Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supporting Information for:

Methyl Red Based Metal-Organic Frameworks for the Selective and Tunable Sensing of Ammonia Gas.

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1. ^{1}H NMR Spectroscopy

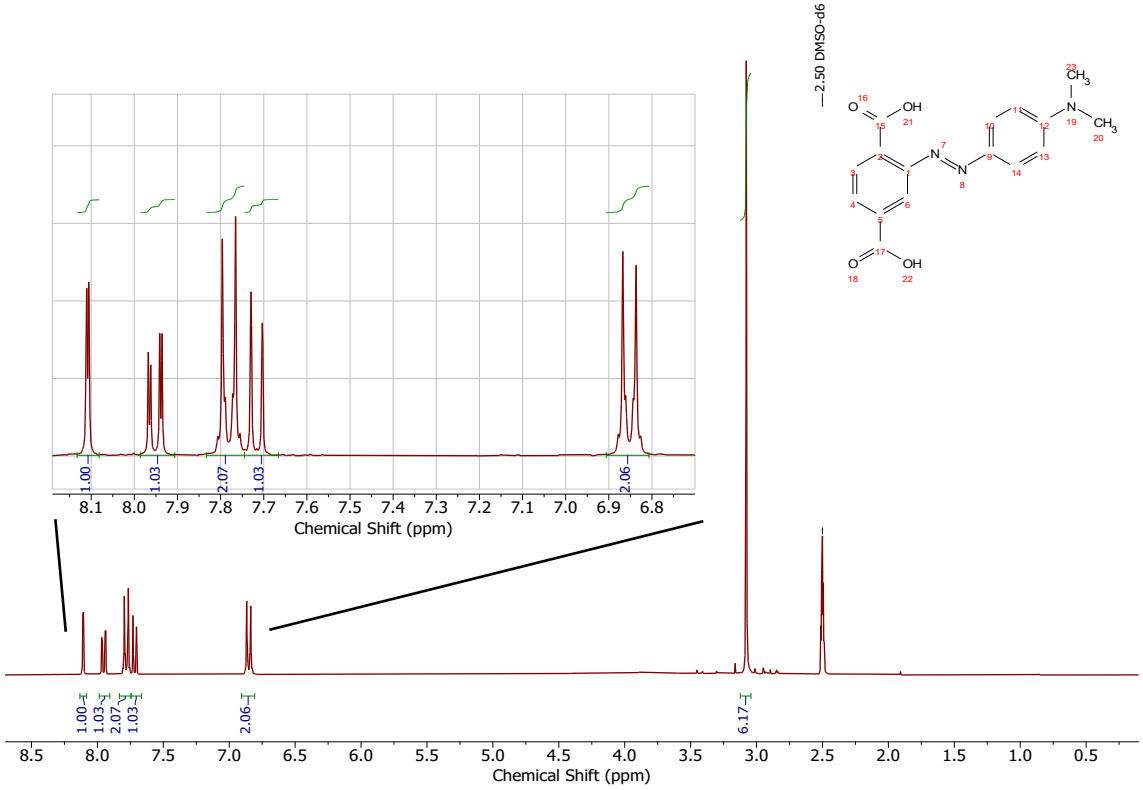

Fig. S1: 1H NMR of 2-[2-[4-(Dimethylamino)phenyl]diazenyl]-1,4-benzenedicarboxylic acid (H_2MRL) measured in DMSO-d_6 on a Bruker AVANCE 500 MHz spectrometer.

