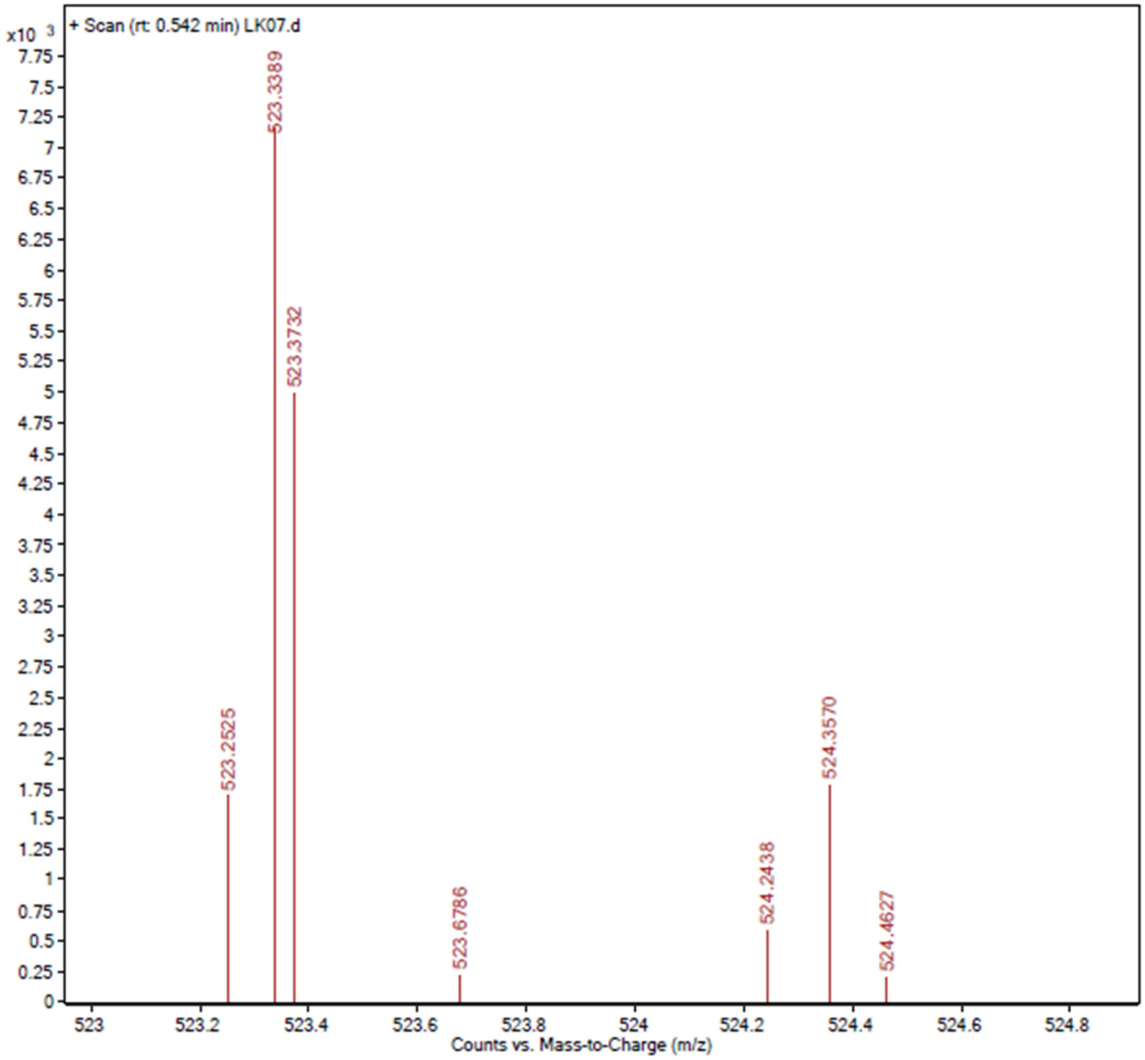


Figure S1. HRESIMS spectrum of **2a**.

