Supporting information

Selective Cu and Ni-MOFs as pre-catalysts for the hydrogenation of furfural to furfuryl alcohol

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Characterisation

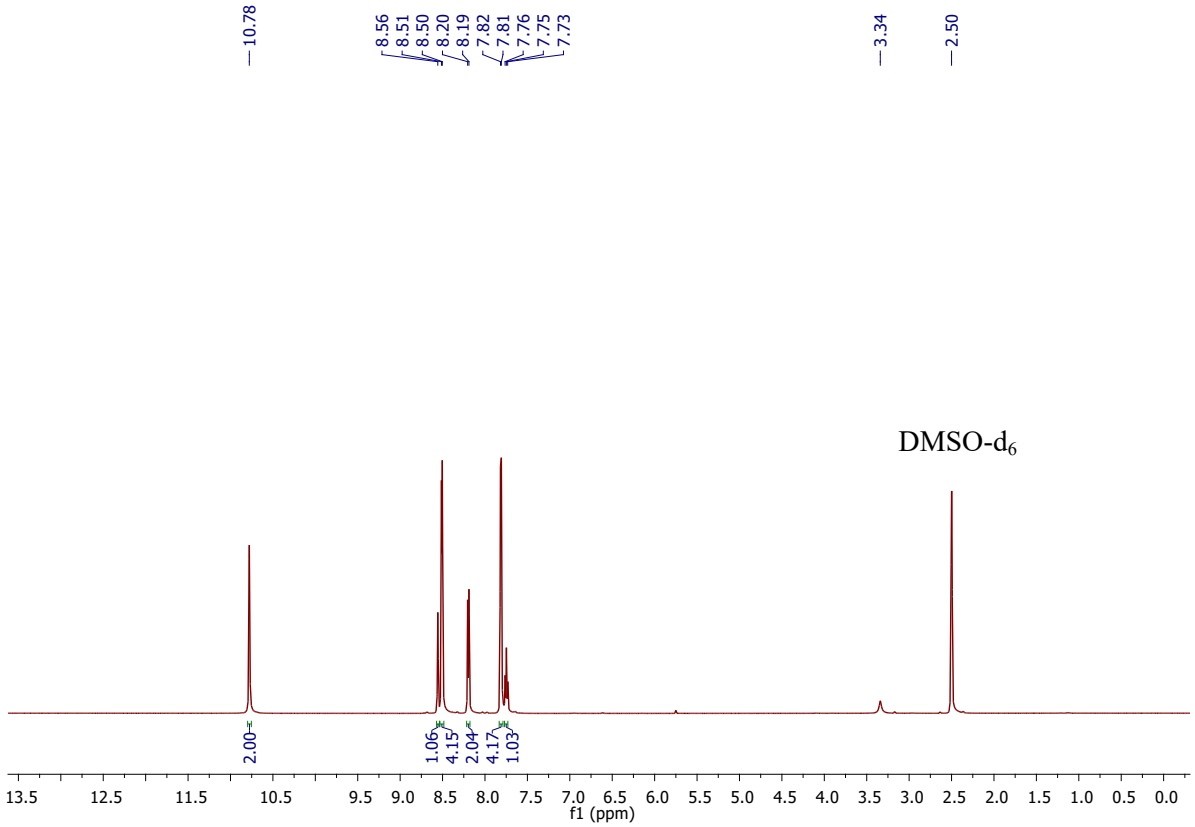

Figure SI 1: ^{1}H NMR spectrum of **L1**, recorded in DMSO-d$_6$.

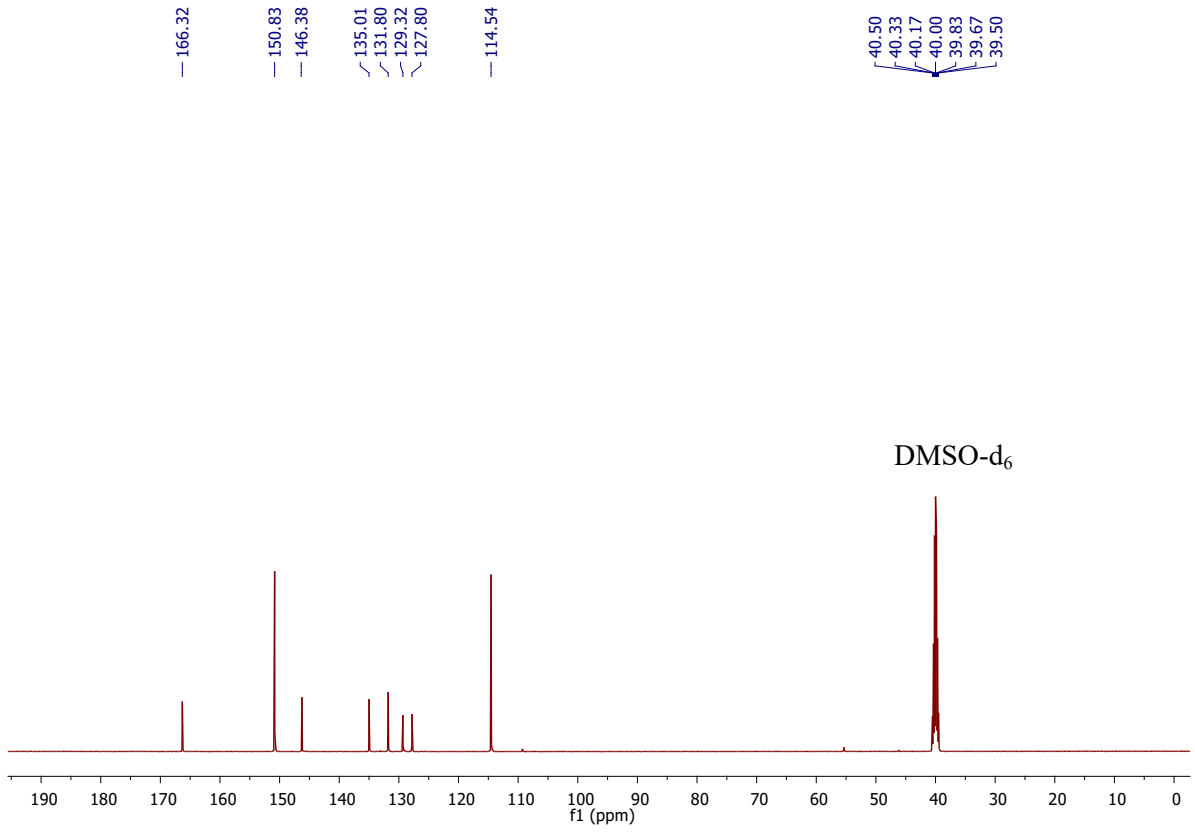

Figure SI 2: ^{13}C{H} NMR spectrum of **L1**, recorded in DMSO-d$_6$.