2. Gas Adsorption Isotherms

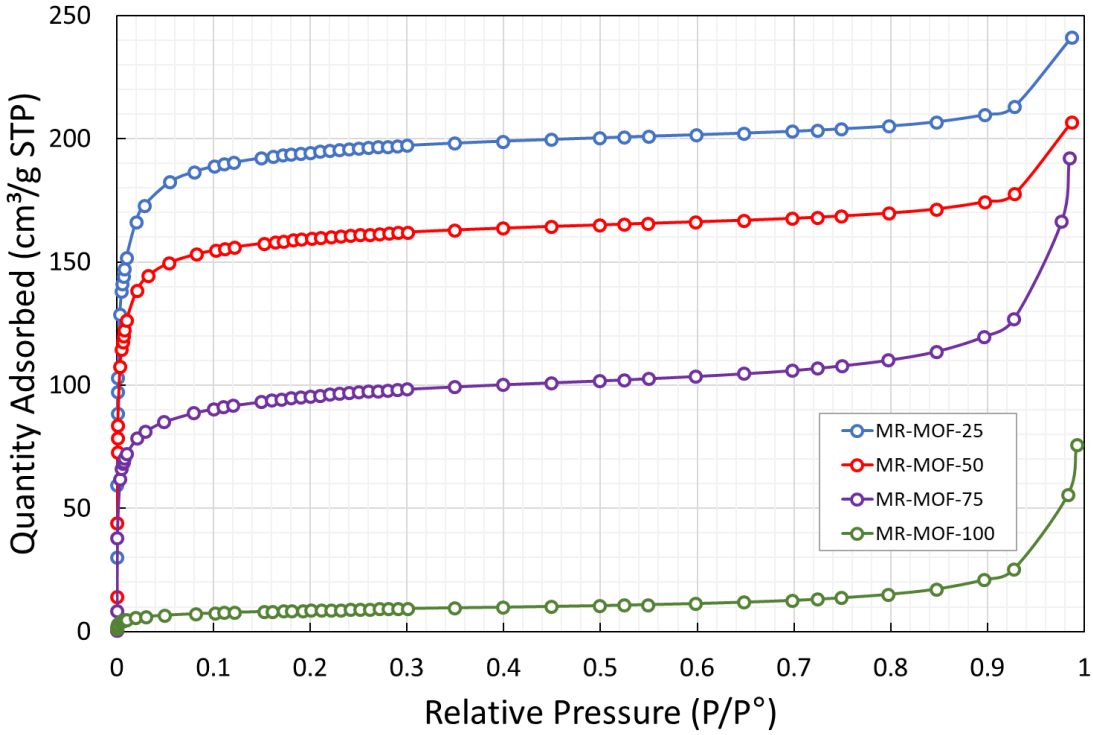

Fig. S2: Nitrogen gas adsorption isotherms measured at 77 K for MR-MOF after 5 adsorption/desorption cycles of ammonia vapour. Sufficient ammonia vapour was utilized to convert all the MOFs from the parent red colour to the yellow colour. Especially for MR-MOF-100, this represented a large amount of ammonia vapour.

