

Figure S1. Chromatogram for CA purity determination (the main peak is CA). CA, 6'-O-Caffeoylarbutin.

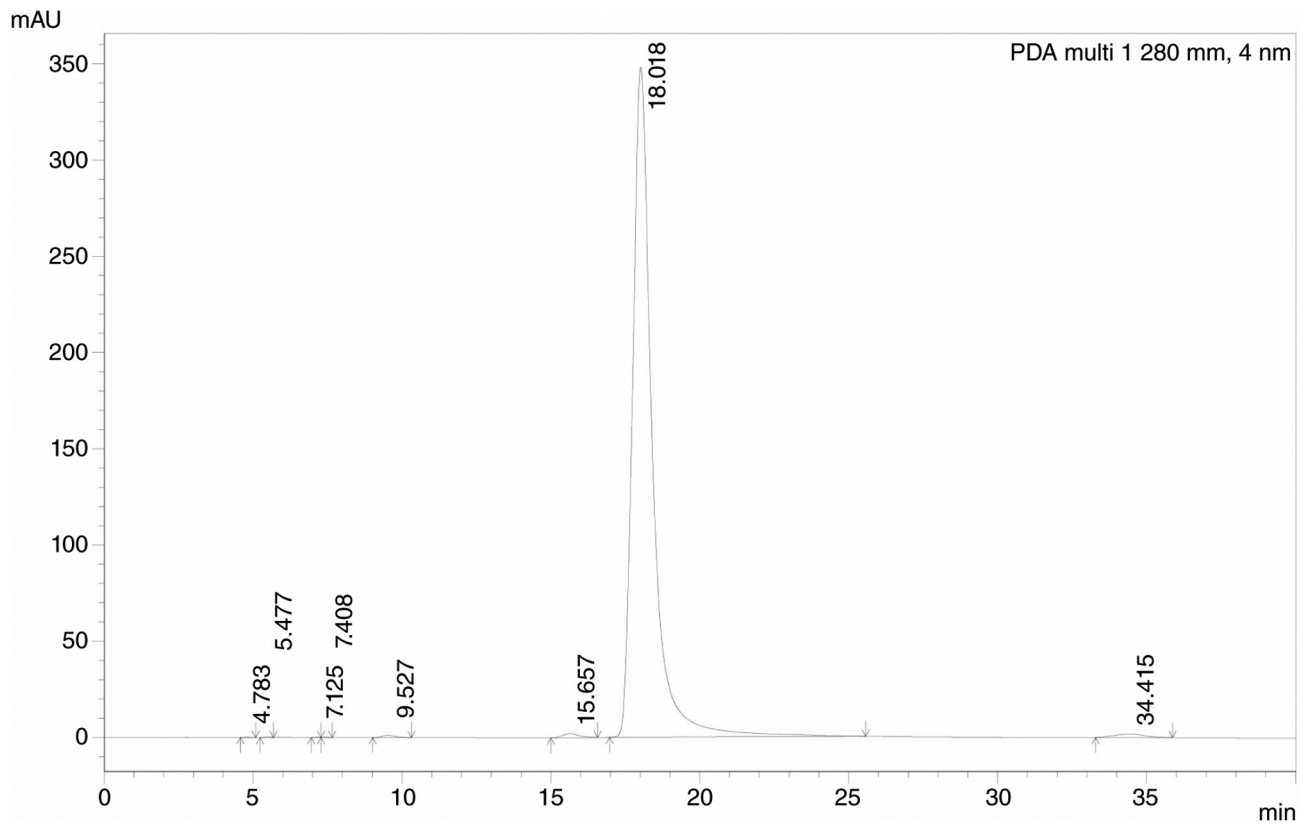


Figure S2. NMR hydrogen spectrum (^1H) of CA. The main signal peaks are distributed in the range of δ .30-7.56, with a strong peak near δ 3.45. The aromatic hydrogen signal peaks are located at δ 6.50-7.50. The green curves represent solvent/impurity peaks. NMR, nuclear magnetic resonance; CA, 6'-O-Caffeoylarbutin.

