Supplementary Materials:

N/N bridge type and substituents effects on chemical and crystallographic properties of Schiff-base (*salen*/salphen) Ni^{II} coordination compounds

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **NiMe*salen***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3492(1)	9677(3)	2525(4)	30(1)
C(2)	3813(1)	8745(3)	2604(4)	32(1)
C(3)	3456(1)	7849(3)	2637(5)	45(1)
C(4)	2808(2)	7890(3)	2566(5)	51(1)
C(5)	2483(1)	8808(3)	2466(5)	44(1)
C(6)	2828(1)	9689(3)	2442(4)	37(1)
C(7)	3814(1)	10628(3)	2574(4)	30(1)
C(8)	4681(1)	11765(2)	2902(4)	30(1)
C(17)	1769(1)	8830(3)	2393(6)	59(1)
O(1)	4431(1)	8667(2)	2671(3)	33(1)
Ni(1)	5000	9715(1)	2500	27(1)
N(1)	4417(1)	10737(2)	2625(3)	25(1)

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **NiMeO*salen***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2755(1)	2077(2)	3857(1)	13(1)
C(2)	3172(1)	1246(2)	3191(1)	12(1)

C(3)	2667(1)	315(2)	2348(1)	15(1)
C(4)	1810(1)	253(2)	2176(1)	17(1)
C(5)	1404(1)	1115(2)	2832(1)	16(1)
C(6)	1871(1)	2016(2)	3660(1)	16(1)
C(7)	3217(1)	2878(2)	4782(1)	13(1)
C(8)	4397(1)	3762(2)	6080(1)	14(1)
C(9)	5255(1)	2946(2)	6475(1)	15(1)
C(10)	6393(1)	2728(2)	5714(1)	14(1)
C(11)	6816(1)	2152(2)	4977(1)	13(1)
C(12)	6378(1)	1192(2)	4110(1)	12(1)
C(13)	6872(1)	319(2)	3537(1)	14(1)
C(14)	7727(1)	520(2)	3770(1)	16(1)
C(15)	8146(1)	1589(2)	4594(1)	17(1)
C(16)	7698(1)	2368(2)	5201(1)	15(1)
C(17)	119(1)	1617(3)	3282(1)	24(1)
C(18)	9443(1)	2762(3)	5576(1)	27(1)
O(1)	3988(1)	1262(1)	3318(1)	14(1)
O(2)	5563(1)	1011(1)	3824(1)	13(1)
O(3)	547(1)	910(2)	2586(1)	22(1)
O(4)	9000(1)	1718(2)	4737(1)	23(1)
Ni(1)	4790(1)	1943(1)	4462(1)	11(1)
N(1)	4022(1)	2890(2)	5100(1)	12(1)
N(2)	5597(1)	2608(2)	5603(1)	13(1)

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **NiMeO*salphen***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	76(1)	4798(2)	7015(1)	16(1)
C(2)	1004(1)	4934(2)	6738(1)	17(1)
C(3)	1830(1)	4052(2)	7183(1)	19(1)
C(4)	1763(1)	3141(2)	7869(1)	18(1)
C(5)	846(1)	3081(2)	8148(1)	17(1)
C(6)	21(1)	3881(2)	7722(1)	18(1)
C(7)	-823(1)	5528(2)	6586(1)	17(1)
C(8)	-1839(1)	7068(2)	5550(1)	16(1)
C(9)	-1787(1)	8020(2)	4864(1)	16(1)
C(10)	-647(1)	8997(2)	4054(1)	17(1)
C(11)	284(1)	9118(2)	3788(1)	17(1)
C(12)	1150(1)	8278(2)	4199(1)	18(1)
C(13)	2030(1)	8363(2)	3862(1)	22(1)
C(14)	2053(1)	9277(2)	3178(1)	23(1)
C(15)	1202(1)	10157(2)	2784(1)	20(1)
C(16)	326(1)	10065(2)	3079(1)	18(1)
C(17)	1548(1)	1381(2)	9284(1)	25(1)

C(18)	476(1)	11666(2)	1603(1)	25(1)
C(19)	-2646(1)	8796(2)	4443(1)	21(1)
C(20)	-3545(1)	8640(2)	4718(1)	22(1)
C(21)	-3597(1)	7684(2)	5402(1)	21(1)
C(22)	-2748(1)	6889(2)	5817(1)	20(1)
N(1)	-899(1)	6384(2)	5923(1)	16(1)
N(2)	-810(1)	8107(2)	4669(1)	16(1)
Ni(1)	146(1)	6909(1)	5385(1)	15(1)
O(1)	1126(1)	5799(1)	6104(1)	20(1)
O(2)	1187(1)	7417(2)	4863(1)	20(1)
O(3)	708(1)	2235(2)	8830(1)	23(1)
O(4)	1347(1)	11055(2)	2115(1)	27(1)

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **Ni*salphen***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	3747(2)	5203(2)	6778(2)	22(1)
C(2A)	2879(2)	4872(2)	5638(2)	21(1)
C(3A)	1866(2)	5175(2)	5475(3)	28(1)
C(4A)	1726(2)	5749(2)	6400(3)	34(1)
C(5A)	2575(3)	6054(2)	7527(3)	34(1)
C(6A)	3571(2)	5789(2)	7709(2)	29(1)
C(7A)	4814(2)	4989(2)	7034(2)	22(1)
C(8A)	6197(2)	4313(2)	6609(2)	21(1)
C(9A)	6353(2)	3719(2)	5682(2)	20(1)
C(10A)	5397(2)	2821(2)	3629(2)	22(1)
C(11A)	4498(2)	2503(2)	2497(2)	21(1)
C(12A)	3474(2)	2787(2)	2296(2)	22(1)
C(13A)	2670(2)	2521(2)	1158(2)	30(1)
C(14A)	2852(2)	1957(2)	259(3)	36(1)
C(15A)	3840(2)	1631(2)	451(3)	37(1)
C(16A)	4644(2)	1906(2)	1548(2)	29(1)
C(19A)	7383(2)	3491(2)	5877(3)	27(1)
C(20A)	8248(2)	3859(2)	6999(3)	31(1)
C(21A)	8098(2)	4455(2)	7921(3)	32(1)
C(22A)	7079(2)	4683(2)	7735(2)	28(1)
O(1A)	2956(1)	4313(1)	4724(2)	22(1)
O(2A)	3236(1)	3285(1)	3110(2)	23(1)
N(1A)	5107(2)	4478(2)	6271(2)	19(1)
N(2A)	5390(2)	3405(2)	4582(2)	19(1)
Ni(1A)	4184(1)	3877(1)	4679(1)	17(1)
C(1B)	6324(2)	9941(2)	7787(2)	21(1)
C(2B)	5288(2)	10201(2)	7600(2)	21(1)

C(3B)	5226(2)	10883(2)	8586(2)	27(1)
C(4B)	6121(2)	11250(2)	9681(2)	33(1)
C(5B)	7131(2)	10970(2)	9866(2)	34(1)
C(6B)	7222(2)	10325(2)	8930(2)	27(1)
C(7B)	6483(2)	9311(2)	6845(2)	21(1)
C(8B)	5997(2)	8342(2)	4880(2)	19(1)
C(9B)	5125(2)	8026(2)	3767(2)	20(1)
C(10B)	3229(2)	8056(2)	2726(2)	21(1)
C(11B)	2225(2)	8359(2)	2589(2)	20(1)
C(12B)	2101(2)	8989(2)	3550(2)	20(1)
C(13B)	1116(2)	9350(2)	3344(2)	24(1)
C(14B)	307(2)	9089(2)	2248(2)	28(1)
C(15B)	412(2)	8444(2)	1292(2)	30(1)
C(16B)	1356(2)	8089(2)	1470(2)	27(1)
C(19B)	5277(2)	7481(2)	2830(2)	27(1)
C(20B)	6295(2)	7257(2)	3019(3)	32(1)
C(21B)	7161(2)	7557(2)	4124(3)	29(1)
C(22B)	7017(2)	8093(2)	5059(2)	25(1)
O(1B)	4394(1)	9845(1)	6573(2)	22(1)
O(2B)	2861(1)	9277(1)	4619(2)	21(1)
N(1B)	5740(2)	8933(2)	5757(2)	17(1)
N(2B)	4137(2)	8327(2)	3716(2)	18(1)
Ni(1B)	4287(1)	9092(1)	5161(1)	17(1)
C(31)	2217(3)	4496(2)	8785(3)	36(1)
Cl(31)	1327(1)	3195(1)	8175(1)	76(1)
Cl(32)	3624(1)	4657(1)	9762(1)	59(1)
Cl(33)	1724(1)	5526(1)	9483(1)	64(1)
C(41)	723(2)	2487(2)	2488(2)	25(1)
Cl(41)	509(1)	1180(1)	1377(1)	37(1)
Cl(42)	214(1)	2317(1)	3321(1)	35(1)
Cl(43)	23(1)	3277(1)	1901(1)	40(1)
C(51)	1942(2)	9249(2)	6173(3)	33(1)
Cl(51)	2526(1)	8847(1)	7221(1)	57(1)
Cl(52)	1730(1)	10535(1)	6754(1)	69(1)
Cl(53)	662(1)	8230(1)	4977(1)	64(1)

Table S5. Bond lengths [Å] and angles [°] for compound **Ni*salphen***.

C(1A)-C(2A)	1.410(4)	C(5A)-H(5A)	0.9500
C(1A)-C(6A)	1.417(3)	C(6A)-H(6A)	0.9500
C(1A)-C(7A)	1.423(3)	C(7A)-N(1A)	1.308(3)
C(2A)-O(1A)	1.306(3)	C(7A)-H(7A)	0.9500
C(2A)-C(3A)	1.421(3)	C(8A)-C(22A)	1.390(4)
C(3A)-C(4A)	1.374(4)	C(8A)-C(9A)	1.395(3)
C(3A)-H(3A)	0.9500	C(8A)-N(1A)	1.417(3)
C(4A)-C(5A)	1.398(4)	C(9A)-C(19A)	1.394(3)
C(4A)-H(4A)	0.9500	C(9A)-N(2A)	1.421(3)
C(5A)-C(6A)	1.373(4)	C(10A)-N(2A)	1.307(3)

C(10A)-C(11A)	1.419(4)	C(12B)-O(2B)	1.309(3)
C(10A)-H(10A)	0.9500	C(12B)-C(13B)	1.418(3)
C(11A)-C(16A)	1.415(3)	C(13B)-C(14B)	1.366(4)
C(11A)-C(12A)	1.417(3)	C(13B)-H(13B)	0.9500
C(12A)-O(2A)	1.312(3)	C(14B)-C(15B)	1.403(4)
C(12A)-C(13A)	1.408(4)	C(14B)-H(14B)	0.9500
C(13A)-C(14A)	1.377(4)	C(15B)-C(16B)	1.366(4)
C(13A)-H(13A)	0.9500	C(15B)-H15B)	0.9500
C(14A)-C(15A)	1.399(4)	C(16B)-H(16B)	0.9500
C(14A)-H(14A)	0.9500	C(19B)-C(20B)	1.378(4)
C(15A)-C(16A)	1.360(4)	C(19B)-H(19B)	0.9500
C(15A)-H(15A)	0.9500	C(20B)-C(21B)	1.383(4)
C(16A)-H(16A)	0.9500	C(20B)-H(20B)	0.9500
C(19A)-C(20A)	1.379(4)	C(21B)-C(22B)	1.382(4)
C(19A)-H(19A)	0.9500	C(21B)-H(21B)	0.9500
C(20A)-C(21A)	1.385(4)	C(22B)-H(22B)	0.9500
C(20A)-H(20A)	0.9500	O(1B)-Ni(1B)	1.8370(17)
C(21A)-C(22A)	1.382(4)	O(2B)-Ni(1B)	1.8360(16)
C(21A)-H(21A)	0.9500	N(1B)-Ni(1B)	1.8567(19)
C(22A)-H(22A)	0.9500	N(2B)-Ni(1B)	1.856(2)
O(1A)-Ni(1A)	1.8398(16)	C(31)-Cl(31)	1.735(3)
O(2A)-Ni(1A)	1.8346(18)	C(31)-Cl(32)	1.751(3)
N(1A)-Ni(1A)	1.857(2)	C(31)-Cl(33)	1.753(3)
N(2A)-Ni(1A)	1.8564(19)	C(31)-H(31)	1.0000
C(1B)-C(6B)	1.409(4)	C(41)-Cl(42)	1.759(3)
C(1B)-C(2B)	1.420(3)	C(41)-Cl(43)	1.761(3)
C(1B)-C(7B)	1.426(3)	C(41)-Cl(41)	1.763(3)
C(2B)-O(1B)	1.306(3)	C(41)-H(41)	1.0000
C(2B)-C(3B)	1.415(3)	C(51)-Cl(52)	1.742(3)
C(3B)-C(4B)	1.367(4)	C(51)-Cl(53)	1.754(3)
C(3B)-H(3B)	0.9500	C(51)-Cl(51)	1.756(3)
C(4B)-C(5B)	1.400(4)	C(51)-H(51)	1.0000
C(4B)-H(4B)	0.9500		
C(5B)-C(6B)	1.367(4)	C(2A)-C(1A)-C(6A)	119.5(2)
C(5B)-H(5B)	0.9500	C(2A)-C(1A)-C(7A)	122.1(2)
C(6B)-H(6B)	0.9500	C(6A)-C(1A)-C(7A)	118.4(2)
C(7B)-N(1B)	1.299(3)	O(1A)-C(2A)-C(1A)	123.8(2)
C(7B)-H(7B)	0.9500	O(1A)-C(2A)-C(3A)	118.2(2)
C(8B)-C(9B)	1.389(4)	C(1A)-C(2A)-C(3A)	118.0(2)
C(8B)-C(22B)	1.396(3)	C(4A)-C(3A)-C(2A)	120.9(3)
C(8B)-N(1B)	1.427(3)	C(4A)-C(3A)-H(3A)	119.5
C(9B)-C(19B)	1.394(3)	C(2A)-C(3A)-H(3A)	119.5
C(9B)-N(2B)	1.420(3)	C(3A)-C(4A)-C(5A)	121.1(3)
C(10B)-N(2B)	1.307(3)	C(3A)-C(4A)-H(4A)	119.5
C(10B)-C(11B)	1.415(3)	C(5A)-C(4A)-H(4A)	119.5
C(10B)-H(10B)	0.9500	C(6A)-C(5A)-C(4A)	119.1(3)
C(11B)-C(16B)	1.411(4)	C(6A)-C(5A)-H(5A)	120.5
C(11B)-C(12B)	1.418(3)	C(4A)-C(5A)-H(5A)	120.5