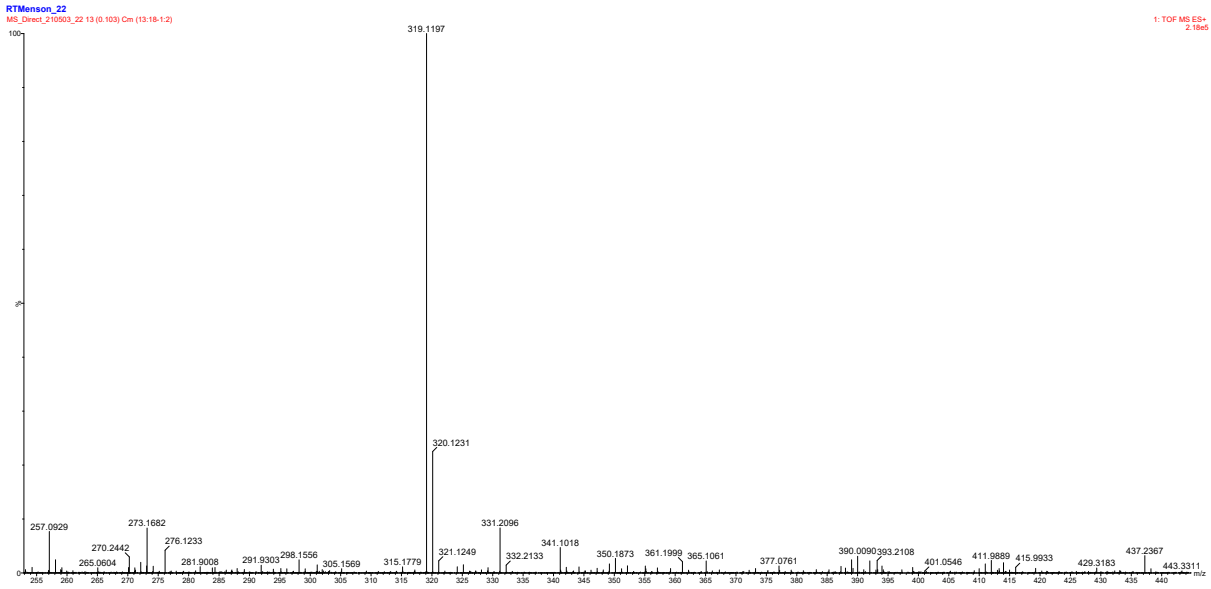

Figure SI 3: High resolution electrospray ionisation-mass spectrum for **L1**.

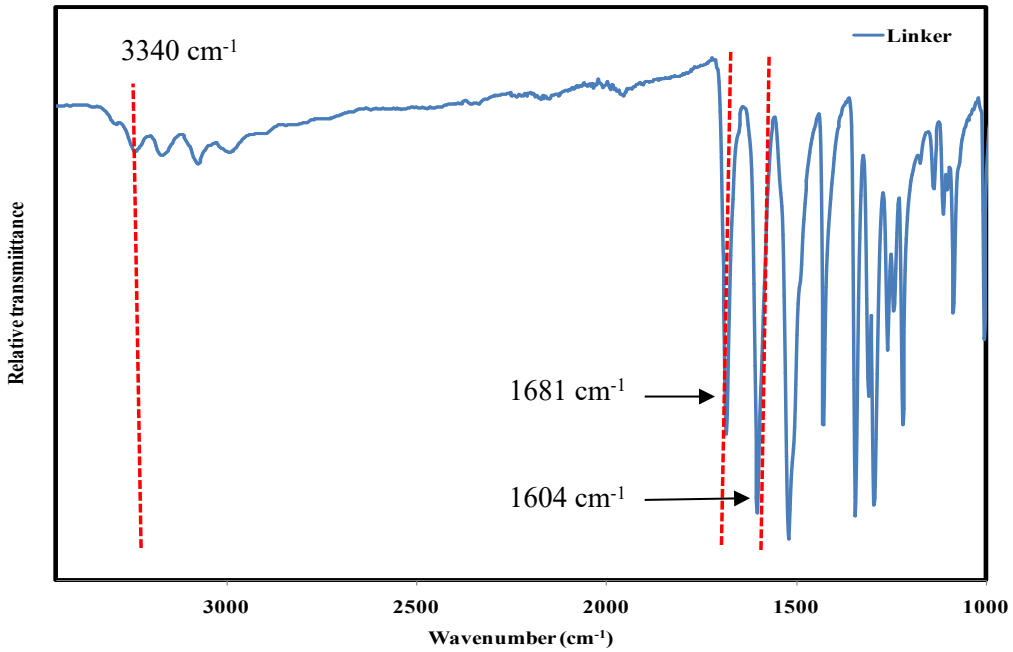

Figure SI 4: FT-IR spectrum of **L1**.

Table SI 1: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for ligand L1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O001	10433.4(18)	1863(2)	9228.7(16)	69.5(7)
N002	9406(2)	3973(3)	8558.7(16)	51.1(6)
N003	5581.0(19)	2567(3)	5425.1(17)	51.8(6)
N004	2891(2)	4412(3)	2873.2(19)	60.6(7)
N005	12002(2)	7275(3)	9582.7(19)	61.3(7)

O006	4523(2)	1063(3)	5951.0(17)	89.4(9)
C007	4665(2)	3177(3)	4587(2)	47.4(7)
C008	7484(2)	2008(3)	7382(2)	49.4(7)
C009	10295(2)	5035(3)	8928(2)	48.3(7)
C00A	8436(2)	1559(3)	8237(2)	48.7(7)
C00B	9517(3)	2469(3)	8723(2)	52.3(8)
C00C	4883(3)	3707(3)	3795(2)	53.1(8)
C00D	6523(2)	1104(3)	6960(2)	50.7(8)
C00E	10028(3)	6515(3)	8671(2)	55.8(8)
C00F	5461(3)	1563(3)	6078(2)	58.0(8)
C00G	6513(3)	-265(3)	7394(2)	58.5(8)
C00H	3558(3)	3308(3)	4514(2)	59.3(8)
C00I	3978(3)	4302(3)	2970(2)	59.5(8)
C00J	10892(3)	7557(3)	9009(2)	59.8(8)
C00K	8405(3)	178(3)	8654(2)	56.8(8)
C00L	11438(3)	4706(4)	9548(2)	61.6(9)
C00M	7456(3)	-718(3)	8238(2)	60.3(8)
C00N	12230(3)	5857(4)	9844(2)	67.4(9)
C00O	2716(3)	3919(4)	3661(3)	63.4(9)

Table SI 2: Anisotropic Displacement Parameters ($Å^2×10^3$) for ligand L1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O001	48.3(14)	61.3(14)	79.6(15)	10.1(11)	7.6(12)	17.6(12)
N002	38.9(14)	47.6(15)	54.7(14)	1.2(11)	7.5(11)	2.4(12)
N003	39.5(14)	54.1(14)	52.5(14)	-4.9(12)	10.1(12)	3.4(12)
N004	48.5(17)	54.2(16)	66.8(17)	-0.4(13)	11.7(14)	4.3(13)
N005	47.3(17)	66.7(19)	64.3(17)	-0.2(13)	17.7(14)	-2.7(14)
O006	55.0(16)	113(2)	79.6(16)	-30.0(14)	7.7(13)	30.0(14)
C007	38.7(17)	46.5(16)	49.1(17)	-3.6(13)	10.5(14)	-4.7(13)
C008	49.4(18)	47.5(17)	48.0(17)	2.6(15)	17.0(15)	4.7(14)
C009	39.4(17)	54.4(18)	45.8(16)	2.7(14)	12.5(13)	-1.4(14)
C00A	47.8(18)	46.1(17)	48.0(16)	4.2(14)	15.7(15)	1.3(14)
C00B	50(2)	54.7(19)	49.0(17)	5.7(16)	17.0(15)	4.5(15)
C00C	42.6(18)	54.3(18)	57.2(18)	0.0(14)	15.7(16)	0.5(15)
C00D	52(2)	47.6(18)	48.1(17)	-1.7(15)	16.2(15)	-0.7(14)
C00E	43.0(19)	55(2)	56.2(18)	6.1(15)	7.7(15)	1.8(15)
C00F	49(2)	60(2)	55.2(19)	-15.7(16)	11.9(16)	0.3(16)
C00G	59(2)	46.9(19)	65(2)	-7.0(15)	22.4(18)	-3.6(16)
C00H	47(2)	70(2)	57.7(19)	-3.7(16)	18.5(16)	3.1(16)
C00I	60(2)	55.9(19)	56.8(19)	-0.8(16)	18.4(17)	3.9(15)
C00J	50(2)	54.4(19)	70(2)	-0.7(17)	20.1(17)	-4.2(16)
C00K	61(2)	47.9(18)	55.2(18)	6.9(16)	17.5(16)	6.7(15)
C00L	41.1(19)	59(2)	71(2)	4.5(16)	9.8(16)	8.0(16)
C00M	68(2)	46.0(18)	63(2)	2.3(17)	23.2(18)	8.9(16)

