

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

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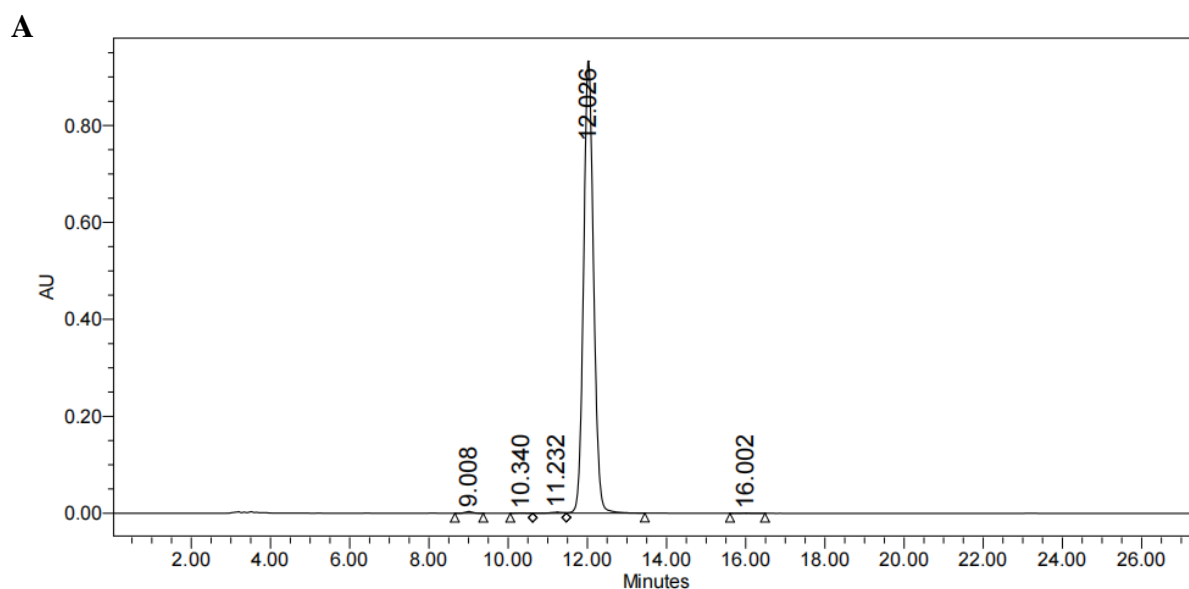
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| | RT | Area | % Area | Height |
|---|--------|----------|--------|--------|
| 1 | 9.008 | 46813 | 0.28 | 3448 |
| 2 | 10.340 | 11434 | 0.07 | 698 |
| 3 | 11.232 | 44928 | 0.27 | 1918 |
| 4 | 12.026 | 16350449 | 99.32 | 934296 |
| 5 | 16.002 | 8704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

B

Display Report

Analysis Info

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Method HPLC - MS - positive.m
Sample Name BA
Comment

