Terephthalate and trimesate metal-organic frameworks of Mn, Co, and Ni: Exploring photostability by spectroscopy

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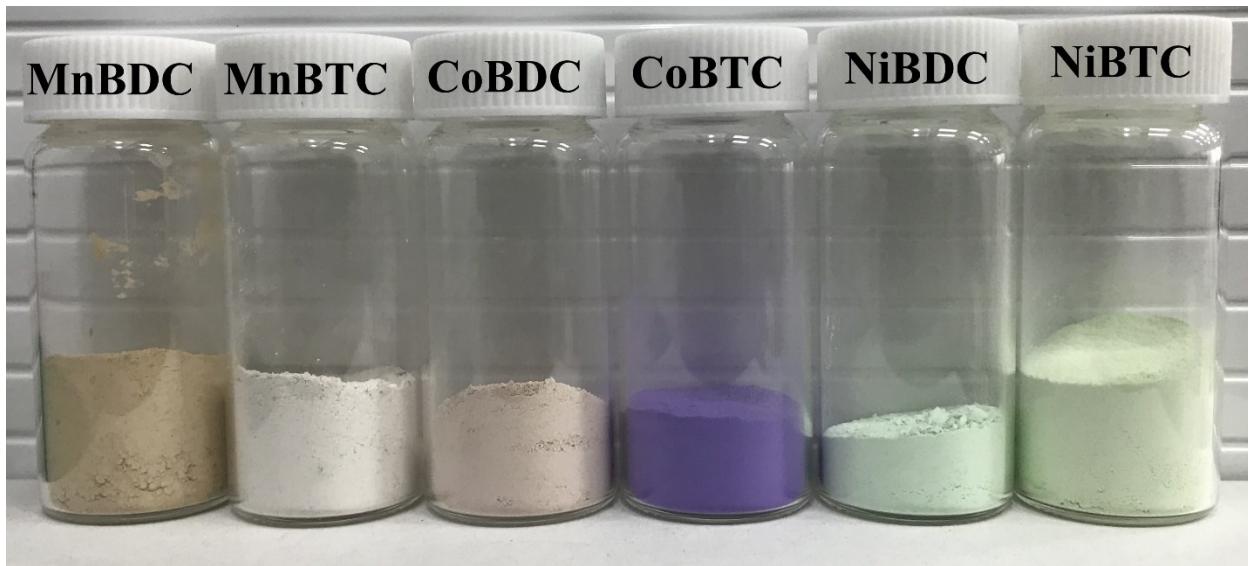
Supplementary figure 1. Photograph of synthesized transition MOFs.
