Supplementary data

Alpha-amylase and Alpha-glucosidase Enzyme Inhibition and Antioxidant Potential of 3-Oxolupenal and Katononic Acid Isolated from *Nuxia oppositifolia*

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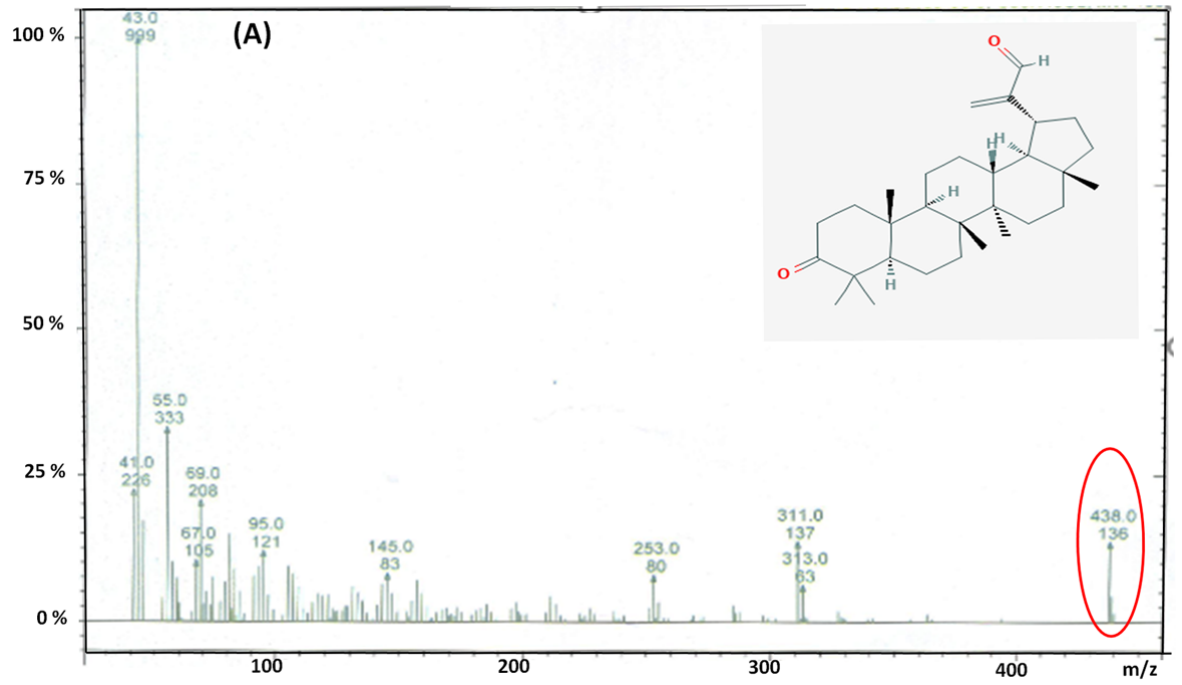


