Bruceine A exerts antitumor effect against colon cancer by accumulating ROS and suppressing PI3K/Akt pathway

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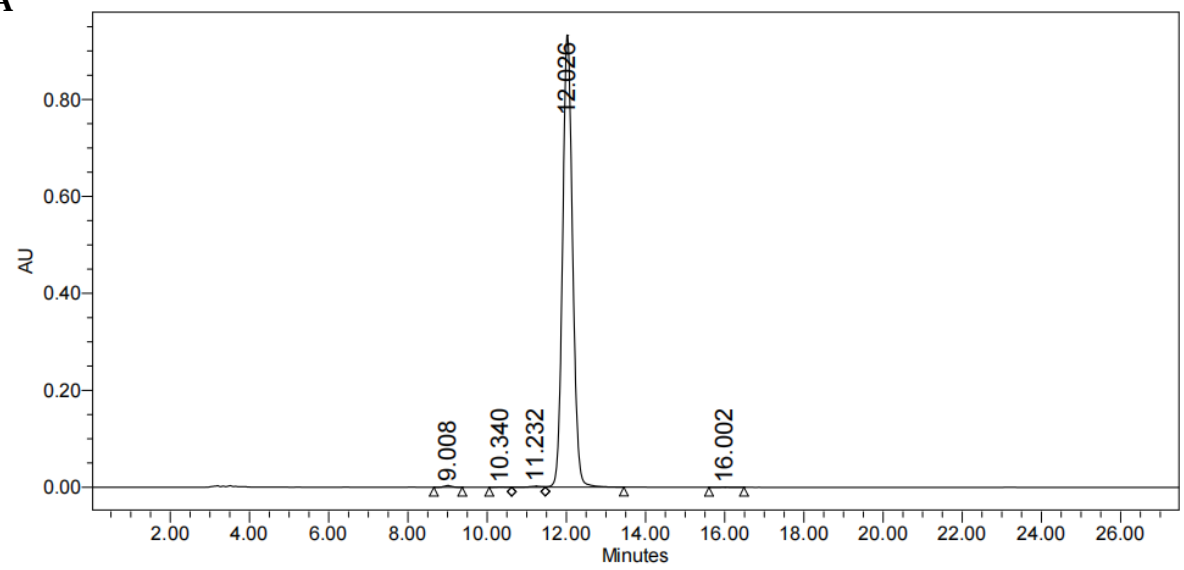
A