C00N	37.3(19)	78(2)	73(2)	6.5(18)	8.5(16)	9.6(19)
C00O	43(2)	66(2)	76(2)	1.0(16)	20.4(18)	0.4(18)

Table SI 3: Bond Lengths for ligand L1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	C00B	1.217(3)	C008	C00D	1.380(4)
N002	C009	1.403(4)	C009	C00E	1.384(4)
N002	C00B	1.369(4)	C009	C00L	1.386(4)
N003	C007	1.403(3)	C00A	C00B	1.499(4)
N003	C00F	1.366(4)	C00A	C00K	1.390(4)
N004	C00I	1.332(4)	C00C	C00I	1.380(4)
N004	C00O	1.336(4)	C00D	C00F	1.485(4)
N005	C00J	1.332(4)	C00D	C00G	1.386(4)
N005	C00N	1.326(4)	C00E	C00J	1.369(4)
O006	C00F	1.213(3)	C00G	C00M	1.375(4)
C007	C00C	1.382(4)	C00H	C00O	1.375(4)
C007	C00H	1.371(4)	C00K	C00M	1.364(4)
C008	C00A	1.388(4)	C00L	C00N	1.380(4)

Table SI 4: Bond Angles for ligand L1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00B	N002	C009	126.5(2)	C00I	C00C	C007	118.7(3)
C00F	N003	C007	125.0(2)	C00F	C00D	C008	122.7(3)
C00O	N004	C00I	114.9(3)	C00G	C00D	C008	119.4(3)
C00N	N005	C00J	114.2(3)	C00G	C00D	C00F	117.8(3)
C00C	C007	N003	118.9(3)	C00J	C00E	C009	119.3(3)
C00H	C007	N003	123.5(3)	O006	C00F	N003	121.7(3)
C00H	C007	C00C	117.5(3)	C00D	C00F	N003	117.6(3)
C00D	C008	C00A	120.6(3)	C00D	C00F	O006	120.6(3)
C00E	C009	N002	118.8(3)	C00M	C00G	C00D	120.2(3)
C00L	C009	N002	124.3(3)	C00O	C00H	C007	119.4(3)
C00L	C009	C00E	116.9(3)	C00C	C00I	N004	124.9(3)
C00B	C00A	C008	123.5(3)	C00E	C00J	N005	125.3(3)
C00K	C00A	C008	118.7(3)	C00M	C00K	C00A	120.9(3)
C00K	C00A	C00B	117.8(3)	C00N	C00L	C009	118.3(3)
N002	C00B	O001	123.4(3)	C00K	C00M	C00G	120.2(3)
C00A	C00B	O001	120.1(3)	C00L	C00N	N005	125.9(3)
C00A	C00B	N002	116.6(3)	C00H	C00O	N004	124.6(3)

Table SI 5: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for ligand L1.

Atom	*x*	*y*	*z*	U(eq)
H00K	9039(3)	-139(3)	9223(2)	68.1(10)
H00M	7447(3)	-1639(3)	8526(2)	72.4(10)

H00G	5867(3)	-878(3)	7115(2)	70.2(10)
H008	7494(2)	2926(3)	7092(2)	59.3(9)
H00N	12991(3)	5617(4)	10265(2)	80.9(11)
H00J	10686(3)	8542(3)	8822(2)	71.7(10)
H00E	9269(3)	6798(3)	8273(2)	67(1)
H00L	11666(3)	3735(4)	9758(2)	73.9(10)
H00I	4139(3)	4652(3)	2444(2)	71.4(10)
H00O	1972(3)	3995(4)	3630(3)	76.1(11)
H00H	3379(3)	2985(3)	5037(2)	71.2(10)
H00C	5624(3)	3664(3)	3817(2)	63.7(9)
H002	8723(2)	4300(3)	8192.3(16)	61.3(8)

Table SI 6 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for MOF 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	9.6(6)	18.3(7)	12.2(6)	0	0	0
N2	13(2)	20(2)	18(2)	-1.6(19)	0.3(17)	2.2(19)
O4	20(2)	56(3)	27(2)	-14(2)	-4.8(18)	14(2)
N3	16(2)	27(3)	25(2)	-7(2)	-4.7(18)	7(2)
C5	14(2)	20(3)	22(3)	-4(2)	1(2)	2(2)
C1	14(2)	23(3)	20(2)	-3(2)	-2(2)	2(2)
C7	17(2)	14(3)	19(2)	-0.1(19)	-1.8(19)	-2(2)
C6	16(2)	22(3)	16(2)	1(2)	-1.0(19)	-1(2)
C2	14(2)	24(3)	21(3)	-6(2)	0(2)	4(2)
C10	18(3)	30(4)	14(3)	0	0	-4(3)
C8	18(3)	19(3)	19(2)	-2(2)	3(2)	1(2)
C4	14(2)	23(3)	27(3)	-7(2)	1(2)	3(2)
C9	24(4)	31(4)	15(3)	0	0	4(4)
N4B	21(5)	34(6)	49(4)	-3(5)	11(4)	1(4)
C3	14(2)	23(2)	21(2)	-3(2)	-1(2)	2(2)
O5B	20(5)	30(5)	40(6)	-9(4)	2(4)	4(4)
C13A	28(9)	34(8)	48(6)	-4(6)	10(7)	6(7)
C11B	20(5)	29(5)	46(5)	-6(4)	7(4)	1(4)
C11A	22(5)	31(6)	45(5)	-7(4)	2(4)	0(4)
O5A	24(4)	29(5)	43(5)	-8(4)	5(4)	4(4)
C13B	30(10)	42(9)	48(7)	-5(6)	17(7)	-6(8)
C12A	28(6)	36(7)	66(7)	-1(6)	11(6)	8(5)
N4A	25(5)	31(6)	47(4)	-5(4)	9(4)	1(4)
C12B	33(7)	52(8)	72(9)	8(7)	15(7)	18(6)
N5	29(4)	17(3)	23(5)	2(3)	-11(3)	0(3)
O1	36(8)	21(3)	42(7)	1(5)	3(6)	-3(4)

Table SI 6 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for MOF 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	47(4)	22(3)	41(13)	2(5)	-27(7)	14(5)
O3	31(4)	26(4)	31(5)	0(4)	-6(4)	-8(3)

Table SI 7: Bond Lengths for MOF 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	$N2^1$	2.029(4)	C2	C3	1.398(8)
Cu1	N2	2.030(4)	C8	C9	1.392(7)
Cu1	$N2^2$	2.029(4)	C4	C3	1.398(8)
Cu1	$N2^3$	2.029(4)	N4B	C11B	1.35(2)
Cu1	O1	2.433(8)	N4B	C13B	1.41(3)
N2	C5	1.351(7)	N4B	C12B	1.39(2)
N2	C1	1.354(7)	O5B	C11B	1.21(2)
O4	C6	1.206(7)	C13A	N4A	1.43(3)
N3	C6	1.379(7)	C11A	O5A	1.26(2)
N3	C3	1.396(7)	C11A	N4A	1.32(2)
C5	C4	1.365(8)	C12A	N4A	1.48(3)
C1	C2	1.377(8)	N5	O1	1.248(12)
C7	C6	1.504(8)	N5	O2	1.244(12)
C7	C10	1.390(7)	N5	O3	1.241(10)
C7	C8	1.389(8)			