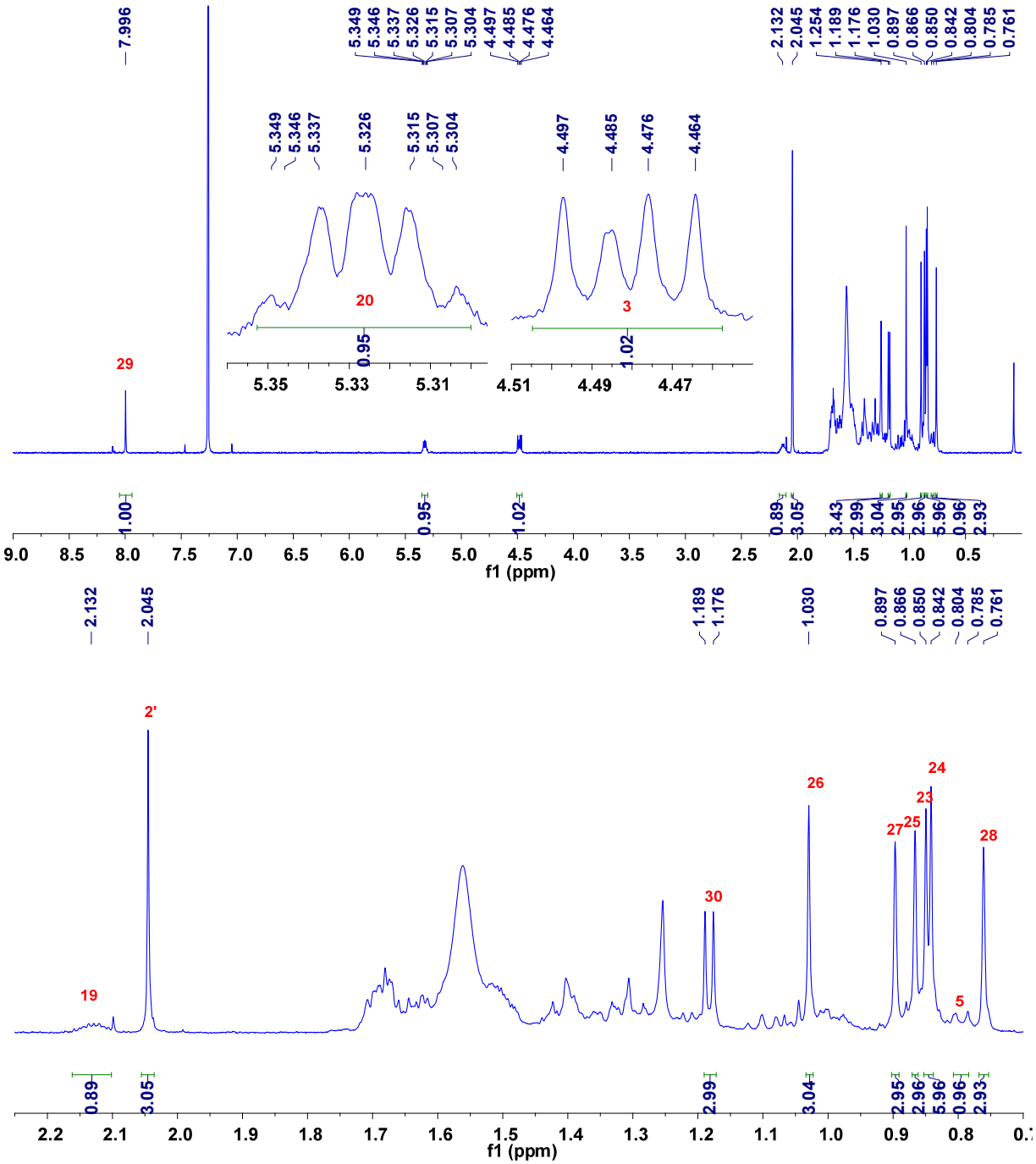


Figure S2. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **2a**.