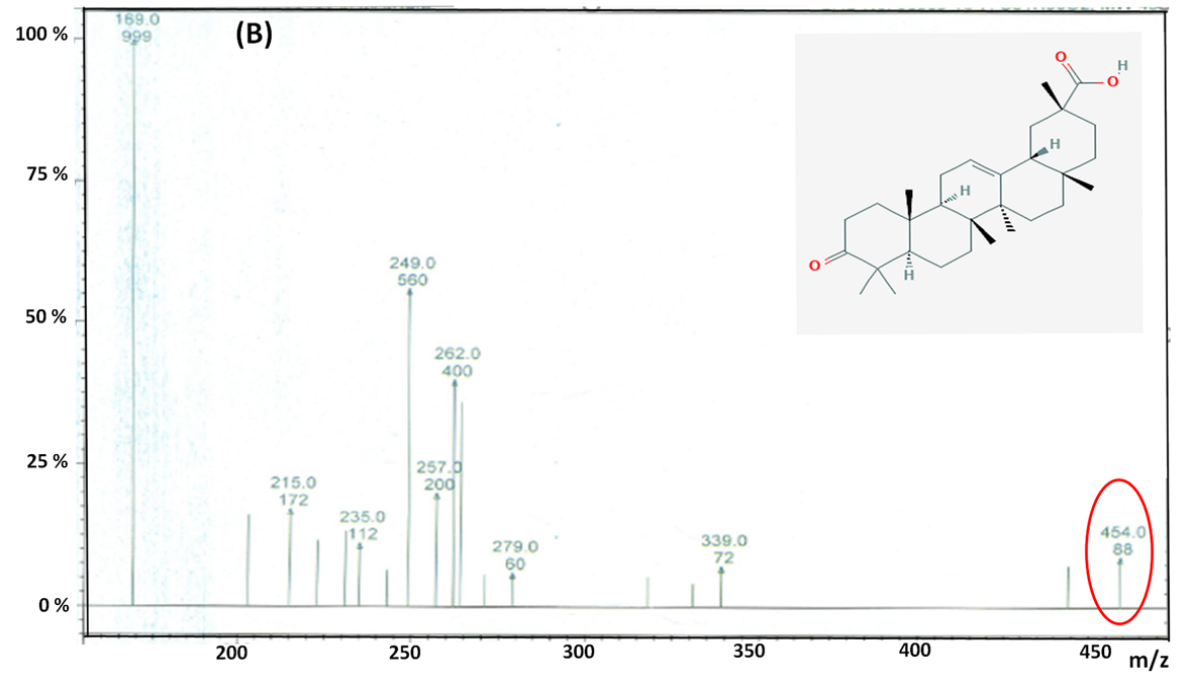
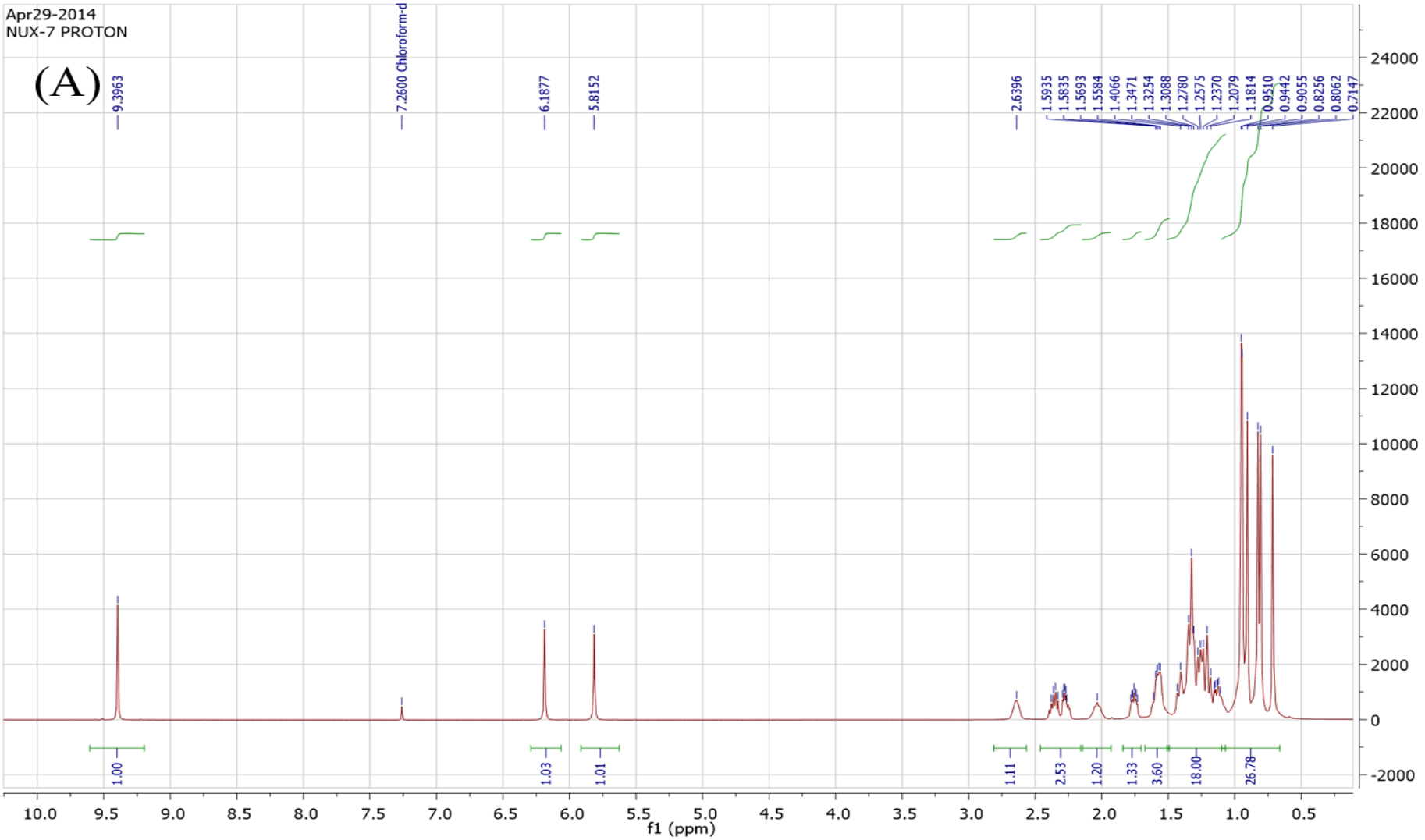