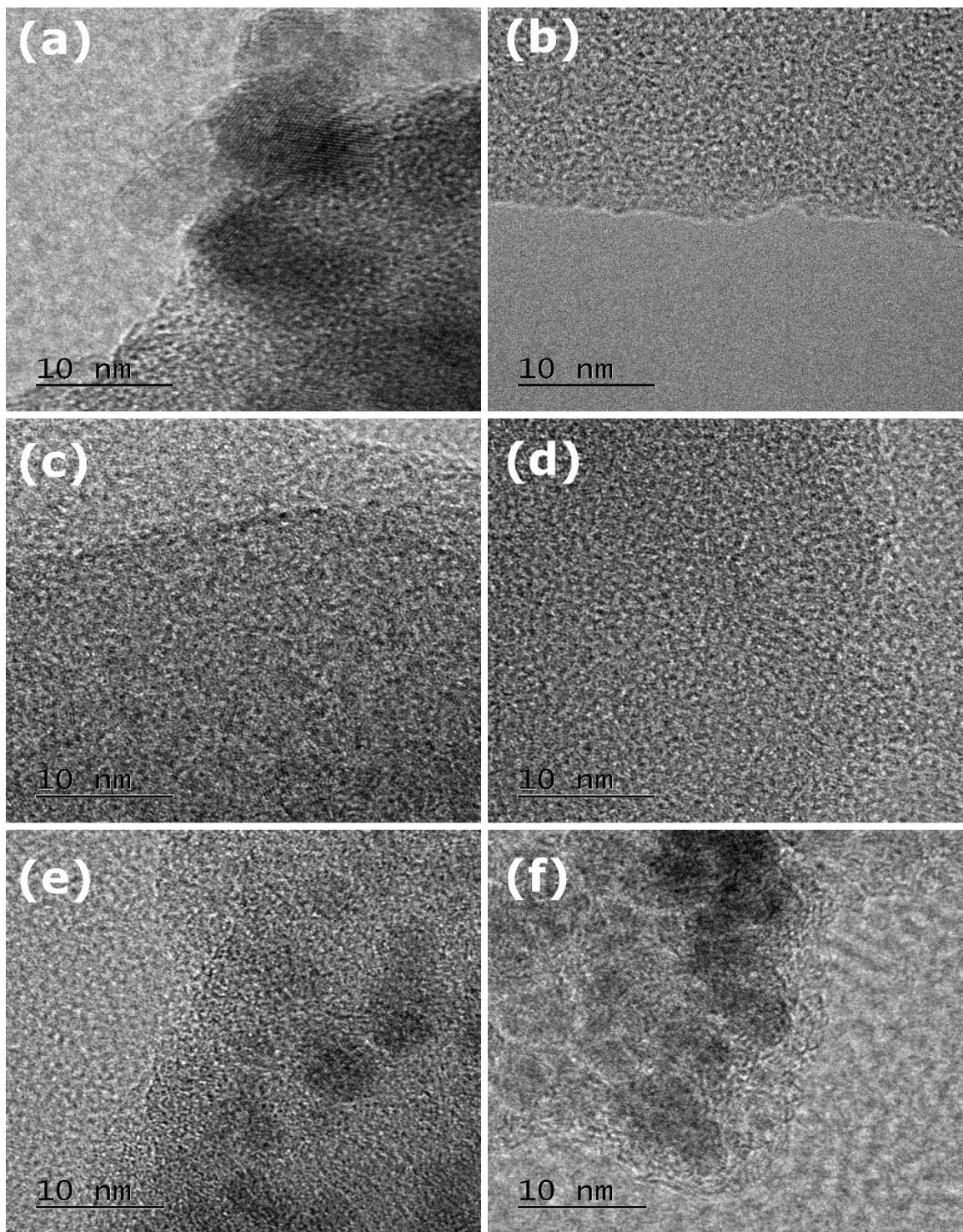
Supplementary figure 2. TEM images of (**a**) MnBDC; (**b**) MnBTC; (**c**) CoBDC; (**d**) CoBTC; (**e**) NiBDC; (**f**) NiBTC at 10 nm resolution.
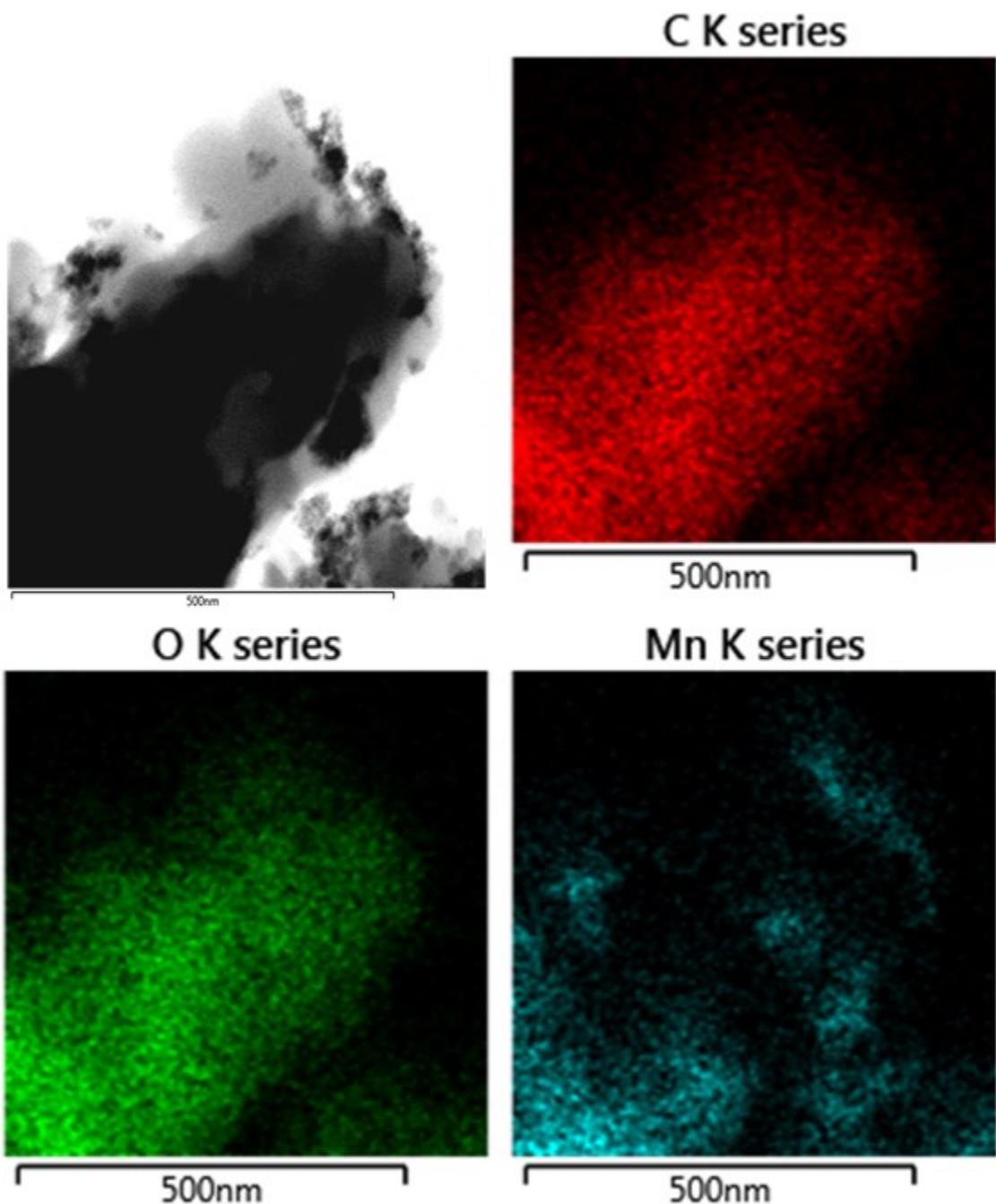
Supplementary figure 3a. 2D elemental mapping of MnBDC.