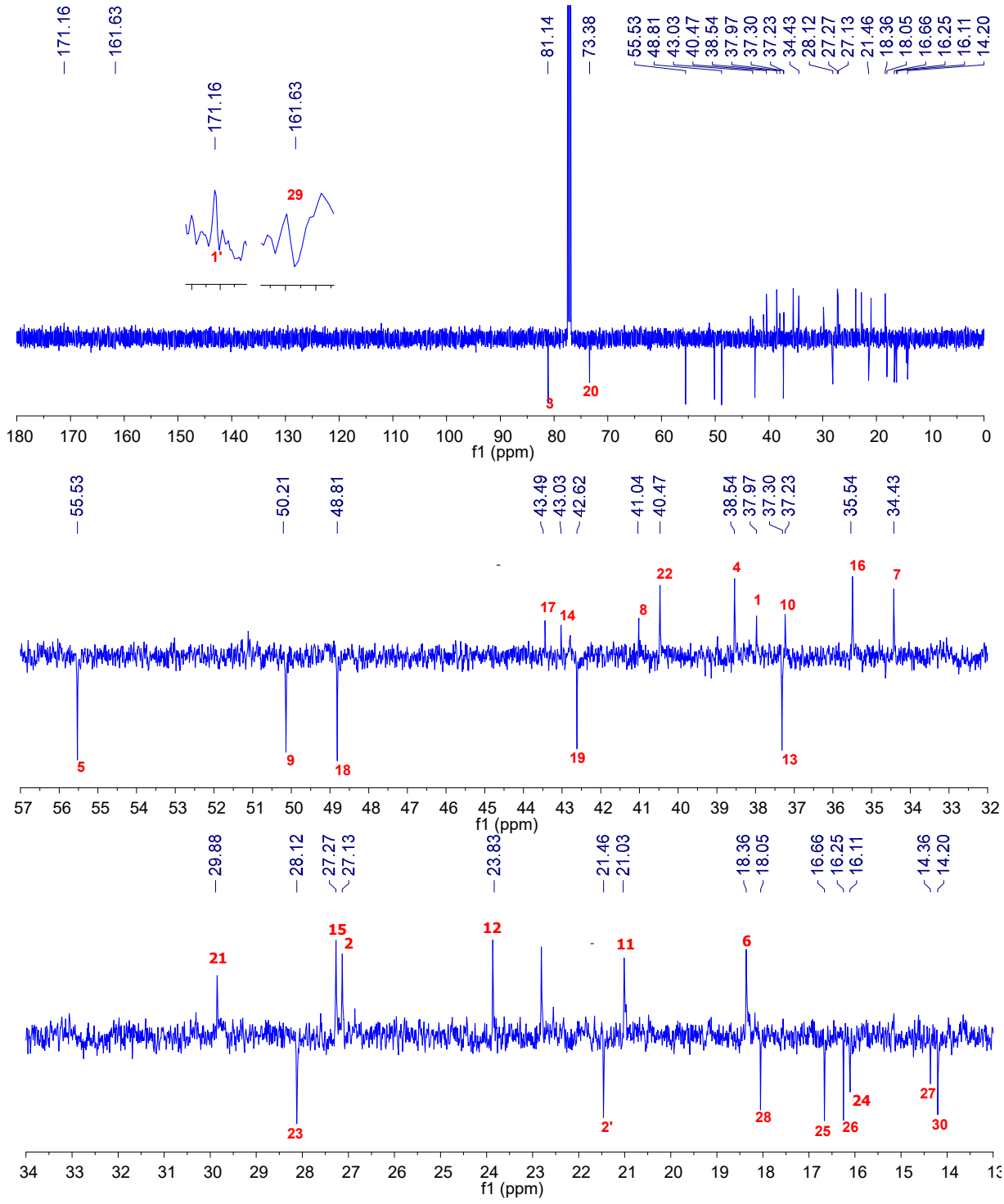


Figure S3. ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **2a.**

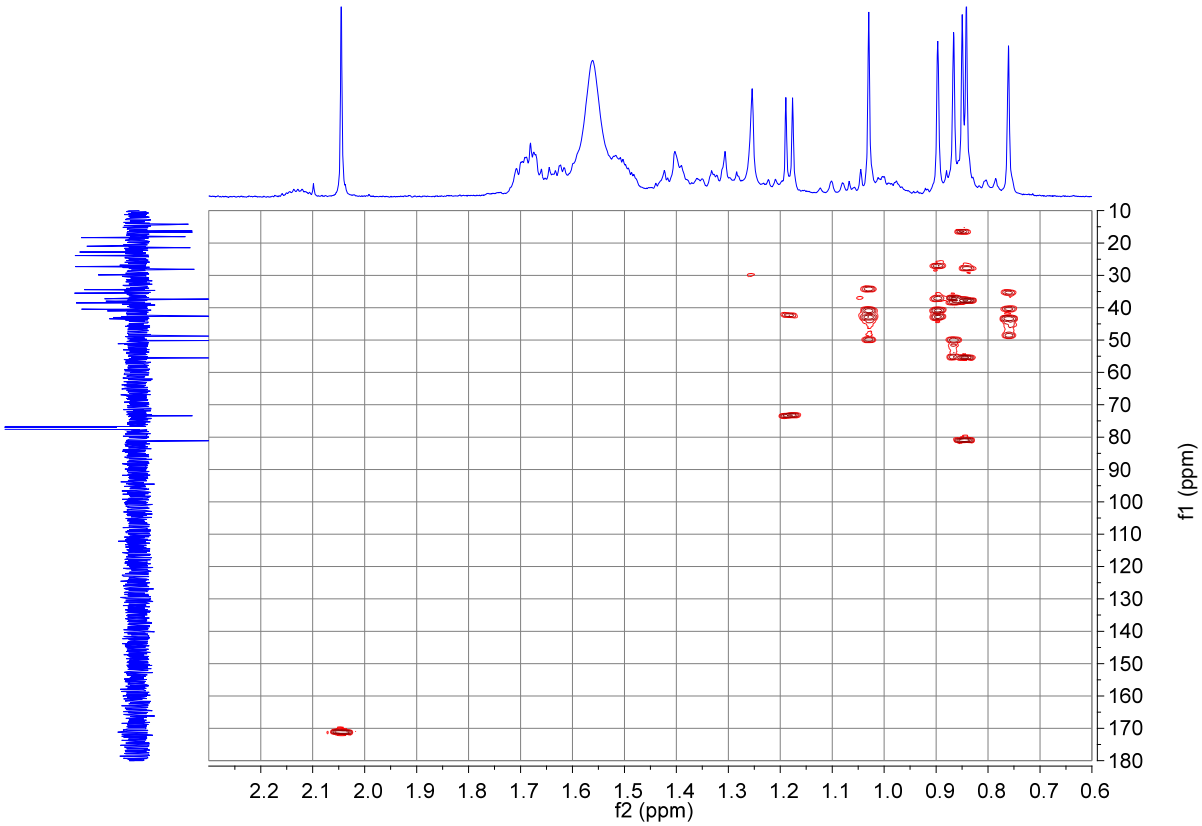


Figure S4. HMBC ($CDCl_3$) spectrum of **2a**.