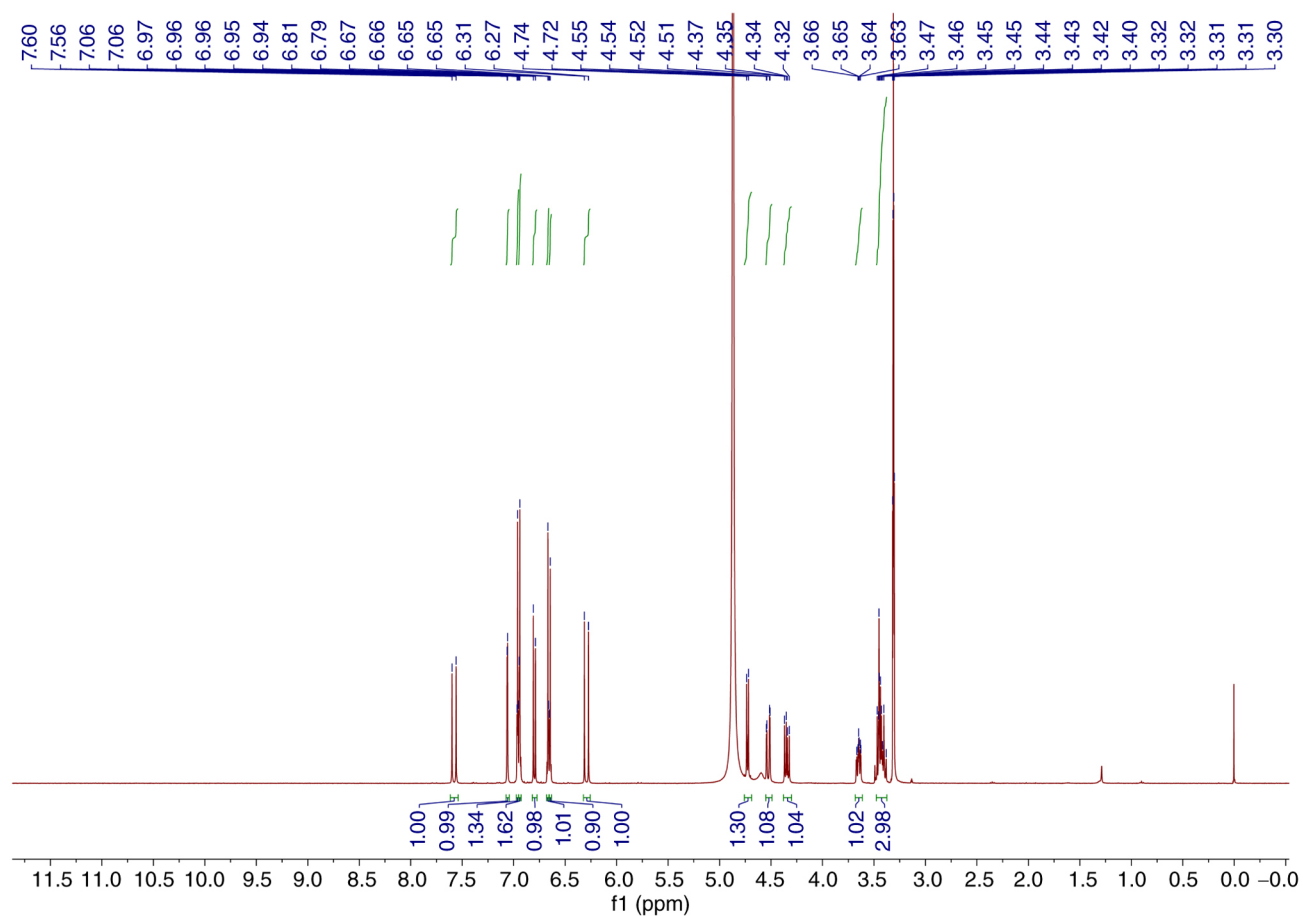


Figure S3. NMR carbon spectrum (^{13}C) of CA. The main signal peaks are distributed in the range of δ 64.7-169.0, with the peak near δ 50 being the solvent peak, and the signal peaks in the range of δ 64.7-169.0 corresponding to carbon atoms in different chemical environments in the molecule. NMR, nuclear magnetic resonance; CA, 6'-O-Caffeoylarbutin.