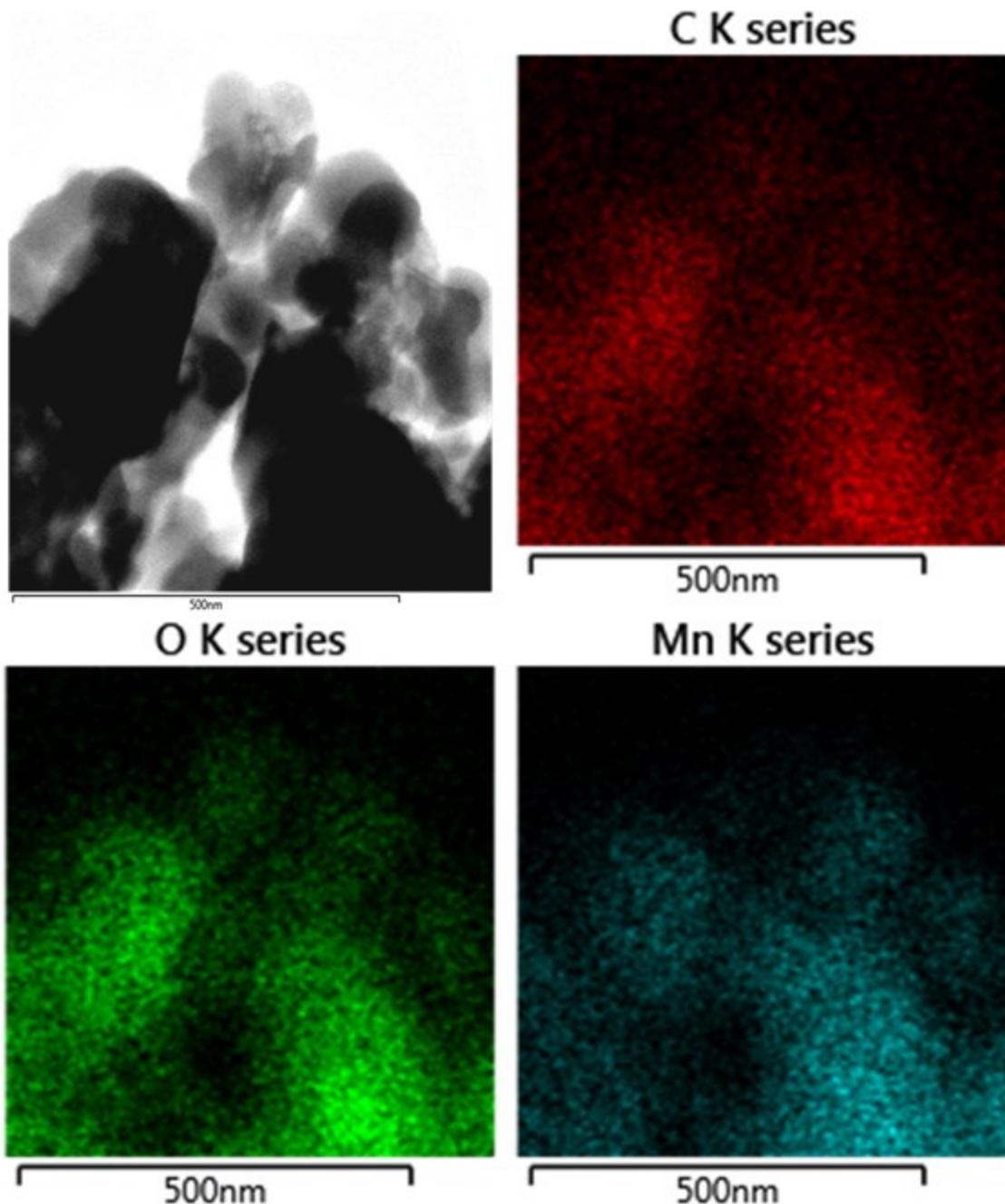
Supplementary figure 3b. 2D elemental mapping of MnBTC.
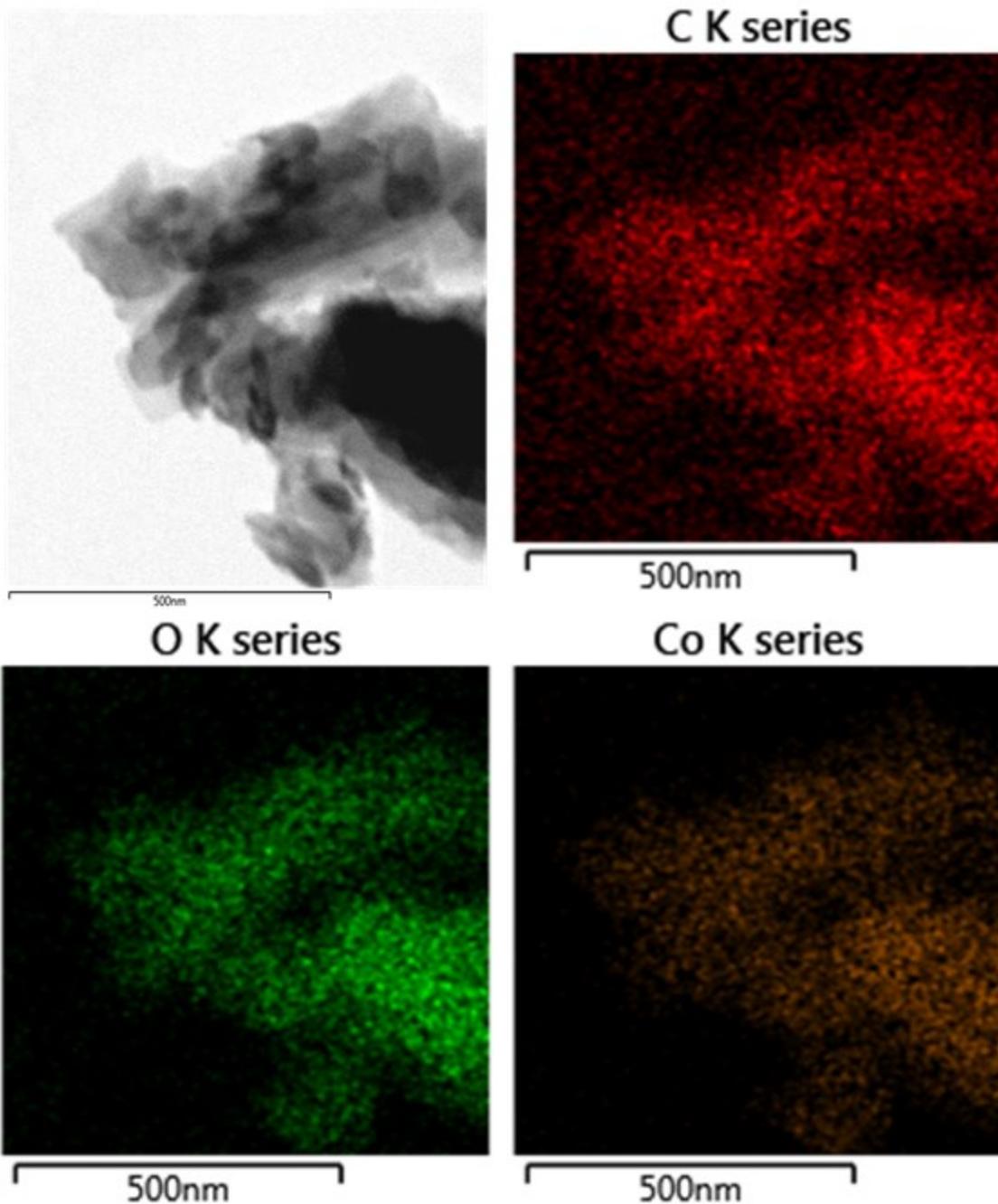
Supplementary figure 3c. 2D elemental mapping of CoBDC.
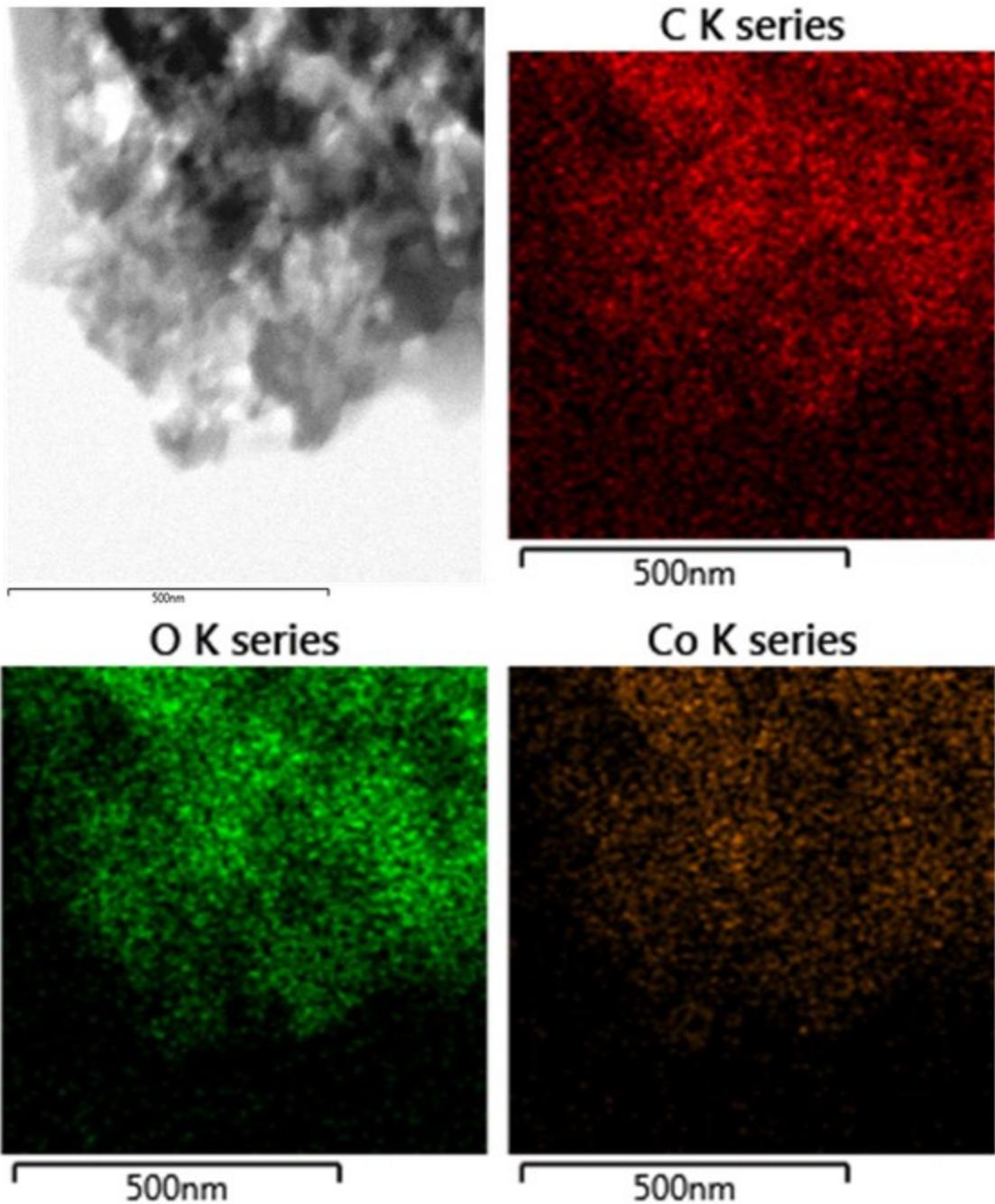
**Supplementary figure 3d.** 2D elemental mapping of CoBTC.
