Supplementary information

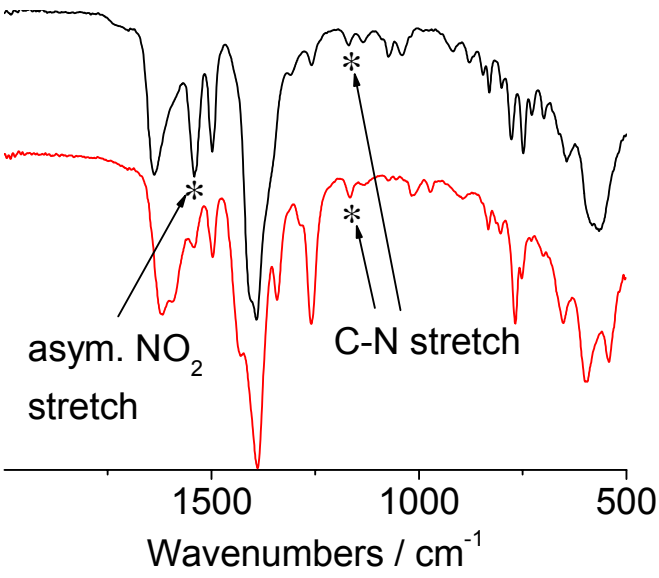

Fig. S1. FTIR spectra of Cr-MIL-101-NO_2 (top) and Cr-MIL-101-NH_2 (bottom). The characteristic signals are marked with an asterisk for clarity.

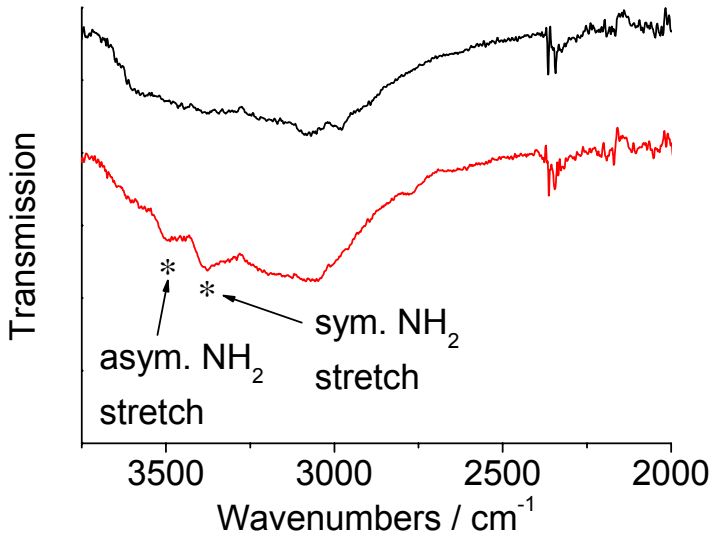

Fig. S2. FTIR spectra of Cr-MIL-101-NO_2 (top) and Cr-MIL-101-NH_2 (bottom). The characteristic signals are marked with an asterisk for clarity.