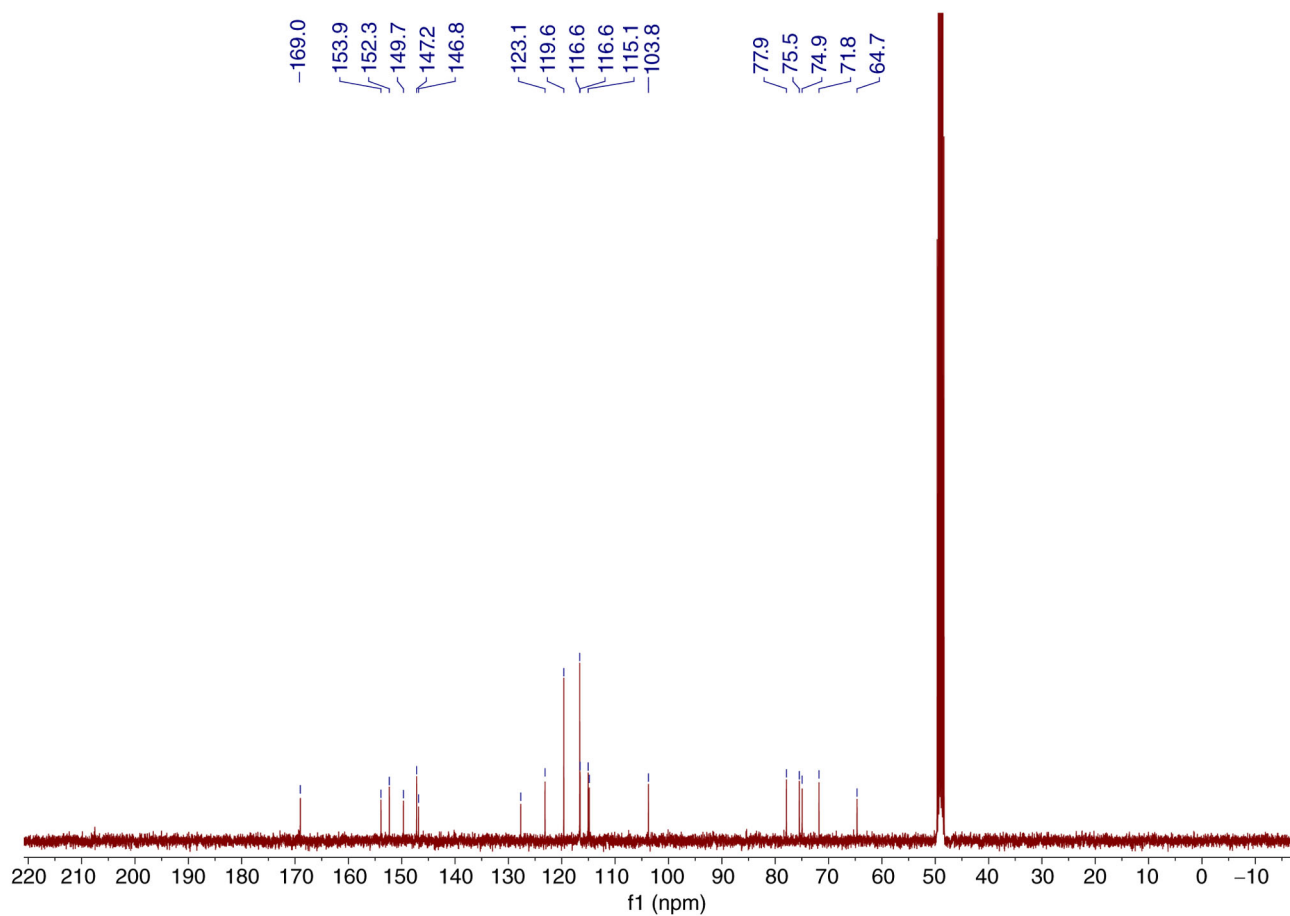


Figure S4. View of the molecules in an asymmetric unit of CA. Red indicates oxygen atoms with high electron cloud density, blue indicates nitrogen atoms, gray indicates carbon atoms, and cyan indicates hydrogen atoms. CA, 6'-O-Caffeoylarbutin.

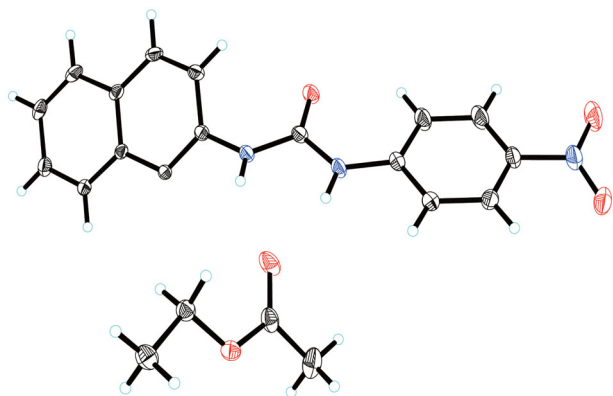


Figure S5. Packing diagram of CA crystals. Gray represents carbon atoms, red represents oxygen atoms, blue represents nitrogen atoms and cyan represents hydrogen atoms. CA, 6'-O-Caffeoylarbutin.