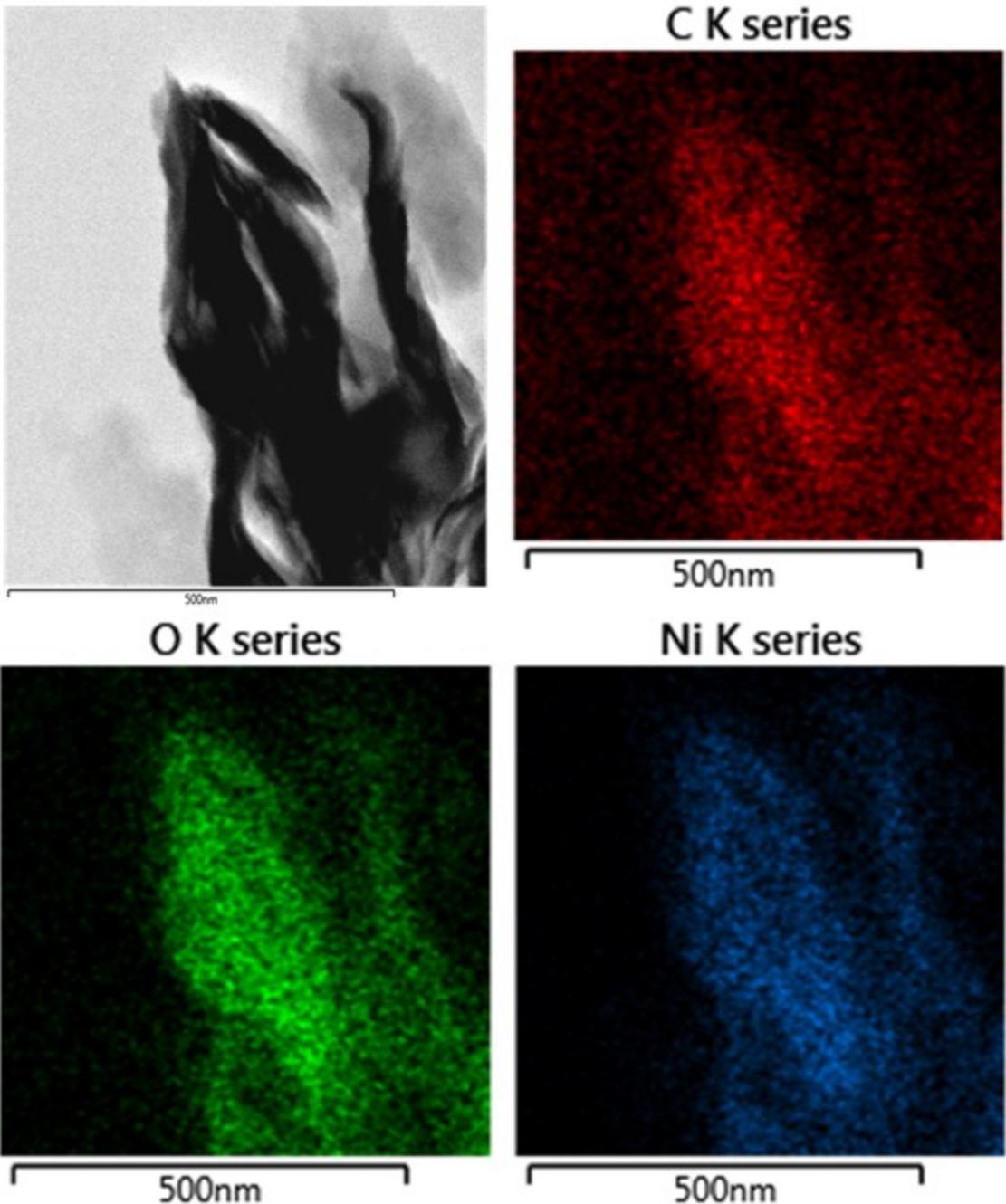
Supplementary figure 3e. 2D elemental mapping of NiBDC.
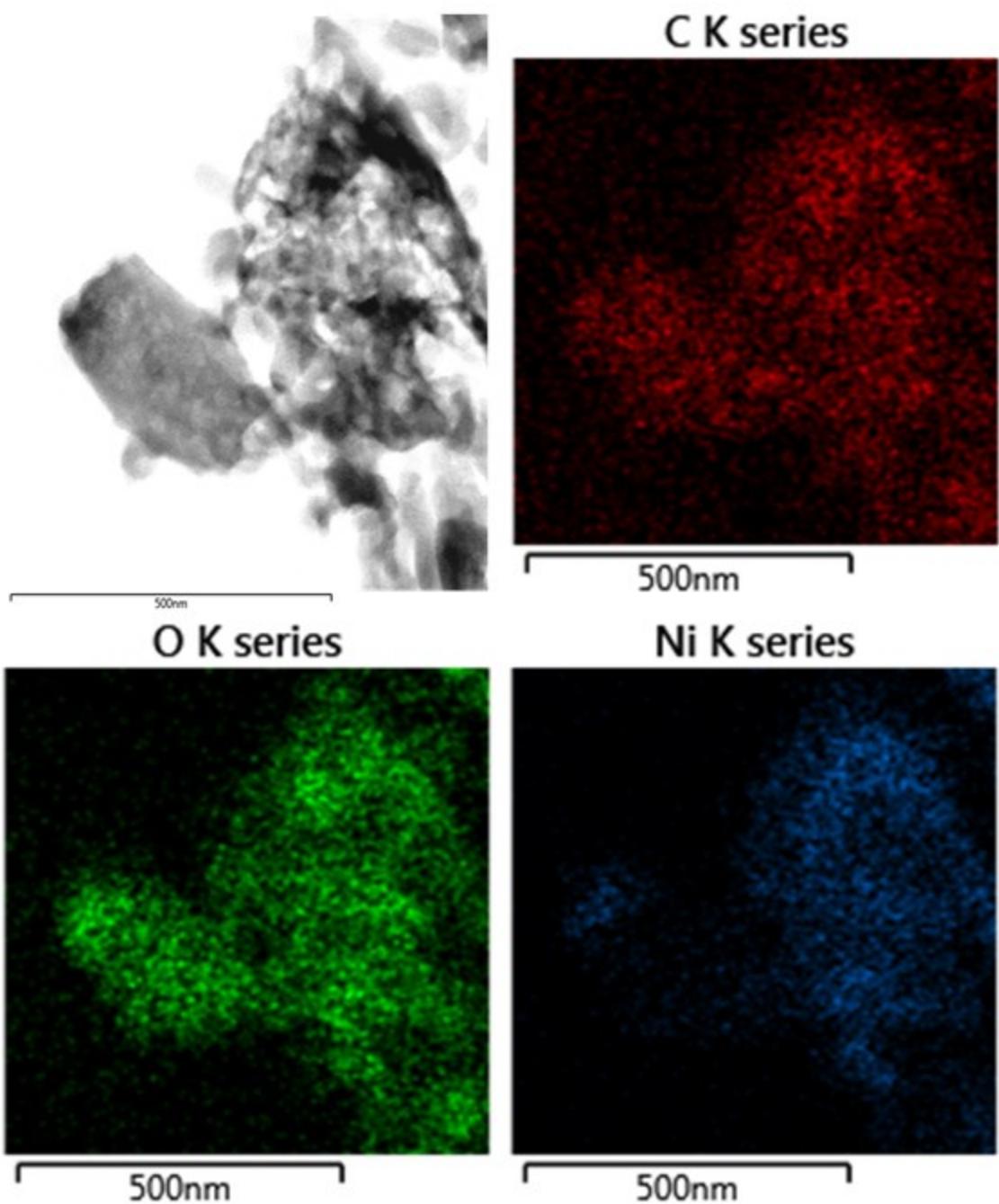
Supplementary figure 3f. 2D elemental mapping of NiBTC.
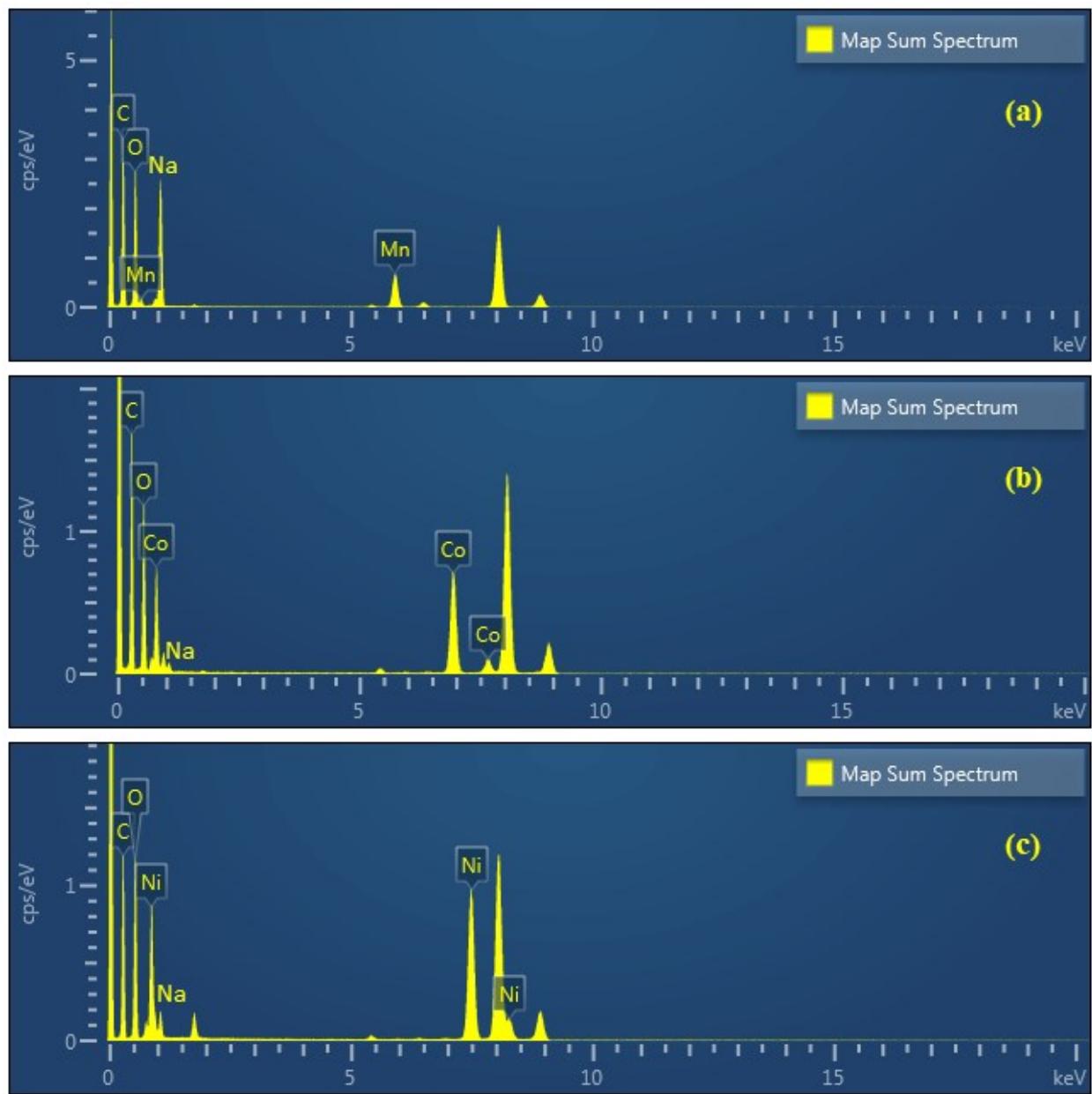