C(5A)-C(6A)-C(1A)	121.4(3)	C(7A)-N(1A)-Ni(1A)	125.54(17)
C(5A)-C(6A)-H(6A)	119.3	C(8A)-N(1A)-Ni(1A)	113.13(16)
C(1A)-C(6A)-H(6A)	119.3	C(10A)-N(2A)-C(9A)	120.9(2)
N(1A)-C(7A)-C(1A)	125.3(2)	C(10A)-N(2A)-Ni(1A)	126.15(18)
N(1A)-C(7A)-H(7A)	117.4	C(9A)-N(2A)-Ni(1A)	112.97(16)
C(1A)-C(7A)-H(7A)	117.4	O(2A)-Ni(1A)-O(1A)	83.05(8)
C(22A)-C(8A)-C(9A)	119.6(2)	O(2A)-Ni(1A)-N(2A)	95.17(8)
C(22A)-C(8A)-N(1A)	126.6(2)	O(1A)-Ni(1A)-N(2A)	178.13(9)
C(9A)-C(8A)-N(1A)	113.8(2)	O(2A)-Ni(1A)-N(1A)	178.42(8)
C(19A)-C(9A)-C(8A)	120.5(2)	O(1A)-Ni(1A)-N(1A)	95.46(8)
C(19A)-C(9A)-N(2A)	125.7(2)	N(2A)-Ni(1A)-N(1A)	86.32(9)
C(8A)-C(9A)-N(2A)	113.8(2)	C(6B)-C(1B)-C(2B)	119.4(2)
N(2A)-C(10A)-C(11A)	125.0(2)	C(6B)-C(1B)-C(7B)	119.1(2)
N(2A)-C(10A)-H(10A)	117.5	C(2B)-C(1B)-C(7B)	121.5(2)
C(11A)-C(10A)-H(10A)	117.5	O(1B)-C(2B)-C(3B)	118.5(2)
C(16A)-C(11A)-C(12A)	119.4(2)	O(1B)-C(2B)-C(1B)	123.7(2)
C(16A)-C(11A)-C(10A)	118.7(2)	C(3B)-C(2B)-C(1B)	117.8(2)
C(12A)-C(11A)-C(10A)	121.9(2)	C(4B)-C(3B)-C(2B)	121.0(2)
O(2A)-C(12A)-C(13A)	118.4(2)	C(4B)-C(3B)-H(3B)	119.5
O(2A)-C(12A)-C(11A)	123.7(2)	C(2B)-C(3B)-H(3B)	119.5
C(13A)-C(12A)-C(11A)	118.0(2)	C(3B)-C(4B)-C(5B)	121.2(3)
C(14A)-C(13A)-C(12A)	120.9(3)	C(3B)-C(4B)-H(4B)	119.4
C(14A)-C(13A)-H(13A)	119.6	C(5B)-C(4B)-H(4B)	119.4
C(12A)-C(13A)-H(13A)	119.6	C(6B)-C(5B)-C(4B)	119.1(3)
C(13A)-C(14A)-C(15A)	121.0(3)	C(6B)-C(5B)-H(5B)	120.5
C(13A)-C(14A)-H(14A)	119.5	C(4B)-C(5B)-H(5B)	120.5
C(15A)-C(14A)-H(14A)	119.5	C(5B)-C(6B)-C(1B)	121.5(2)
C(16A)-C(15A)-C(14A)	119.2(3)	C(5B)-C(6B)-H(6B)	119.3
C(16A)-C(15A)-H(15A)	120.4	C(1B)-C(6B)-H(6B)	119.3
C(14A)-C(15A)-H(15A)	120.4	N(1B)-C(7B)-C(1B)	125.4(2)
C(15A)-C(16A)-C(11A)	121.4(2)	N(1B)-C(7B)-H(7B)	117.3
C(15A)-C(16A)-H(16A)	119.3	C(1B)-C(7B)-H(7B)	117.3
C(11A)-C(16A)-H(16A)	119.3	C(9B)-C(8B)-C(22B)	120.0(2)
C(20A)-C(19A)-C(9A)	119.2(3)	C(9B)-C(8B)-N(1B)	113.8(2)
C(20A)-C(19A)-H(19A)	120.4	C(22B)-C(8B)-N(1B)	126.1(2)
C(9A)-C(19A)-H(19A)	120.4	C(8B)-C(9B)-C(19B)	120.0(2)
C(19A)-C(20A)-C(21A)	120.3(2)	C(8B)-C(9B)-N(2B)	113.8(2)
C(19A)-C(20A)-H(20A)	119.8	C(19B)-C(9B)-N(2B)	126.2(2)
C(21A)-C(20A)-H(20A)	119.8	N(2B)-C(10B)-C(11B)	125.4(2)
C(22A)-C(21A)-C(20A)	120.9(3)	N(2B)-C(10B)-H(10B)	117.3
C(22A)-C(21A)-H(21A)	119.6	C(11B)-C(10B)-H(10B)	117.3
C(20A)-C(21A)-H(21A)	119.6	C(16B)-C(11B)-C(10B)	118.7(2)
C(21A)-C(22A)-C(8A)	119.4(3)	C(16B)-C(11B)-C(12B)	119.1(2)
C(21A)-C(22A)-H(22A)	120.3	C(10B)-C(11B)-C(12B)	122.0(2)
C(8A)-C(22A)-H(22A)	120.3	O(2B)-C(12B)-C(13B)	118.3(2)
C(2A)-O(1A)-Ni(1A)	127.71(16)	O(2B)-C(12B)-C(11B)	123.5(2)
C(12A)-O(2A)-Ni(1A)	127.68(16)	C(13B)-C(12B)-C(11B)	118.2(2)
C(7A)-N(1A)-C(8A)	121.3(2)	C(14B)-C(13B)-C(12B)	120.7(2)

C(14B)-C(13B)-H(13B)	119.7	C(10B)-N(2B)-C(9B)	121.2(2)
C(12B)-C(13B)-H(13B)	119.7	C(10B)-N(2B)-Ni(1B)	125.59(16)
C(13B)-C(14B)-C(15B)	121.3(2)	C(9B)-N(2B)-Ni(1B)	113.22(16)
C(13B)-C(14B)-H(14B)	119.3	O(2B)-Ni(1B)-O(1B)	83.03(7)
C(15B)-C(14B)-H(14B)	119.3	O(2B)-Ni(1B)-N(2B)	95.47(8)
C(16B)-C(15B)-C(14B)	119.0(3)	O(1B)-Ni(1B)-N(2B)	178.47(8)
C(16B)-C(15B)-H(15B)	120.5	O(2B)-Ni(1B)-N(1B)	178.24(9)
C(14B)-C(15B)-H(15B)	120.5	O(1B)-Ni(1B)-N(1B)	95.23(8)
C(15B)-C(16B)-C(11B)	121.7(2)	N(2B)-Ni(1B)-N(1B)	86.27(9)
C(15B)-C(16B)-H(16B)	119.2	Cl(31)-C(31)-Cl(32)	111.15(16)
C(11B)-C(16B)-H(16B)	119.2	Cl(31)-C(31)-Cl(33)	110.49(17)
C(20B)-C(19B)-C(9B)	119.5(3)	Cl(32)-C(31)-Cl(33)	110.13(17)
C(20B)-C(19B)-H(19B)	120.3	Cl(31)-C(31)-H(31)	108.3
C(9B)-C(19B)-H(19B)	120.3	Cl(32)-C(31)-H(31)	108.3
C(19B)-C(20B)-C(21B)	120.7(2)	Cl(33)-C(31)-H(31)	108.3
C(19B)-C(20B)-H(20B)	119.6	Cl(42)-C(41)-Cl(43)	110.22(13)
C(21B)-C(20B)-H(20B)	119.6	Cl(42)-C(41)-Cl(41)	109.42(14)
C(22B)-C(21B)-C(20B)	120.3(2)	Cl(43)-C(41)-Cl(41)	110.78(15)
C(22B)-C(21B)-H(21B)	119.8	Cl(42)-C(41)-H(41)	108.8
C(20B)-C(21B)-H(21B)	119.8	Cl(43)-C(41)-H(41)	108.8
C(21B)-C(22B)-C(8B)	119.4(3)	Cl(41)-C(41)-H(41)	108.8
C(21B)-C(22B)-H(22B)	120.3	Cl(52)-C(51)-Cl(53)	111.51(16)
C(8B)-C(22B)-H(22B)	120.3	Cl(52)-C(51)-Cl(51)	110.74(17)
C(2B)-O(1B)-Ni(1B)	127.75(15)	Cl(53)-C(51)-Cl(51)	108.88(16)
C(12B)-O(2B)-Ni(1B)	127.63(15)	Cl(52)-C(51)-H(51)	108.5
C(7B)-N(1B)-C(8B)	121.1(2)	Cl(53)-C(51)-H(51)	108.5
C(7B)-N(1B)-Ni(1B)	126.00(16)	Cl(51)-C(51)-H(51)	108.5
C(8B)-N(1B)-Ni(1B)	112.87(16)		

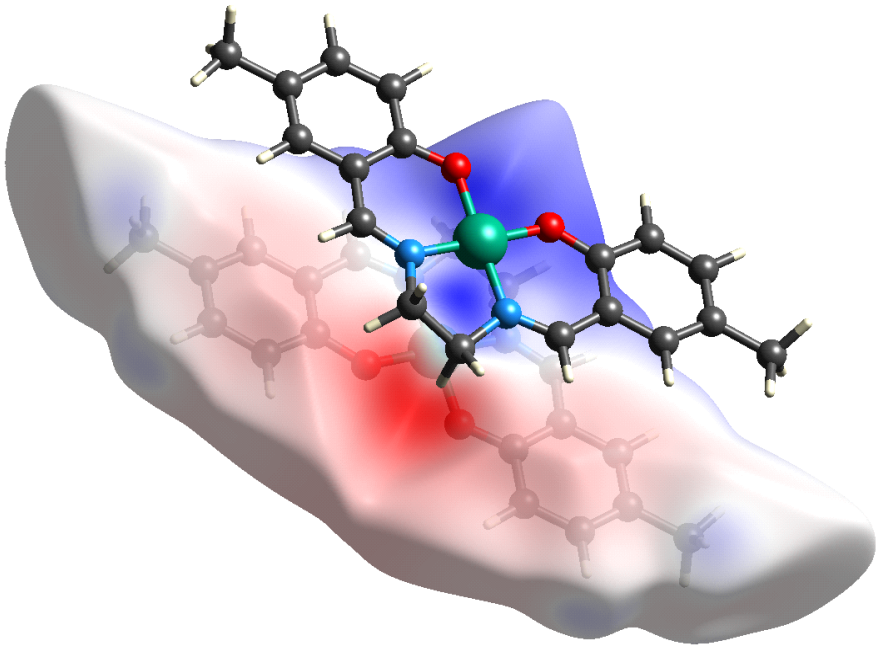


Figure S1. Normalized contact distance ($\mathbf{d_{norm}}$, defined in terms of $\mathbf{d_e}$, $\mathbf{d_i}$, and the van der Waals radii of the atoms) mapped on the Hirshfeld surface of the compound **NiMeO*salen***, represented together with one surrounding moiety to visualize the intermolecular interaction.

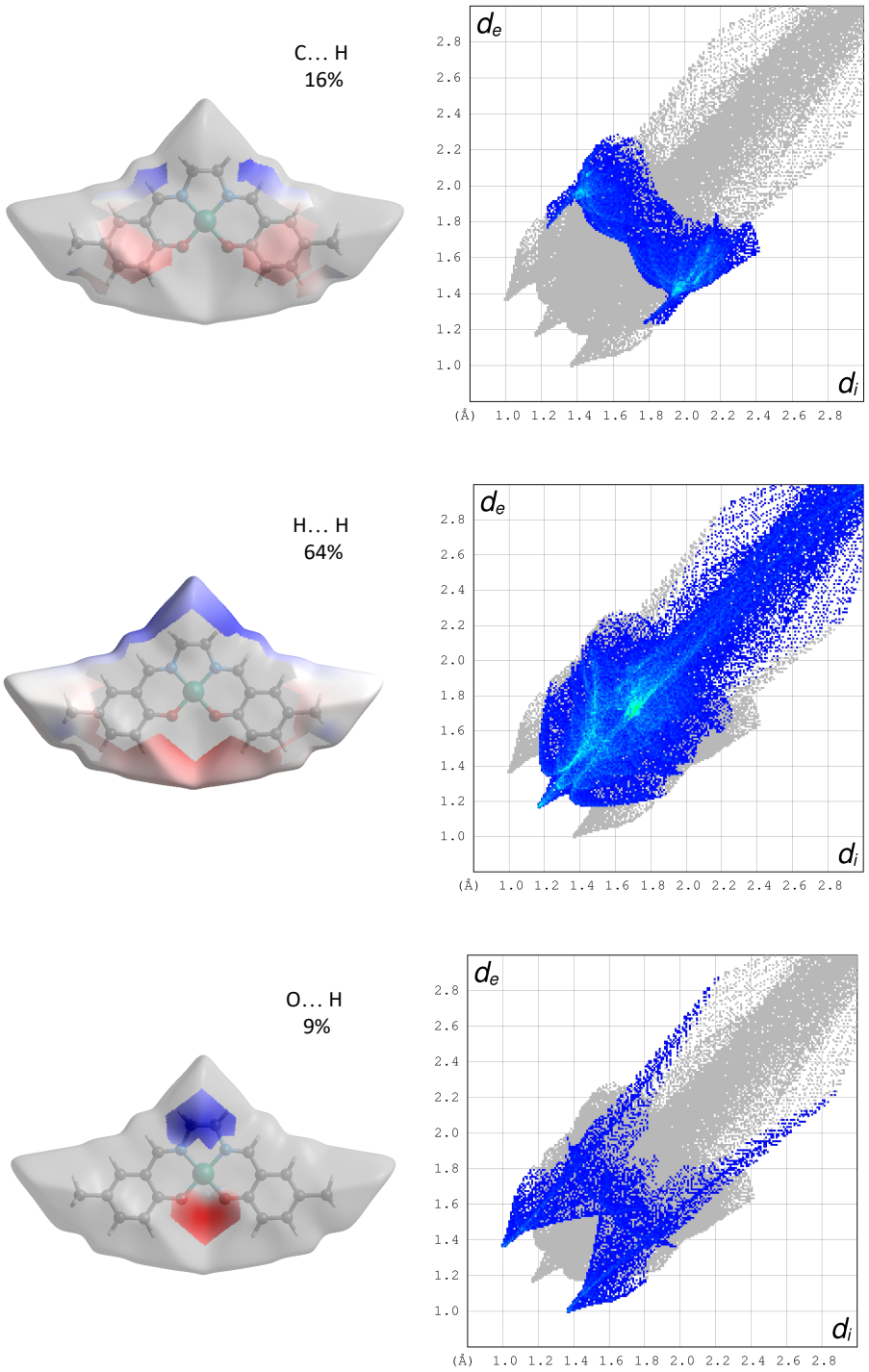


Figure S2. Hirshfeld surface with $\mathbf{d}_{norm}$ mapped and fingerprint plots for compound **NiMe*salen*,** with C…H interaction (first row) and H···H, O···H interactions (row 2–3). The color ranges from dark blue to red with increasing frequency (relative area of the surface) corresponding to each kind of interaction.

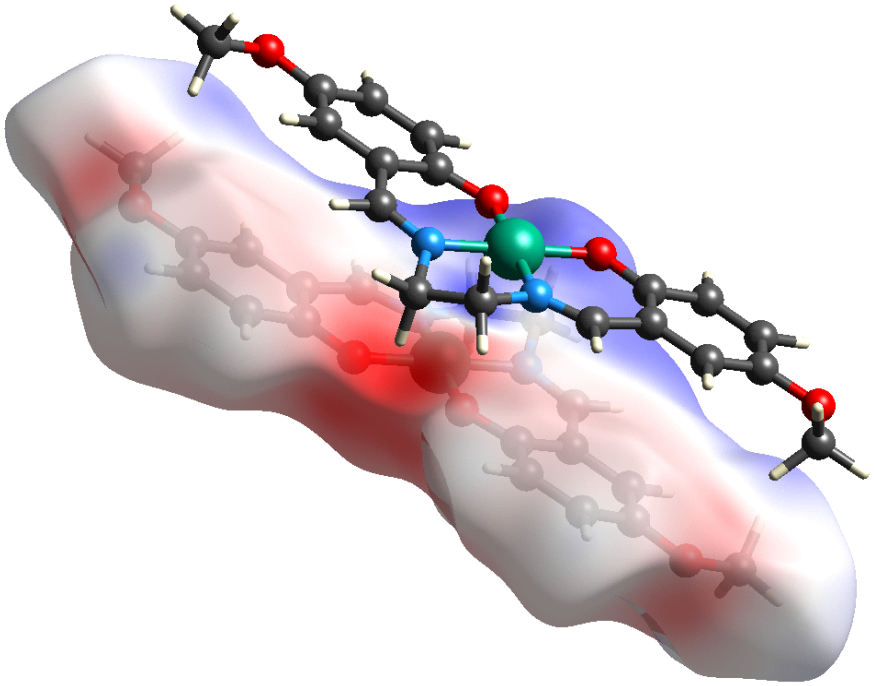


Figure S3. Normalized contact distance ($\mathbf{d_{norm}}$, defined in terms of $\mathbf{d_e}$, $\mathbf{d_i}$, and the van der Waals radii of the atoms) mapped on the Hirshfeld surface of the compound **NiMeO*salen***, represented together with one surrounding moiety to visualize the intermolecular interaction.