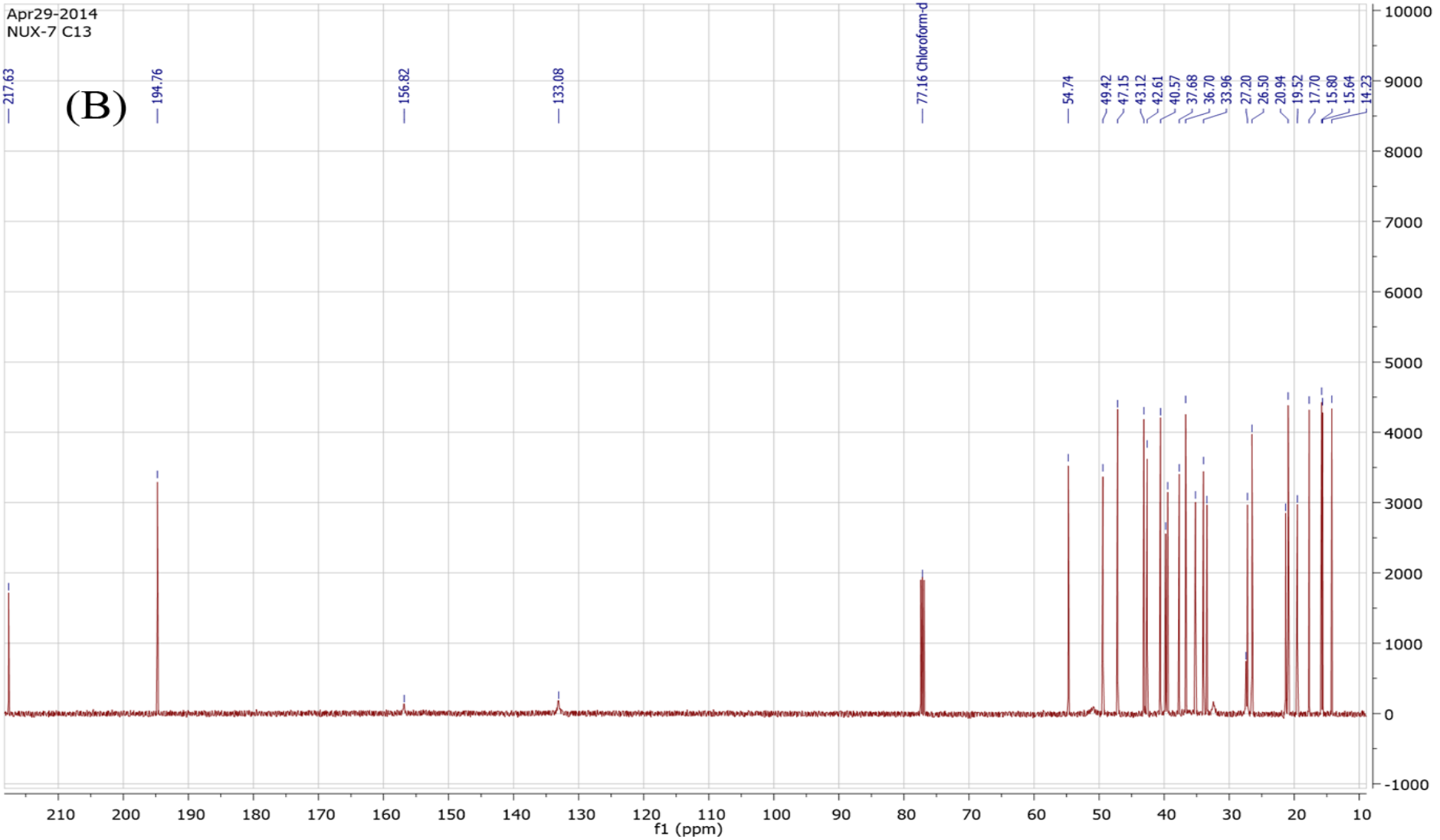