Table SI 8: Bond Angles for MOF 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$N2^1$	Cu1	$N2^2$	89.1(3)	N3	C6	C7	114.7(5)
$N2^3$	Cu1	N2	89.1(3)	C1	C2	C3	118.9(5)
$N2^1$	Cu1	N2	179.6(3)	$C7^4$	C10	C7	120.6(7)
$N2^1$	Cu1	$N2^3$	90.9(3)	C7	C8	C9	120.1(5)
$N2^2$	Cu1	$N2^3$	179.6(3)	C5	C4	C3	119.8(5)
$N2^2$	Cu1	N2	90.9(3)	C8	C9	$C8^4$	120.0(7)
$N2^1$	Cu1	O1	91.5(8)	C11B	N4B	C12B	125(2)
$N2^3$	Cu1	O1	94.2(5)	C13B	N4B	C11B	133.9(19)
$N2^2$	Cu1	O1	85.4(5)	C13B	N4B	C12B	101.0(17)
N2	Cu1	O1	88.9(8)	N3	C3	C2	125.4(5)
C5	N2	Cu1	120.1(4)	N3	C3	C4	116.9(5)
C5	N2	C1	117.0(5)	C2	C3	C4	117.7(5)
C1	N2	Cu1	122.8(4)	O5B	C11B	N4B	129(2)
C6	N3	C3	127.2(5)	O5A	C11A	N4A	124(2)
N2	C5	C4	123.2(5)	C11A	N4A	C13A	104(2)
N2	C1	C2	123.4(5)	C11A	N4A	C12A	121(2)
C10	C7	C6	121.4(5)	C12A	N4A	C13A	134.6(16)
C8	C7	C6	119.0(5)	O2	N5	O1	119.0(14)
C8	C7	C10	119.6(5)	O3	N5	O1	121.7(10)

Table SI 8: Bond Angles for MOF 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	C6	N3	123.7(5)	O3	N5	O2	119.3(15)
O4	C6	C7	121.6(5)	N5	O1	Cu1	137.8(10)

Table SI 9: Torsion Angles for MOF 1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	N2	C5	C4	-179.6(5)	C10	C7	C6	O4	-149.4(5)
Cu1	N2	C1	C2	178.5(5)	C10	C7	C6	N3	30.5(7)
N2	C5	C4	C3	0.8(9)	C10	C7	C8	C9	-1.2(8)
N2	C1	C2	C3	1.3(9)	C8	C7	C6	O4	30.5(9)
C5	N2	C1	C2	0.5(9)	C8	C7	C6	N3	-149.7(5)
C5	C4	C3	N3	-178.1(6)	C8	C7	C10	C7[1]	0.6(4)
C5	C4	C3	C2	1.0(9)	C3	N3	C6	O4	2.4(10)
C1	N2	C5	C4	-1.6(9)	C3	N3	C6	C7	-177.5(5)
C1	C2	C3	N3	177.1(6)	O5A	C11A	N4A	C13A	172.8(18)
C1	C2	C3	C4	-2.0(9)	O5A	C11A	N4A	C12A	-1(3)
C7	C8	C9	C8[1]	0.6(4)	C13B	N4B	C11B	O5B	0(4)
C6	N3	C3	C2	12.0(10)	C12B	N4B	C11B	O5B	-172(2)
C6	N3	C3	C4	-168.9(6)	O2	N5	O1	Cu1	-170(3)
C6	C7	C10	C7[1]	-179.6(6)	O3	N5	O1	Cu1	11(4)
C6	C7	C8	C9	178.9(4)					

Table SI 10: Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for MOF 1.

Atom	*x*	*y*	*z*	U(eq)
H3	7392.56	3382.74	4762.13	27
H5	5473.42	2894.41	3928.02	22
H1	4263.14	4595.18	4369.87	23
H2	5385.72	4576.09	4785.18	24
H10	8749.97	3750.02	4895.12	25
H8	7341.37	3987.76	5757.76	22
H4	6648.74	2850.25	4318.95	25
H9	8749.99	3749.99	6046.13	28
H13D	9424.37	2992.99	3875.47	55
H13E	10010.04	2242.84	3827.57	55
H13F	10519.56	2955.03	3980.37	55
H11B	8933.15	2192.42	4656.5	38
H11A	8606.04	3107.39	4175.8	39
H13A	10178.43	2188.66	3822.58	60
H13B	10888.01	2692.27	4033.44	60
H13C	9876.19	3010.71	3922.84	60
H12D	9780.5	2025.83	4751.88	65
H12E	10735.75	1962.17	4539.87	65
H12F	9867.92	1413.1	4469.38	65

Table SI 10: Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for MOF 1.

Atom	*x*	*y*	*z*	U(eq)
H12A	11047.06	1837.12	4354.35	78
H12B	10288.43	1322.14	4171.29	78
H12C	10201.69	1464.59	4559.12	78

Table SI 11: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for MOF 2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ni01	12533.5(4)	10000	6666.666667	48.84(16)
Cl1	12215.6(7)	9381.0(6)	5419.4(4)	56.1(2)
N3	4108(2)	6695(2)	7280.3(15)	53.5(7)
N4	3001(2)	8853(2)	6871.6(14)	54.4(7)
N1	10937(2)	8877(2)	6899.1(16)	54.9(7)
O2	3082(2)	5711(2)	8208.6(16)	81.8(8)
N2	7737(2)	6702(2)	7442.1(16)	57.5(8)
O1	7424(2)	5107(2)	6978.3(18)	91.1(9)
C12	5388(3)	4077(3)	7738(2)	60.8(9)
C7	5962(3)	5169(3)	7519(2)	55.0(9)
C13	3802(3)	5932(3)	7781(2)	58.0(9)
C16	3667(3)	7376(3)	7155.2(19)	56.0(9)
C6	7072(3)	5611(3)	7294(2)	61.3(9)
C14	2656(3)	8205(3)	7444.8(18)	56.4(9)
C24	4382(3)	5320(2)	7772.1(17)	48.2(8)
C3	8796(3)	7379(3)	7255.7(18)	51.5(8)
C5	10456(3)	7864(3)	6674(2)	62.7(9)
C17	4021(3)	8005(3)	6564(2)	62.8(10)
C15	2961(3)	7464(3)	7595.7(19)	58.0(9)
C4	9398(3)	7101(3)	6829(2)	64.8(10)
C8	5434(3)	5766(2)	7543.6(17)	54.3(8)
C11	4364(3)	3666(3)	8010(2)	79.3(12)
C10	3857(3)	4260(3)	8036(2)	63.4(10)
C1	10333(3)	9124(3)	7326(2)	66.4(10)
C18	3666(3)	8738(3)	6431.9(19)	66.2(10)
C2	9269(3)	8407(3)	7500(2)	65.1(10)

Table SI 12: Anisotropic Displacement Parameters (Å²×10³) for MOF 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni01	41.9(2)	48.7(3)	58.3(3)	24.34(16)	4.62(14)	9.2(3)
Cl1	57.9(5)	52.1(4)	59.8(4)	28.7(4)	6.7(4)	9.9(4)
N3	51.4(16)	56.6(17)	60.1(17)	32.7(14)	-3.5(13)	4.7(14)