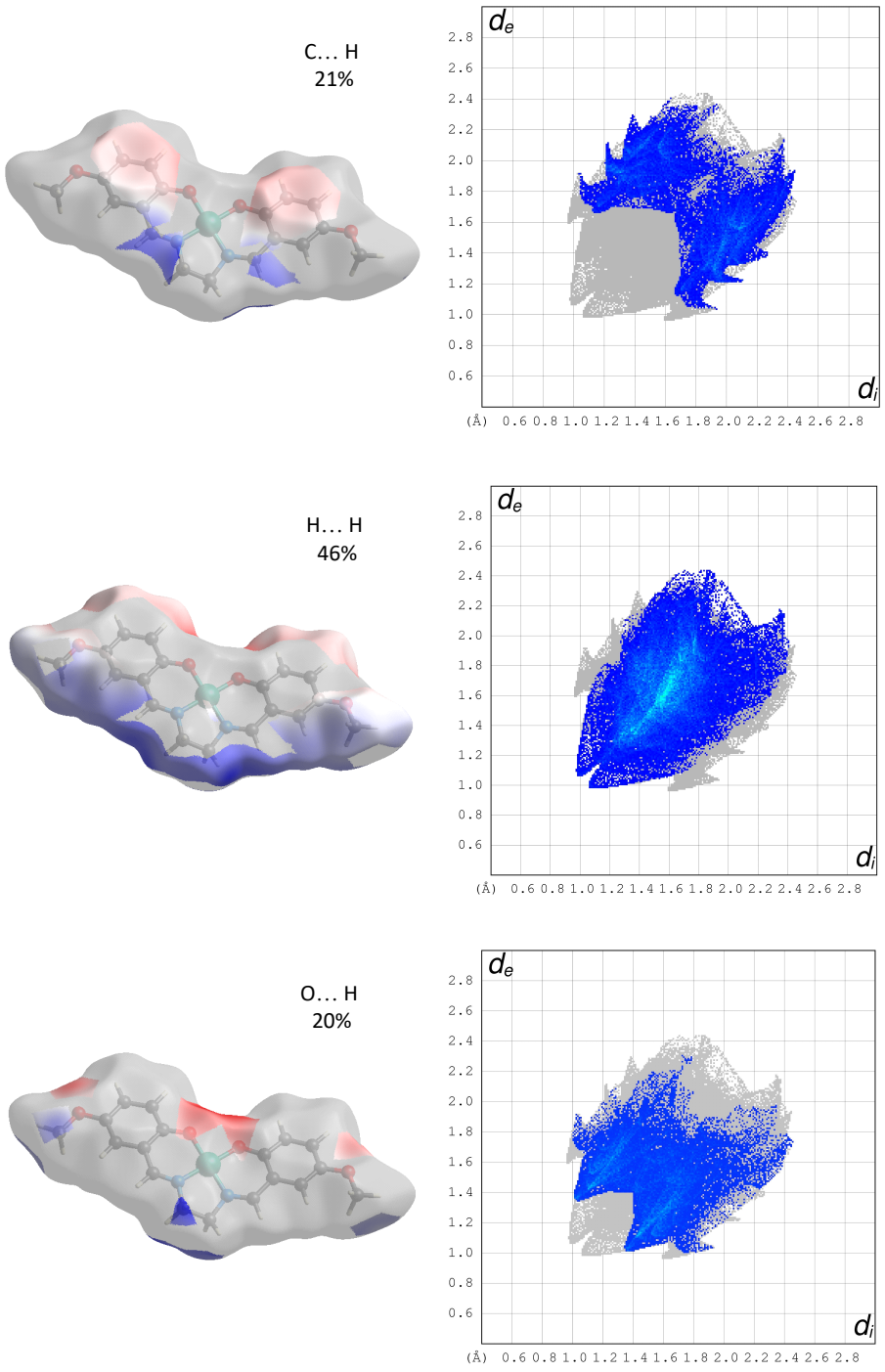


Figure S4. Hirshfeld surface with $\mathbf{d_{norm}}$ mapped and fingerprint plots for compound **NiMeO*salen***, with C···H interaction (first row) and H···H, O···H interactions (row 2–3). The color ranges from dark blue to red with increasing frequency (relative area of the surface) corresponding to each kind of interaction.

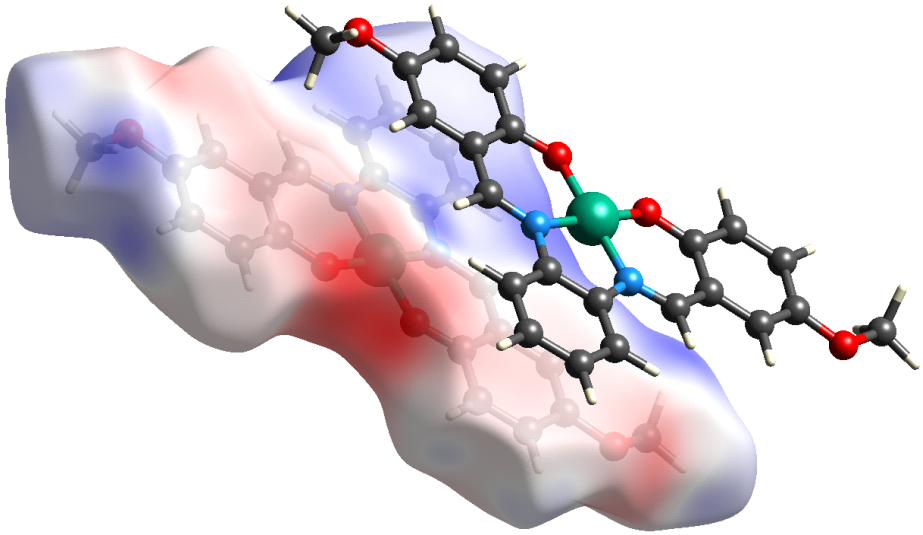


Figure S5. Normalized contact distance ($\mathbf{d_{norm}}$, defined in terms of $\mathbf{d_e}$, $\mathbf{d_i}$, and the van der Waals radii of the atoms) mapped on the Hirshfeld surface of the compound **NiMeO*salphen***, represented together with one surrounding moiety to visualize the intermolecular interaction.

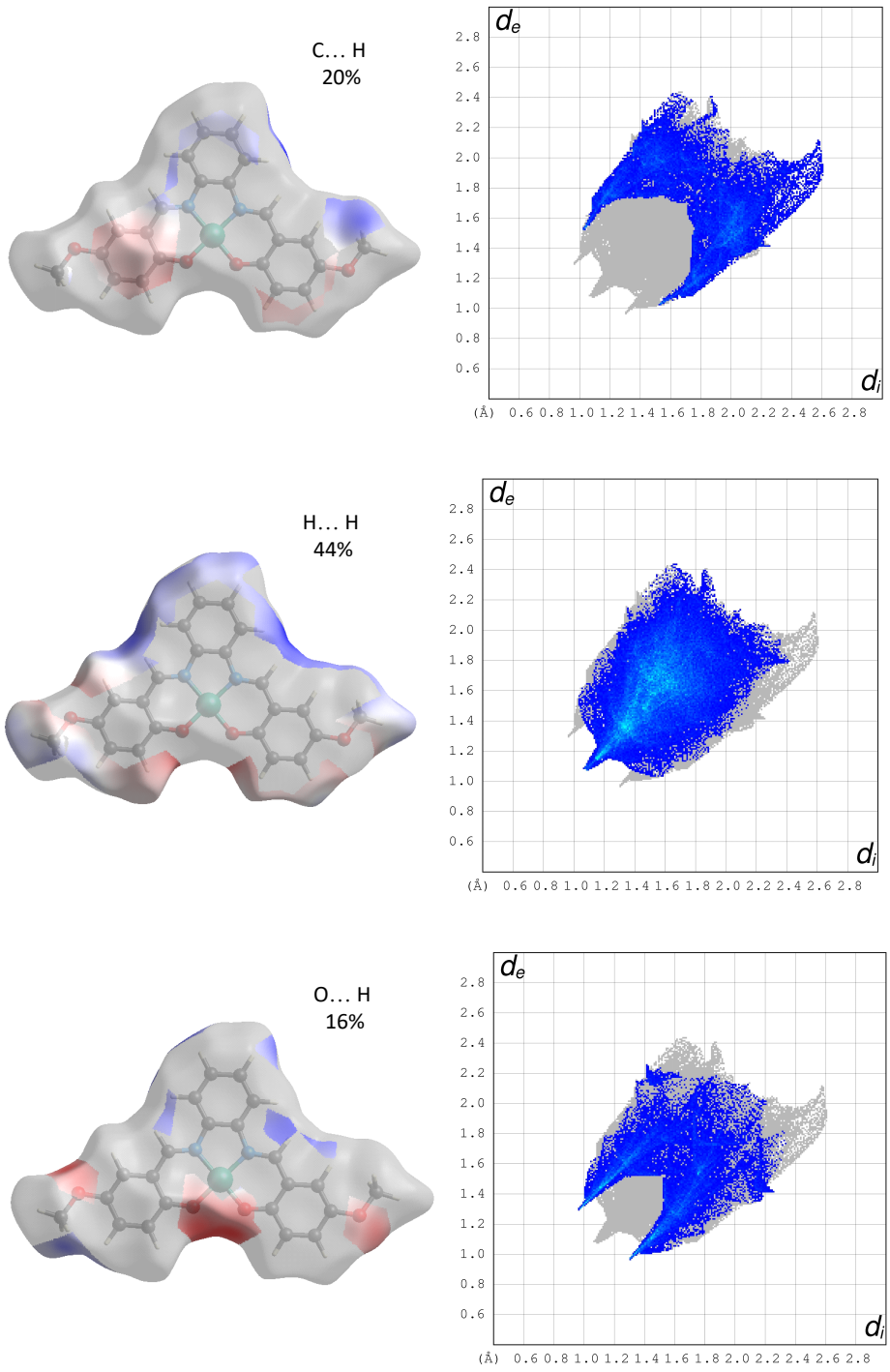


Figure S6. Hirshfeld surface with $\mathbf{d_{norm}}$ mapped and fingerprint plots for compound **NiMeO*salphen*,** with C···H interaction (first row) and H···H, O···H interactions (row 2–3). The color ranges from dark blue to red with increasing frequency (relative area of the surface) corresponding to each kind of interaction.

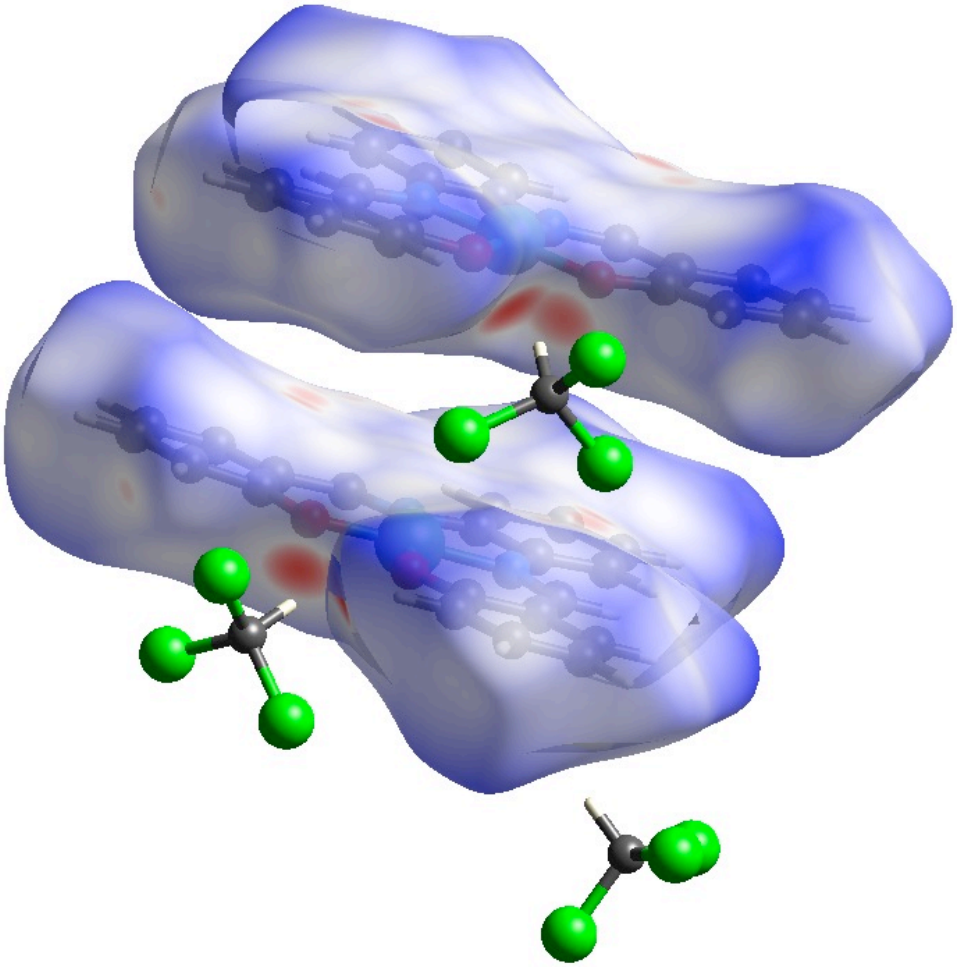
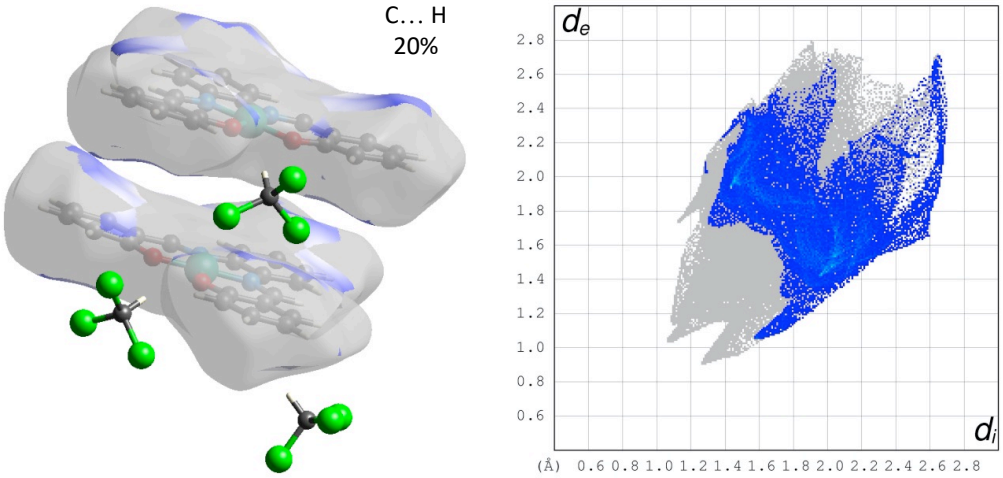


Figure S7. Normalized contact distance (d_{norm}, defined in terms of d_e, d_i, and the van der Waals radii of the atoms) mapped on the Hirshfeld surface of the compound **Ni*salphen***, represented together with one surrounding moiety to visualize the intermolecular interaction.



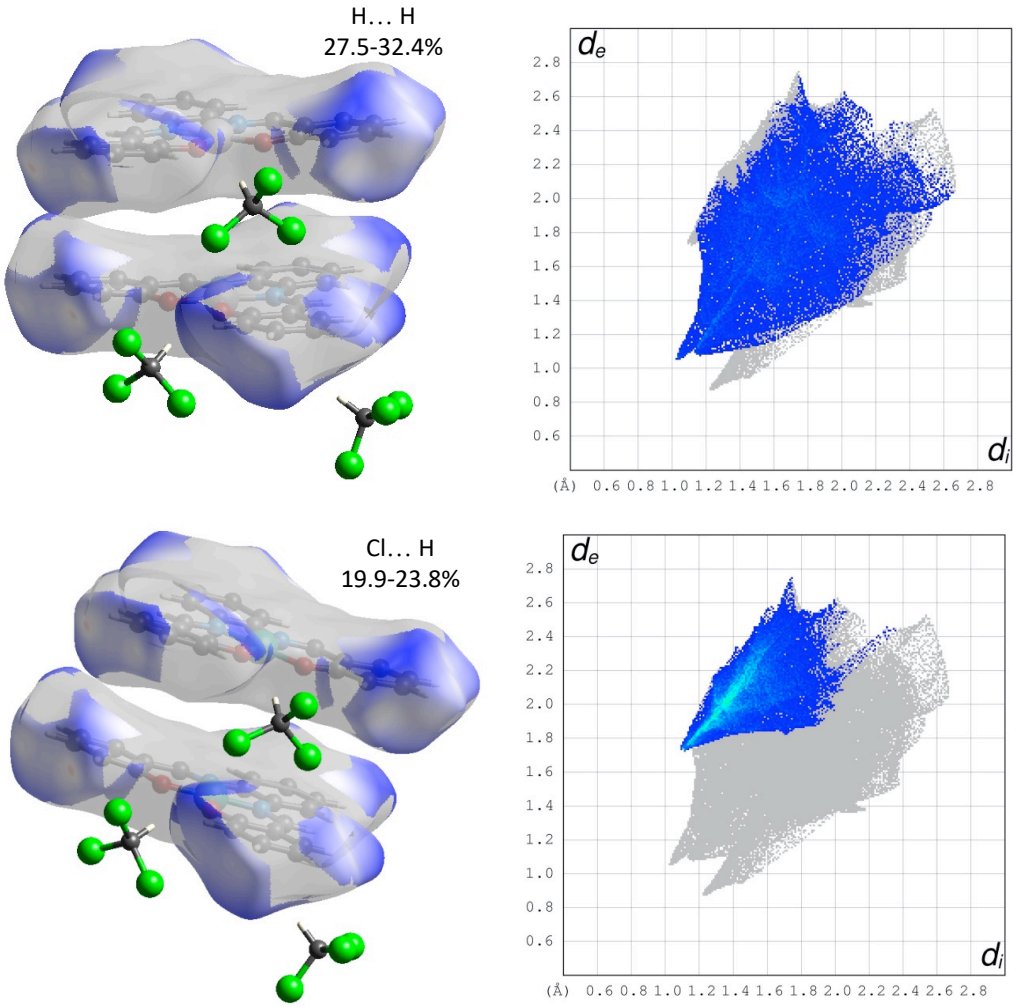
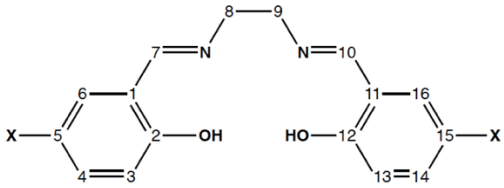


Figure S8. Hirshfeld surface with $\mathbf{d_{norm}}$ mapped and fingerprint plots of the two molecules name A and B in compound **Nis*alphen*** for C···H interaction (first row) and H···H, Cl···H interactions (row 2–3). The color ranges from dark blue to red with increasing frequency (relative area of the surface) corresponding to each kind of interaction.