Figure S1. GC-MS analysis of (A) 3-oxolupenal (m/z = 438.0136 calculated for $C_{30}H_{46}O_2$, 438.3498), and (B) katononic acid (m/z 454.0880 calculated for $C_{30}H_{46}O_3$, 454.3603).


Apr29-2014
NUX-7 PROTON
(A)
9.3963
7.2600 Chloroform-d
6.1877
5.8152
2.6396
1.5935
1.5835
1.5693
1.5584
1.4066
1.3471
1.3254
1.3088
1.2780
1.2575
1.2370
1.2079
1.1814
0.9510
0.9442
0.9055
0.8256
0.8062
0.7147
1.00
1.03
1.01
1.11
2.53
1.20
1.33
3.60
18.00
26.78
f1 (ppm)

27


Apr29-2014
NUX-7 C13
(B)
217.63
194.76
156.82
133.08
77.16 Chloroform-d
54.74
49.42
47.15
43.12
42.61
40.57
37.68
36.70
33.96
27.20
26.50
20.94
19.52
17.70
15.80
15.64
14.23
f1 (ppm)

28

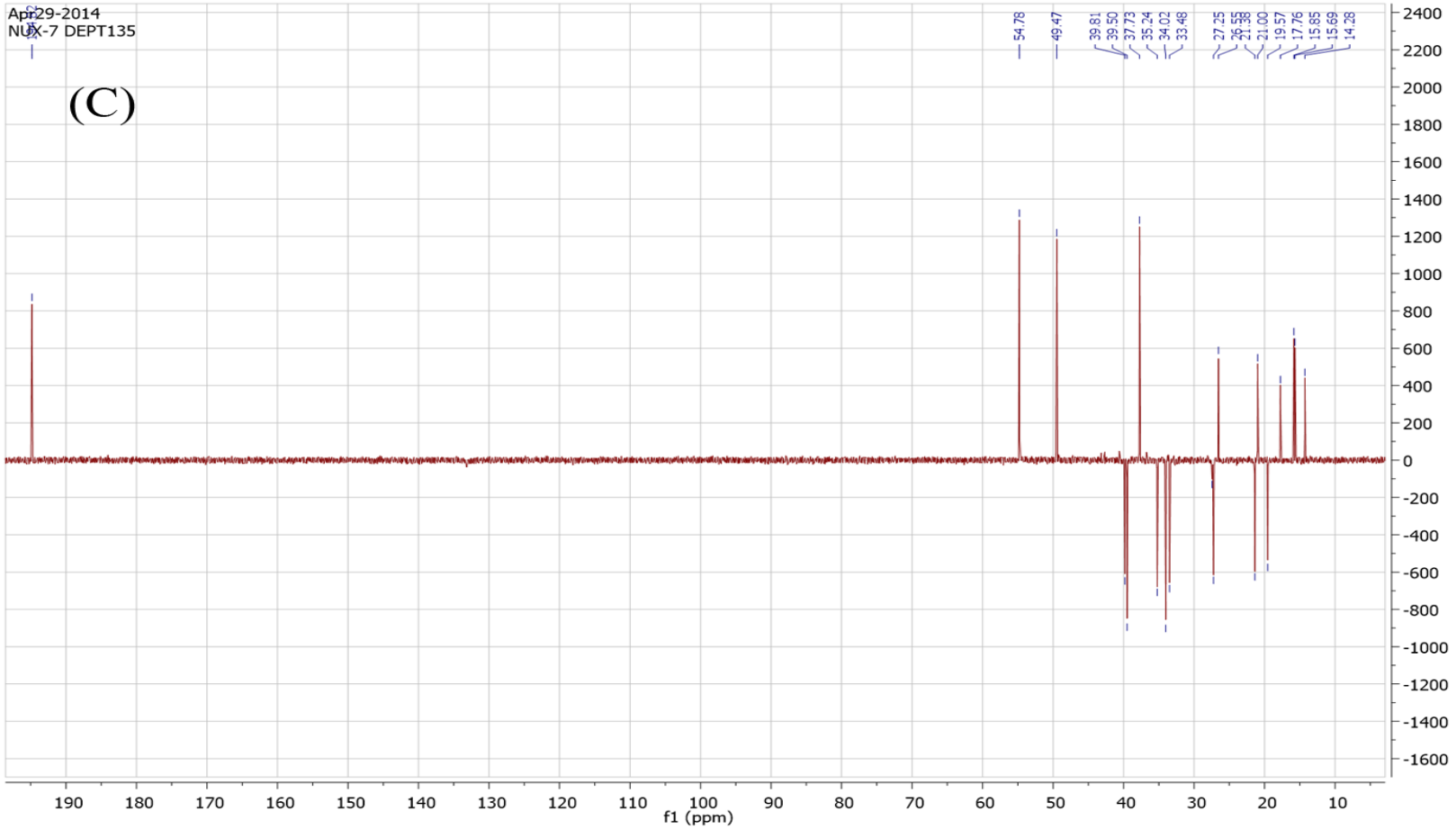
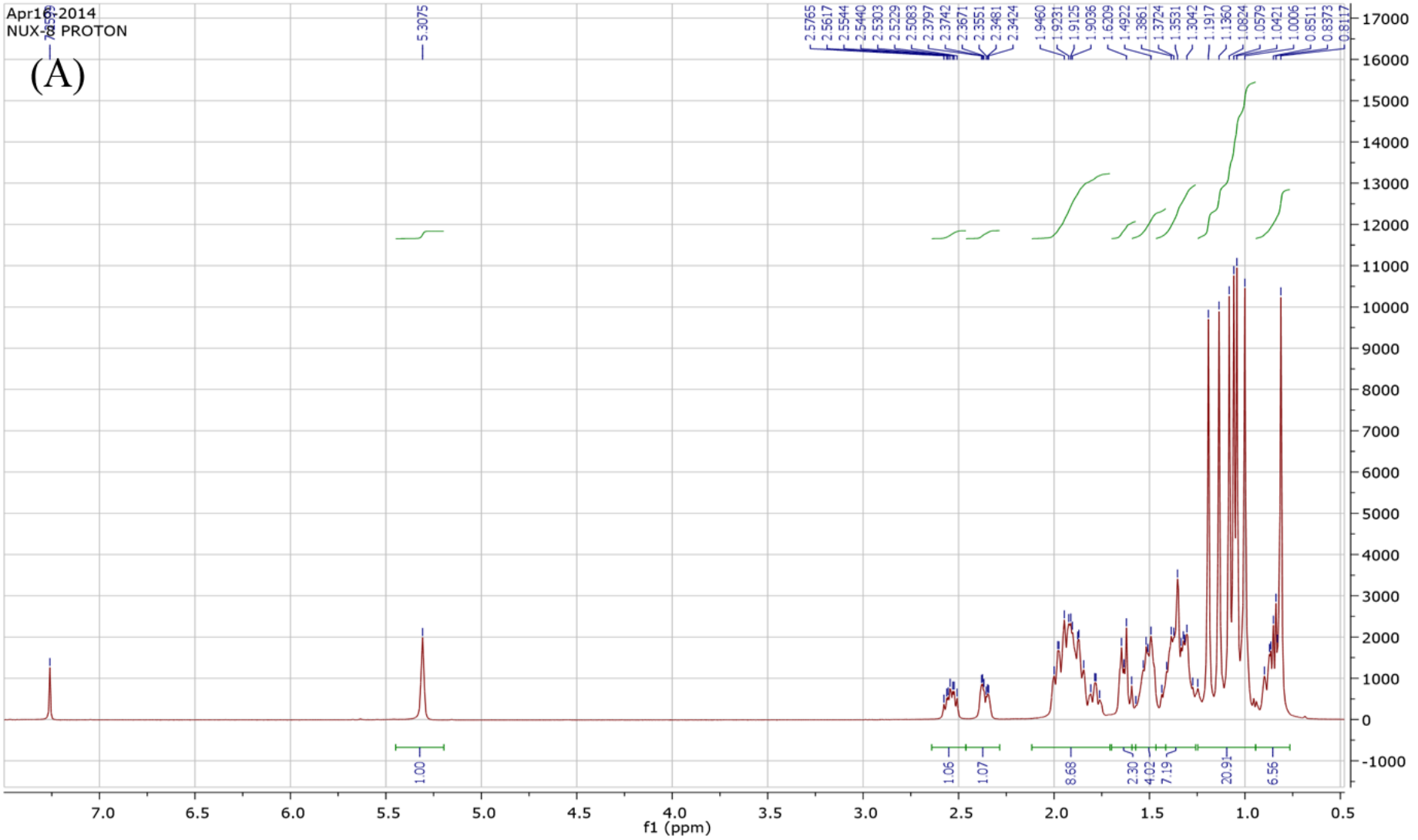