N4	45.7(15)	57.7(17)	59.8(16)	25.9(14)	6.8(12)	9.7(13)
N1	46.8(16)	56.5(19)	66.0(18)	29.3(14)	6.1(14)	-1.7(14)
O2	80.0(19)	75.5(18)	97(2)	43.9(16)	16.6(17)	31.0(17)
N2	47.6(17)	42.6(16)	79.6(19)	20.6(14)	3.9(14)	-10.8(13)
O1	70.1(19)	60.4(16)	144(3)	33.3(14)	4.8(18)	-30.9(19)
C12	56(2)	43.8(19)	81(2)	23.9(17)	-13.1(19)	4.2(18)
C7	51(2)	42.6(18)	68(2)	20.8(16)	-10.9(16)	-9.1(16)
C13	52(2)	52(2)	68(2)	23.9(17)	-2.5(18)	2.5(17)
C16	54(2)	57(2)	62(2)	31.1(18)	-11.3(17)	-7.7(17)
C6	49(2)	50(2)	81(2)	22.2(17)	6.9(19)	-3.0(19)
C14	64(2)	59(2)	61(2)	41.8(18)	5.1(17)	2.8(17)
C24	43.4(19)	37.7(17)	59.1(19)	16.9(14)	-7.3(15)	0.5(15)
C3	46(2)	43.2(18)	60(2)	18.7(16)	2.9(16)	1.6(16)
C5	57(2)	65(2)	72(2)	35(2)	14.4(18)	-11(2)
C17	56(2)	78(3)	72(2)	47(2)	12.7(17)	23.4(19)
C15	65(2)	57(2)	57(2)	34.2(19)	6.7(18)	6.5(17)
C4	62(2)	51(2)	76(2)	23.5(19)	9.5(18)	-9.0(18)
C8	56(2)	39.9(16)	65.4(19)	22.6(17)	-13.8(18)	0.6(14)
C11	65(3)	34.5(18)	124(4)	15(2)	-18(3)	4(2)
C10	46.0(19)	51(2)	82(3)	16.2(17)	-9.8(17)	5.8(18)
C1	49(2)	56(2)	90(3)	22.7(17)	-1.6(19)	-11.1(19)
C18	74(2)	79(3)	67(2)	54(2)	19(2)	24(2)
C2	53(2)	53(2)	75(2)	15.8(18)	11.3(17)	-20.3(19)

Table SI 13: Bond Lengths for MOF 2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni01	Cl1	2.4733(9)	C12	C7	1.420(5)
Ni01	Cl11	2.4733(9)	C12	C11	1.382(5)
Ni01	N42	2.103(3)	C7	C6	1.454(5)
Ni01	N43	2.103(3)	C7	C8	1.403(5)
Ni01	N1	2.088(3)	C13	C24	1.485(5)
Ni01	N11	2.088(3)	C16	C17	1.363(5)
N3	C13	1.343(4)	C16	C15	1.364(5)
N3	C16	1.426(4)	C14	C15	1.368(4)
N4	C14	1.349(4)	C24	C8	1.383(5)
N4	C18	1.336(4)	C24	C10	1.409(5)
N1	C5	1.330(4)	C3	C4	1.379(5)

N1	C1	1.355(4)	C3	C2	1.362(5)
O2	C13	1.220(4)	C5	C4	1.389(5)
N2	C6	1.397(4)	C17	C18	1.404(5)
N2	C3	1.379(4)	C11	C10	1.373(5)
O1	C6	1.225(4)	C1	C2	1.389(4)

Table SI 14: Bond Angles for MOF 2.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Cl1	Ni01	Cl11	179.44(5)	O2	C13	N3	124.4(3)
N42	Ni01	Cl11	88.09(8)	C24	C13	N3	115.1(3)
N43	Ni01	Cl11	92.31(8)	C24	C13	O2	120.4(3)
N43	Ni01	Cl1	88.09(8)	C17	C16	N3	116.3(3)
N42	Ni01	Cl1	92.31(8)	C15	C16	N3	124.6(3)
N42	Ni01	N43	89.35(14)	C15	C16	C17	119.0(3)
N11	Ni01	Cl1	90.32(8)	O1	C6	N2	120.5(3)
N1	Ni01	Cl1	89.27(8)	C7	C6	N2	114.7(3)
N11	Ni01	Cl11	89.27(8)	C7	C6	O1	124.8(3)
N1	Ni01	Cl11	90.32(8)	C15	C14	N4	123.7(3)
N1	Ni01	N43	90.78(10)	C8	C24	C13	122.4(3)
N11	Ni01	N43	178.41(11)	C10	C24	C13	118.7(3)
N1	Ni01	N42	178.41(11)	C10	C24	C8	118.8(3)
N11	Ni01	N42	90.78(10)	C4	C3	N2	125.1(3)
N11	Ni01	N1	89.13(15)	C2	C3	N2	117.1(3)
C16	N3	C13	126.9(3)	C2	C3	C4	117.8(3)
C14	N4	Ni014	122.5(2)	C4	C5	N1	124.2(3)
C18	N4	Ni014	120.8(2)	C18	C17	C16	119.1(3)
C18	N4	C14	116.7(3)	C14	C15	C16	119.2(3)
C5	N1	Ni01	123.3(2)	C5	C4	C3	119.4(3)

C1	N1	Ni01	121.5(2)	C24	C8	C7	121.8(3)
C1	N1	C5	115.2(3)	C10	C11	C12	122.0(3)
C3	N2	C6	129.4(3)	C11	C10	C24	119.7(3)
C11	C12	C7	119.1(3)	C2	C1	N1	123.8(3)
C6	C7	C12	118.2(3)	C17	C18	N4	122.3(3)
C8	C7	C12	118.2(3)	C1	C2	C3	119.5(3)

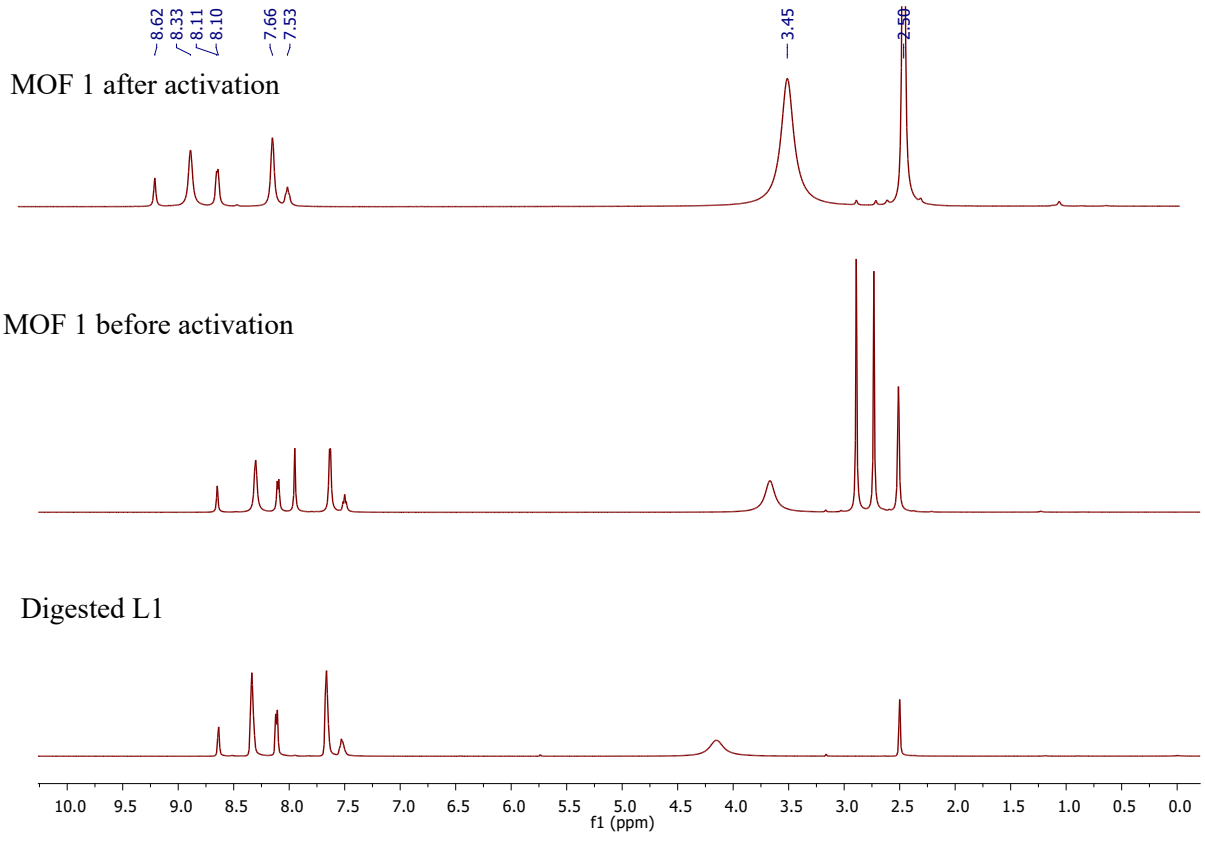

Figure SI 5: ^{1}H NMR spectra of digested ligand **L1**, **MOF 1** before and after activation recorded in DMSO-d_6.