Table S6. Effective magnetic moment, and number of unpaired electrons of Ni^{II} complexes.

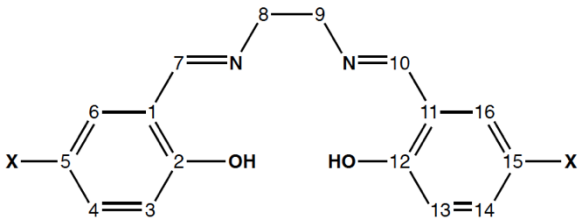
Compound	X_m (cm^3/mol)	X_{corr} (cm^3/mol)	μ_{eff} (MB)	# unpaired e^-
NiMeO*salen*	$5.03x10^{-5}$	$1.76 x10^{-4}$	0.65	0
NiMe*salen*	$6.05x10^{-5}$	$1.56 x10^{-4}$	0.61	0
NiOH*salen*	$7.44x10^{-5}$	$1.28 x10^{-4}$	0.55	0
Ni*salen*	$1.23x10^{-4}$	$6.51x10^{-5}$	0.39	0
NiCl*salen*	$1.05 x10^{-4}$	$1.22 x10^{-4}$	0.54	0
NiBr*salen*	$1.76 x10^{-4}$	$7.24x10^{-5}$	0.41	0
NiNO$_2$*salen*	$1.88 x10^{-4}$	$3.22 x10^{-4}$	0.27	0
NiMeO*salphen*	$1.79x10^{-5}$	$3.61x10^{-3}$	0.17	0
NiMe*salphen*	$2.22x10^{-5}$	$4.88 x10^{-3}$	0.20	0
NiOH*salphen*	$-5.44x10^{-5}$	$1.46x10^{-2}$	0.34	0
Ni*salphen*	$-1.09 x10^{-4}$	$3.16x10^{-2}$	0.51	0
NiCl*salphen*	$-1.47 x10^{-4}$	$4.68x10^{-2}$	0.61	0
NiBr*salphen*	$2.78 x10^{-4}$	$8.69x10^{-2}$	0.84	0

Table S7. [1]H-NMR values for the ligands and nickel complexes.



	Key	Solvent	δ_{OH} (ppm)	$\delta_{7,10}$ (ppm)	$\delta_{Aromatic}$ (ppm)	$\delta_{8,9}$ (ppm)	δ_{X}(ppm)
Ligands	**MeO*salen***	Chloroform	12.63 (s)	8.30 (s)	6.73-6.89	3.94 (s)	3.74 (s)
	Me*salen*	Chloroform	12.95 (s)	8.29 (s)	6.84-7.08	3.92 (s)	2.26 (s)
	OH*salen*	Acetone-d6	12.40 (s)	8.46 (s)	6.66-6.73	3.35 (s)	12.40 (s)
	Salen	Chloroform	13.19 (s)	8.36 (s)	6.88-7.29	3.43 (s)	---
	Cl*salen*	Chloroform	13.08 (s)	8.29 (s)	6.90-7.24	3.95 (s)	---
	Br*salen*	Chloroform	13.10 (s)	8.28 (s)	6.84- 7.34	3.95 (s)	---
	NO_2*salen*	DMSO-d6	---	8.77 (s)	6.79-7.40	4.01 (s)	---
	MeO*salphen*	Acetone-d6	12.46 (s)	8.85 (s)	6.88-7.44	---	3.78 (s)
	Me*salphen*	Acetonitrile	12.86 (s)	8.70 (s)	6.88-7.41	---	2.37 (d)
	OH*salphen*	Acetone-d6	12.30 (s)	8.76 (s)	6.94-7.41	---	12.32(s)
	Br*salphen*	Acetone-d6	13.09 (s)	8.91 (s)	6.95-7.78	---	---
Complexes	**NiMeO*salen***	DMSO-d6	---	7.80 (s)	6.62-6.85	3.62 (s)	3.33 (s)
	NiMe*salen*	Chloroform	---	7.25 (s)	6.64-6.94	3.38 (s)	2.58 (s)
	NiOH*salen*	DMSO-d6	7.75 (s)	7.75 (s)	6.53-6.71	3.35 (s)	8.52 (s)
	Ni*salen*	Chloroform	---	7.38 (s)	6.99-7.27	3.43 (s)	---
	NiCl*salen*	Chloroform	---	7.44 (s)	6.95-7.13	3.47 (s)	---
	NiBr*salen*	Chloroform	---	7.45 (s)	6.91-7.26	3.46 (s)	---
	NiNO_2*salen*	DMSO-d6	---	7.95 (s)	---	3.53 (s)	---
	NiMeO*salphen*	Chloroform	---	8.23(s)	6.69-7.14	---	3.78 (s)
	NiOH*salphen*	DMF-d7	---	8.00 (s)	6.79-7.28	---	8.97(s)

Table S8. ^{13}C-NMR values for the ligands and nickel complexes.



	Key	Solvent	(ppm)	(ppm)	(ppm)	(ppm)	(ppm)	(ppm)	(ppm)	(ppm)
Ligands	**MeO*salen***	Chloroform	118	151	155	119	117	118	166	60
	Mes*alen*	Chloroform	130	133	159	132	128	118	166	60
	Salen	Chloroform	116	132	161	131	118	118	166	60
	Cls*alen*	Chloroform	118	132	159	130	123	119	165	59
	Brs*alen*	Chloroform	110	135	160	133	120	119	165	59
	MeO*salphen*	Acetone-d6	115	119	155	117	118	152	166	143
	Mes*alphen*	Acetonitrile	133	120	159	118	135	128	165	143
	Brs*alphen*	Acetone-d6	135	121	160	119	136	110	164	142
	OHs*alphen*	DMF-d7	117	117	155	119	121	150	165	143
Complexes	**NiMeOs*alen***	DMSO-d6	113	120	162	119	124	149	160	55
	NiMes*alen*	Chloroform	123	121	163	119	135	131	161	58
	NiOHs*alen*	DMSO-d6	115	119	162	120	124	146	159	55
	Nis*alen*	Chloroform	134	121	165	131	121	115	162	58