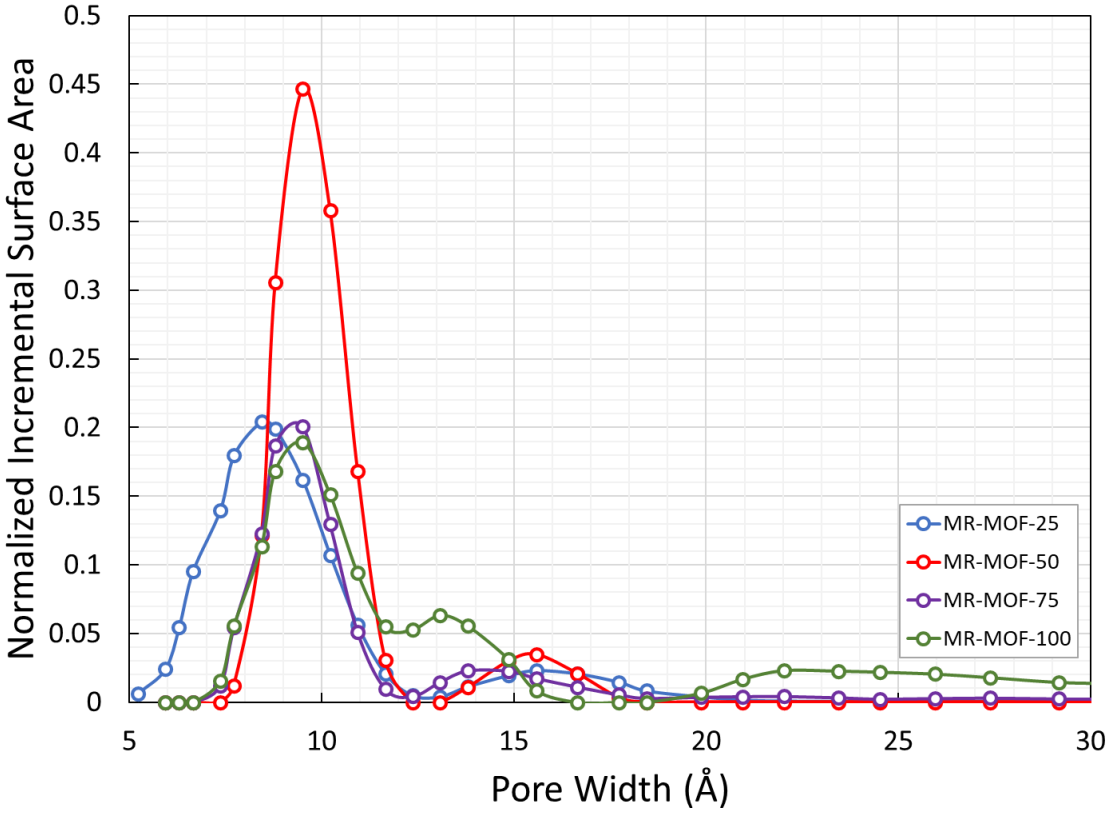

Fig. S3: BET surface area normalized pore size distributions for MR-MOF after 5 adsorption/desorption cycles of ammonia vapour. Pore size distribution was determined using the Tarazona NLDFT (Esf = 30.0K) model. The standard deviations for the fits are 2.87350 (MR-MOF-25), 2.62504 (MR-MOF-50), 1.30490 (MR-MOF-75), and 0.05079 cm^3/g (MR-MOF-100).

3. Infrared Spectroscopy

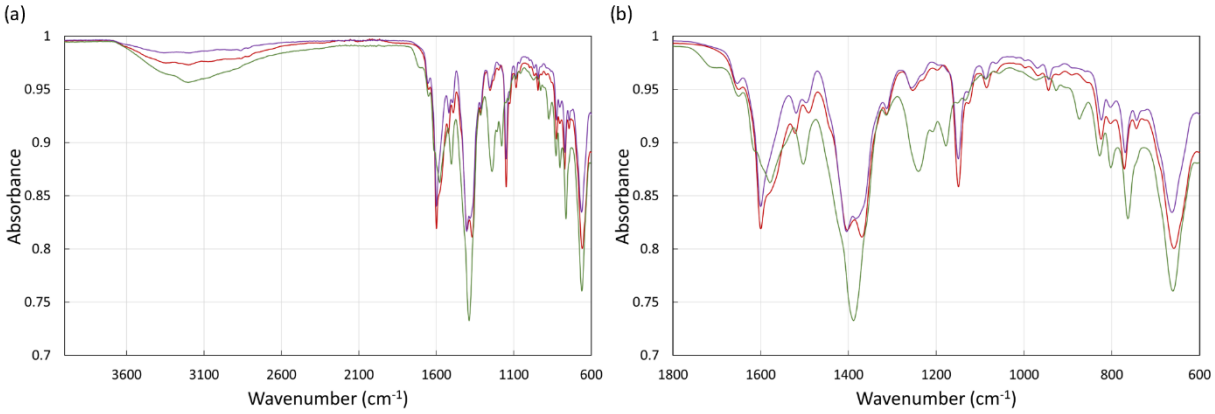

Fig. S4: Full (a) and zoom-in (b) IR spectroscopy of as-synthesized MR-MOF-100 (purple), MR-MOF-100 after hydrochloric acid vapor exposure (green), MR-MOF-100 after ammonia vapor exposure (red).