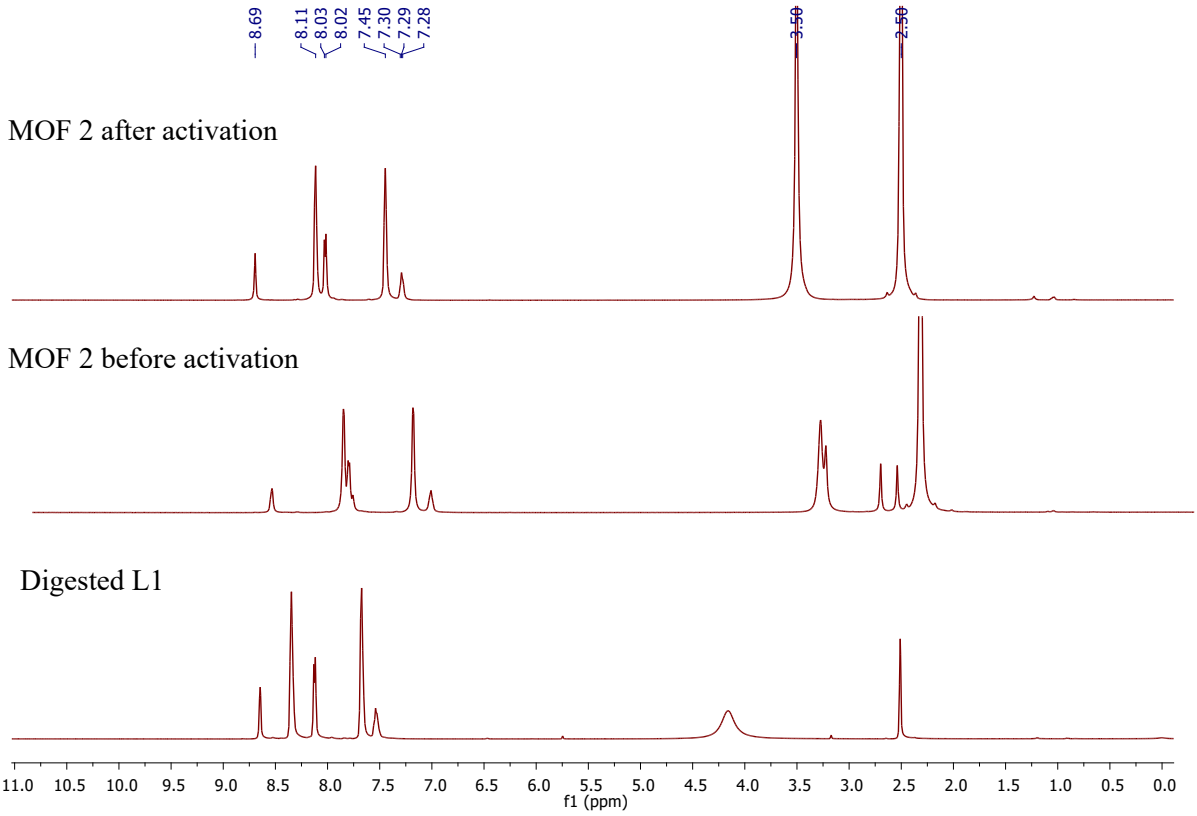

Figure SI 6: ^{1}H NMR spectra of digested ligand **L1**, **MOF 2** before and after activation recorded in DMSO-d_6.

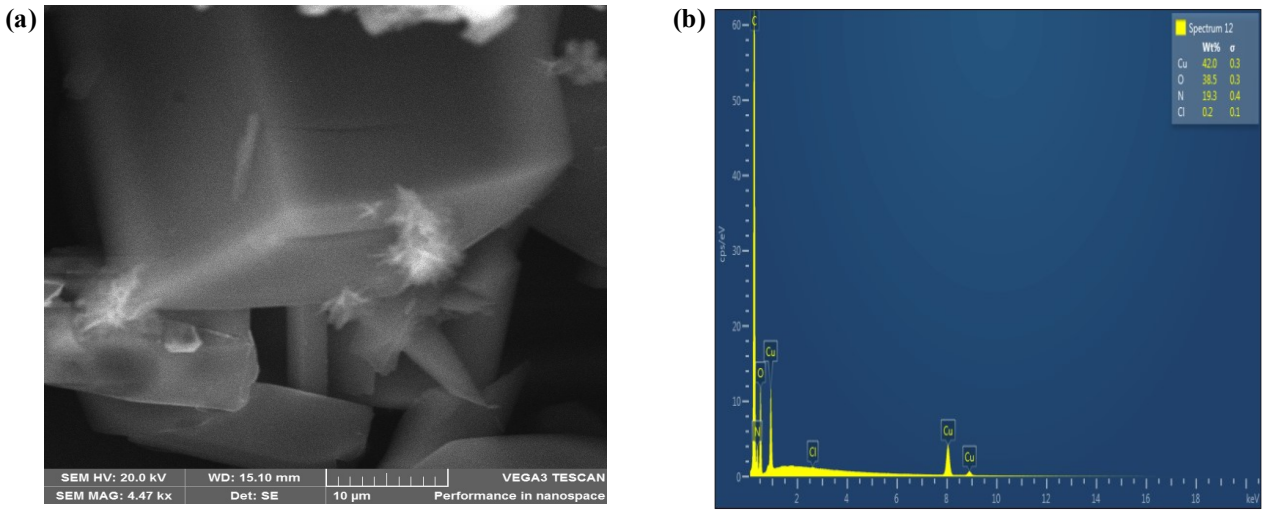

Figure SI 7: SEM-EDX images for **MOF 1**.

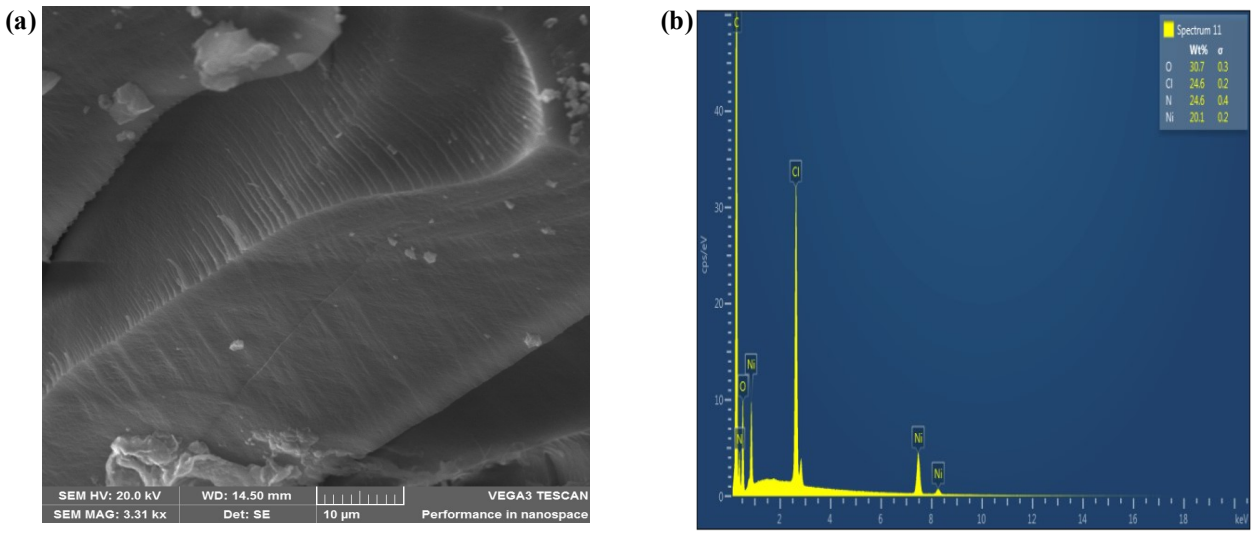

Figure SI 8: SEM-EDX images for **MOF 2**.