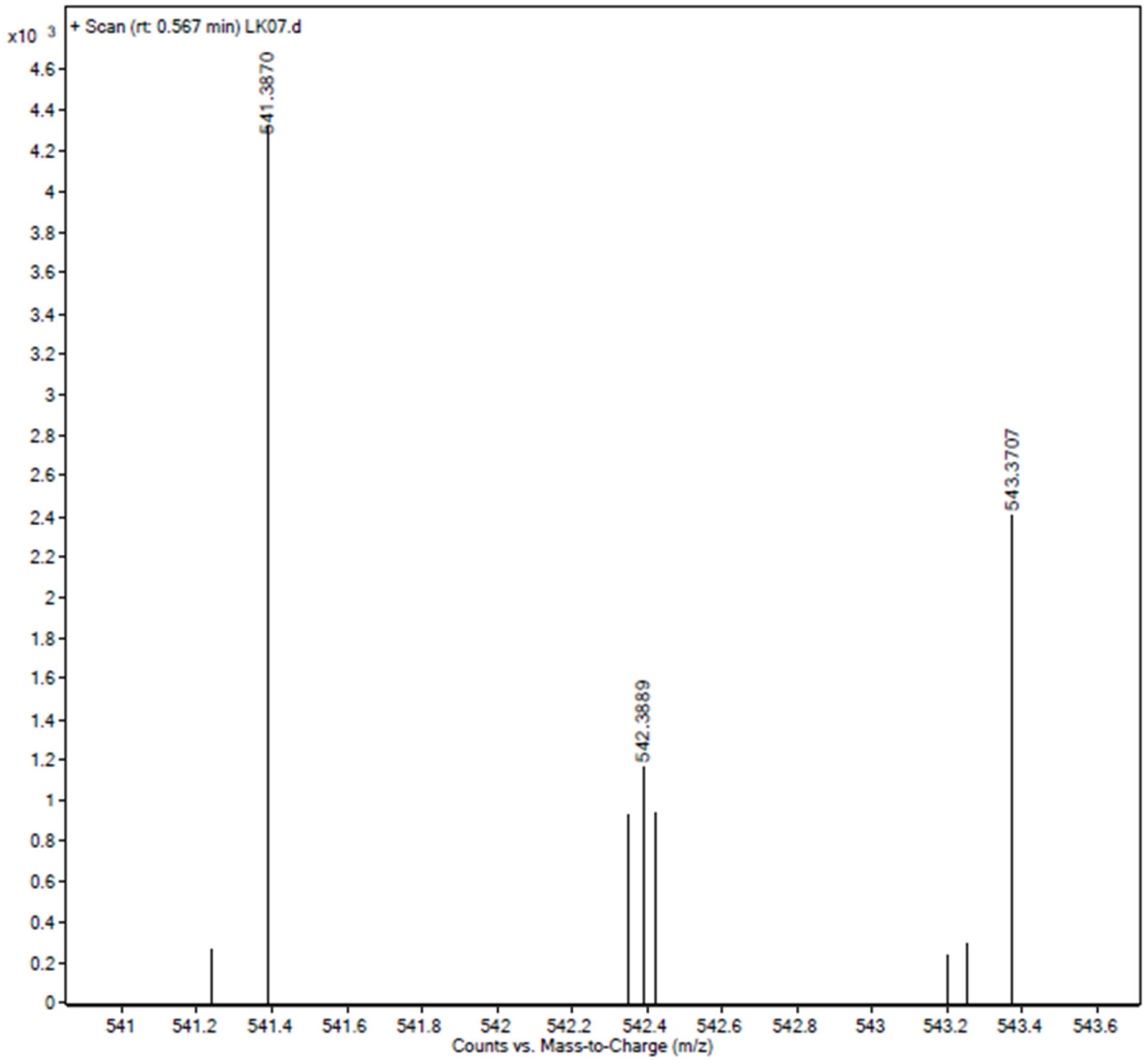


Figure S5. HRESIMS spectrum of **2b**.

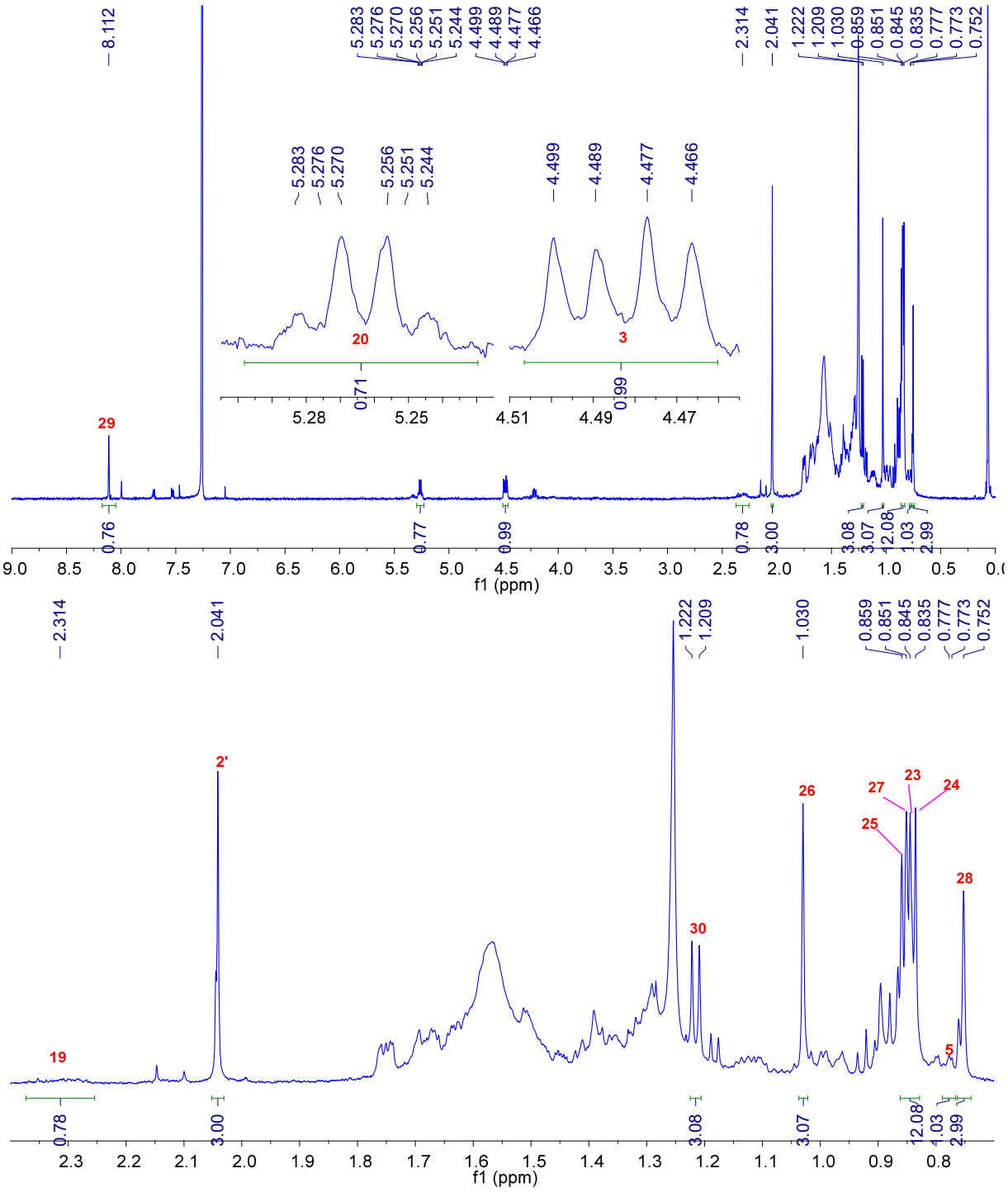


Figure S6. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **2b**.