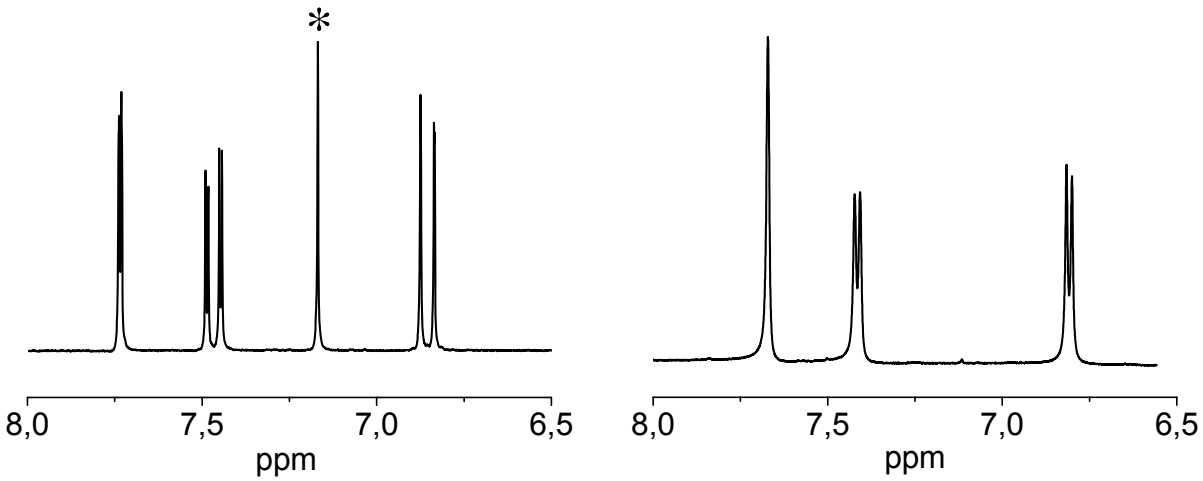

Fig. S3. ^{1}H-NMR spectra of the linker molecules. Left: after 10 minutes nitration time, the signal at 7.3 ppm (marked by an asterisk) belongs to unreacted terephthalic acid. Integration of the signals show a molar ratio terephthalic acid : nitroterephthalic acid = 1:6. Right: after five hours reaction time. There is no signal of the terephthalic acid left. Expanding the reaction time up to 48 h no multiple nitration products were observed.

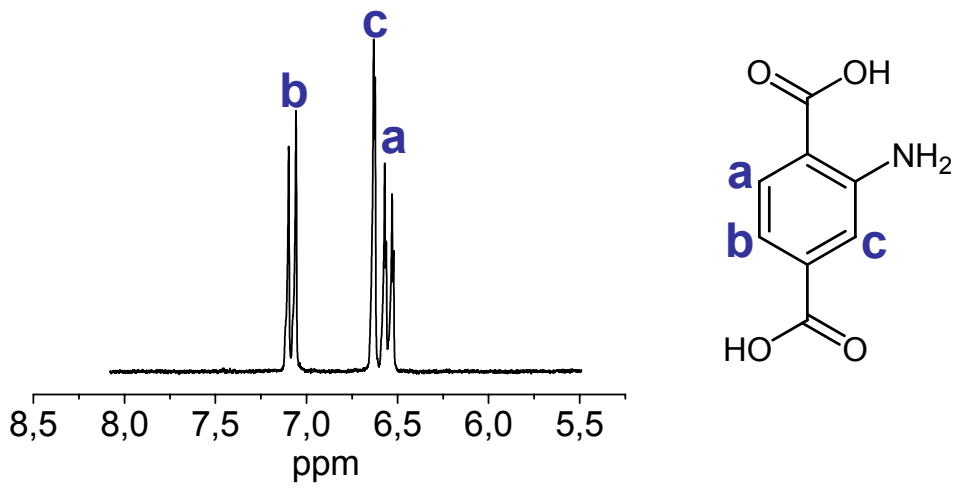

Fig. S4. ^{1}H-NMR spectrum of the linker after the reduction of Cr-MIL-101-NO_2 to Cr-MIL-101-NO_2. Only aminoterephthalic acid is observed.

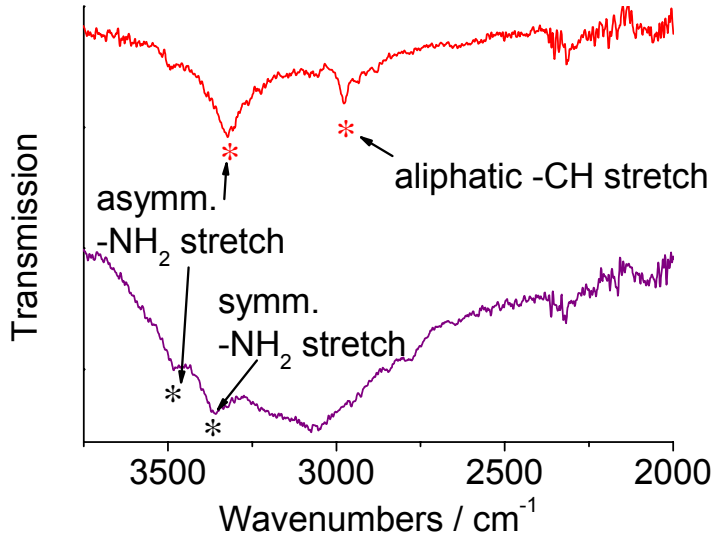

Fig. S5 IR spectra of Cr-MIL-101-NH_2 (bottom) and the urea form Cr-MIL-101-UR2 (top). The characteristic signals are marked with asterisks for clarity

