Supporting Information

Structure features of a chiral supramolecular organic framework self-assembled from natural compound

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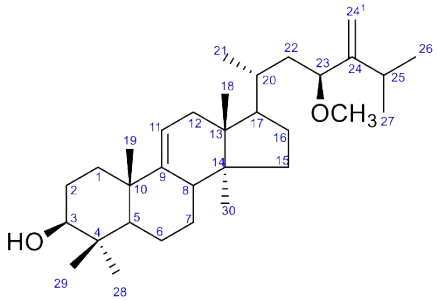
Extraction and isolation

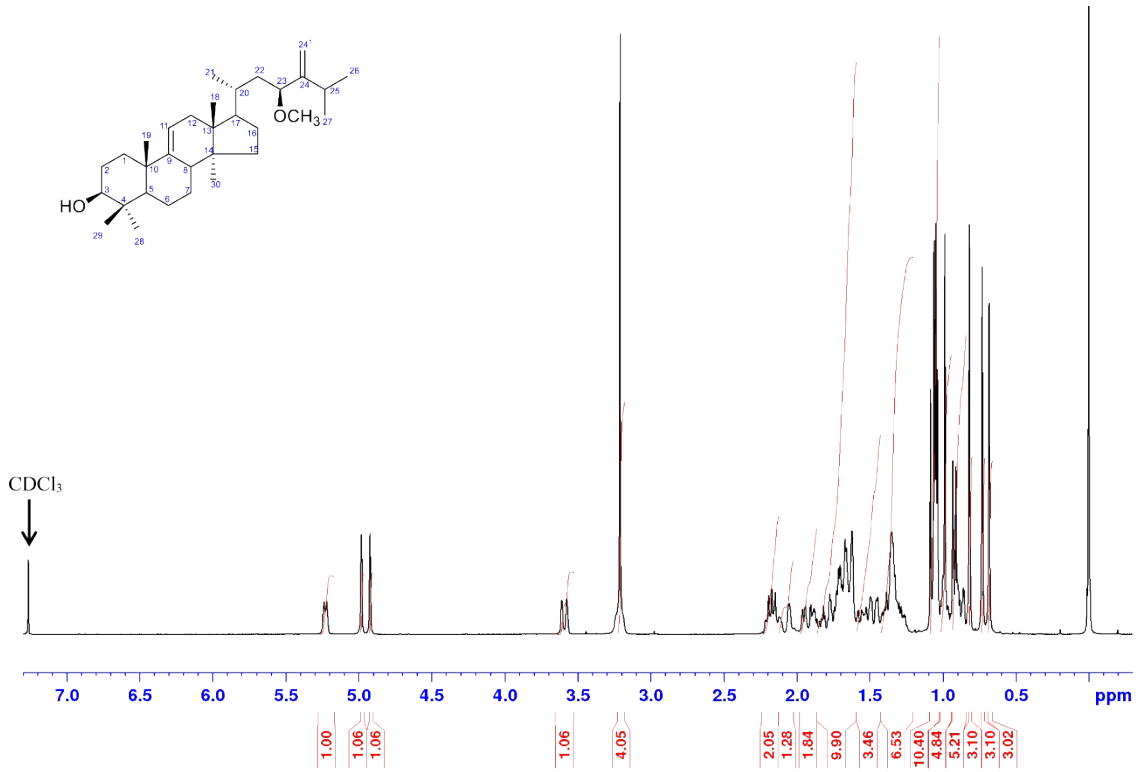
The dried twigs of *Miliusa sessilis* (2.4 kg) were extracted using 95% ethanol at room temperature. After evaporating the solvent under vacuum, a crude ethanolic extract (503.2 g) was obtained. This crude extract was then diluted with water and partitioned into hexane, resulting in a hexane extract (50.4 g) after evaporating the hexane under reduced pressure. The hexane extract was further purified using flash column chromatography with a gradient of hexane and ethyl acetate, yielding 10 fractions. Fraction 8 (1.85 g) was subjected to column chromatography with silica gel and a 1-45% ethyl acetate in hexane eluent, resulting in the isolation of **SOF-**1 as a white solid (43.3 mg), which was recrystallized in hexane-ethyl acetate to obtain colorless crystals.