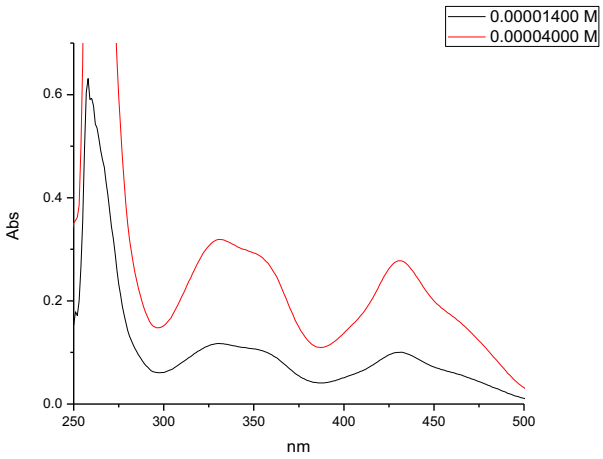


Figure S9. UV-vis of Ni*MeOsalen* in DMSO solution

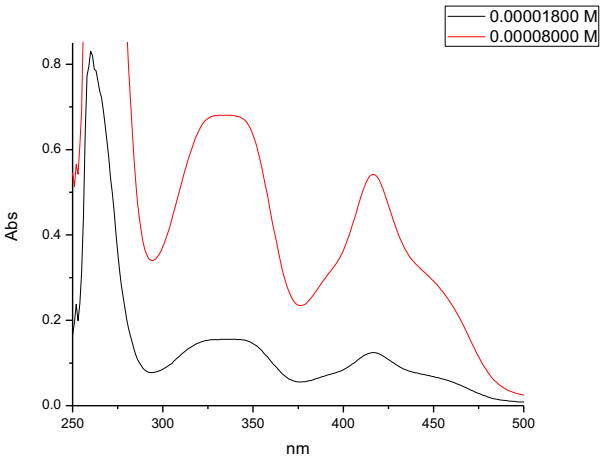


Figure S10. UV-vis Ni*Mesalen* in DMSO solution

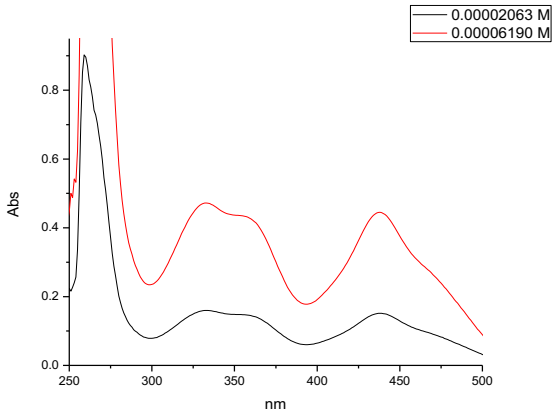


Figure S11. UV-vis NiOH*salen* in DMSO solution

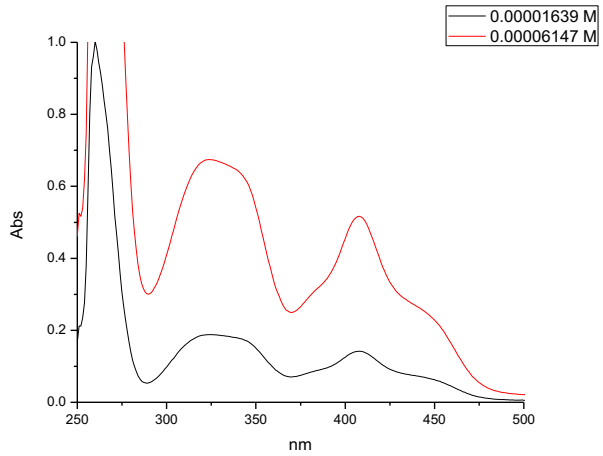


Figure S12. UV-vis of Ni*salen* in DMSO solution

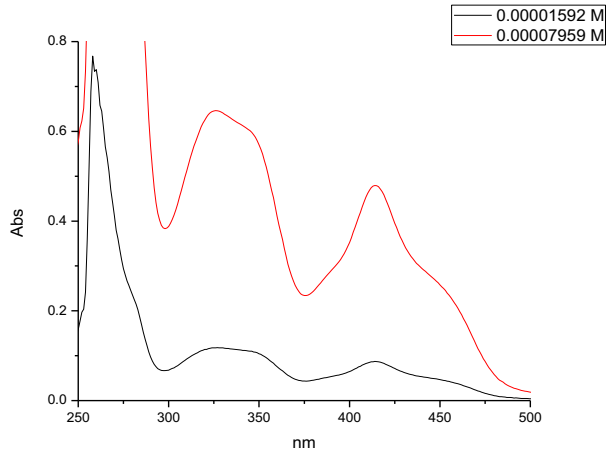


Figure S13. UV-vis of NiCl*salen* in DMSO solution

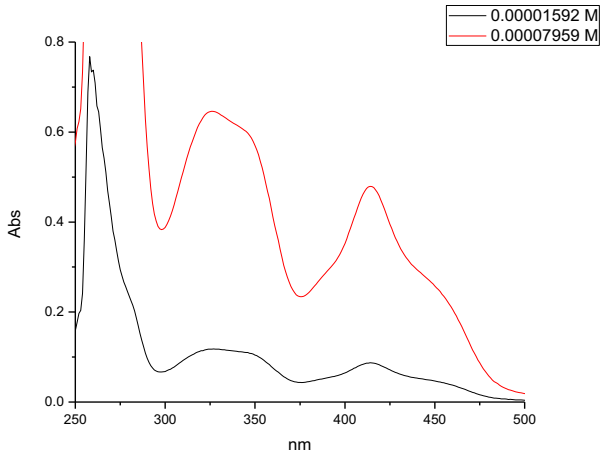


Figure S14. UV-vis of NiBr*salen* in DMSO solution

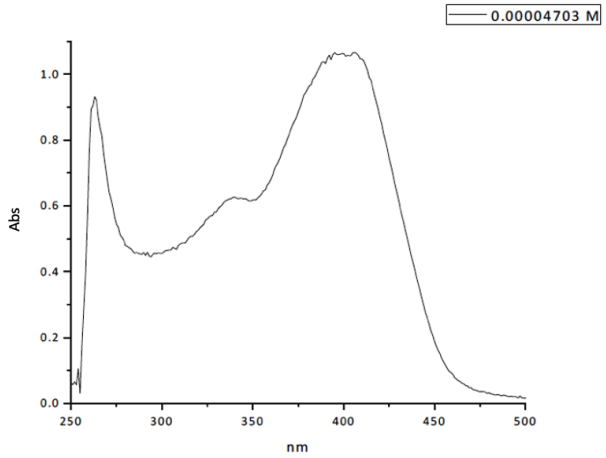


Figure S15. UV-vis $NiNO_2$*salen* in DMSO solution

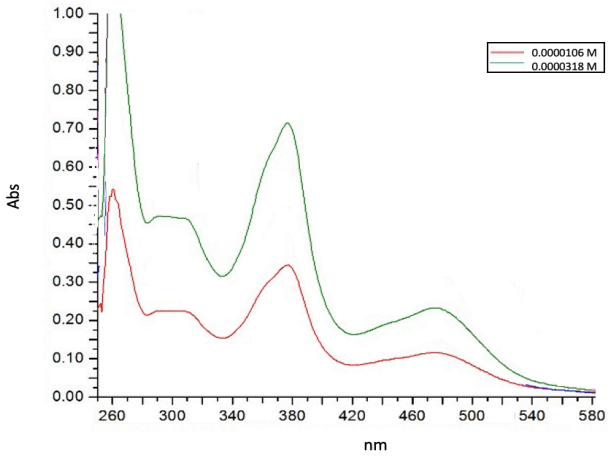


Figure S18. UV-vis Ni*salphen* in DMSO solution

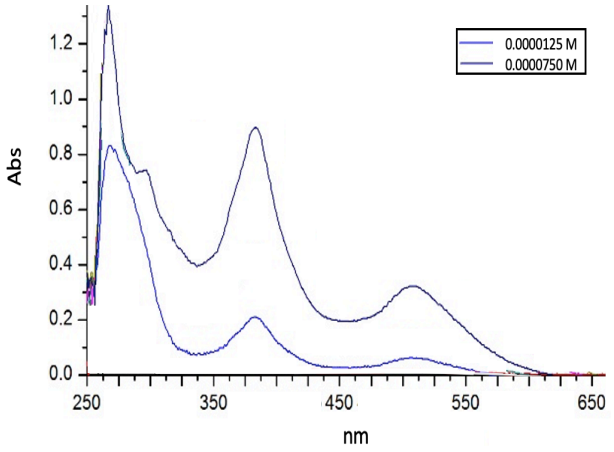


Figure S16. UV-vis NiMeO*salphen* in DMSO solution

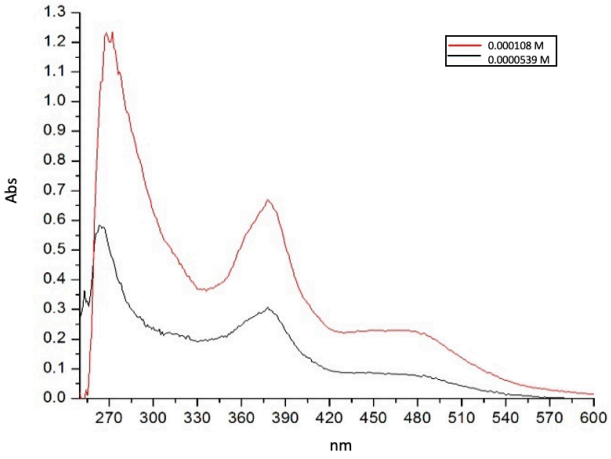


Figure S19. UV-vis NiCl*salphen* in DMSO solution

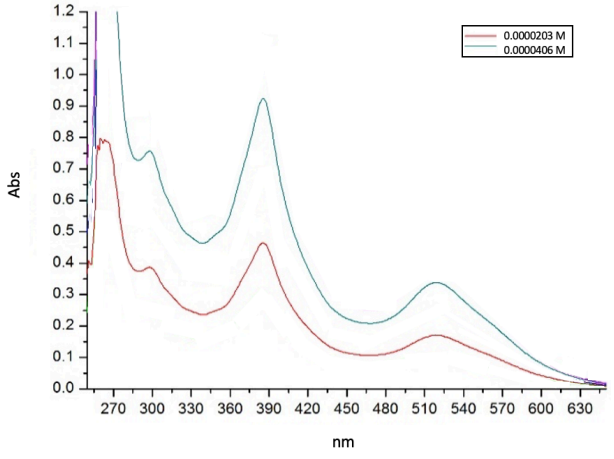


Figure S17. UV-vis NiOH*salphen* in DMSO solution

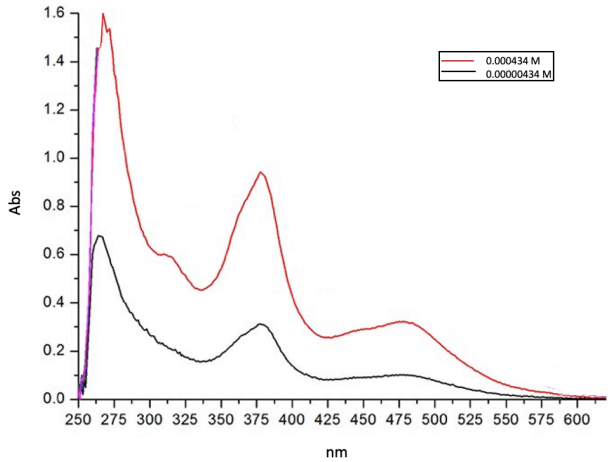


Figure S20. UV-vis NiBr*salphen* in DMSO solution

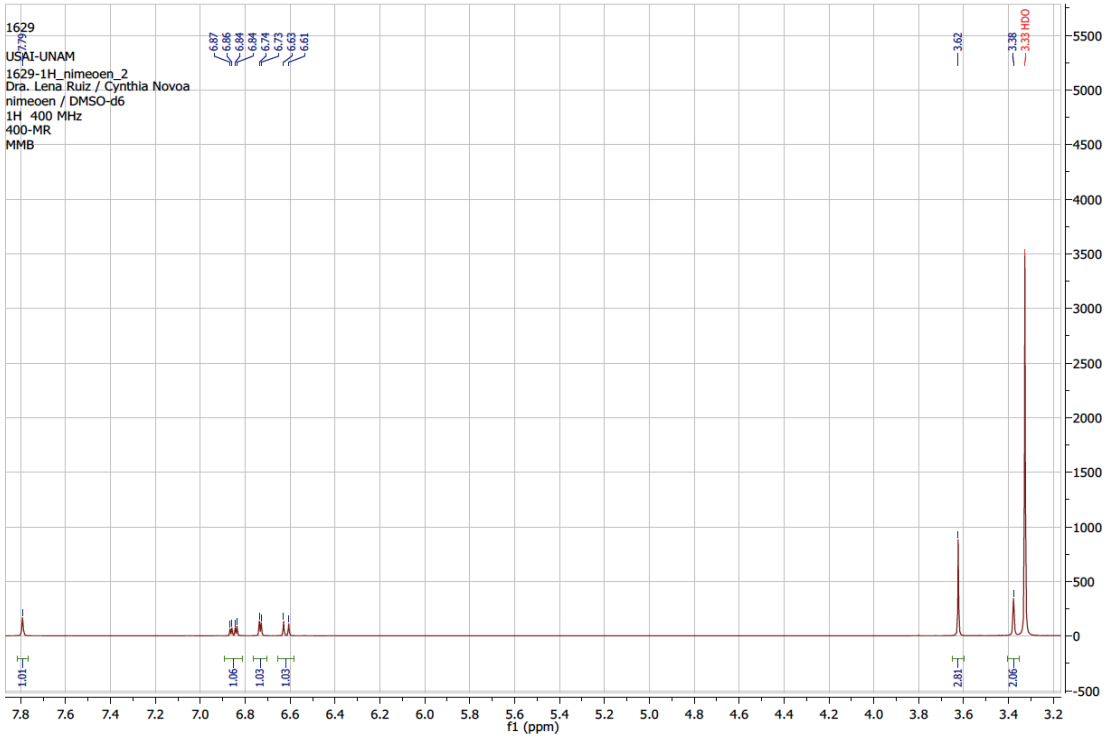


Figure S21. ^{1}H-NMR of NiMeO*salen* in DMSO-d6.

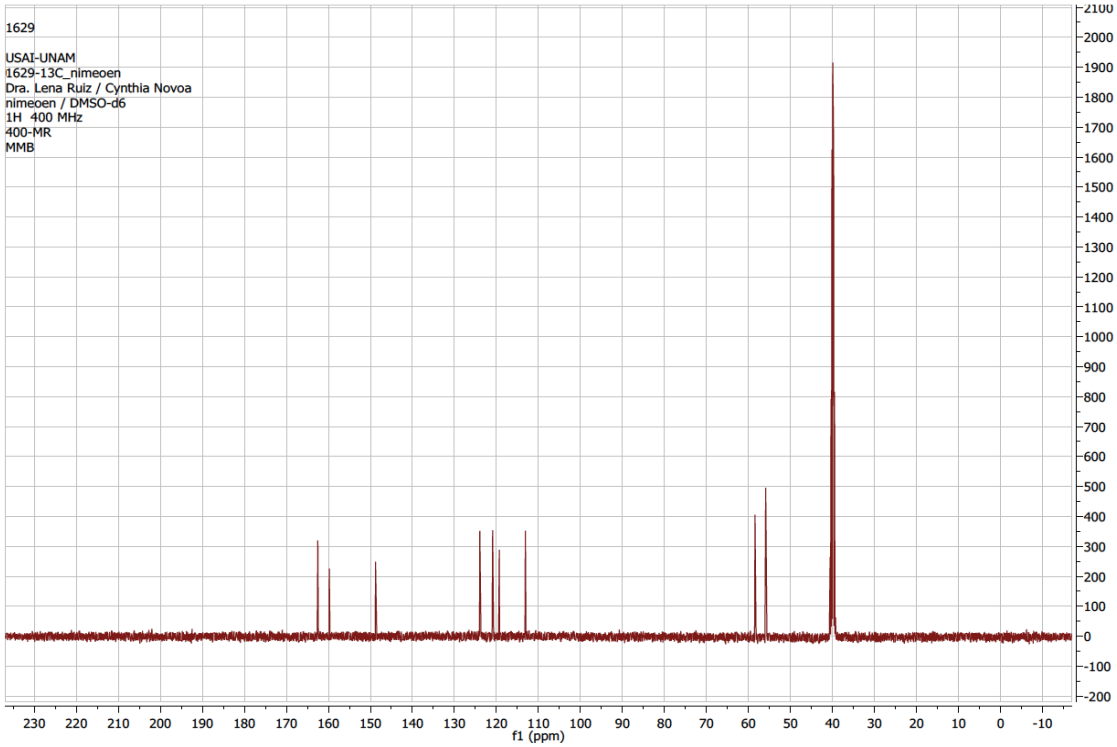


Figure S22. ^{13}C-NMR of NiMeO*salen* in DMSO-d6.

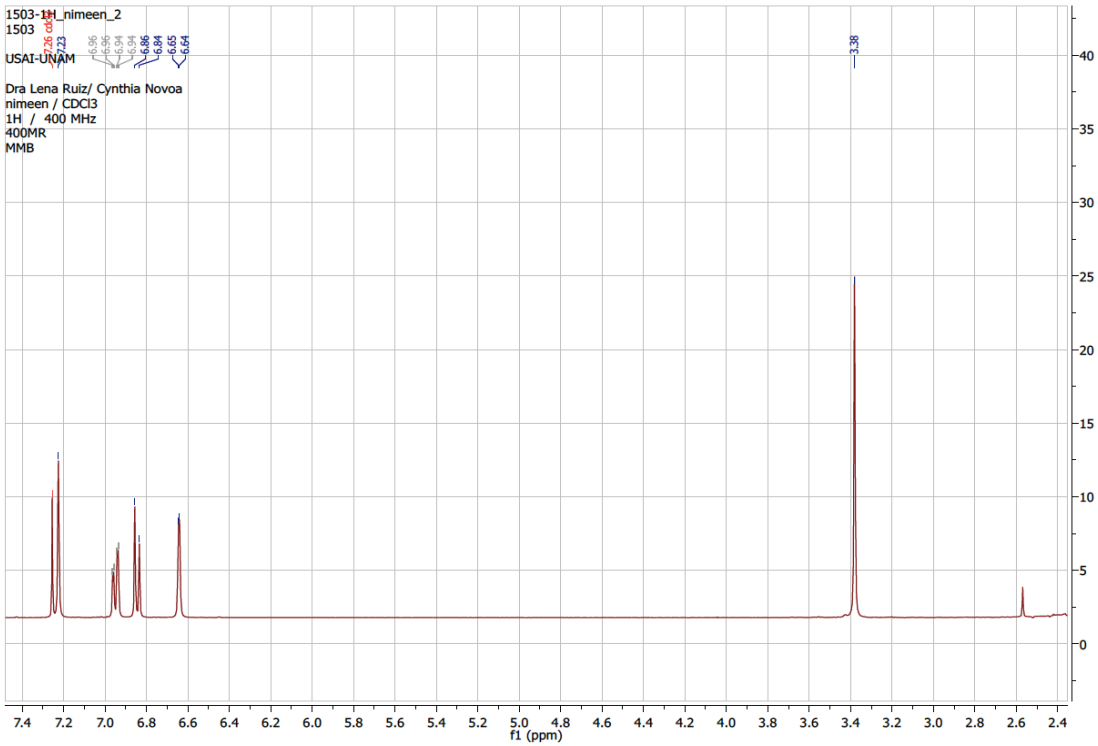


Figure S23. [1]H-NMR of NiMe*salen* in chloroform.

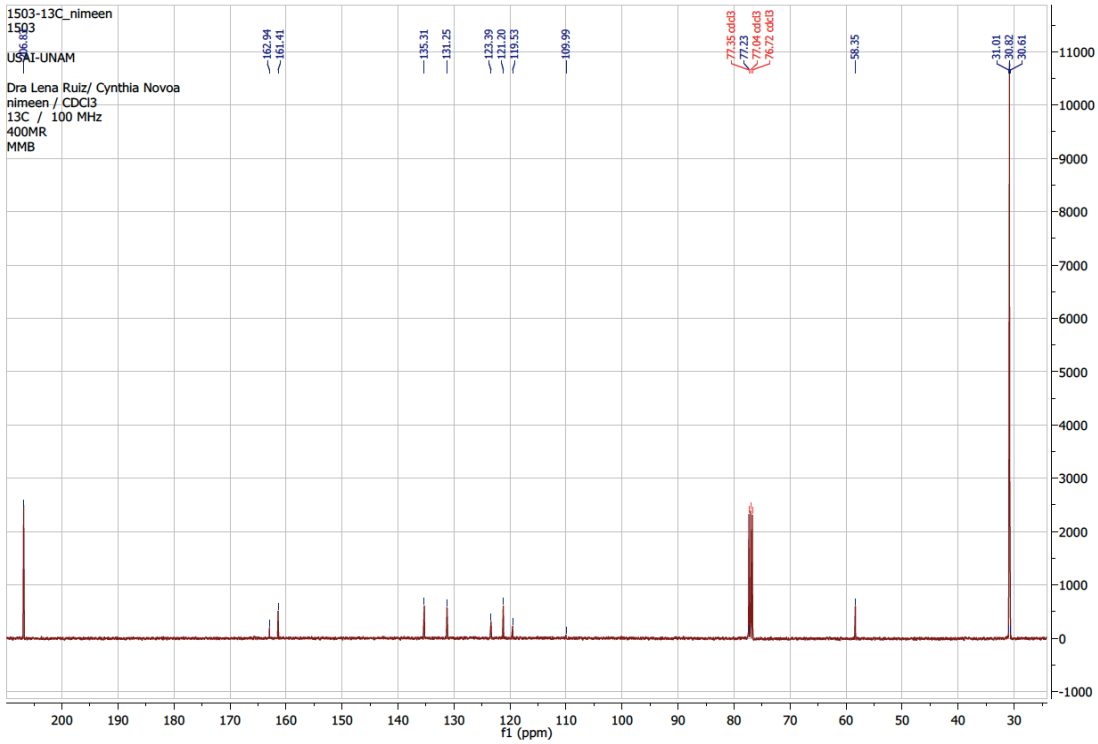


Figure S24. [13]C-NMR of NiMe*salen* in chloroform.

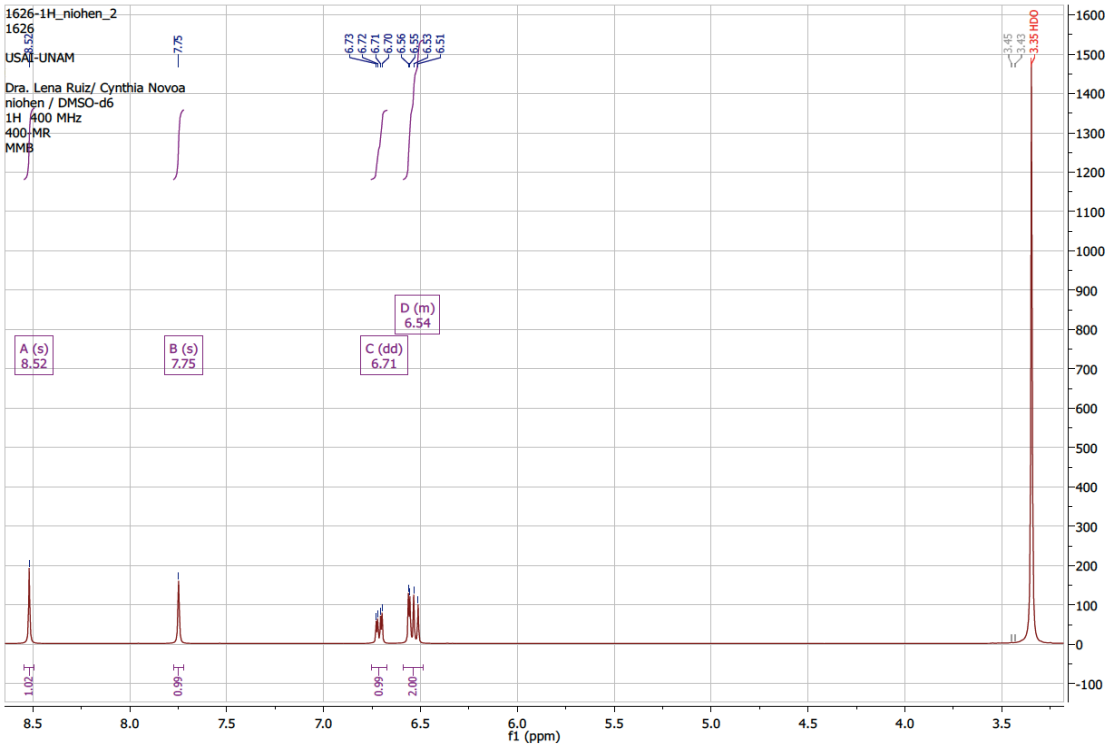


Figure S25. [1]H-NMR of NiOH*salen* in DMSO-d6.

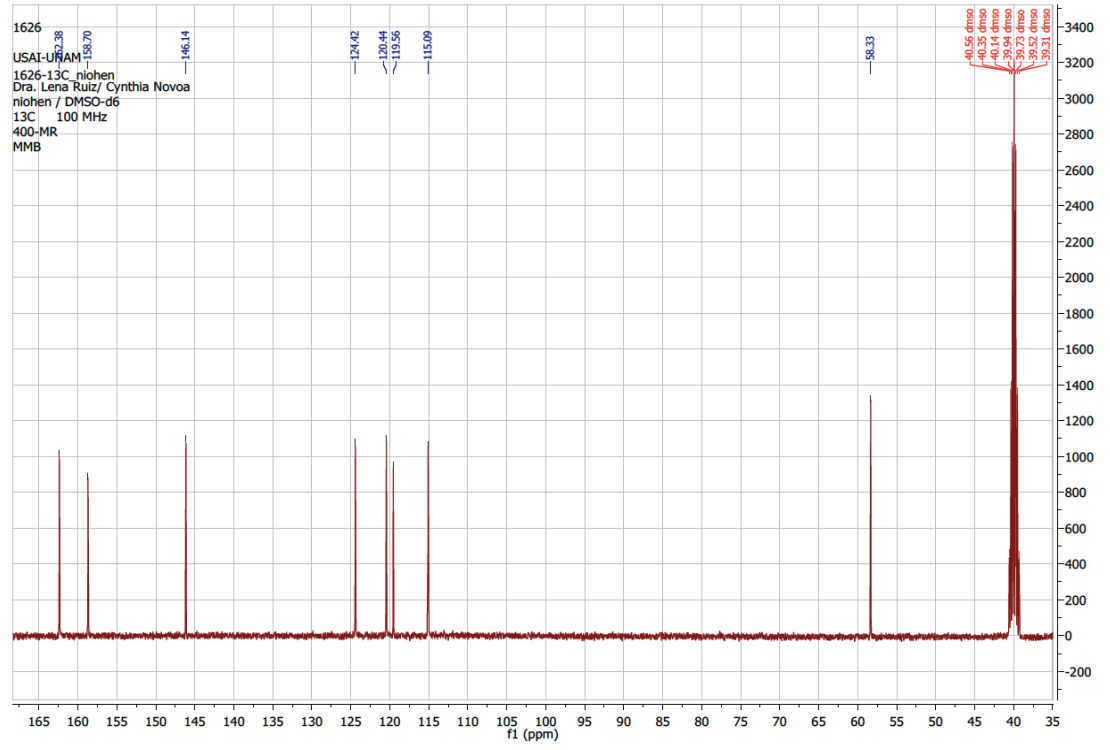


Figure S26. [13]C-NMR of NiOH*salen* in DMSO-d6.