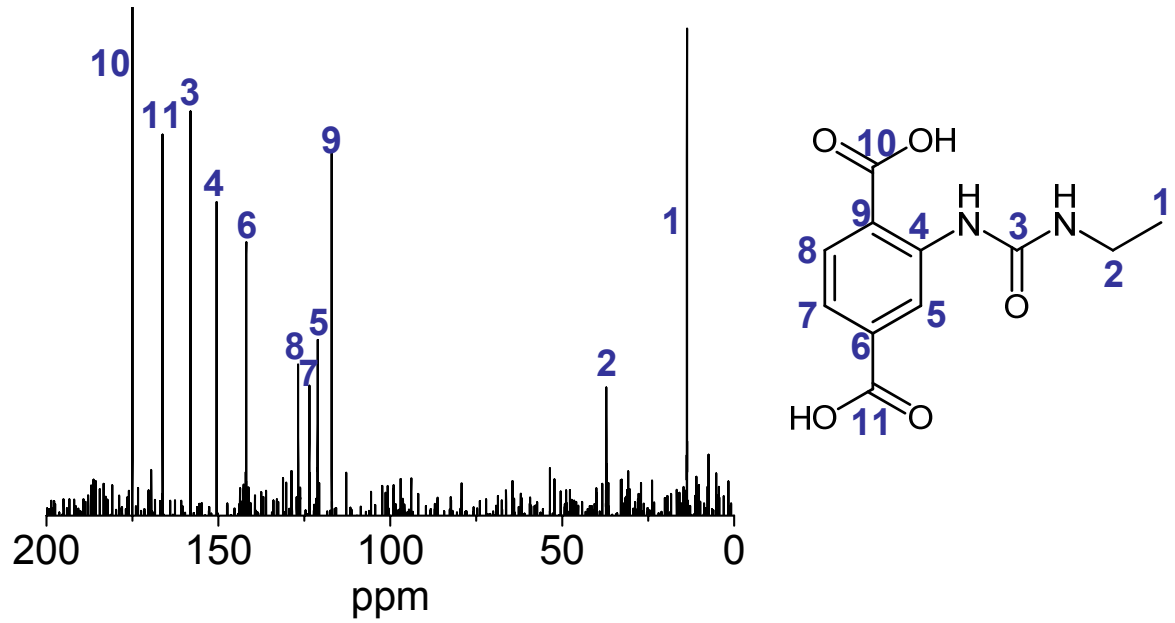

Fig. S6. ^{13}C-NMR spectrum of the linker from the product (Cr-MIL-101-UR2) which was obtained from the reaction of Cr-MIL-101-NH_2 with ethyl isocyanate. The spectrum was recorded in NaOD/D_2O (20%). All signals can be clearly assigned.