Characterization

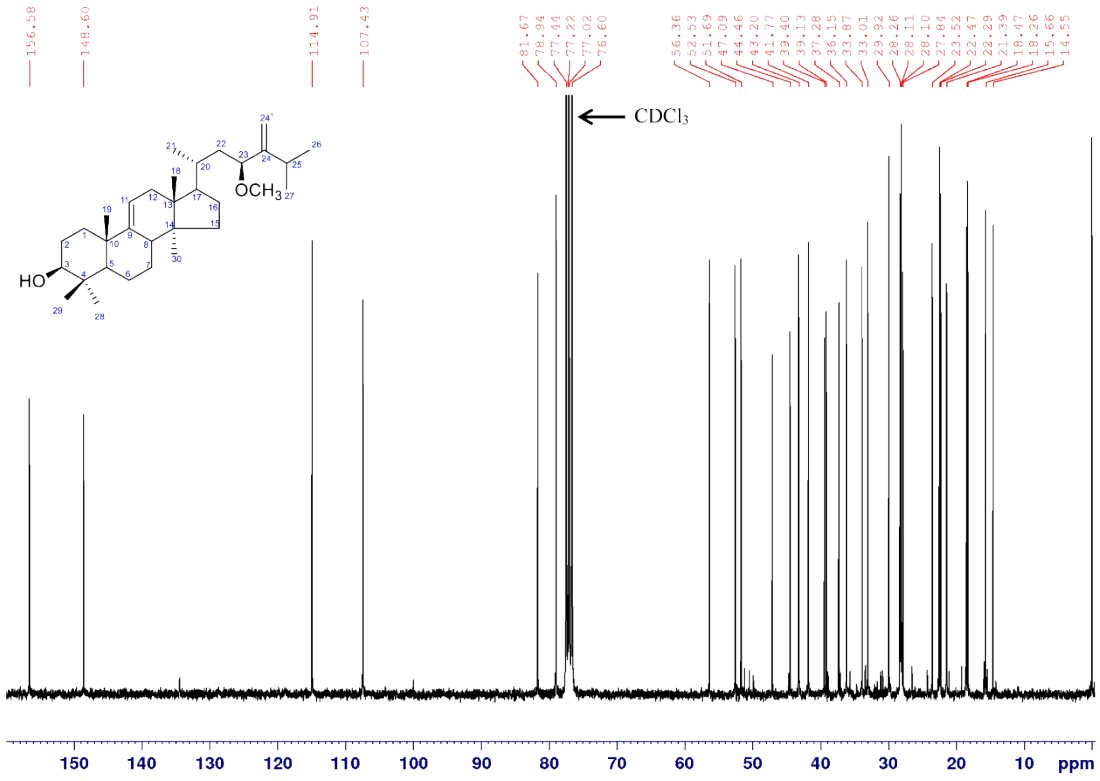
^{1}H NMR (300 MHz, $CDCl_3$): δ 1.45 (1H, m, H-1a), 1.78 (1H, m, H-1b), 1.33 (1H, m, H-2a), 1.65 (1H, m, H-2a), 3.21 (1H, overlapped, H-3), 0.87 (1H, overlapped, H-5), 1.48 (1H, m, H-6a), 1.69 (1H, m, H-6b), 1.65 (1H, m, H-7a), 1.77 (1H, m, H-7b), 2.19 (1H, t, *J* = 6.8 Hz, H-8), 5.23 (1H, *br*d, *J* = 5.9 Hz, H-11), 1.92 (1H, m, H-12a), 2.08 (1H, m, H-12b), 1.34 (1H, m, H-15a), 1.43 (1H, m, H-15b), 1.33 (1H, m, H-16a), 1.87 (2H, m, H-16b), 1.56 (1H, m, H-17), 0.68 (3H, s, H-18), 1.05 (3H, s, H-19), 1.67 (1H, m, H-20), 0.92 (3H, d, *J* = 6.3 Hz H-21), 1.01 (1H, m, H-22a), 1.66 (1H, m, H-22b), 3.59 (1H, dd, *J* = 10.3, 1.2 Hz, H-23), 4.92 (1H, s, H-24^{1}a), 4.98 (1H, s, H-24^{1}b), 2.17 (1H, m, H-25), 1.05 (3H, d, *J* = 7.1 Hz, H-26), 1.88 (3H, d, *J* = 7.1 Hz, H-27), 0.99 (3H, s, H-28), 0.82 (3H, s, H-29), 0.73 (3H, s, H-30). ^{13}C NMR (75 MHz, $CDCl_3$): δ 36.2 (C-1), 28.1 (C-2), 78.9 (C-3), 39.1 (C-4), 52.5 (C-5), 21.4 (C-6), 27.8 (C-7), 41.8 (C-8), 148.6 (C-9), 39.4 (C-10), 114.9 (C-11), 37.3 (C-12), 44.6 (C-13), 47.1 (C-14), 33.9 (C-15), 28.1 (C-16) , 51.7 (C-17), 14.5 (C-18), 22.3 (C-19), 33.0 (C-20), 18.3 (C-21), 43.2 (C-22), 81.7 (C-23), 56.3 (O$\underline{CH_3}$-23), 156.6 (C-24), 107.4 (C-24^{1}), 29.9 (C-25), 23.5 (C-26), 22.5 (C-27), 28.3 (C-28), 15.7 (C-29), 18.5 (C-30). HRESIMS $[M+NH_4]^+$ *m*/*z* 488.4462 (calcd. for $C_{32}H_{58}NO_2$, 488.4467).