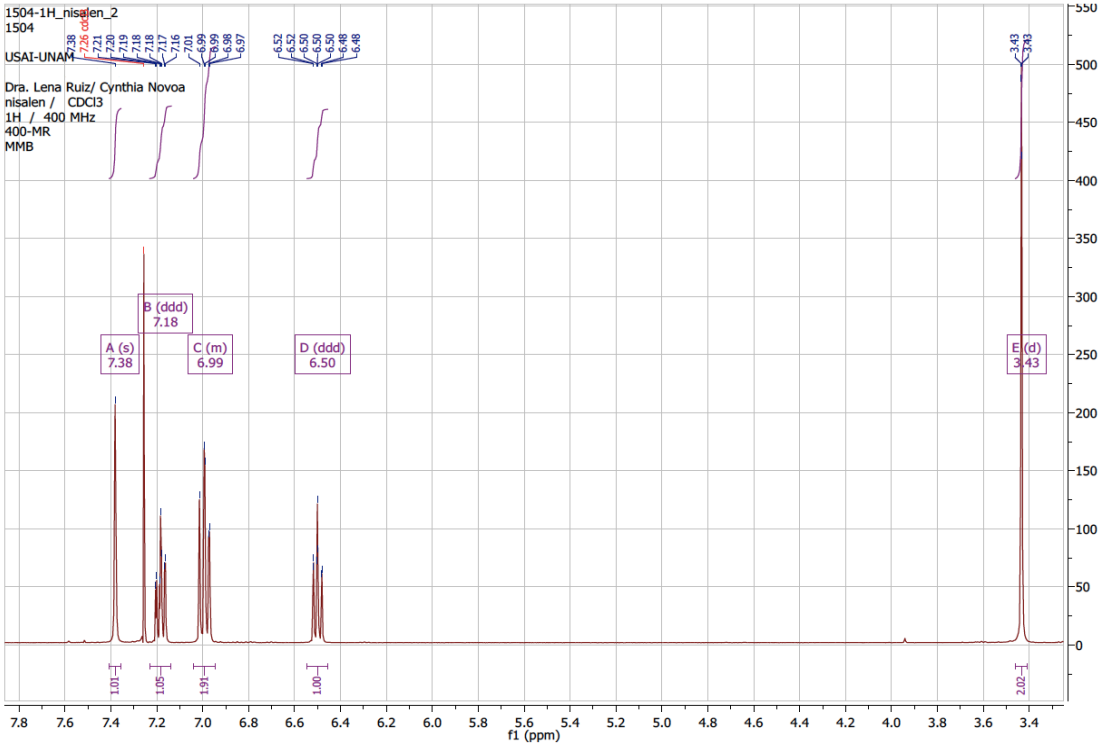


Figure S27. ^{1}H-NMR of Ni*salen* in chloroform.

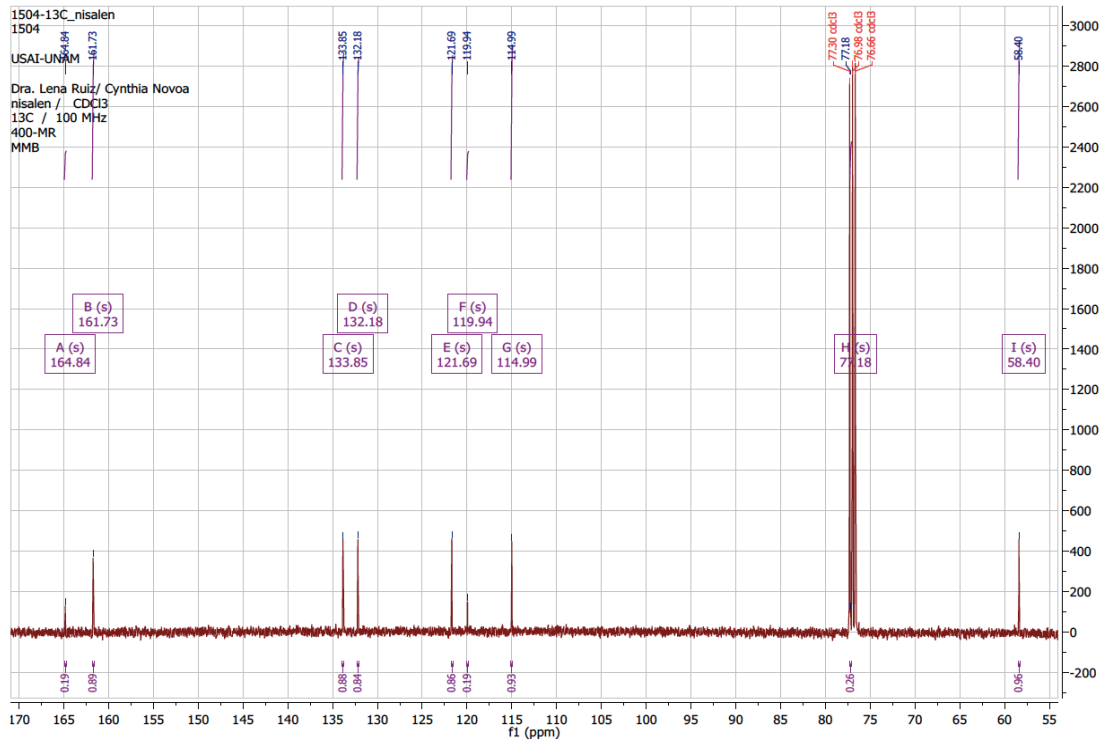


Figure S28. ^{13}C-NMR of Ni*salen* in chloroform.

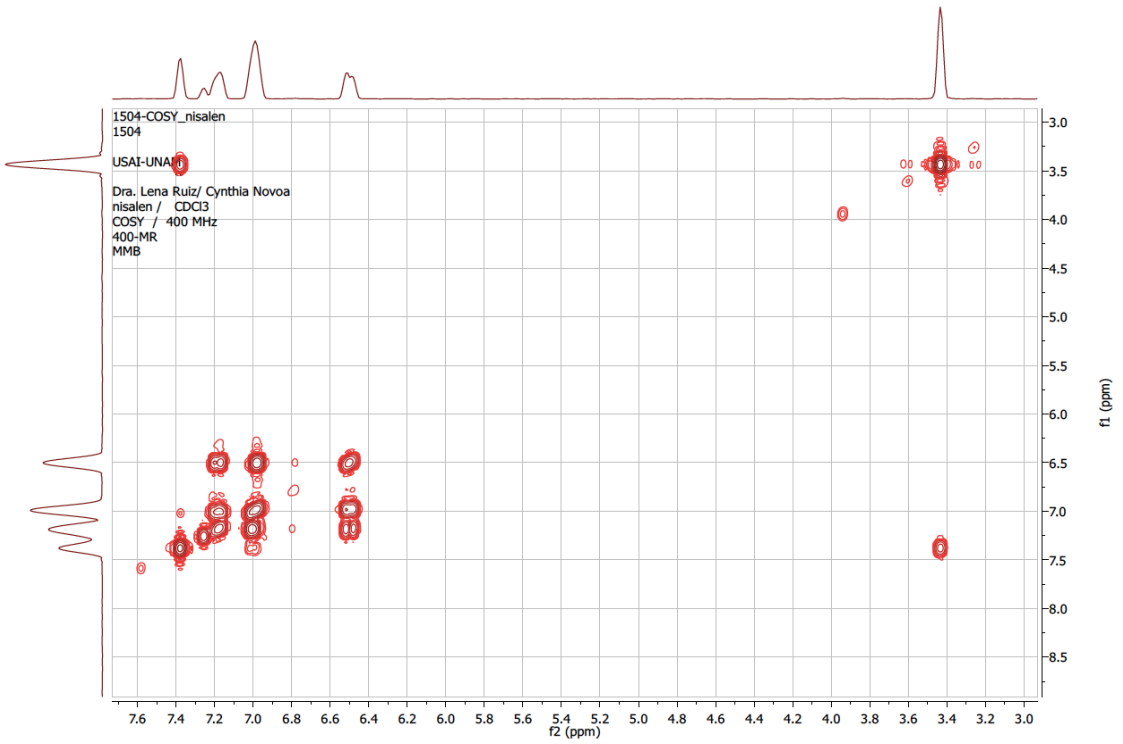


Figure S29. COSY spectrum of Ni*salen* in chloroform.

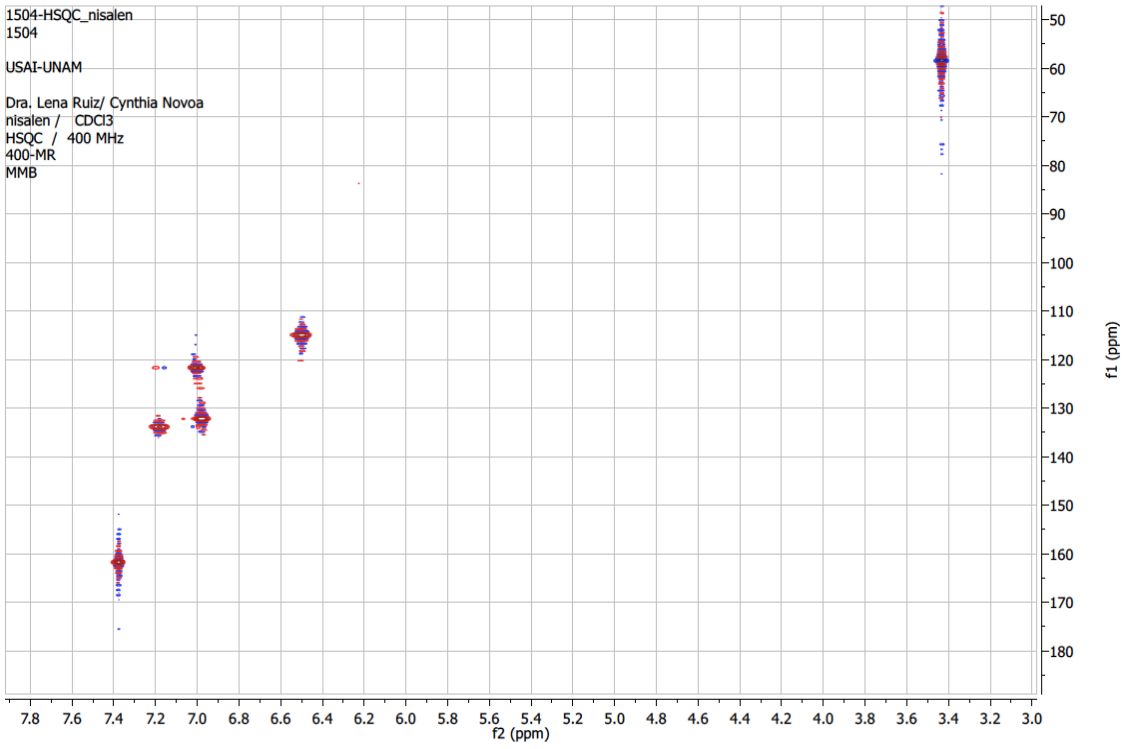


Figure S30. HSQC spectrum of Ni*salen* in choloform.

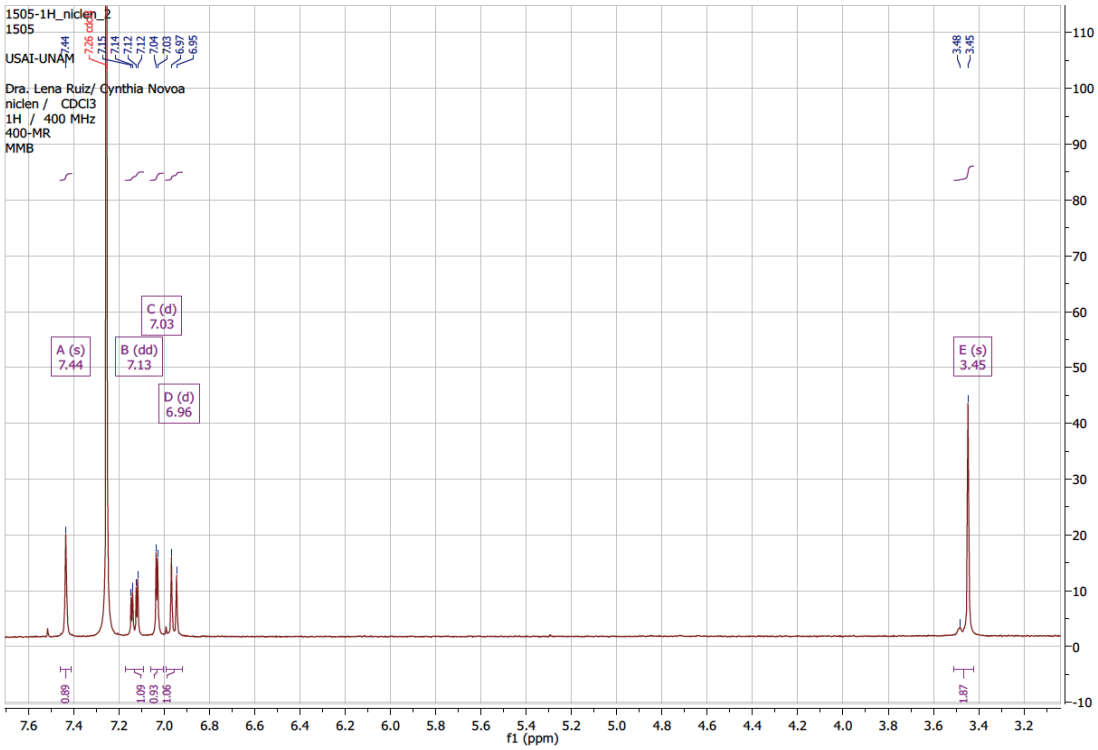


Figure S31. ^{1}H-NMR of NaCl*salen* in chloroform.

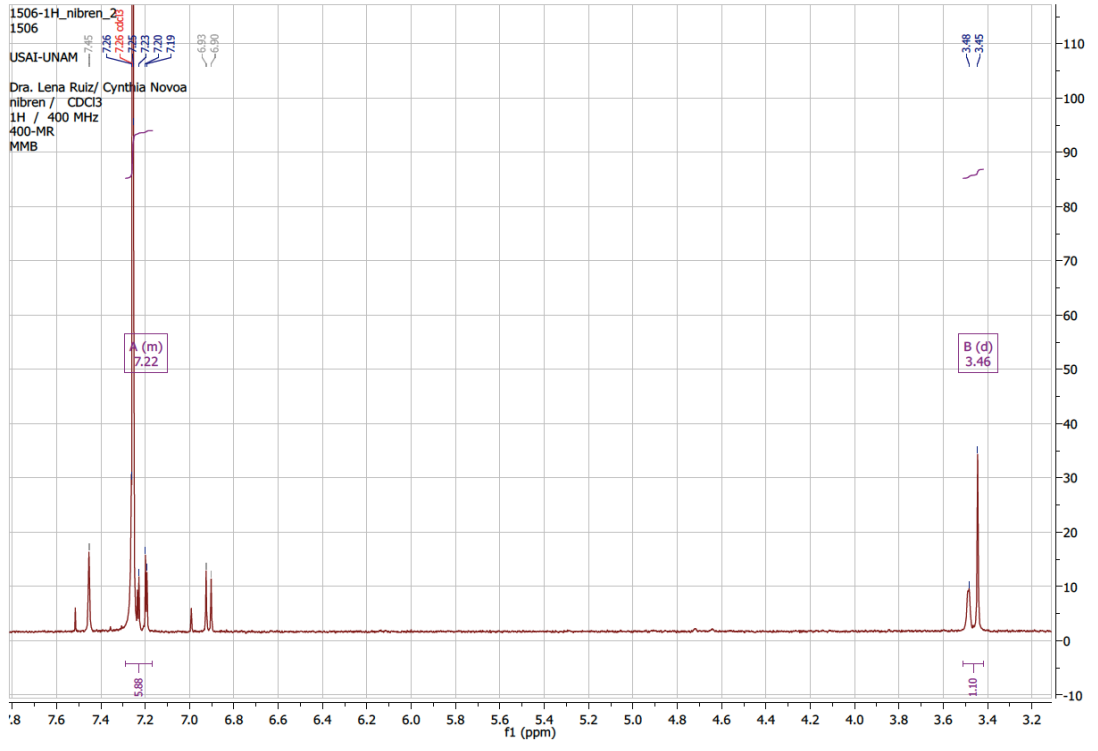


Figure S32. ^{1}H-NMR of NiBr*salen* in chloroform.