Supplementary Figure 4. TEM-EDS analysis of (**a**) MnBDC; (**b**) CoBDC; (**c**) NiBDC.
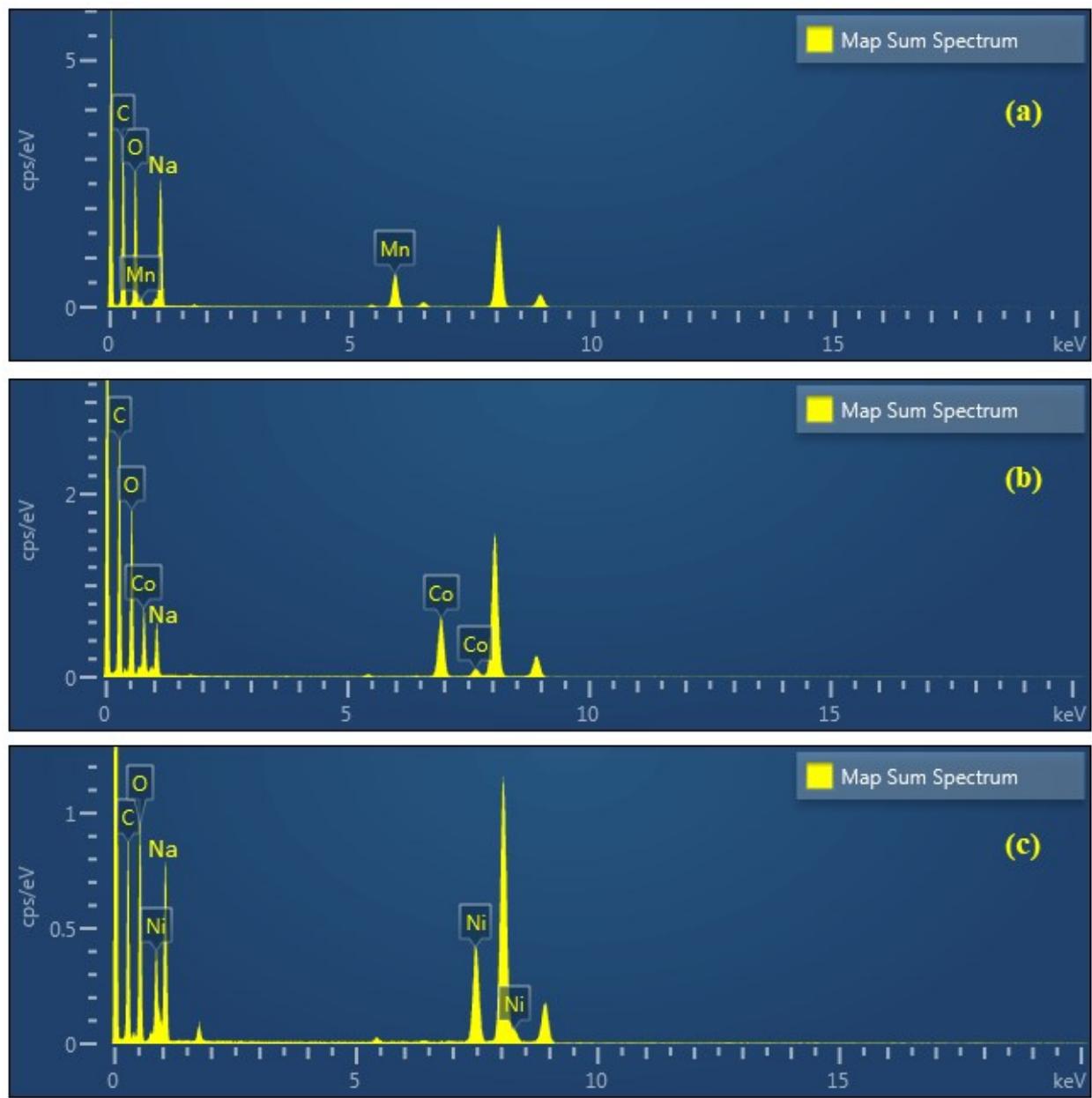
Supplementary Figure 5. TEM-EDS analysis of (**a**) MnBTC; (**b**) CoBTC; (**c**) NiBTC.
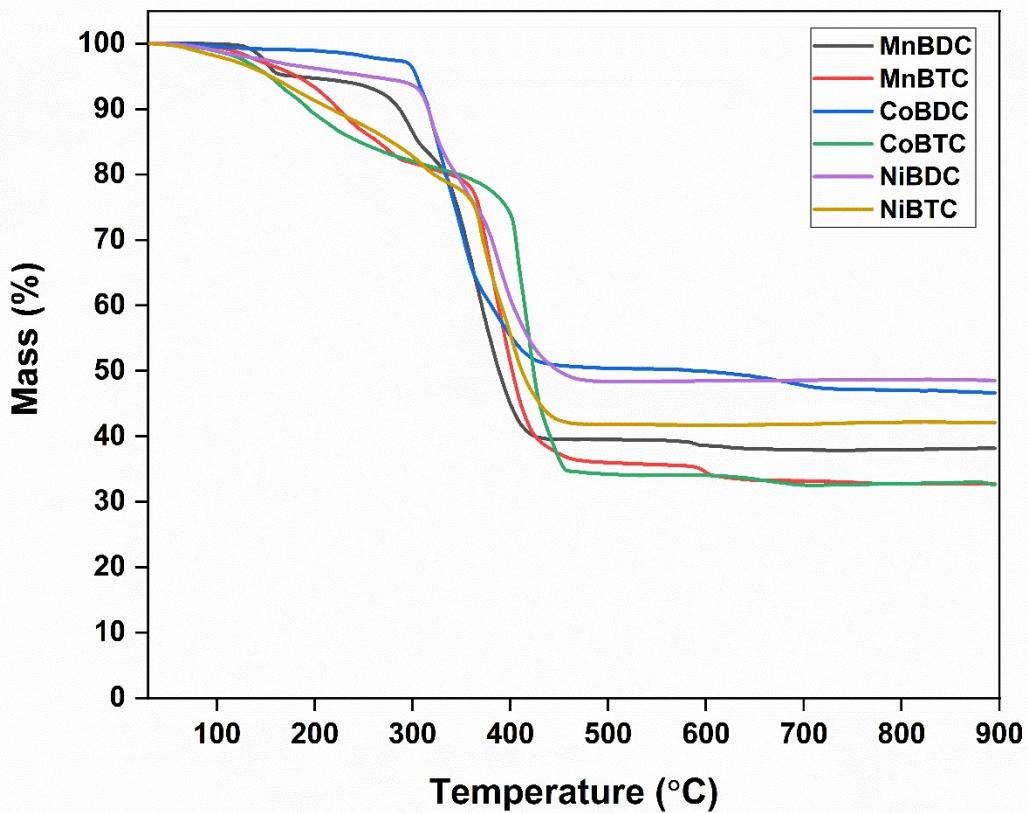
Supplementary Figure 6. TGA profiles of MOFs.