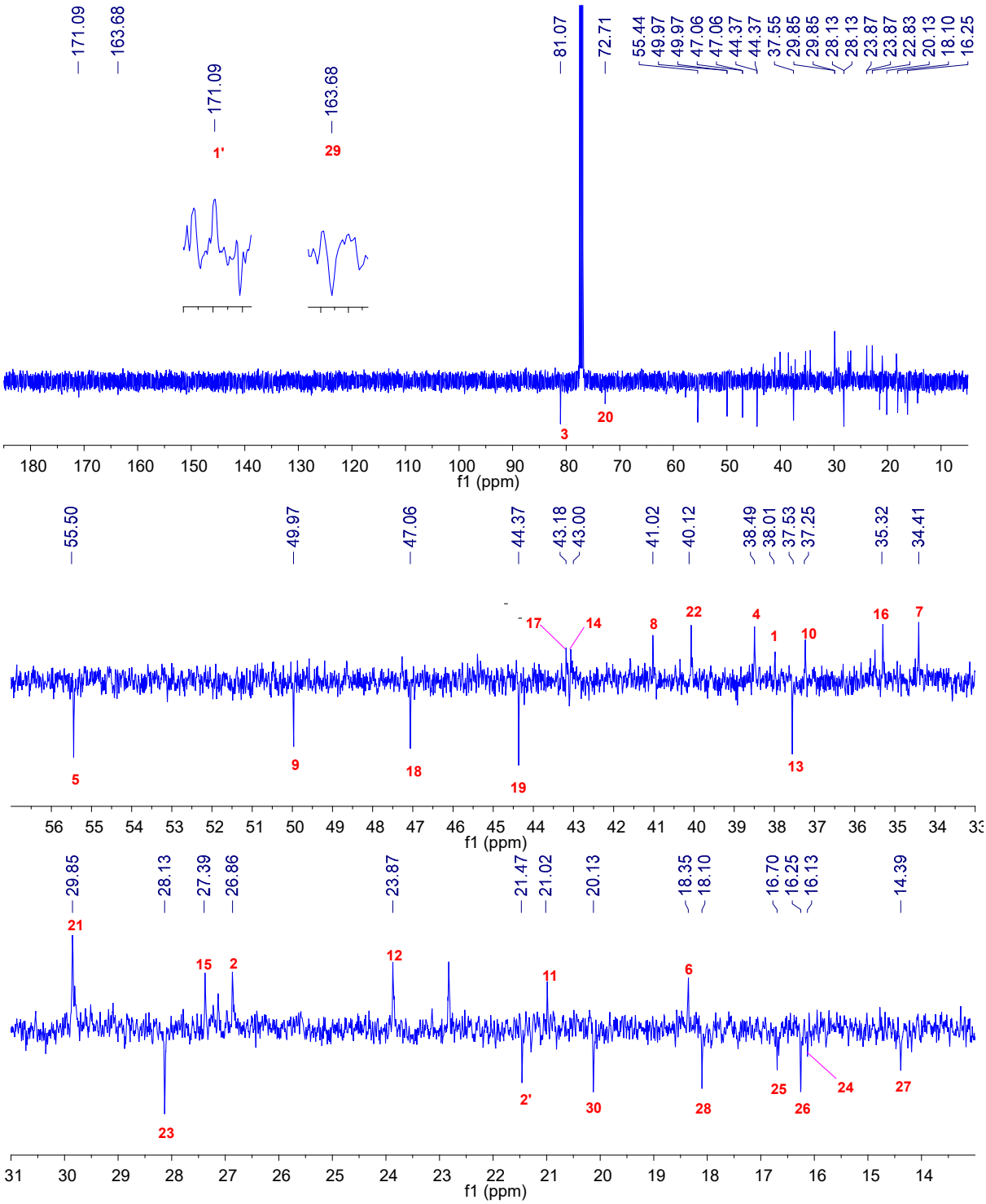


Figure S7. ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **2b.**

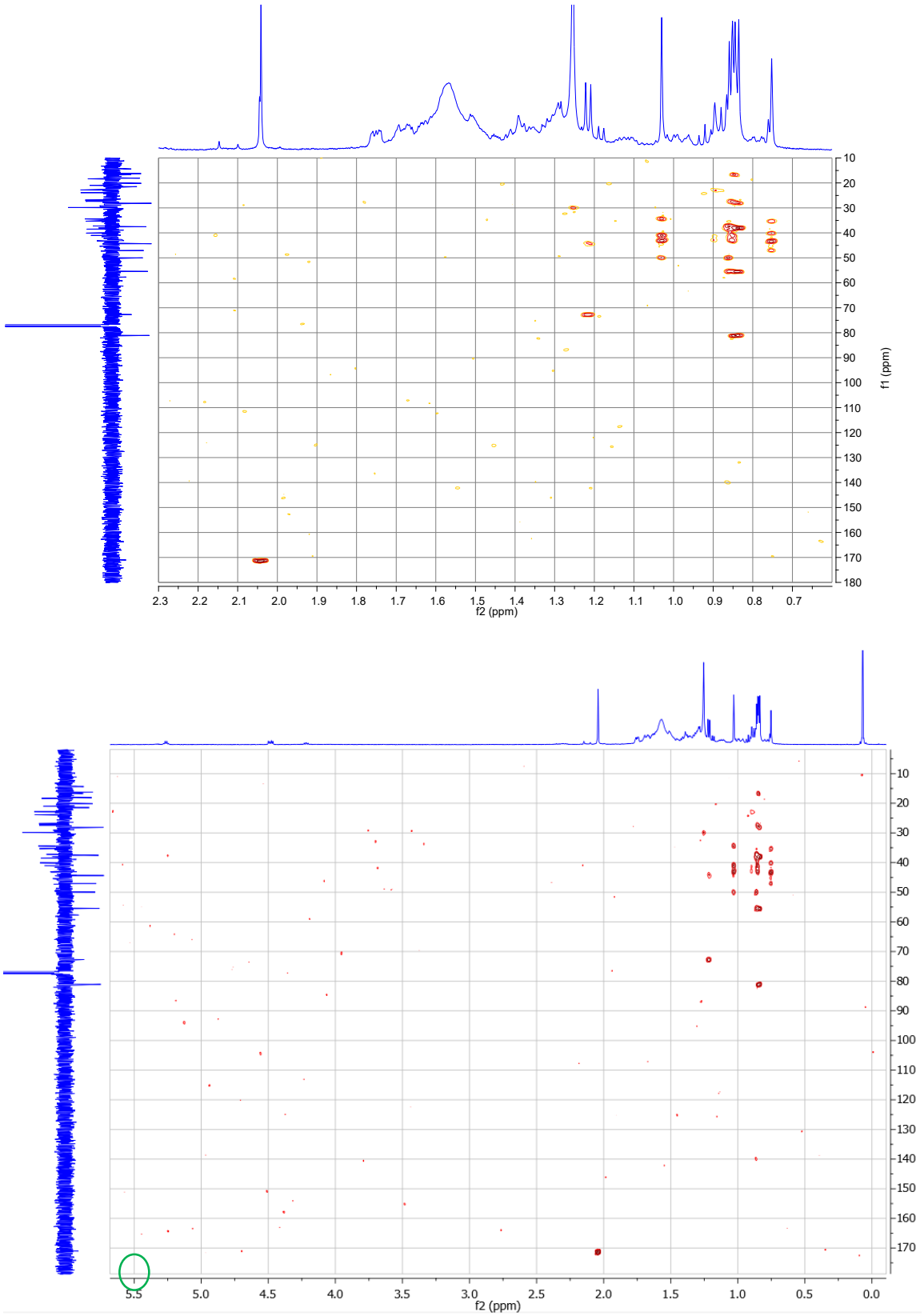


Figure S8. HMBC ($CDCl_3$) spectrum of **2b**.