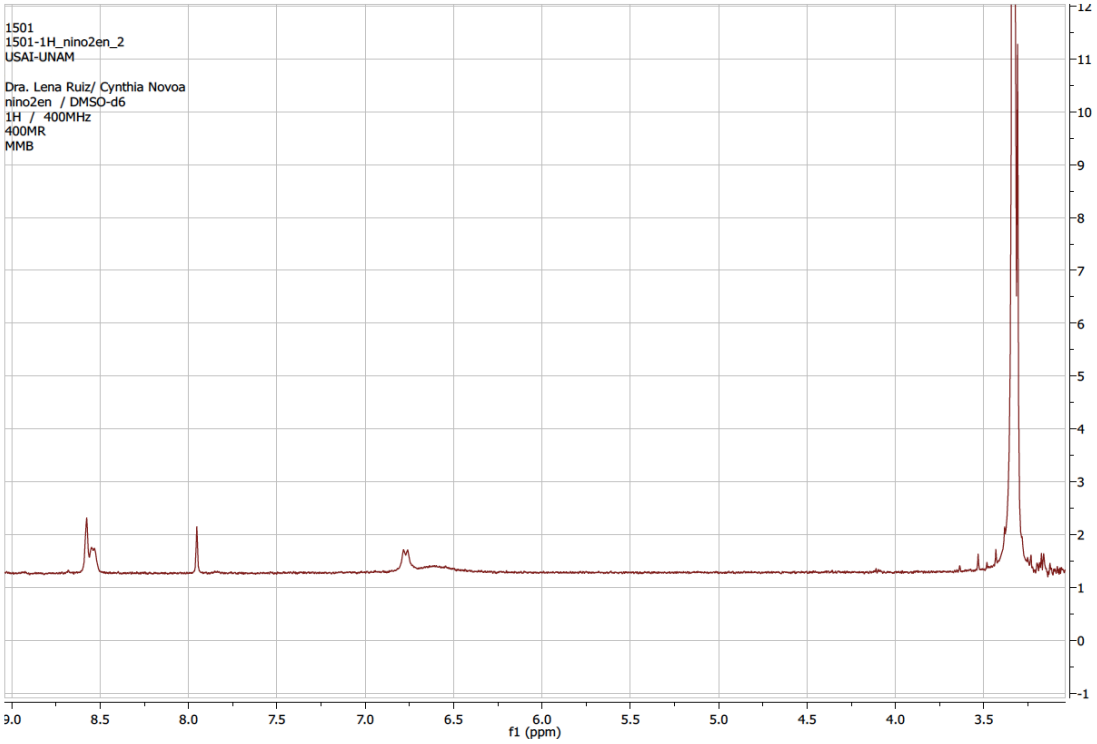


Figure S33. ^{1}H-NMR of NiNO$_2$*salen* in DMSO-d6.

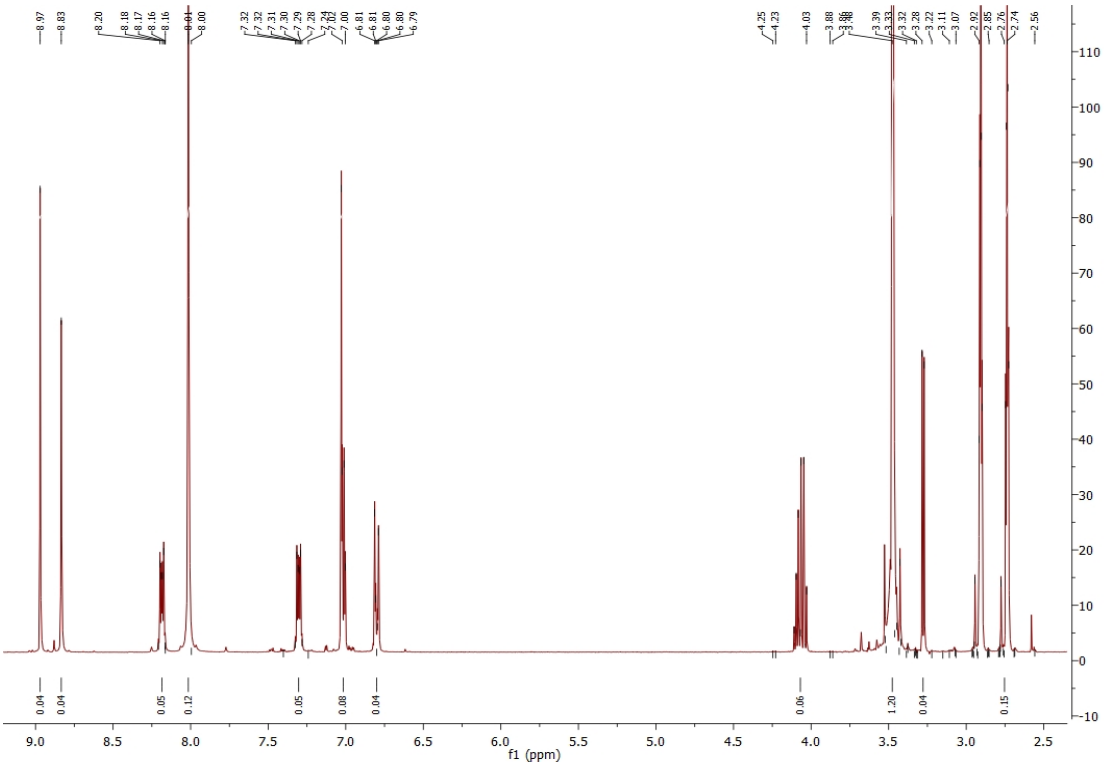


Figure S34. ^{1}H-NMR of NiOH*salphen* in DMF-d7.

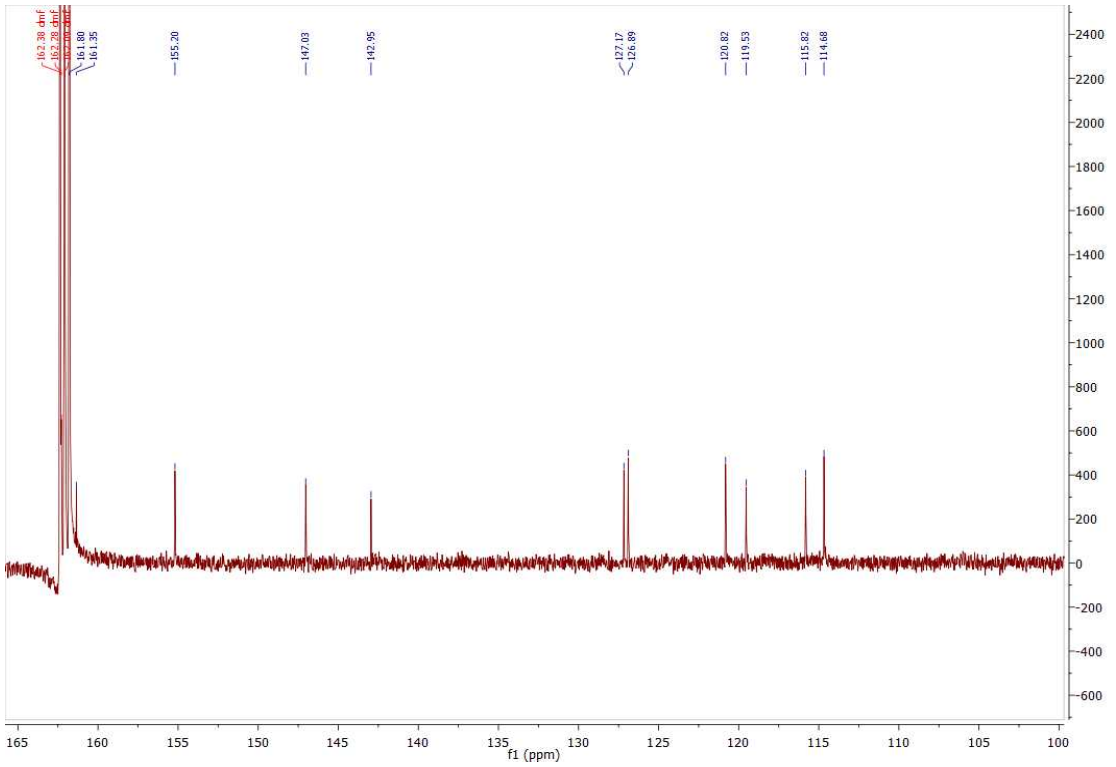


Figure S35. ^{13}C-NMR of NiOH*salphen* in DMF-d7.

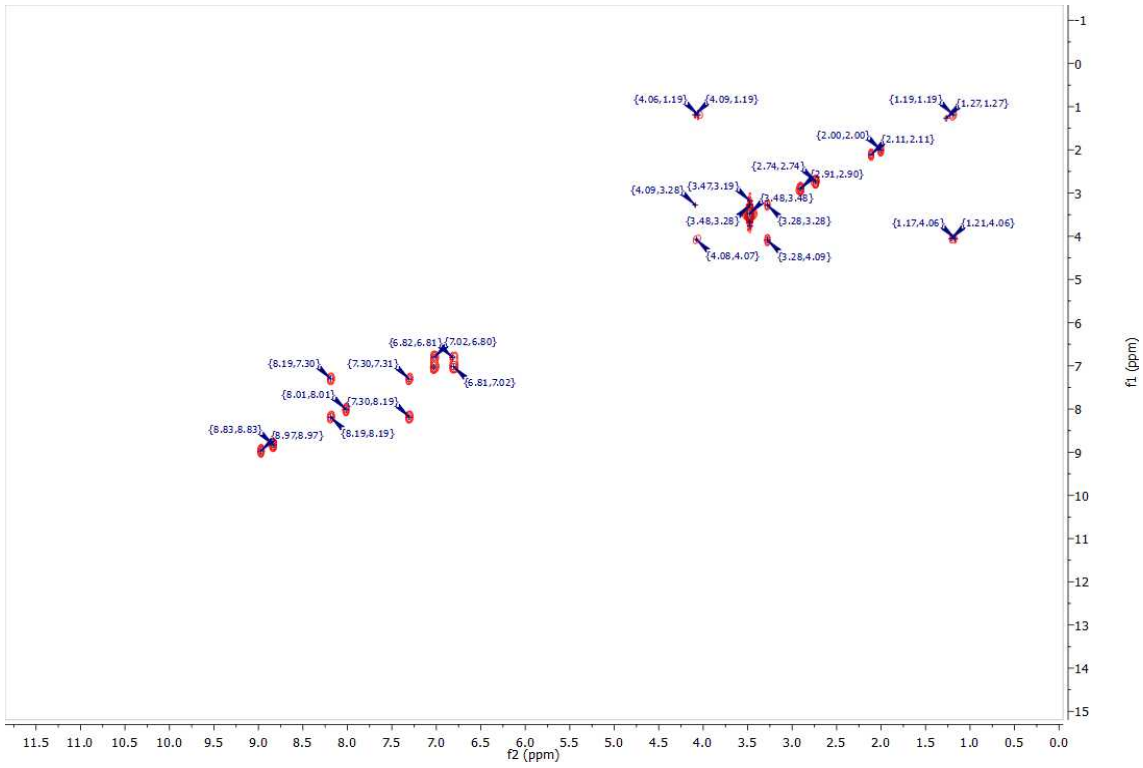


Figure S36. COSY spectrum of NiOH*salphen* in DMF-d7.

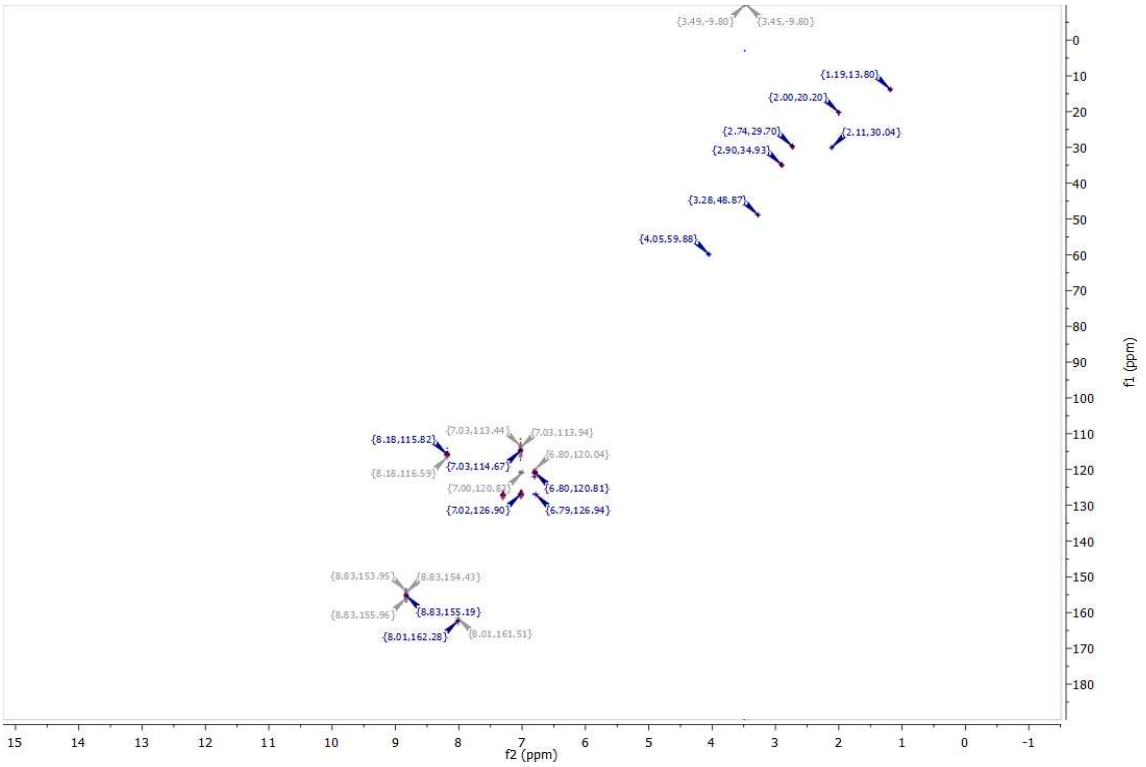


Figure S37. HSQC spectrum of NiOH*salphen* in DMF-d7.

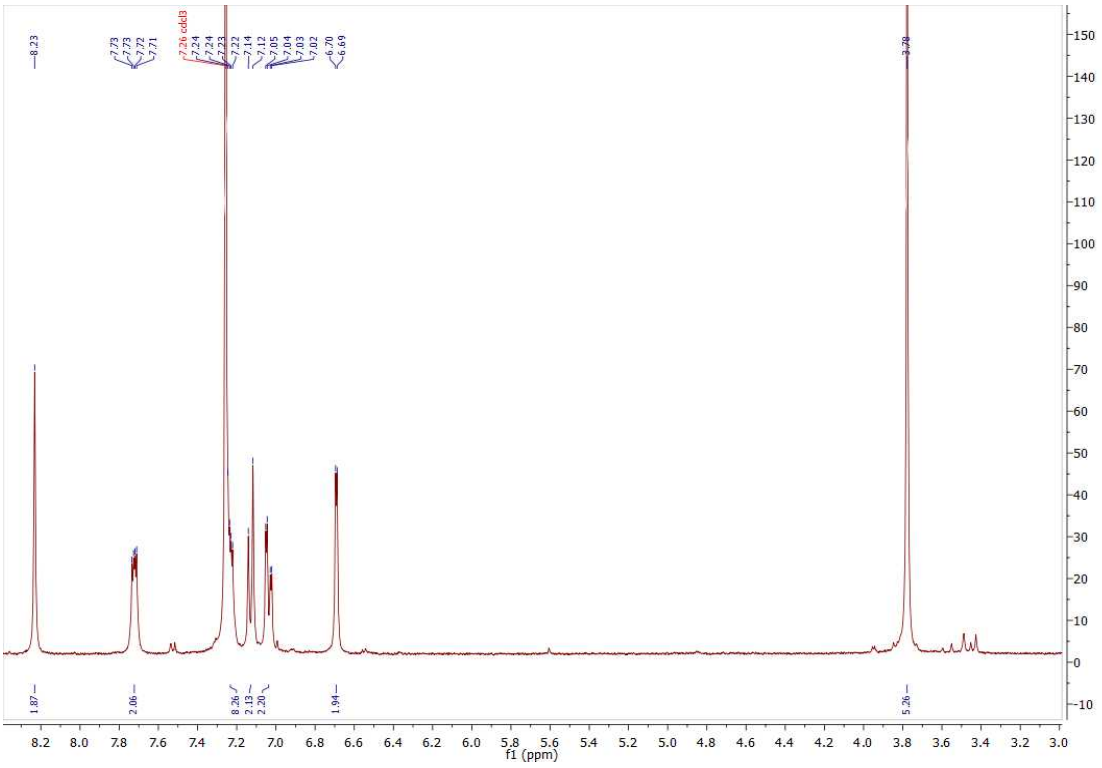


Figure S38. [1]H-NMR of NiMeO*salphen* in chloroform.