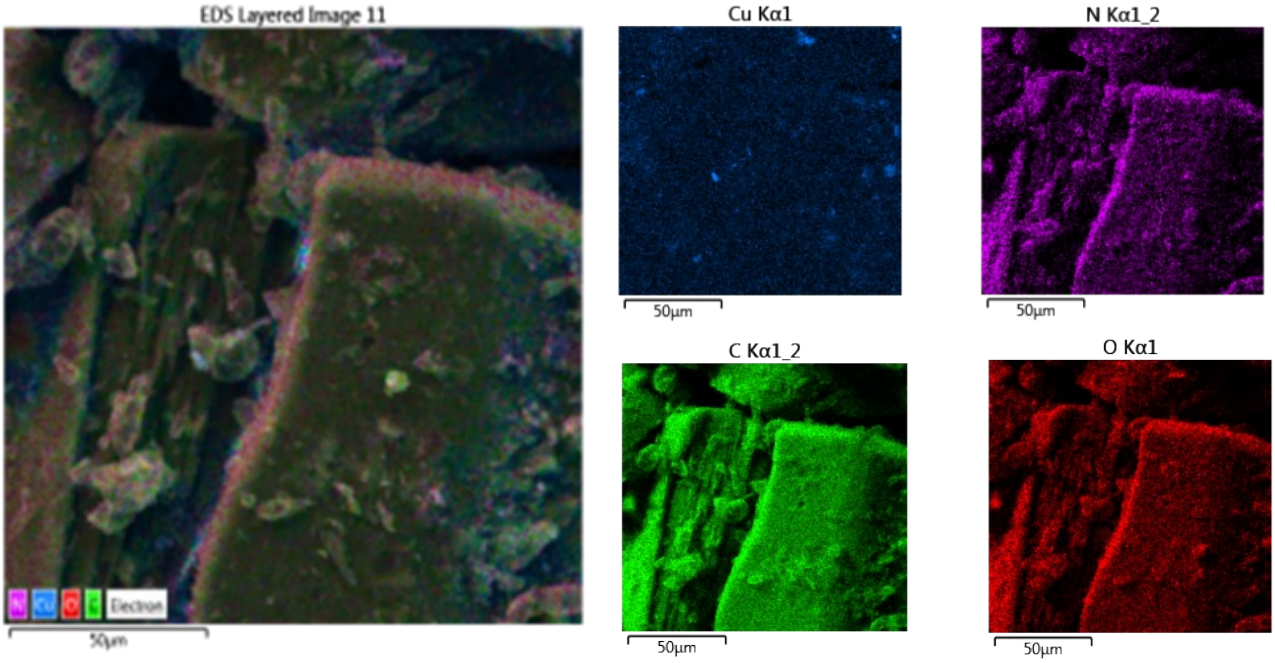

Figure SI 9: EDX mapping images for **MOF 1**.

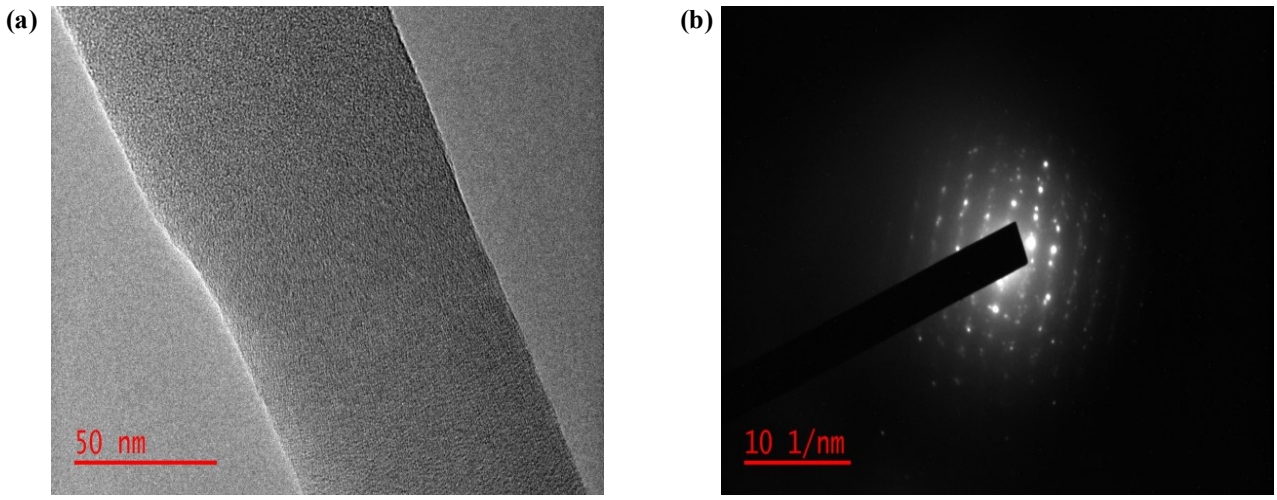

Figure SI 10: HR-TEM and SAED images of **MOF 1**.