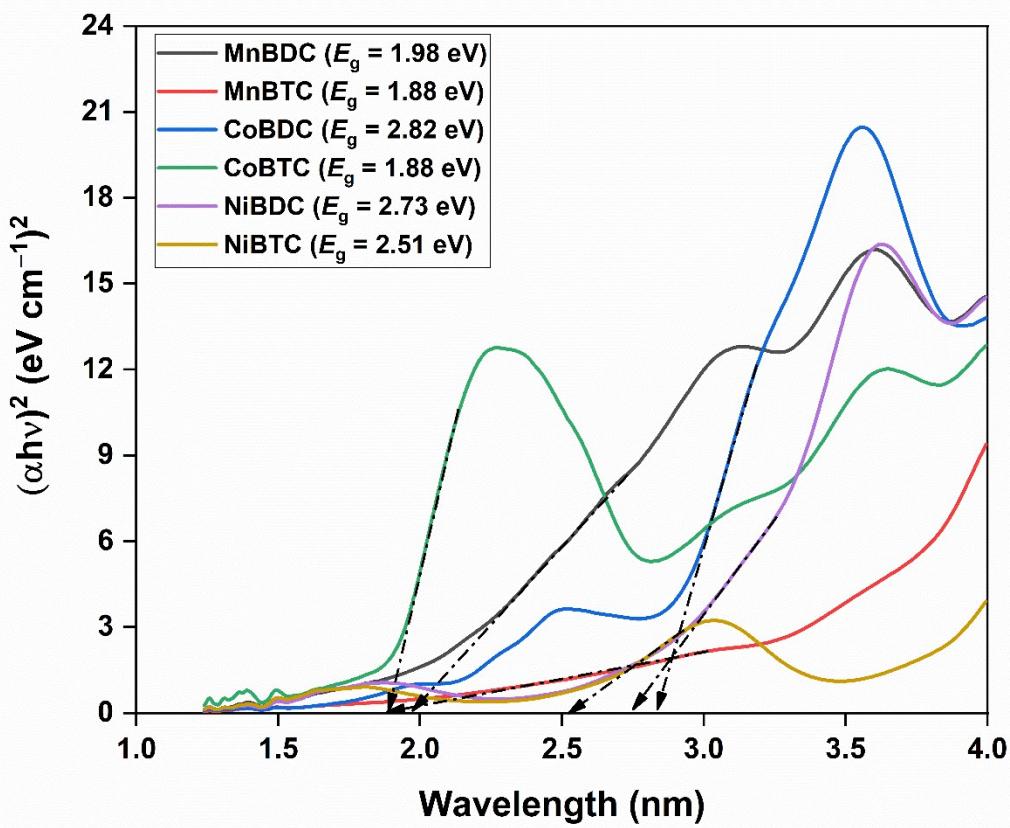
Supplementary Figure 7. Tauc plots for MOFs.
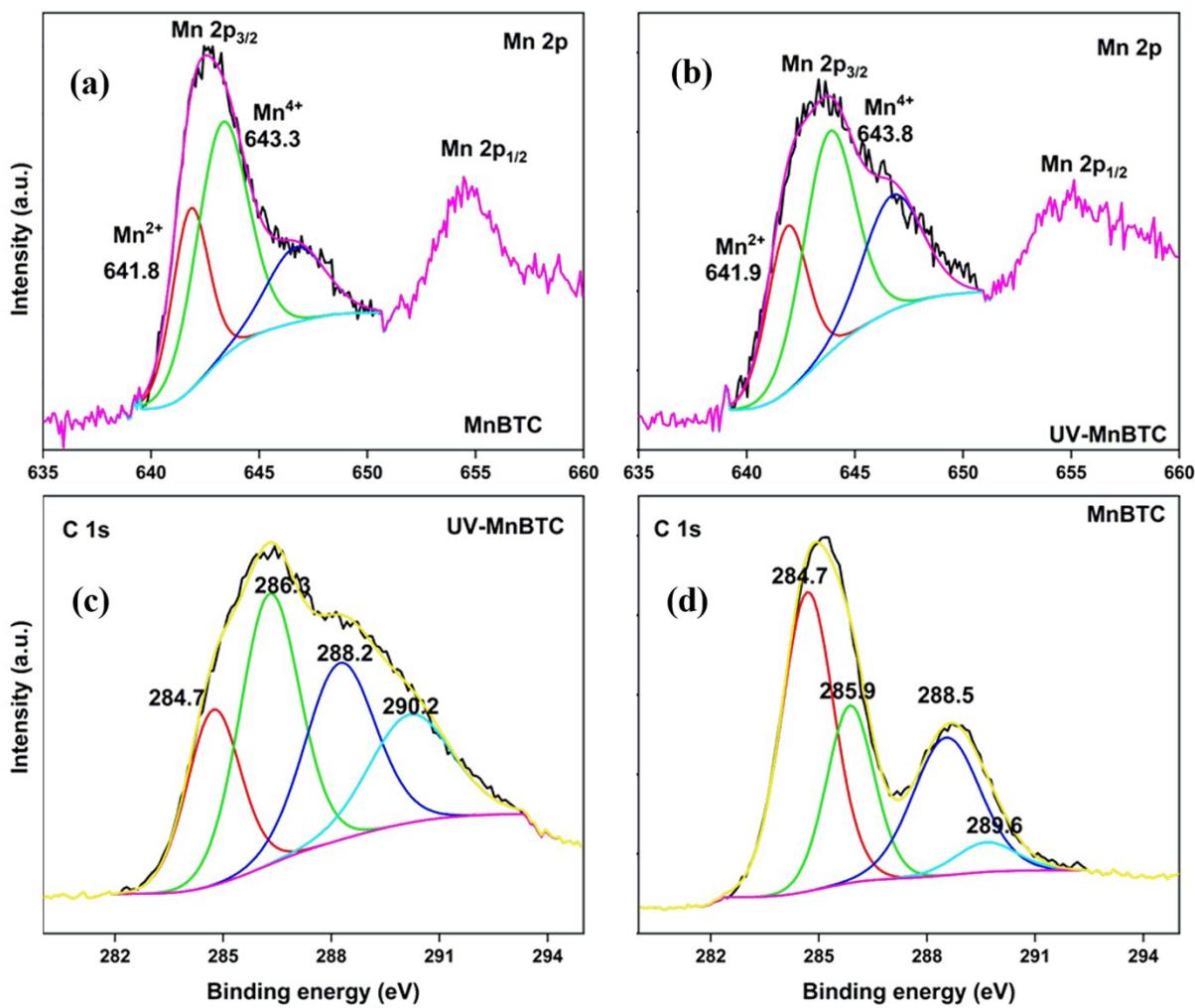
Supplementary Figure 8. HRXPS Mn 2p spectra of (**a**) MnBTC; (**b**) UV-MnBTC; HRXPS C 1s spectra of (**c**) MnBTC; (**d**) UV-MnBTC
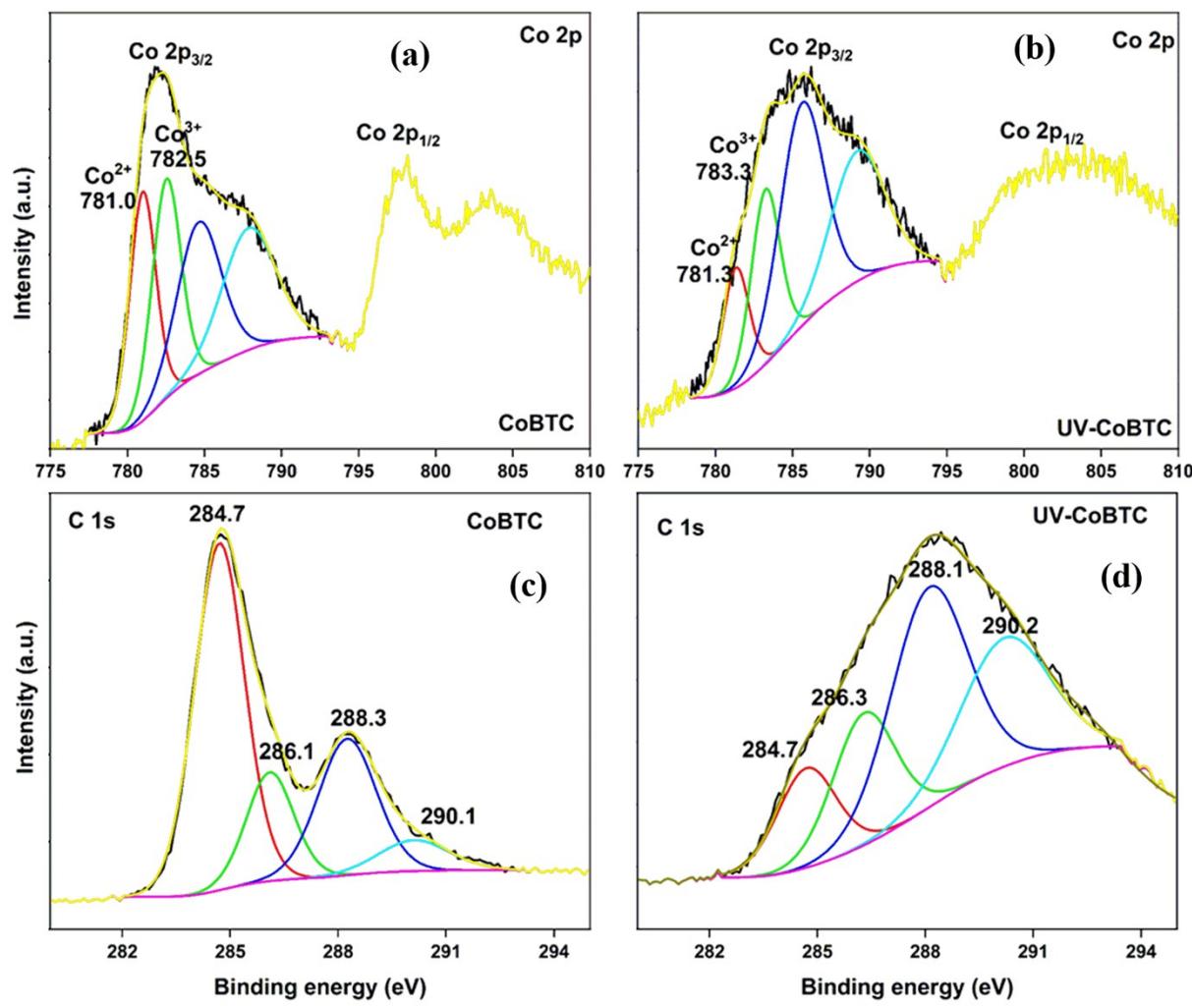