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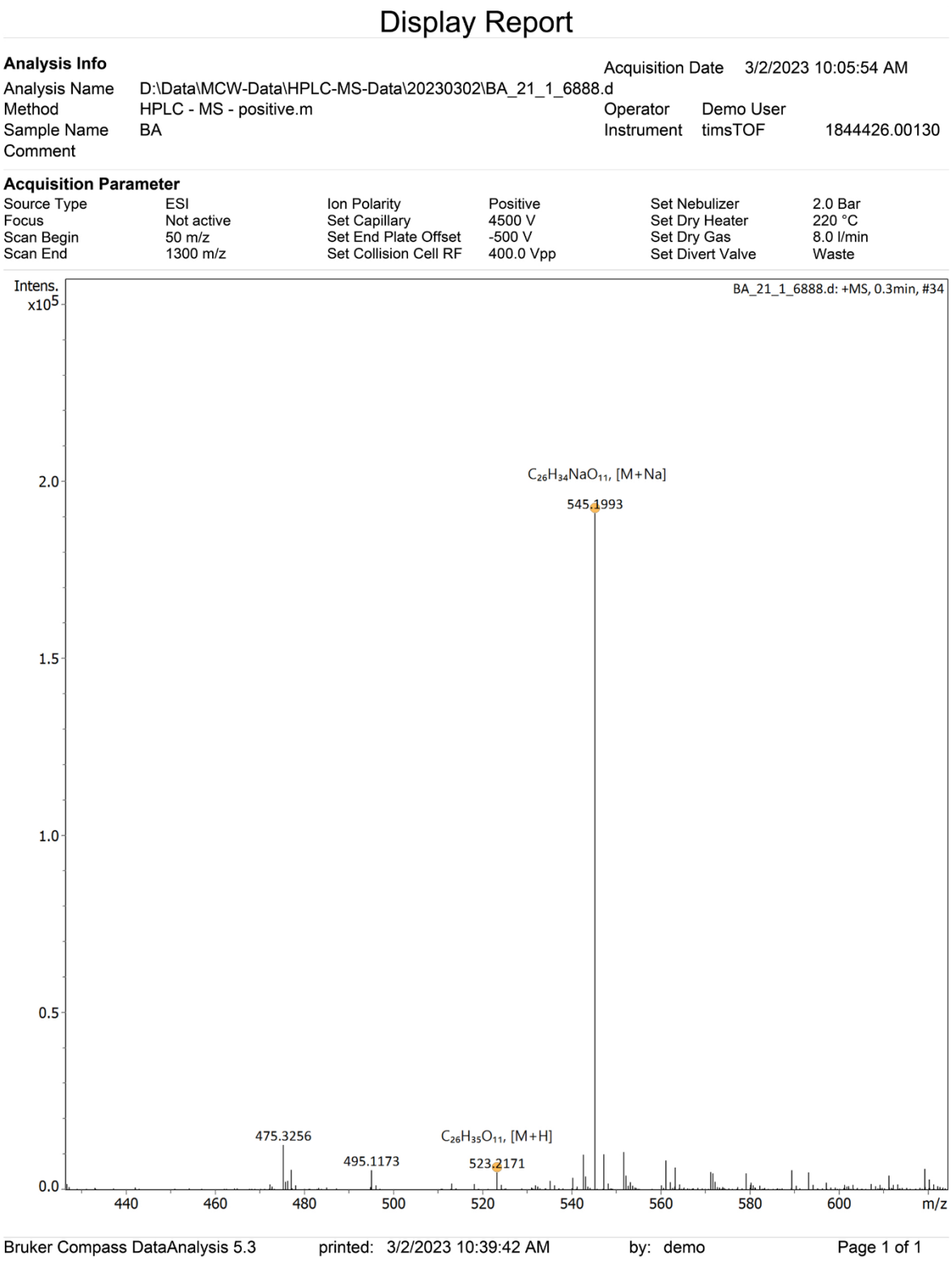
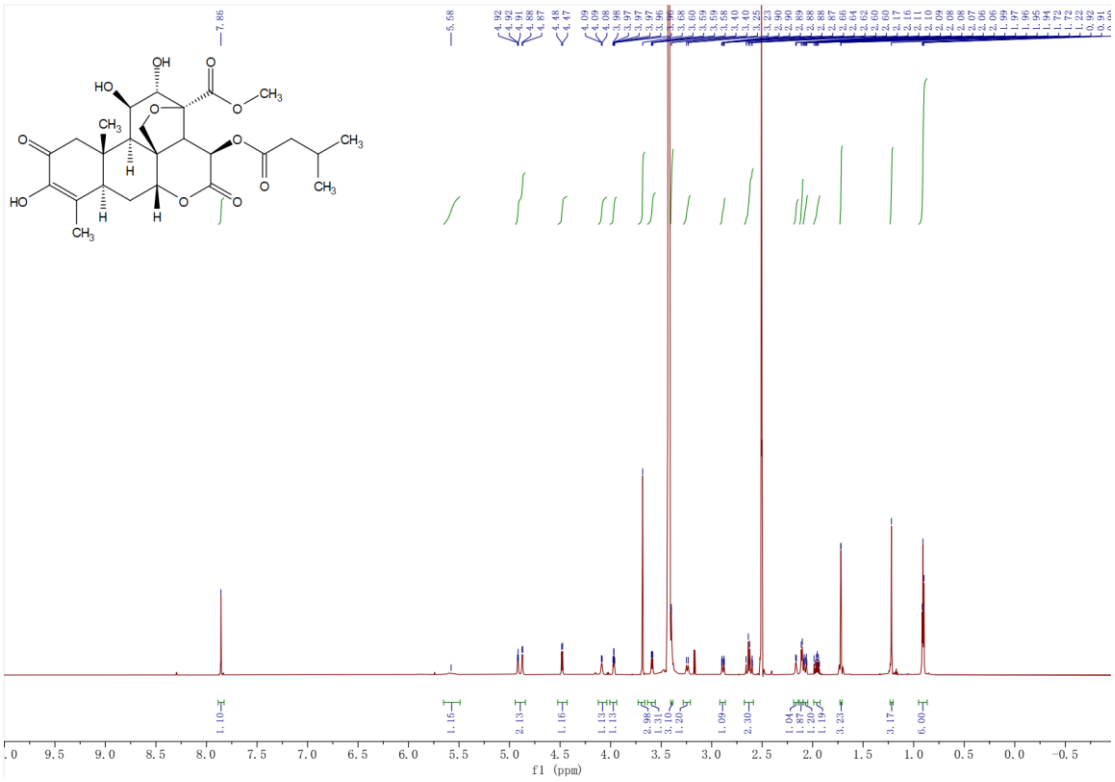
1	9.008	46813	0.28	3448
2	10.340	11434	0.07	698
3	11.232	44928	0.27	1918
4	12.026	16350449	99.32	934296
5	16.002	8704	0.05	393

B



SI Figure 1 HPLC（**A**） and HRMS（**B**） spectra of BA.