Figure S2. NMR spectra of 3-oxolupenal (A) ^{1}H, (B) ^{13}C, and (C) Depth. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 0.71 (s, Me-24), 0.80 (s, Me-28), 0.82 (s, Me-25), 0.90 (s, Me-27), 0.95 (s, Me-23), 1.18 (s, Me-26), 9.39 (s, H-30), 6.1,5.8 (s, H-29a.29b). ^{13}C-NMR($CDCl_3$, 125 MHz): δ 39.5(C-1), 34.0(C-2), 217.6(C-3), 47.2(C-4), 54.8(C-5), 19.6(C-6), 33.5(C-7), 40.6(C-8), 49.5(C-9), 36.7(C-10), 21.7(C-11), 27.5(C-12), 37.7(C-13), 42.7(C-14), 27.5(C-15), 35.2(C-16), 43.2(C-17), 51.0(C-18), 51.0(C-19), 157.2(C-20), 32.7(C-21), 39.8(C-22), 26.6(C-23), 21.0(C-24), 15.6(C-25), 16.0(C-26), 14.7(C-27), 17.8(C-28), 133.2(C-29), 194.8(C-30).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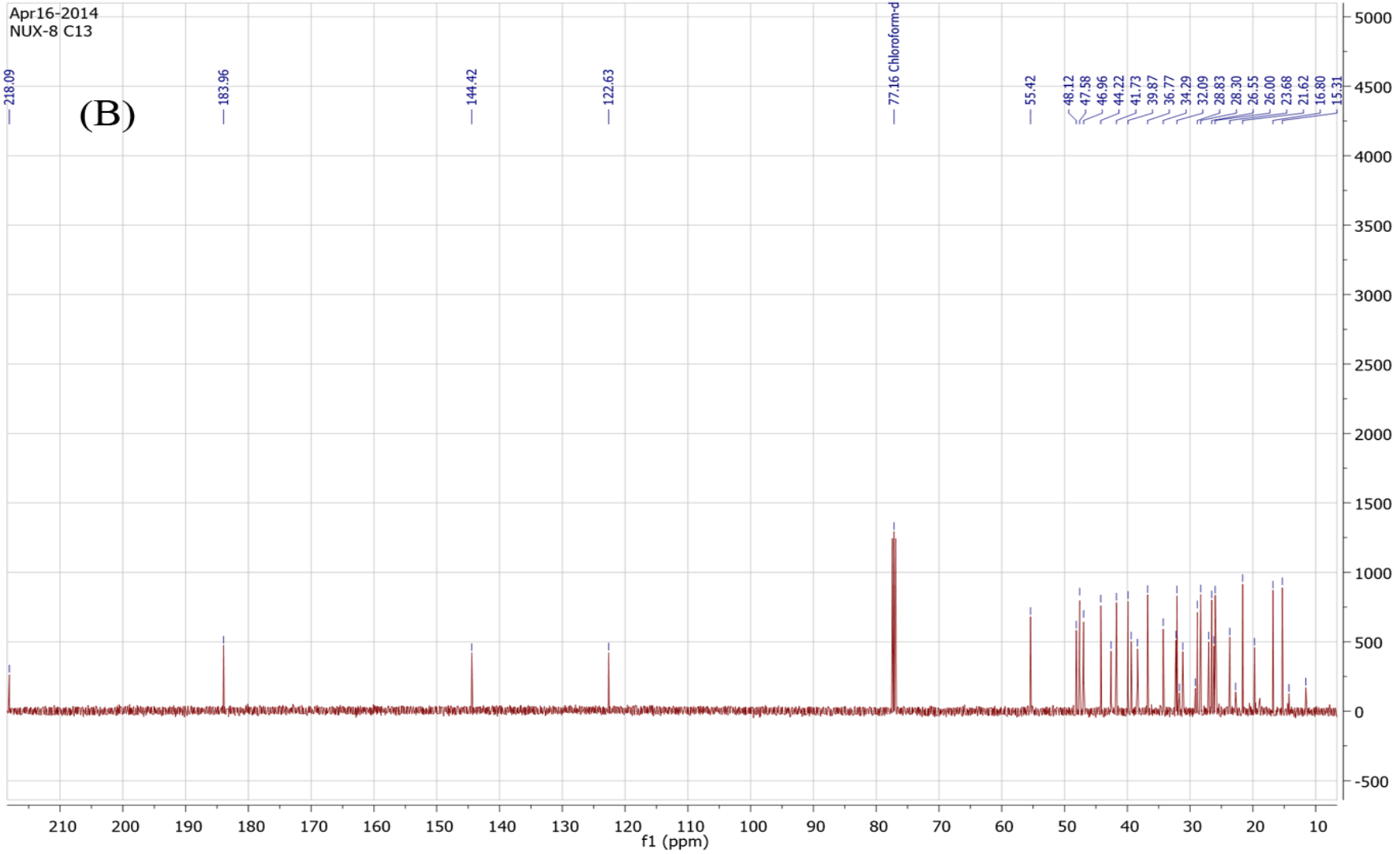
NUX-8 PROTON
(A)
7.2599
5.3075
2.5765
2.5617
2.5544
2.5440
2.5303
2.5229
2.5083
2.3797
2.3742
2.3671
2.3551
2.3481
2.3424
1.9460
1.9231
1.9125
1.9036
1.6209
1.4922
1.3861
1.3724
1.3531
1.3042
1.1917
1.1360
1.0824
1.0579
1.0421
1.0006
0.8511
0.8373
0.8117
1.00
1.06
1.07
8.68
2.30
4.02
7.19
20.91
6.56
f1 (ppm)

