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Supporting information for article:

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Water-mediated intermolecular interactions in 1,2-*O*-cyclohexylidene-*myo*-inositol: A quantitative analysis

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S1. Synthesis of 1,2:4,5-di-O-cyclohexylidene-myo-inositol (2):

1,2:4,5-di-*O*-cyclohexylidene-myo-inositol was obtained as a side product during the synthesis of title compound 1,2-*O*-cyclohexylidene-*myo*-inositol. The dichloromethane filtrate obtained after the filtration of precipitated 1, was further concentrated and purified using flash chromatography with gradient n-hexane: ethyl acetate (up to 40%) mobile phase. The separated fraction was concentrated to get side product 1,2:4,5-di-*O*-cyclohexylidene-*myo*-inositol (2) as a pale yellow oily compound (105 mg, 5.5%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.63 (dd, *J* = 5.3, 3.1 Hz, 1H), 4.21 (t, *J* = 5.5 Hz, 1H), 3.97 (t, *J* = 9.5 Hz, 1H), 3.84 – 3.65 (m, 3H), 1.68 (dddd, *J* = 44.1, 24.4, 16.3, 7.9 Hz, 16H), 1.41 (s, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 112.74, 112.70, 80.80, 78.78, 75.12, 74.91, 74.46, 71.97, 37.38, 36.46, 36.01, 34.92, 24.95, 23.88, 23.69, 23.47.

Figure S1 **^{1}H NMR spectra for 1,2-*O*-cyclohexylidene-*myo*-inositol (1)**

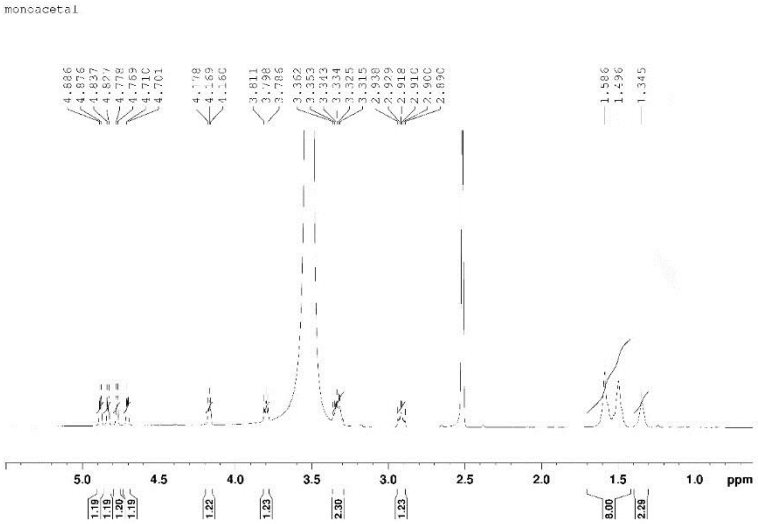
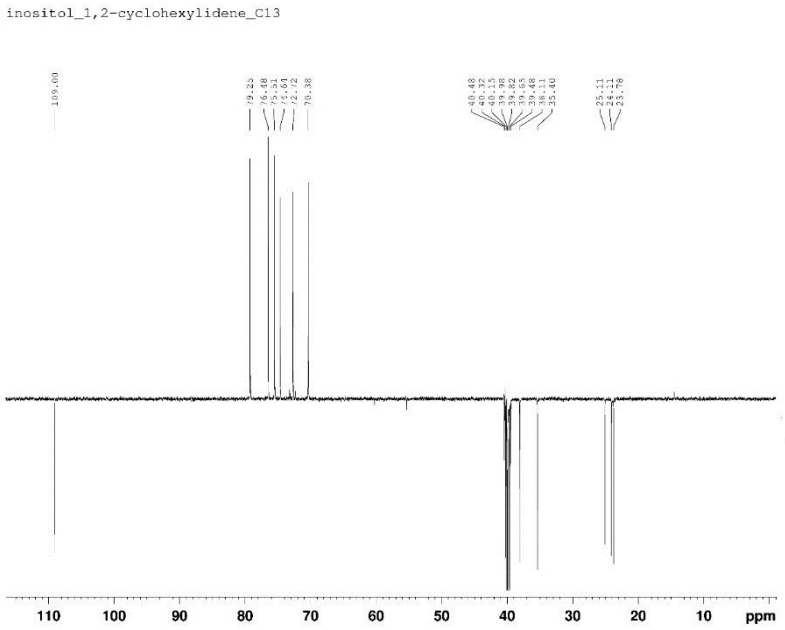


Figure S2 **^{13}C (APT) spectra for 1,2-*O*-cyclohexylidene-*myo*-inositol (1)**



**Atomic coordinates for this structure have been deposited in the Cambridge Crystallographic Data Centre with CCDC number 1404340