Supplementary Figure 9. HRXPS Co 2p spectra of (a) CoBTC; (b) UV-CoBTC; HRXPS C 1s spectra of (c) CoBTC; (d) UV-CoBTC
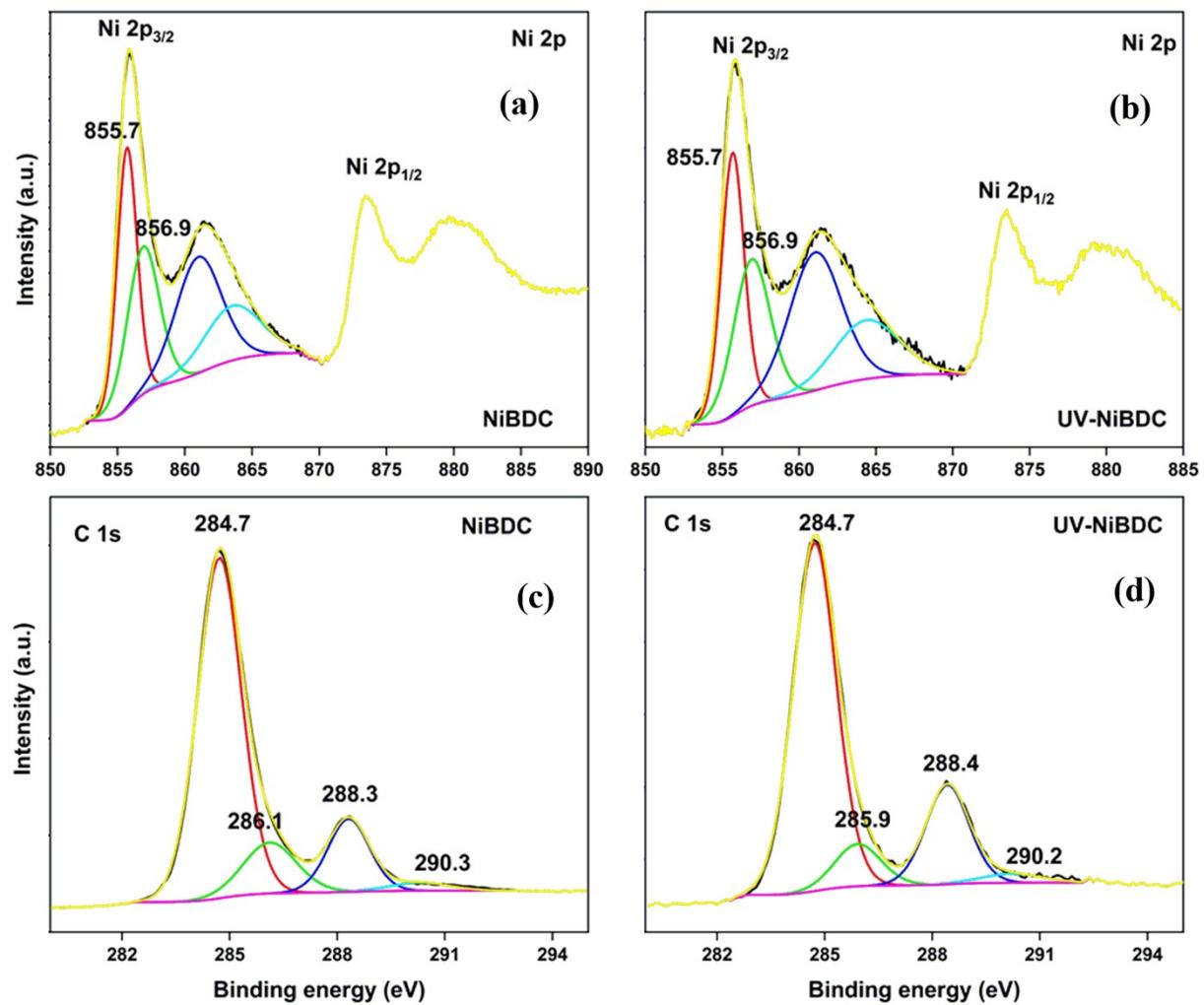
Supplementary Figure 10. HRXPS Ni 2p spectra of (a) NiBDC; (b) UV-NiBDC; HRXPS C 1s spectra of (c) NiBDC; (d) UV-NiBDC