35


Apr16-2014
NUX-8 C13
(B)
218.09
183.96
144.42
122.63
77.16 Chloroform-d
55.42
48.12
47.58
46.96
44.22
41.73
39.87
36.77
34.29
32.09
28.83
28.30
26.55
26.00
23.68
21.62
16.80
15.31
f1 (ppm)

36

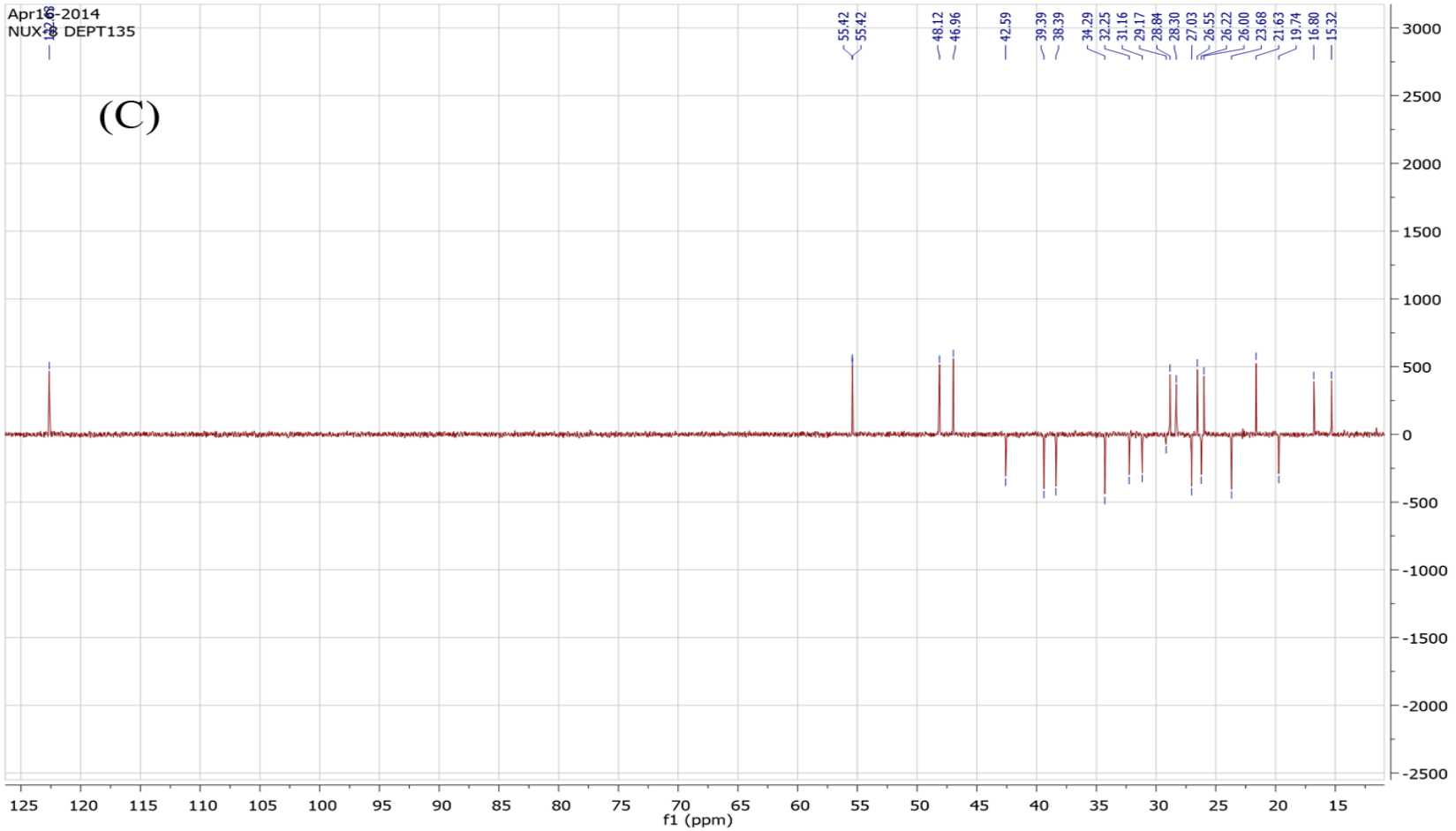
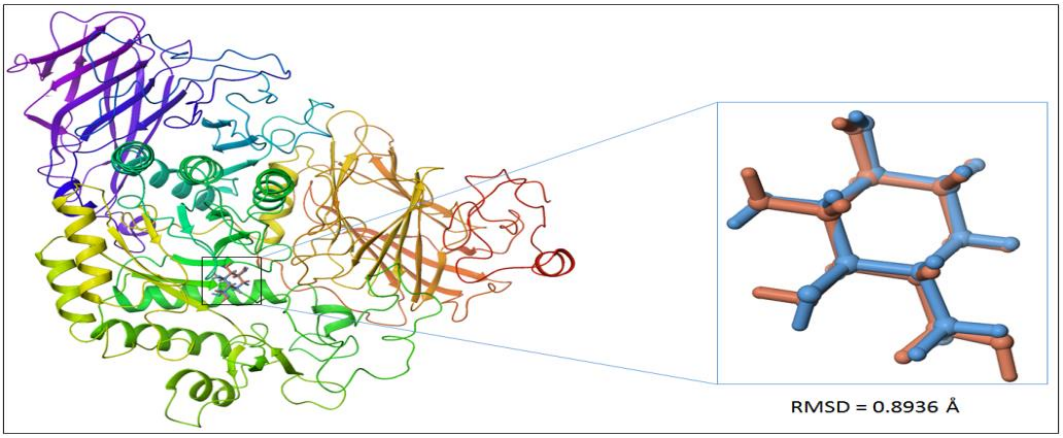
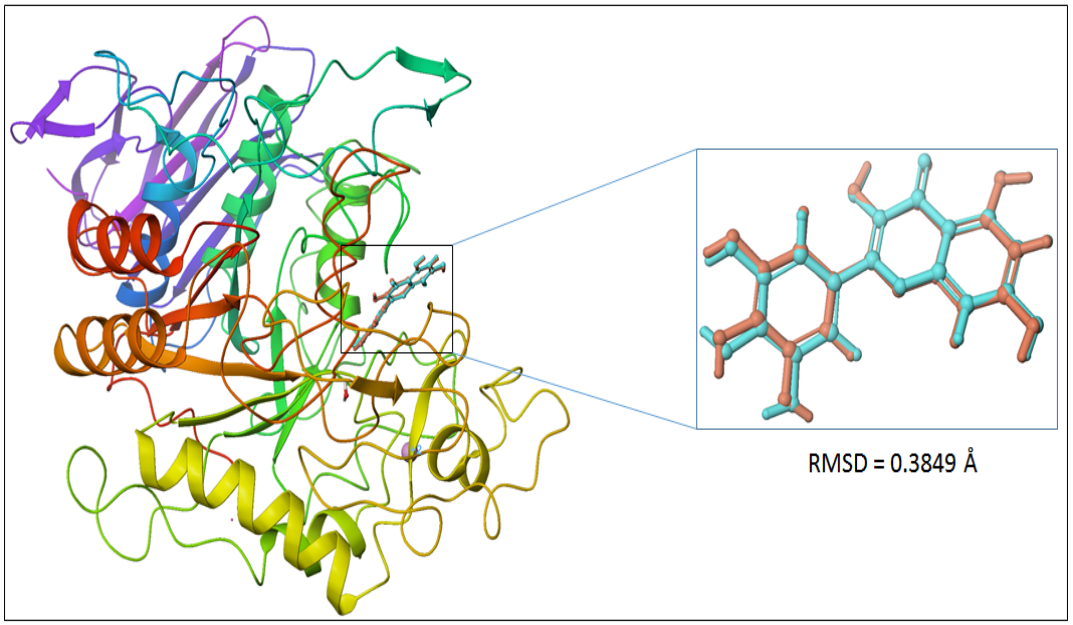