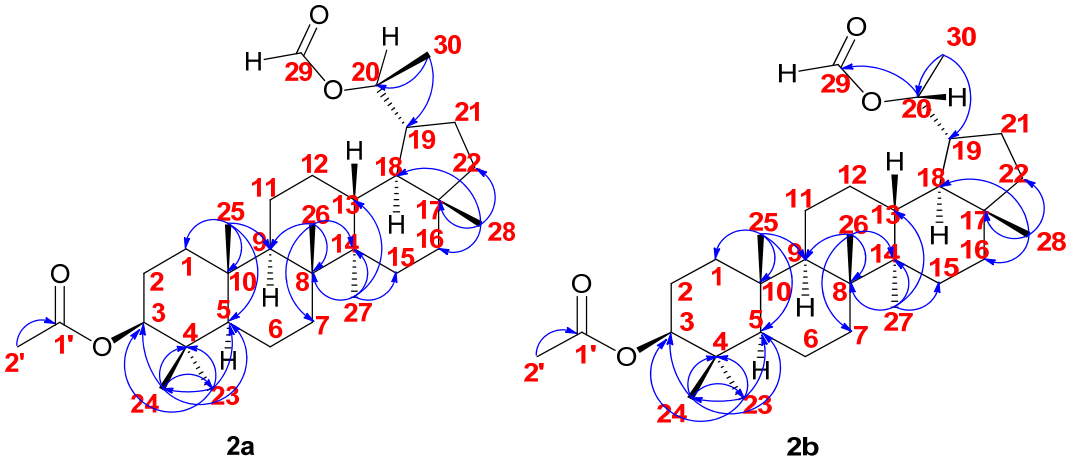


Figure S9. HMBC correlations of **2a** and **2b**.

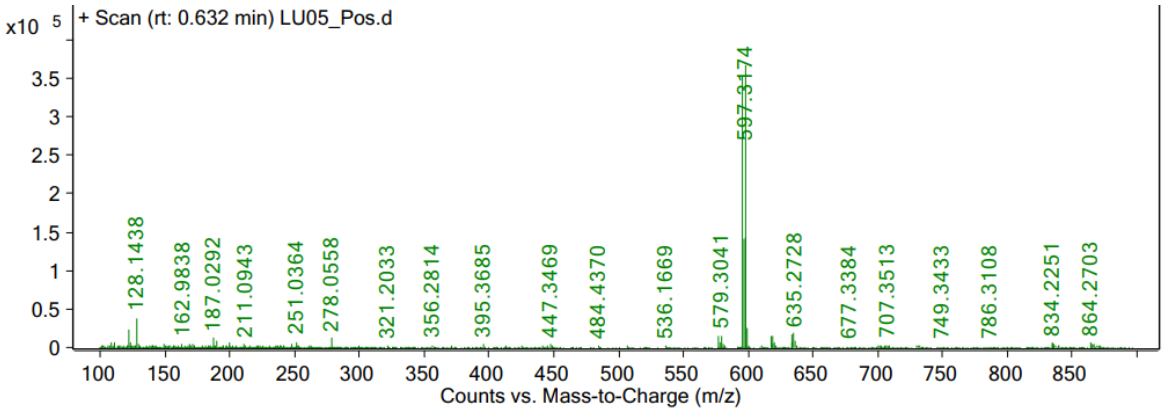


Figure S10. HRESIMS spectrum of **3**.