Supplementary Table 1. Curve fitting parameters from Mn 2p spectra of Mn-MOFs

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
MnBDC	Mn2p$_{3/2}$ Mn2+	641.6	2.2	22.5
	Mn2p$_{3/2}$ Mn4+	643.6	2.8	77.5
	Mn2p$_{3/2}$ Satellite	646.0	3.2	-
UV-MnBDC	Mn2p$_{3/2}$ Mn2+	641.0	1.8	30.4
	Mn2p$_{3/2}$ Mn4+	642.5	2.8	69.6
	Mn2p$_{3/2}$ Satellite	645.9	3.2	-
MnBTC	Mn2p$_{3/2}$ Mn2+	641.8	2.0	35.4
	Mn2p$_{3/2}$ Mn4+	643.3	2.8	64.6
	Mn2p$_{3/2}$ Satellite	646.7	3.2	-
UV-MnBTC	Mn2p$_{3/2}$ Mn2+	641.9	2.2	37.0
	Mn2p$_{3/2}$ Mn4+	643.8	2.8	63.0
	Mn2p$_{3/2}$ Satellite	646.7	3.2	-

Supplementary Table 2. Curve fitting parameters from C 1s spectra of Mn-MOFs

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
MnBDC	C1s $_{C=C,C-H}$	284.7	1.9	11.6
	C1s $_{C-O}$	286.4	2.4	47.2
	C1s $_{-COOMn}$	288.2	2.2	31.3
	C1s $_{-COONa}$	290.2	2.4	10.0
UV-MnBDC	C1s $_{C=C,C-H}$	284.7	1.5	48.4

	C1s $_{C-O}$	286.1	1.7	27.3
	C1s $_{-COOMn}$	288.4	1.9	17.5
	C1s $_{-COONa}$	290.2	2.2	6.8
MnBTC	C1s $_{C=C,C-H}$	284.7	1.7	44.4
	C1s $_{C-O}$	285.9	1.5	23.9
	C1s $_{-COOMn}$	288.5	2.2	26.4
	C1s $_{-COONa}$	289.6	2.0	5.2
UV-MnBTC	C1s $_{C=C,C-H}$	284.7	1.7	20.0
	C1s $_{C-O}$	286.3	1.9	34.4
	C1s $_{-COOMn}$	288.2	2.3	26.5
	C1s $_{-COONa}$	290.2	2.7	19.0

Supplementary Table 3. Curve fitting parameters from Co 2p spectra of Co-MOFs

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
CoBDC	Co2p$_{3/2}$ $_{Co3+}$	781.1	2.0	49.1
	Co2p$_{3/2}$ $_{Co2+}$	782.7	2.2	50.9
	Co2p$_{3/2}$ $_{Satellite}$	785.0	3.2	-
	Co2p$_{3/2}$ $_{Satellite}$	788.2	3.9	-
UV-CoBDC	Co2p$_{3/2}$ $_{Co3+}$	781.1	2.0	48.2
	Co2p$_{3/2}$ $_{Co2+}$	782.6	2.2	51.8
	Co2p$_{3/2}$ $_{Satellite}$	784.8	3.2	-
	Co2p$_{3/2}$ $_{Satellite}$	788.0	3.9	-

Samples	Assignment			
CoBTC	**Co2p$_{3/2}$** Co3+	781.0	2.0	48.7
	Co2p$_{3/2}$ Co2+	782.5	2.2	51.3
	Co2p$_{3/2}$ Satellite	784.6	3.4	-
	Co2p$_{3/2}$ Satellite	787.9	4.1	-
UV-CoBTC	**Co2p$_{3/2}$** Co3+	781.3	2.0	38.5
	Co2p$_{3/2}$ Co2+	783.3	2.2	61.5
	Co2p$_{3/2}$ Satellite	785.6	3.4	-
	Co2p$_{3/2}$ Satellite	789.2	4.1	-

Supplementary Table 4. Curve fitting parameters from C 1s spectra of Co-MOFs

Samples	Assignment	E$_B$ (eV)	FWHM (eV)	At. %
CoBDC	**C1s** C=C,C–H	284.7	1.6	45.4
	C1s C–O	286.2	1.9	27.9
	C1s –COOCo	288.2	1.9	18.5
	C1s –COONa	290.2	2.2	8.2
UV-CoBDC	**C1s** C=C,C–H	284.7	1.5	50.1
	C1s C–O	286.0	1.8	28.1
	C1s –COOCo	288.4	1.7	13.4
	C1s –COONa	289.6	2.4	8.4
CoBTC	**C1s** C=C,C–H	284.7	1.6	53.2
	C1s C–O	286.1	1.6	15.8
	C1s –COOCo	288.3	1.9	24.3

	C1s _–COONa_	290.1	2.3	6.7
UV-CoBTC	**C1s** _C=C,C–H_	284.7	1.9	13.9
	C1s _C–O_	286.3	2.0	19.4
	C1s _–COOCo_	288.1	2.5	40.0
	C1s _–COONa_	290.2	2.9	26.7

Supplementary Table 5. Curve fitting parameters from Ni 2p spectra of Ni-MOFs

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
NiBDC	**Ni2p$_{3/2}$** _Ni2+_	855.7	1.7	52.5
	Ni2p$_{3/2}$ _Ni3+_	856.9	2.8	47.5
	Ni2p$_{3/2}$ _Satellite_	861.0	4.0	-
	Ni2p$_{3/2}$ _Satellite_	863.5	5.0	-
UV-NiBDC	**Ni2p$_{3/2}$** _Ni2+_	855.7	1.7	52.8
	Ni2p$_{3/2}$ _Ni3+_	856.9	2.8	47.2
	Ni2p$_{3/2}$ _Satellite_	861.0	4.0	-
	Ni2p$_{3/2}$ _Satellite_	864.4	5.0	-
NiBTC	**Ni2p$_{3/2}$** _Ni2+_	855.7	1.7	52.1
	Ni2p$_{3/2}$ _Ni3+_	856.9	2.8	47.9
	Ni2p$_{3/2}$ _Satellite_	861.1	4.2	-
	Ni2p$_{3/2}$ _Satellite_	864.3	5.5	-
UV-NiBTC	**Ni2p$_{3/2}$** _Ni2+_	853.2	1.5	4.1
	Ni2p$_{3/2}$ _Ni3+_	856.1	2.3	95.9

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
	Ni2p$_{3/2}$ Satellite	860.4	4.5	-
	Ni2p$_{3/2}$ Satellite	863.9	5.2	-

Supplementary Table 6. Curve fitting parameters from C 1s spectra of Ni-MOFs

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
NiBDC	**C1s** C=C,C–H	284.7	1.4	74.9
	C1s C–O	286.1	1.7	11.5
	C1s –COONi	288.3	1.3	11.3
	C1s –COONa	290.3	1.9	2.3
UV-NiBDC	**C1s** C=C,C–H	284.7	1.4	68.8
	C1s C–O	285.9	1.5	12.6
	C1s –COONi	288.4	1.4	16.1
	C1s –COONa	290.2	2.0	2.5
NiBTC	**C1s** C=C,C–H	284.7	1.4	66.3
	C1s C–O	286.2	1.4	7.5
	C1s –COONi	288.3	1.4	23.2
	C1s –COONa	290.3	1.8	3.0
UV-NiBTC	**C1s** C=C,C–H	284.7	1.6	12.2
	C1s C–O	286.3	1.8	54.0
	C1s –COONi	288.3	1.9	14.6
	C1s –COONa	290.0	1.9	19.2