Figure S3. NMR spectra of katononic acid (A) ^{1}H, (B) ^{13}C, and (C) Depth. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 0.81 (s, Me-24), 0.83 (s, Me-28), 0.85 (s, Me-25), 1.00 (s, Me-27), 1.04 (s, Me-23), 1.13 (s, Me-26), 1.19 (s H-29), 5.30 (s, H-12). ^{13}C-NMR ($CDCl_3$, 125 MHz): δ 39.3(C-1), 34.2(C-2), 217.6(C-3), 47.5(C-4), 55.3(C-5), 19.6(C-6), 32.2(C- 7), 39.7(C-8), 48.0(C-9), 36.7(C-10), 23.6(C-11), 122.5(C-12), 144.3(C-13), 41.6(C-14), 26.1(C-15), 26.9(C-16), 32.0(C-17), 47.0(C-18), 42.5(C-19), 44.1(C-20), 31.1(C-21), 38.3(C-22), 26.4(C-23), 21.5(C-24), 15.2(C-25), 16.7(C-26), 25.9(C-27), 28.2(C-28), 28.7(C-29), 183.9(C-30).



(A)



(B)

Figure S4. Validation of molecular docking protocol by re-docking (A) myricetin at the active site of α-amylase, and (B) 1-deoxynojirimycin at the active site of α-glucosidase.