Catalytic hydrogenation of furfural

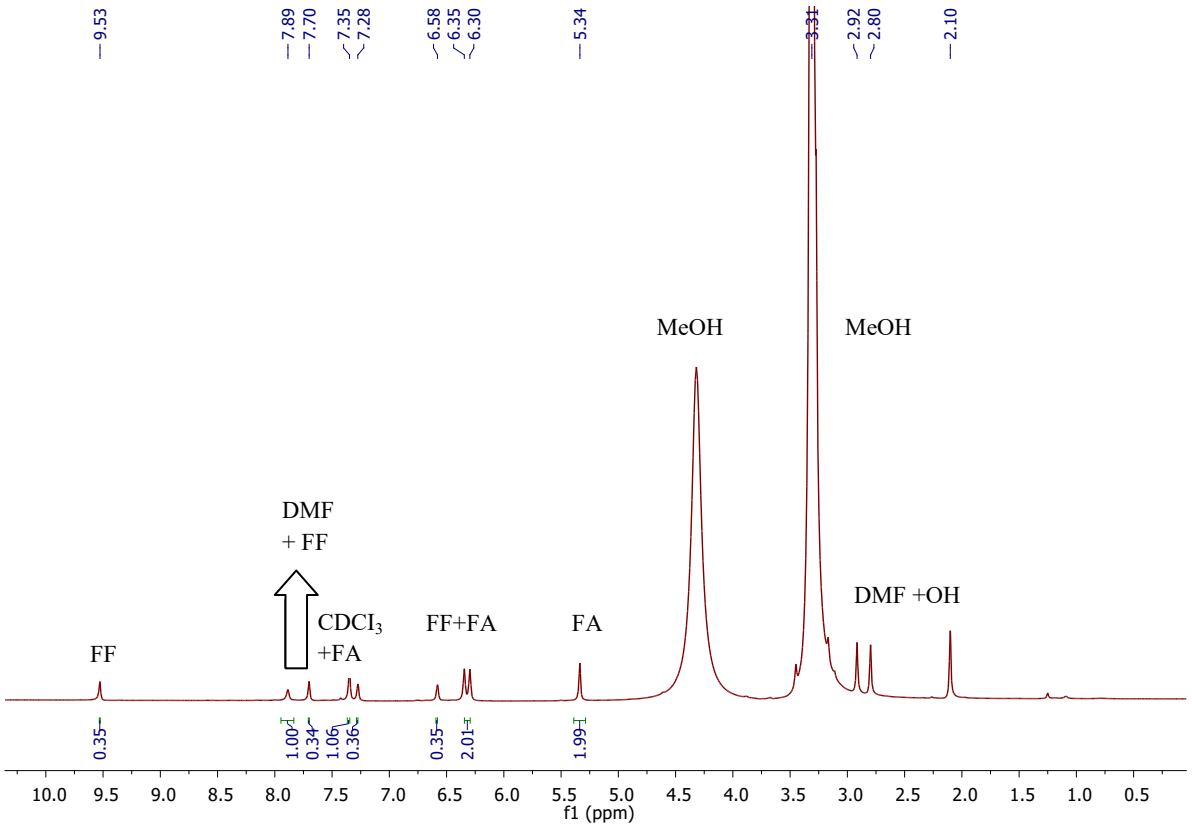

Figure SI 11: Representative ^{1}H NMR of the hydrogenation of FF reaction using molecular H_2, 140 ^{o}C, methanol (5 mL), substrate (FF, 2.5 mmol), pre-catalyst (**MOF 2**), time (24 hours), showing product of FA only, recorded in $CDCl_3$.

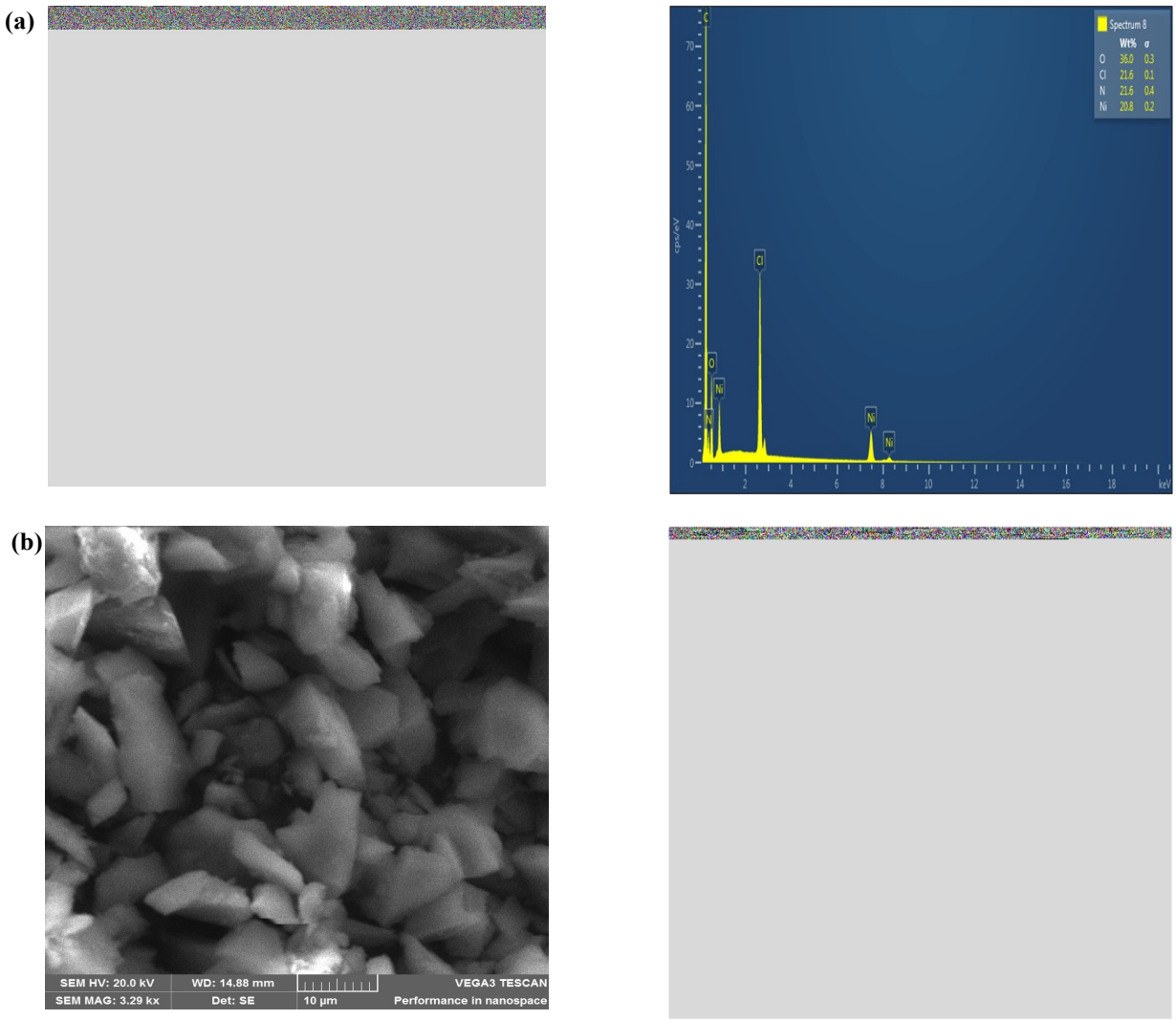

Figure SI 12: SEM-EDX images for (a) **MOF 2** before catalysis and (b) **MOF 2** after the 4th recycle.

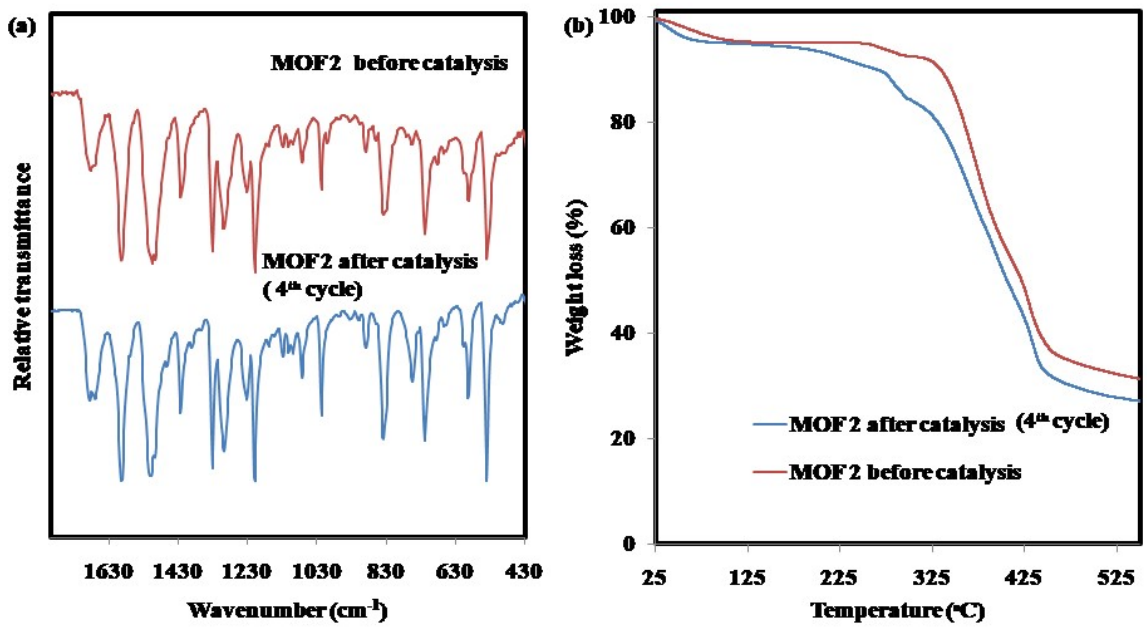

Figure SI 13: (a) FT-IR spectra and (b) TGA curves of the **MOF 2** before and after the 4th recycle.