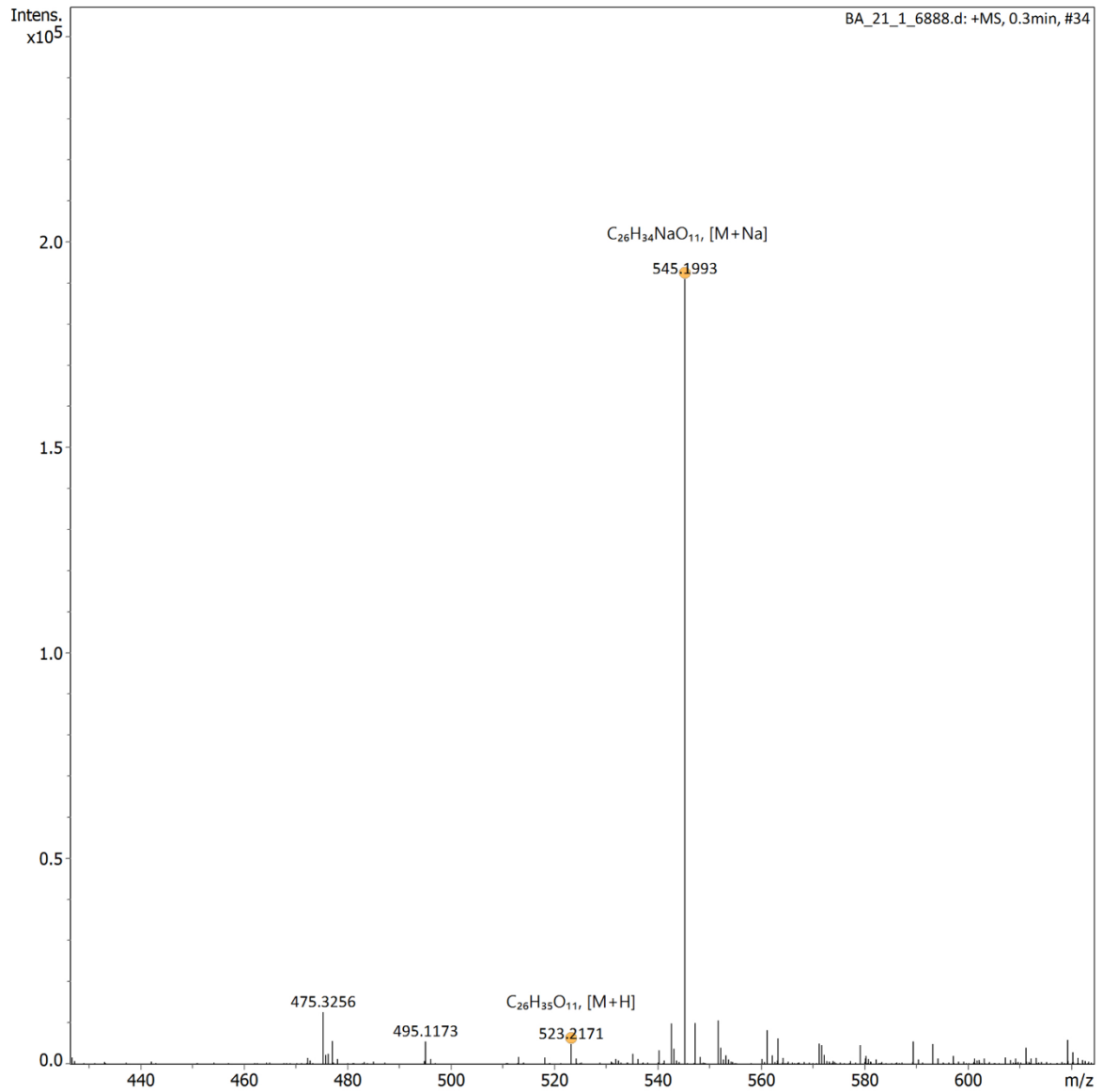
Acquisition Date 3/2/2023 10:05:54 AM

Operator Demo User

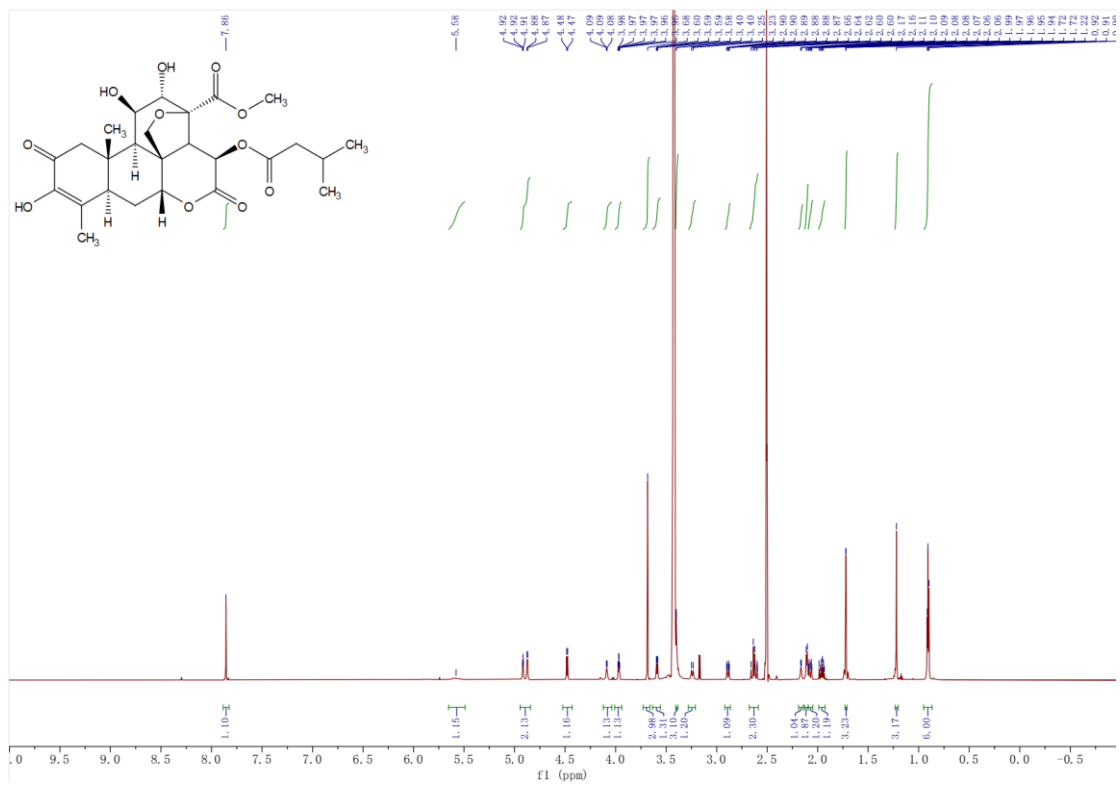
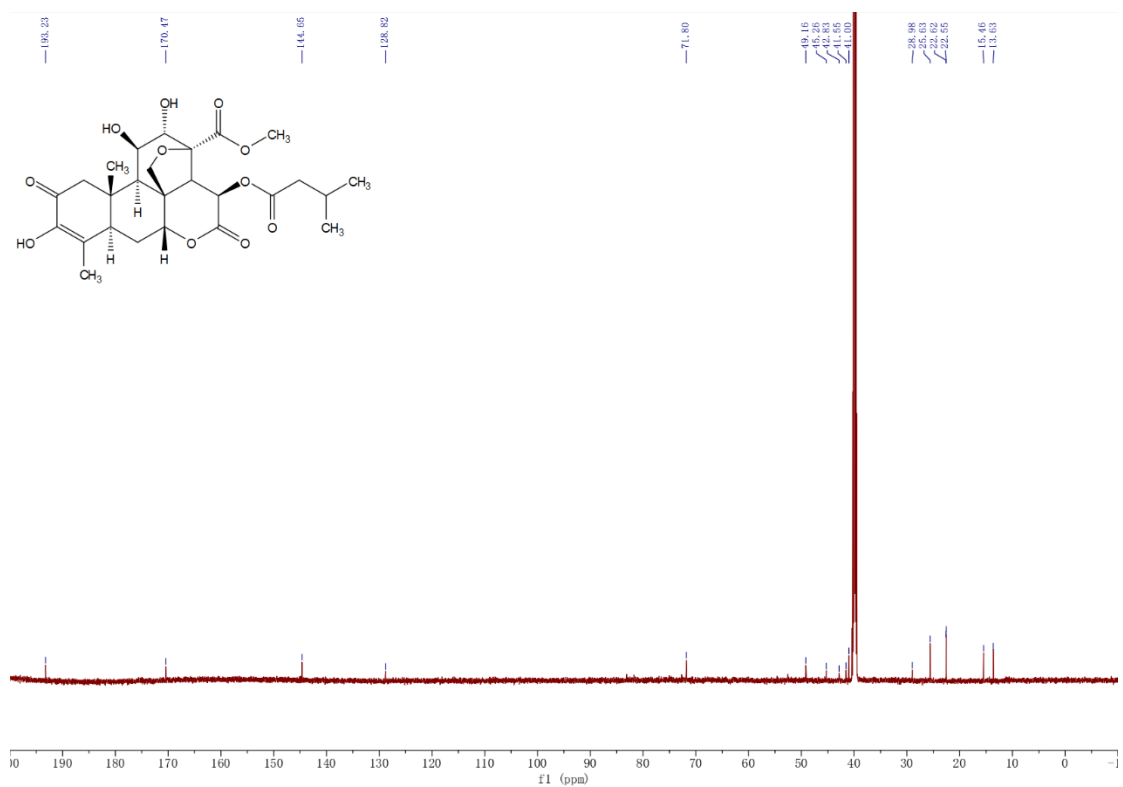
Instrument timsTOF 1844426.00130

Acquisition Parameter

| | | | | | |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 220 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 8.0 l/min |
| Scan End | 1300 m/z | Set Collision Cell RF | 400.0 Vpp | Set Divert Valve | Waste |



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

A**B**

SI Figure 2 ^1H -NMR and ^{13}C -NMR spectra of Bruceine A. (A) ^1H 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-*d*₆) 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 literature values.