4. ^{13}C Magic Angle Spinning Solid-State NMR

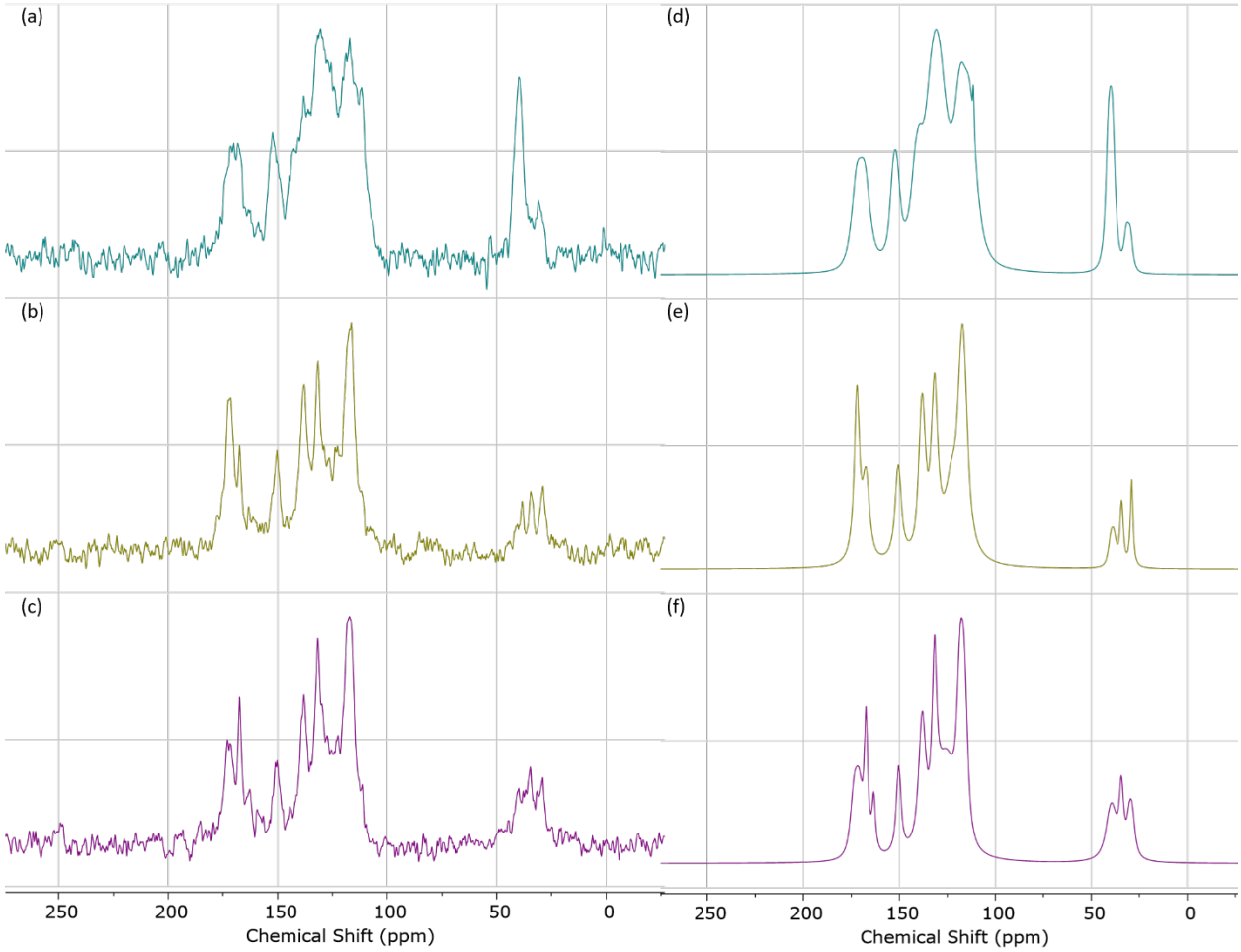

Fig. S5: ^{13}C Magic Angle Spinning Solid-State NMR (151 MHz) of (a) MR-MOF-100 post five cycles of ammonia exposure, (b) MR-MOF-100 post hydrochloric acid exposure, (c) MR-MOF-100, and the respective deconvoluted spectrum (d: δ 30.75, 39.95, 111.37, 115.67, 130.88, 140.78, 152.24, 170.03 ppm), (e: δ 28.98, 34.22, 39.01, 117.01, 122.83, 131.66, 138.14, 150.57, 167.31, 172.07 ppm), and (f: δ 29.35, 34.34, 39.62, 117.26, 125.65, 131.68, 138.09, 150.35, 163.34, 167.34, 172.28 ppm). The integrated intensities of the deconvoluted resonance in the methyl region (25-50 ppm) to the remaining resonances is 2.46:14 for MR-MOF-100 (c/f), 1.32:14 for acid-exposed MR-MOF-100, and 2:14 for ammonia-exposed MR-MOF-100; these values are consistent with one another given the level of noise in the spectra.