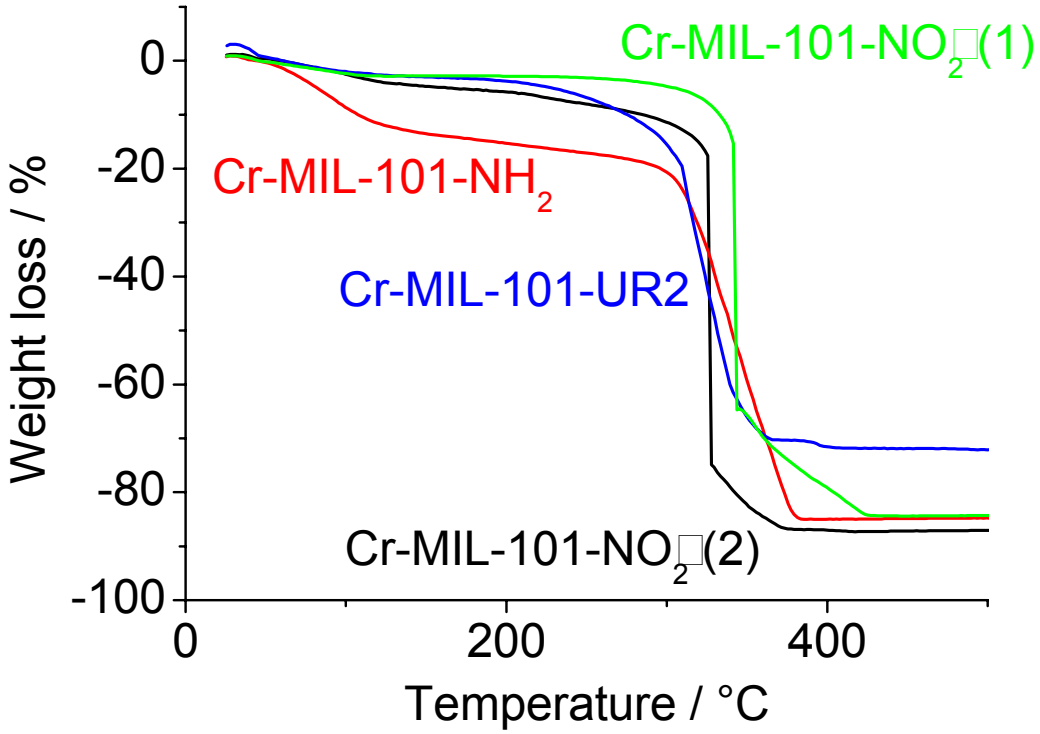

Fig. S7. TGA data of the investigated compounds Cr-MIL-101-NO_2(1), Cr-MIL-101-NO_2(2), Cr-MIL-101-NH_2 and Cr-MIL-101-UR2.

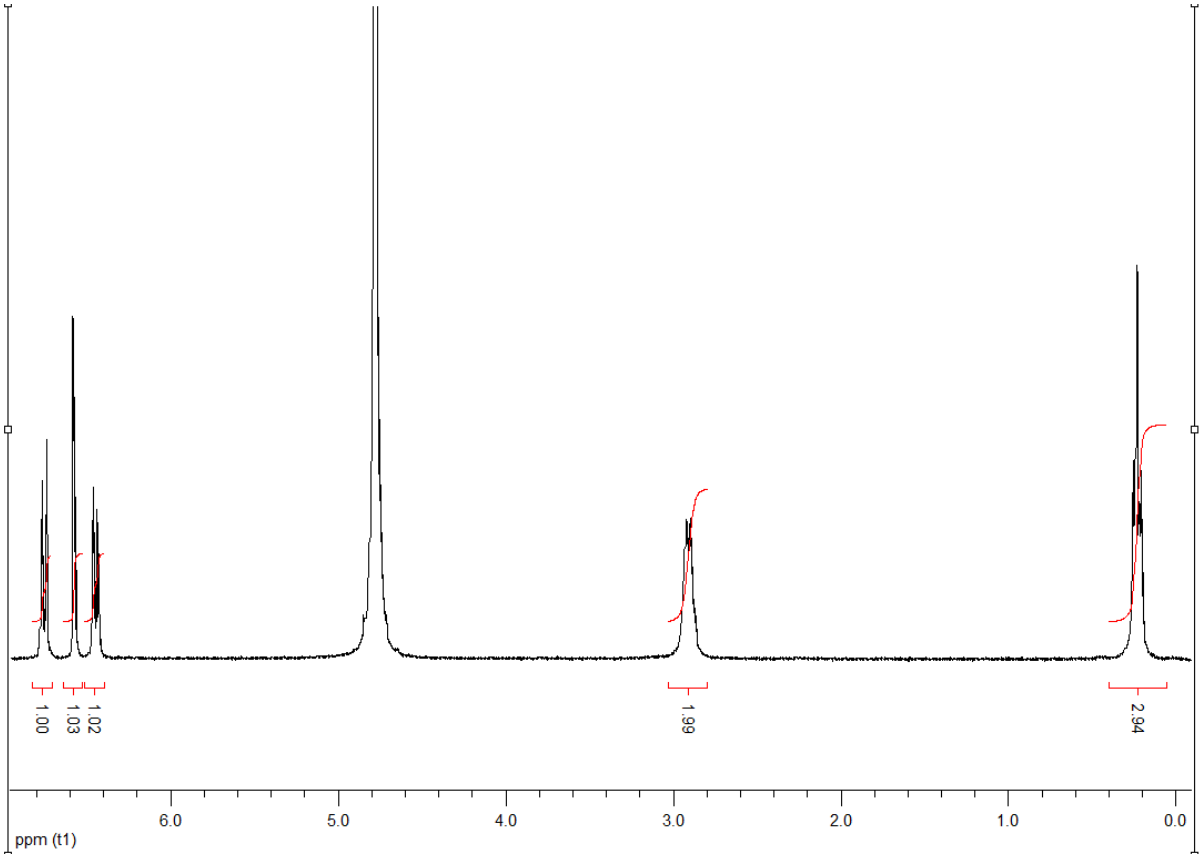

Fig. S8. ^{1}H-NMR spectrum of the linker of Cr-MIL-101-UR measured in NaOD/D_2O (20%). The assignments of the signals can be found in Fig. 5. The integrals can be clearly assigned to the corresponding protons.