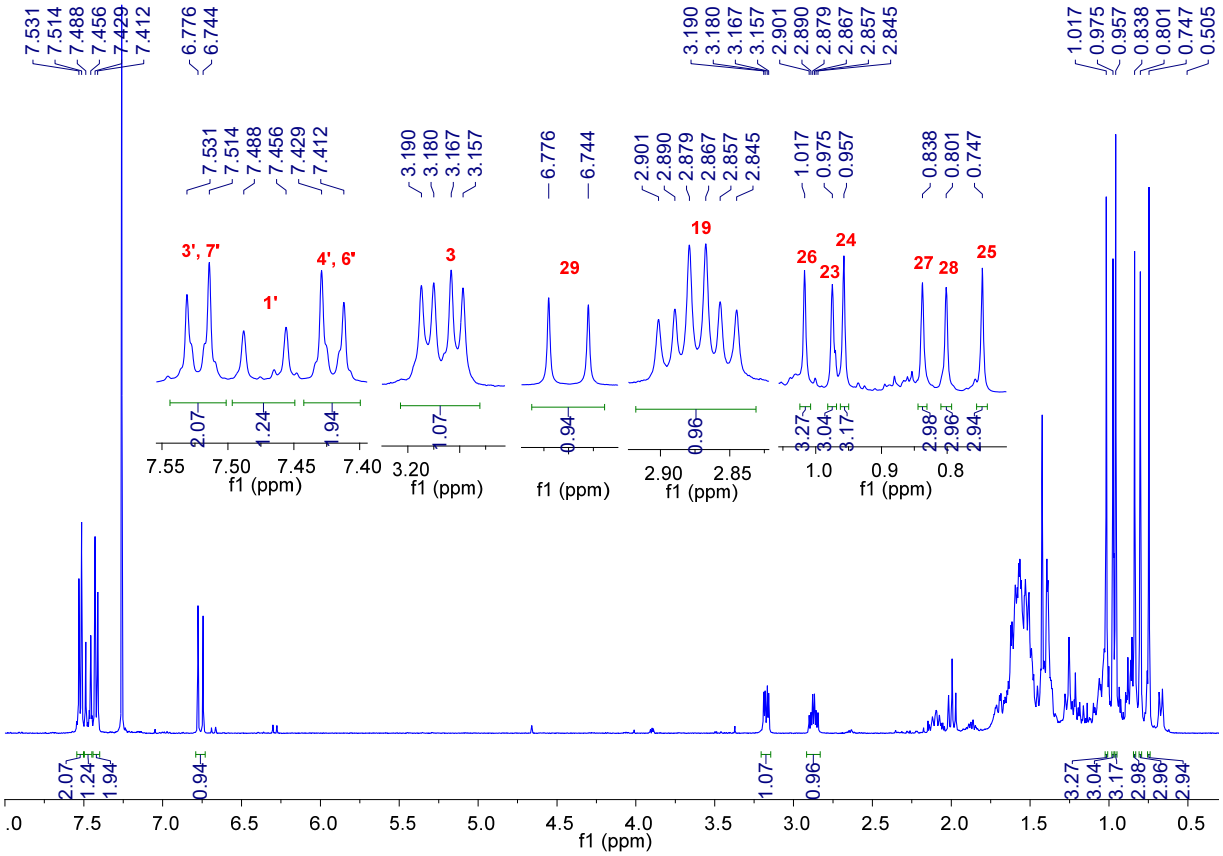


Figure S11. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **3**.

