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Supporting information for article:

Synthesis, crystal structure and bioactivities of α-asaronol

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S1. ¹H NMR spectral analysis

The ¹H NMR spectrum of α -asaronol is shown in Figure S1. Peaks between 3.72 ppm and 3.79 ppm are due to the three methoxy groups. The multiple peaks lying at 4.09-4.10 ppm are attributed to the two methylene hydrogens. The triplet peaks observed around 4.75 ppm are due to the hydrogen on the hydroxyl group. The multiple peaks located at 6.18-6.27 ppm are ascribed to the olefinic hydrogens near methylene. The two peaks at 6.65 ppm and 7.03ppm belong to the two hydrogens of the para hydrogen on the benzene ring. The doublet peaks lying at 6.68-6.74 ppm are ascribed to the olefinic hydrogen near the benzene ring.

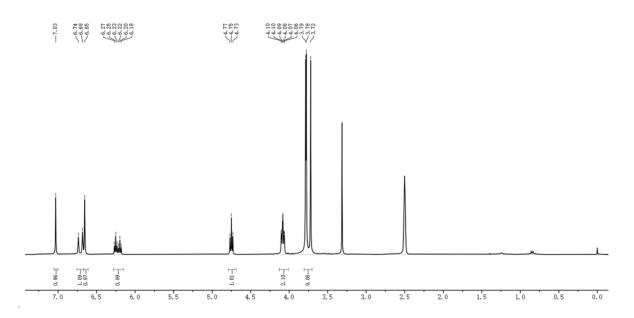


Figure S1 ¹H NMR spectrum of α -asaronol (2) dissolved in DMSO- d_6 .

S2. ¹³C NMR spectral analysis

The ¹³C NMR spectrum of α -asaronol is shown in Figure S2. The peaks at 56.198 ppm, 56.658 ppm and 56.731 ppm confirm the three methoxy groups, and 62.513 ppm is assigned to the methylene group. The olefinic carbons are observed from the peaks at 123.395 ppm and 129.067 ppm. The benzene ring carbons are shown at 98.830 ppm, 110.701 ppm, 117.437 ppm, 143.425 ppm, 149.618 ppm and 151.277 ppm.

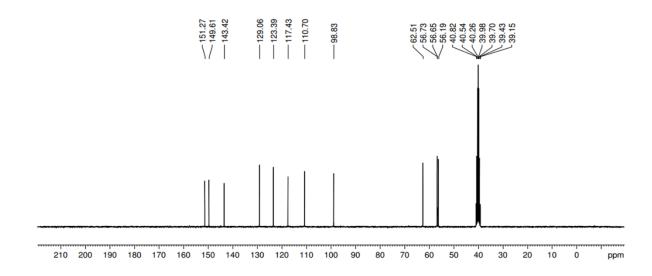


Figure S2 ¹³C NMR spectrum of α -asaronol (2) dissolved in DMSO- d_6 .

S3. FT-IR spectral analysis

To confirm the presence of the functional groups in the α-asaronol crystal, the FT-IR spectrum was recorded, as depicted in Figure S3. The broad band at 3425.47 cm⁻¹ represents O-H asymmetric stretching vibration, where the band shifts to a lower wavenumber due to the formation of intermolecular hydrogen bonds. The =C-H stretching vibration is exhibited at 3052.89 cm^{-1} . The absorption bands at 2931.36 cm⁻¹ and 2827.62 cm⁻¹ correspond to the C-H stretching vibration. The aromatic C=C stretching vibration is exhibited at 1642.97 cm⁻¹. The absorption band between 1614.75 and 1518.98 cm⁻¹ corresponds to the aromatic skeleton C=C stretching vibration. The -OCH₃ stretching vibration is exhibited at 1456.98 cm^{-1} . The aromatic =C-H out-of-plane deformation vibration appears at 965.32 cm⁻¹. The bands at 856.68 cm⁻¹ and 818.01 cm⁻¹ are due to the C-H asymmetric bending vibration.

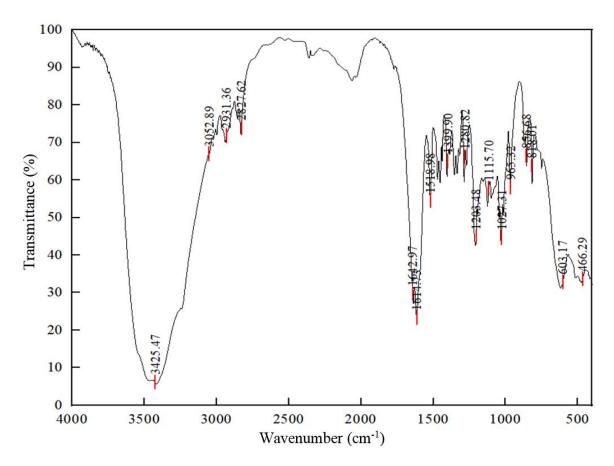


Figure S3 FT-IR spectrum of α -asaronol (2).