IUPAC mame:	(3*β*,23*S*)-23-methoxy-24-methylenelanost-9-en-3-ol
Common name:	-
Appearance:	colorless rod (ethanol/ethyl acetate)
Melting Point:	192-193 °C
Optical rotation:	$[\alpha]_D^{23}$ +84.2 (c 0.06, $CHCl_3$)
CD:	-
UV:	-
IR:	(thin film): υ_{max}, cm^{-1};
	3323, 2917, 2866, 1639, 1462, 1369, 1111, 1087, 1040, 901, 757
HRESIMS:	*m/z* (relative intensiy), 70 eV;
	488.4462 $[M+NH_4]^-$ (calcd. for $C_{32}H_{58}NO_2$, 488.4467)
Chemical Formula:	$C_{31}H_{52}O_2$
Exact Mass:	456.3967 g/mol
^{1}H NMR spectroscopic data	δ ppm, 300 Hz in $CDCl_3$



1H NMR spectrum for **1** (300 MHz, $CDCl_3$)



^{13}C NMR spectrum for **1** (75 MHz, $CDCl_3$)

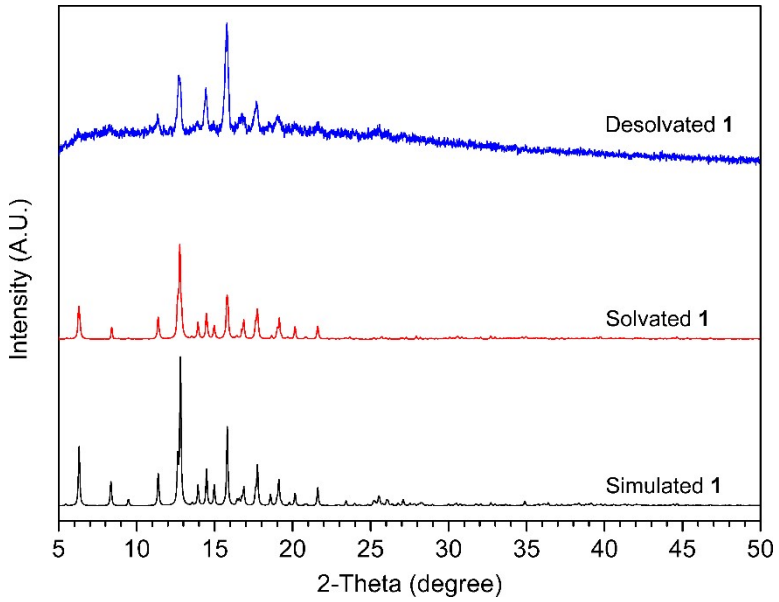


Fig. S1 Comparison of the simulated, 1 and desolvated PXRD patterns for **SOF-1**.

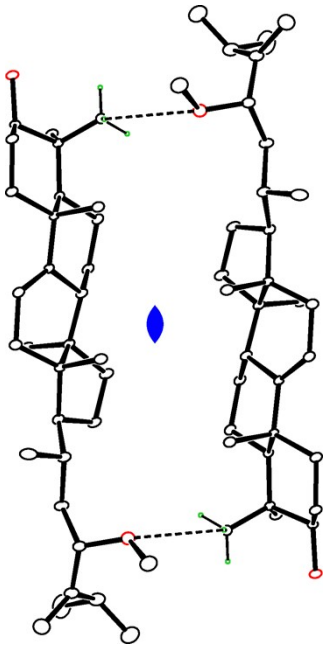


Fig. S2 Symmetry-related molecules form a C−H···O hydrogen bond **SOF-1**.

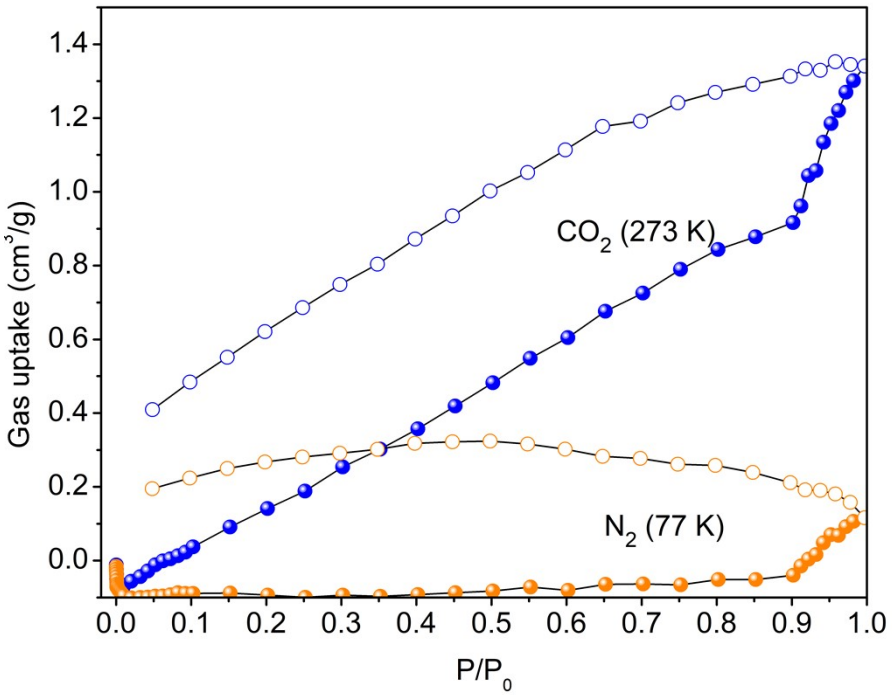


Fig. S3 N_2 (77 K) and CO_2 (273 K) adsorption isotherms of **SOF-1**.