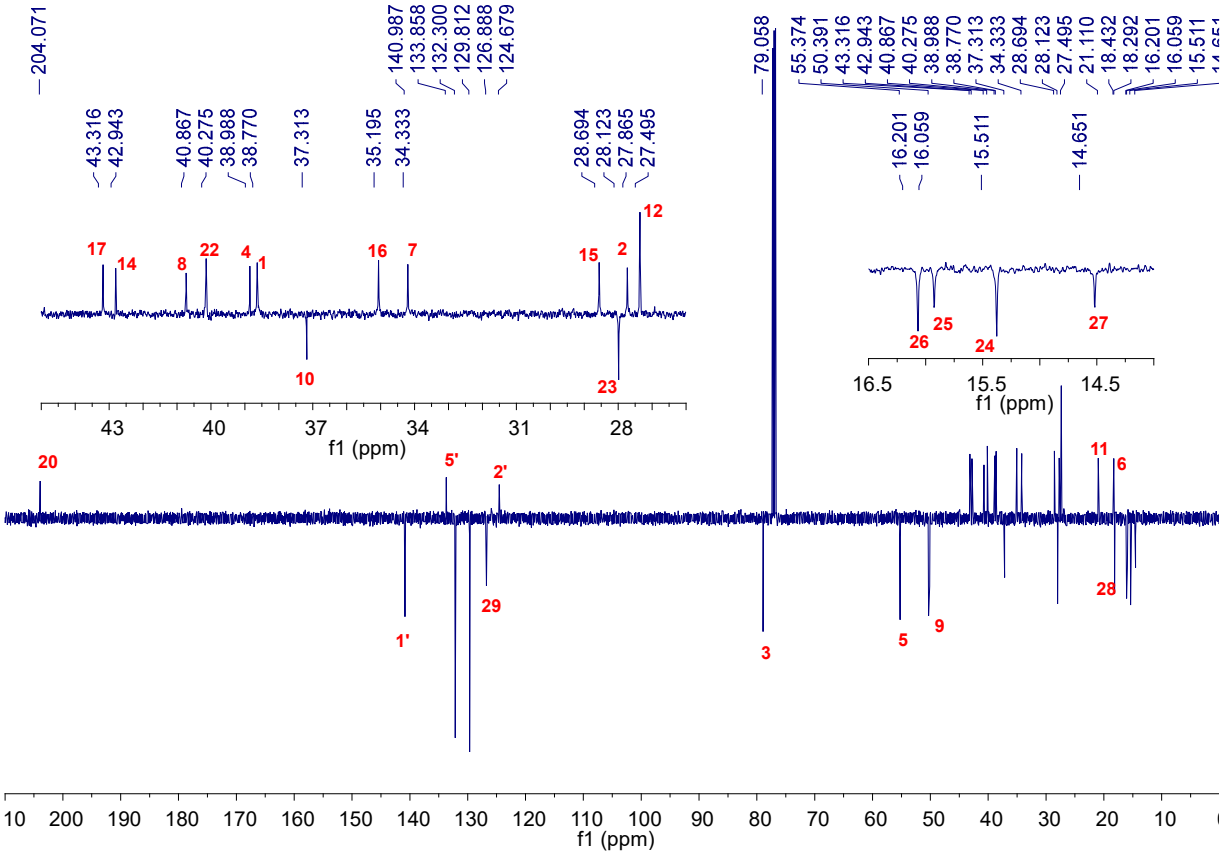
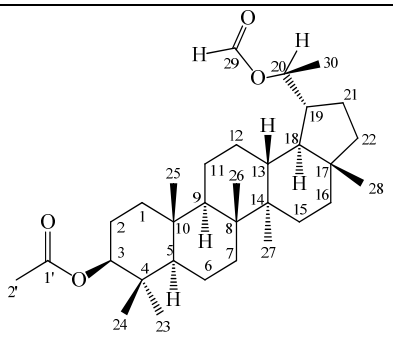
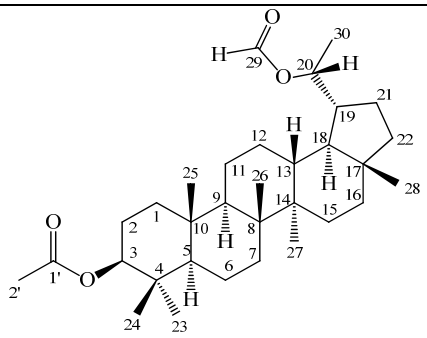


Figure S12. ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **3**.

Table S1. ^{1}H-NMR ($CDCl_3$) and ^{13}C-NMR ($CDCl_3$) data of **2a** and **2b.**

N	2a ($CDCl_3$)		2b ($CDCl_3$)	
	^{1}H-NMR δ_H	**^{13}C-NMR δ_C**	**^{1}H-NMR δ_H**	**^{13}C-NMR δ_C**
				
1	-	38.0	-	38.0
2	-	27.1	-	26.9
			4.48 (1H, *dd*, *J* = 11.5, 5.5 Hz)	
3	4.48 (1H, *dd*, *J* = 10.5, 6.0 Hz)	81.1		81.1
			0	
4	-	38.5	-	38.5
5	0.79 (1H, *d*, *J* = 9.5 Hz)	55.5	0.77 (1H, *d*, *J* = 2.0 Hz)	55.5
6	-	18.4	-	18.4
7	-	34.4	-	34.4
8	-	41.0	-	41.0
9	-	50.2	-	50.0
10	-	37.2	-	37.3
11	-	21.0	-	21.0
12	-	23.8	-	23.9
13	-	37.3	-	37.5
14	-	43.0	-	43.0
15	-	27.3	-	27.4
16	-	35.5	-	35.3
17	-	43.5	-	43.2
18	-	48.8	-	47.1
19	2.13 (1H, *m*)	42.6	2.31 (1H, *m*)	44.4
20	5.33 (1H, *m*)	73.4	5.26 (1H, *m*)	72.7
21	-	29.9	-	29.9
22	-	40.5	-	40.1
23	0.85 (3H, *s*)	28.1	0.85 (3H, *s*)	28.1
24	0.84 (3H, *s*)	16.1	0.84 (3H, *s*)	16.1
25	0.87 (3H, *s*)	16.7	0.86 (3H, *s*)	16.7
26	1.03 (3H, *s*)	16.3	1.03 (3H, *s*)	16.3
27	0.90 (3H, *s*)	14.4	0.85 (3H, *s*)	14.4
28	0.76 (3H, *s*)	18.1	0.75 (3H, *s*)	18.1
29	8.00 (1H, *s*)	161.6	8.11 (1H, *s*)	163.7
30	1.18 (3H, *d*, *J* = 6.5 Hz)	14.2	1.22 (3H, *d*, *J* = 6.5 Hz)	20.1
1′	-	171.2	-	171.1
2′	2.05 (3H, *s*)	21.5	2.04 (3H, *s*)	21.5