A



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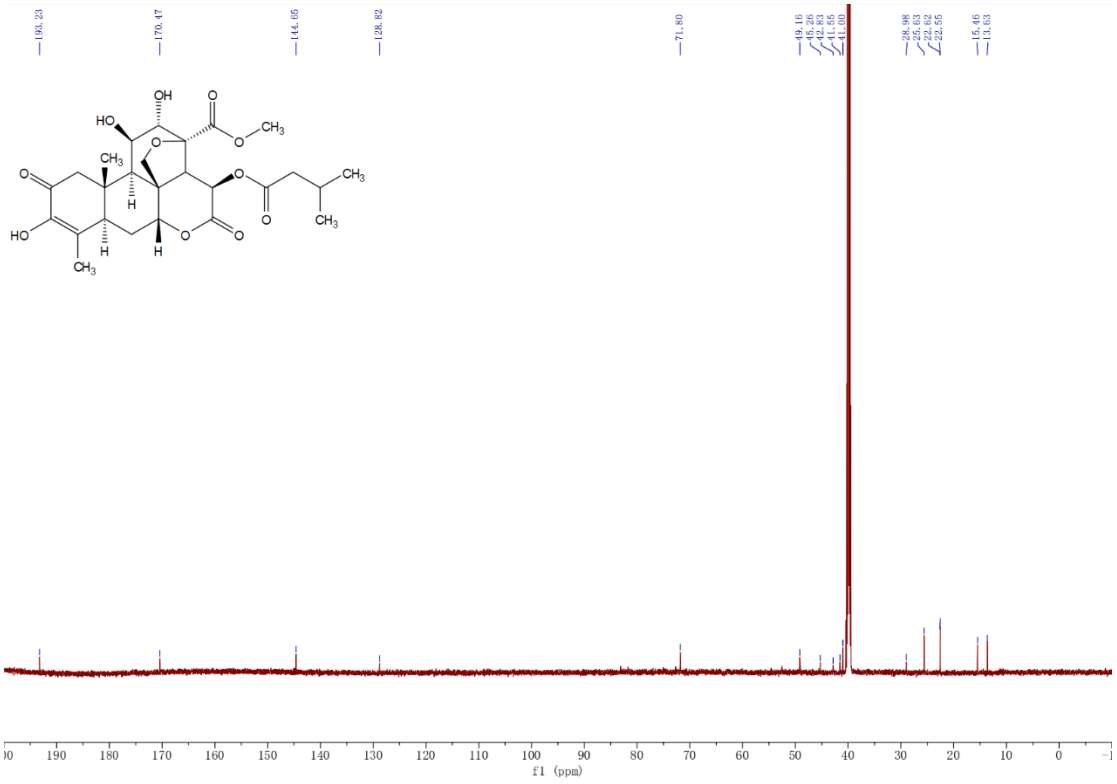

SI Figure 2 ^{1}H-NMR and ^{13}C-NMR spectra of Bruceine A. **（A） ^{1}H NMR (700 MHz, DMSO-*d*$_6$)** δ 7.86 (s, 1H, 3-OH), 5.58 (s, 1H, H-15), 4.95 – 4.84 (m, 2H, H-7, H-20a), 4.48 (d, *J* = 7.3 Hz, 1H, H-11), 4.12 – 4.04 (m, 1H, H-20b), 3.97 (td, *J* = 4.9, 1.6 Hz, 1H, H-12), 3.68 (s, 3H, 22-OMe), 3.59 (dd, *J* = 7.4, 1.7 Hz, 1H, 11-OH), 3.40 (m, 2H, H-9, H-14,), 3.24 (d, *J* = 13.0 Hz, 1H, H-1b), 2.89 (dt, *J* = 13.2, 2.3 Hz, 1H, H-1a), 2.68 – 2.59 (m, 2H, H-5, H-2'b), 2.16 (d, *J* = 4.9 Hz, 1H, 12-OH), 2.11 (d, *J* = 7.3 Hz, 2H, H-2'a, H-3'), 2.07 (dt, *J* = 14.8, 3.0 Hz, 1H, H-6b), 1.99 – 1.93 (m, 1H, H-6a), 1.72 (d, *J* = 1.9 Hz, 3H, 18-Me), 1.22 (s, 3H, 19-Me), 0.91 (t, *J* = 6.1 Hz, 6H, 4'/5'-Me). **（B） ^{13}C NMR (176 MHz, DMSO-*d6*)** δ 193.23 (C-2), 170.47 (C-16, C-21, C-1'), 144.65 (C-3), 128.82(C-4), 82.90(C-7), 80.76(C-13), 71.8(C-11, C-20), 49.16(C-22, C-14), 45.26(C-9), 42.83(C-2'), 41.55(C-5), 41.00(C-10), 28.98(C-6), 25.63(C-3'), 22.62(C-5'), 22.55(C-4'), 15.46(C-19), 13.63(C-18). Based on the above data, The compound was identified as bruceine A, which was consistent with the reported litera ture values.