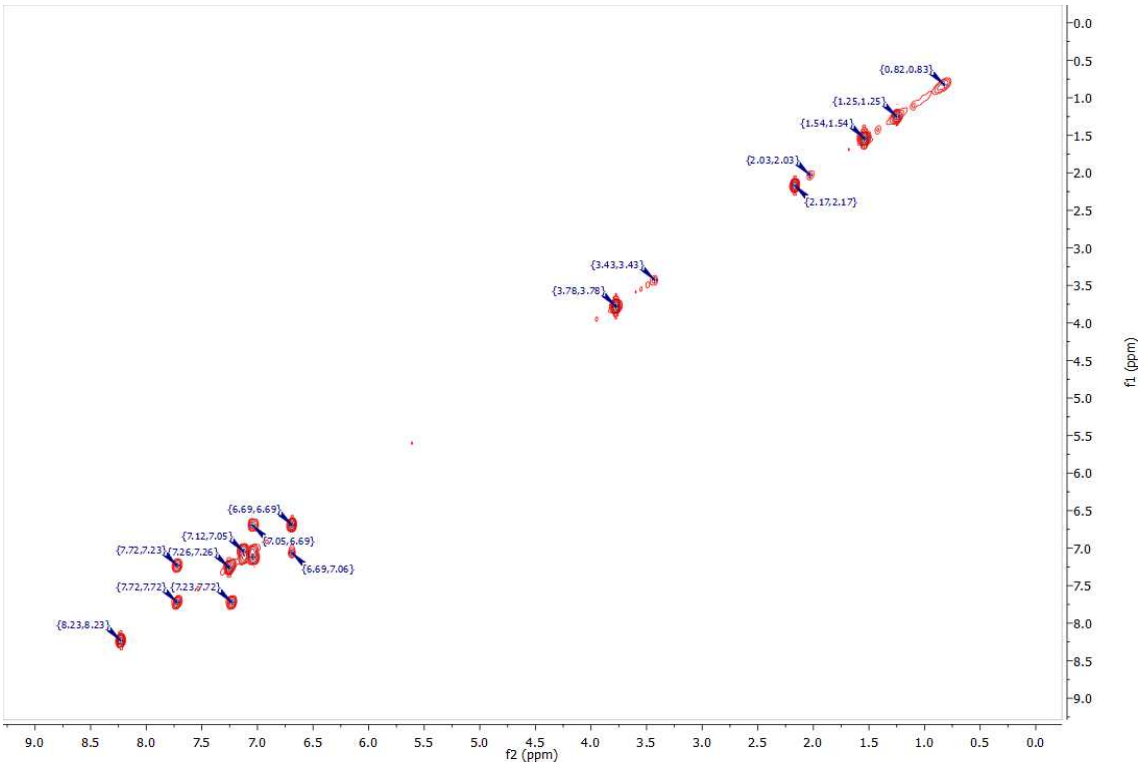


Figure S39. COSY spectrum of NiMeO*salphen* in chloroform.

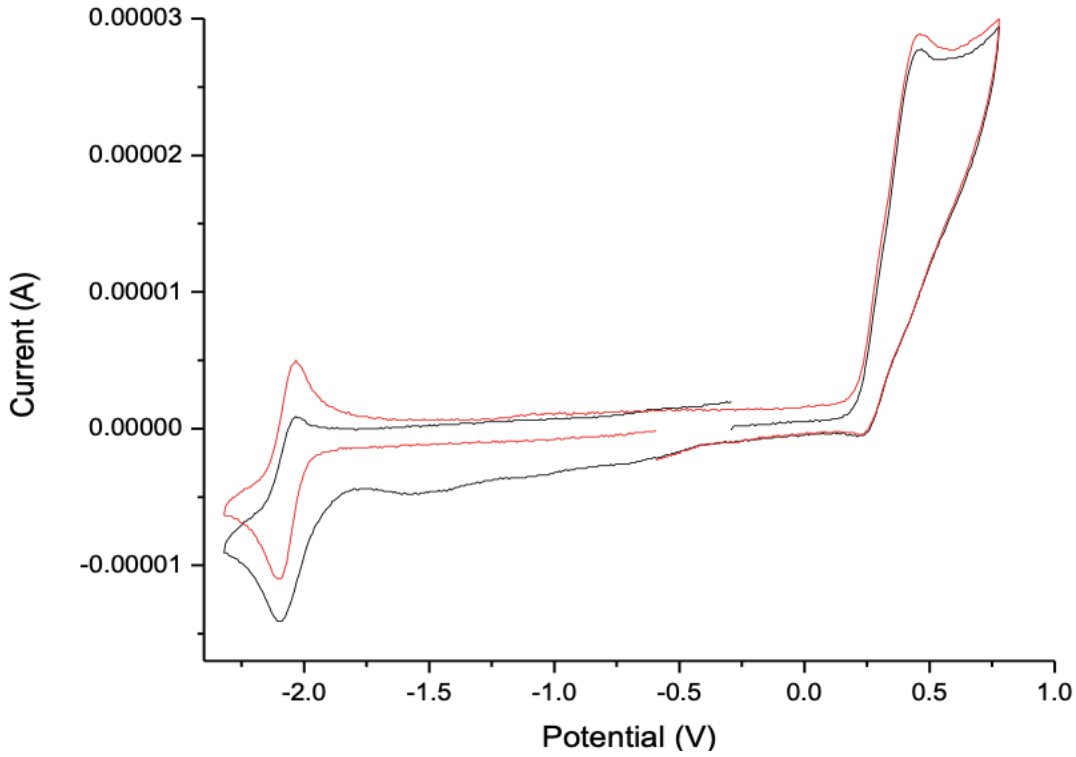


Figure S40. Voltammogram of NiMeO*salen* 1 mM in DMSO at 100 mV.

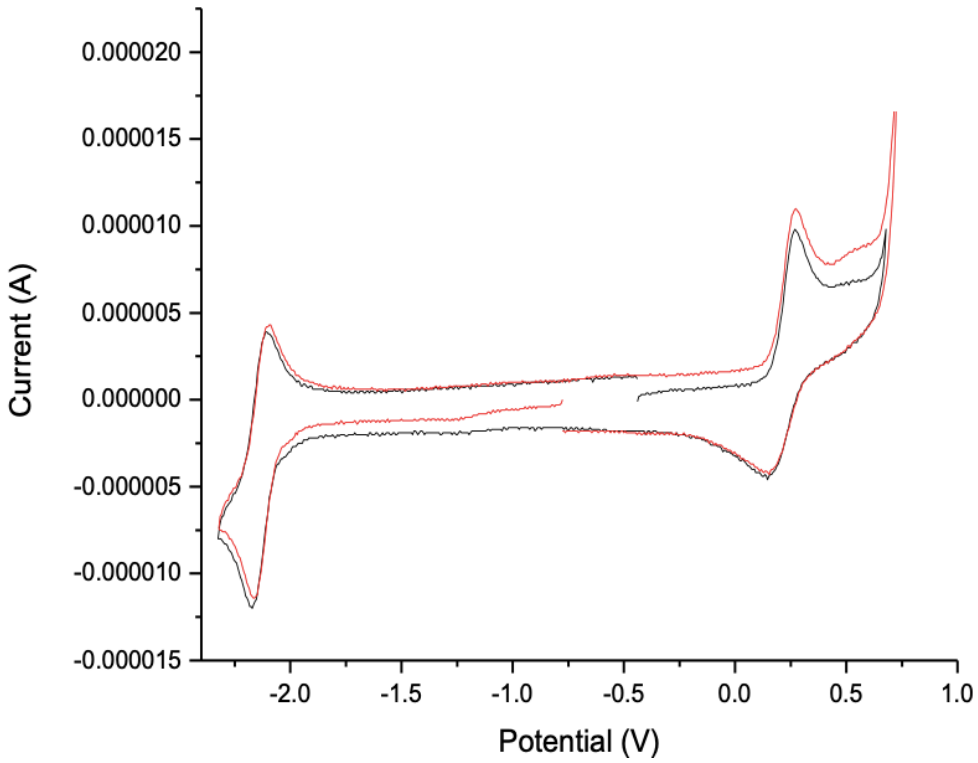


Figure S41. Voltammogram of NiMe*salen* 1 mM in DMSO at 100 mV.

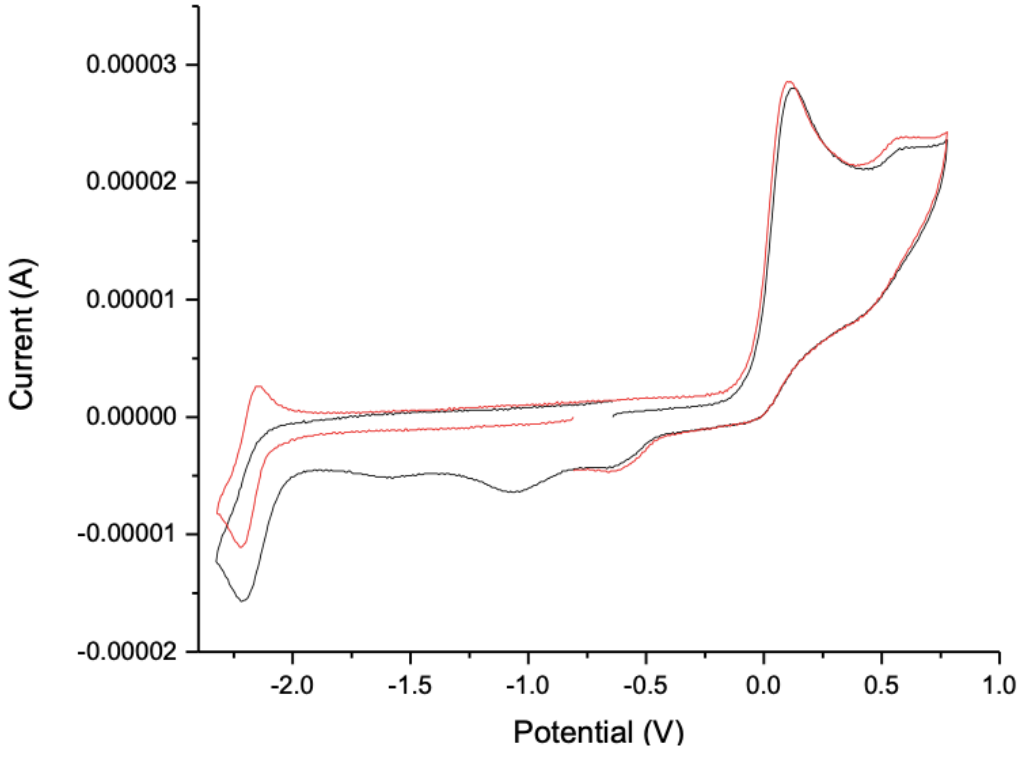


Figure S42. Voltammogram of NiOH*salen* 1 mM in DMSO at 100 mV.

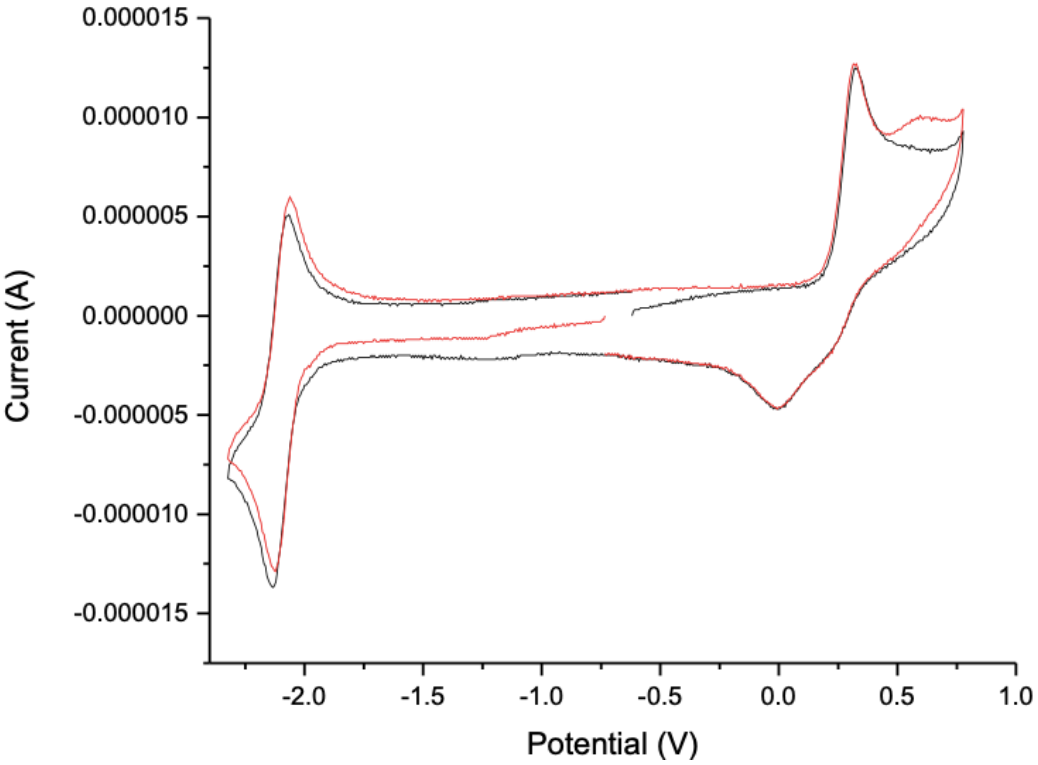


Figure S43. Voltammogram of Ni*salen* 1 mM in DMSO at 100 mV.

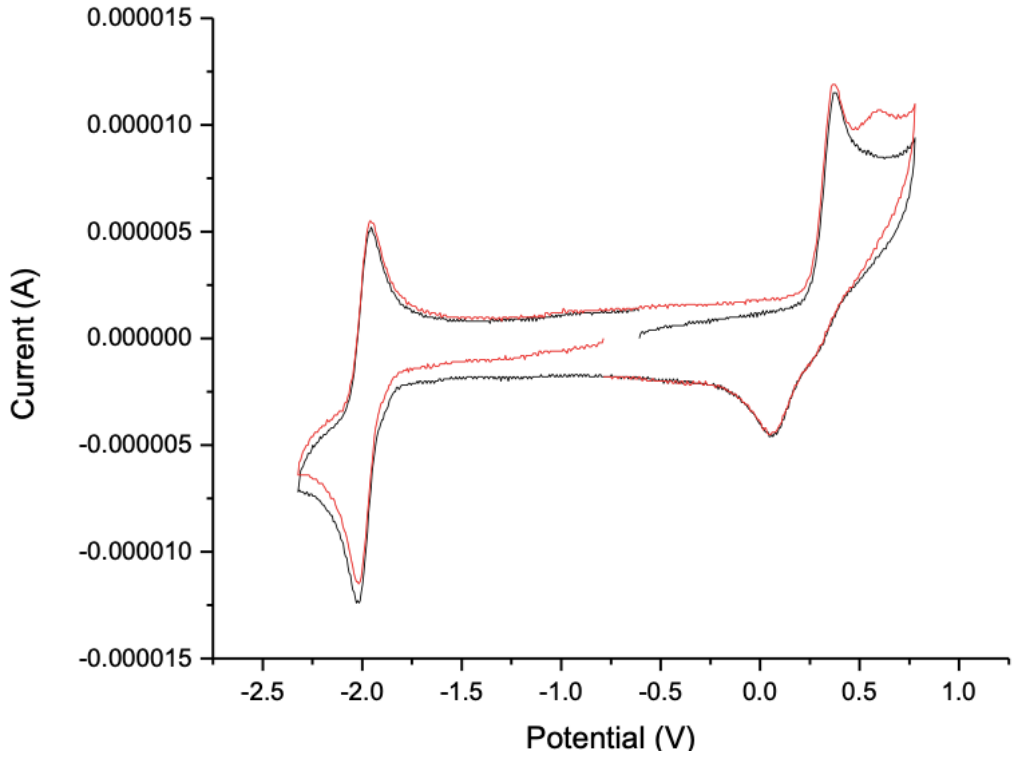


Figure S44. Voltammogram of NiCl*salen* 1 mM in DMSO at 100 mV.

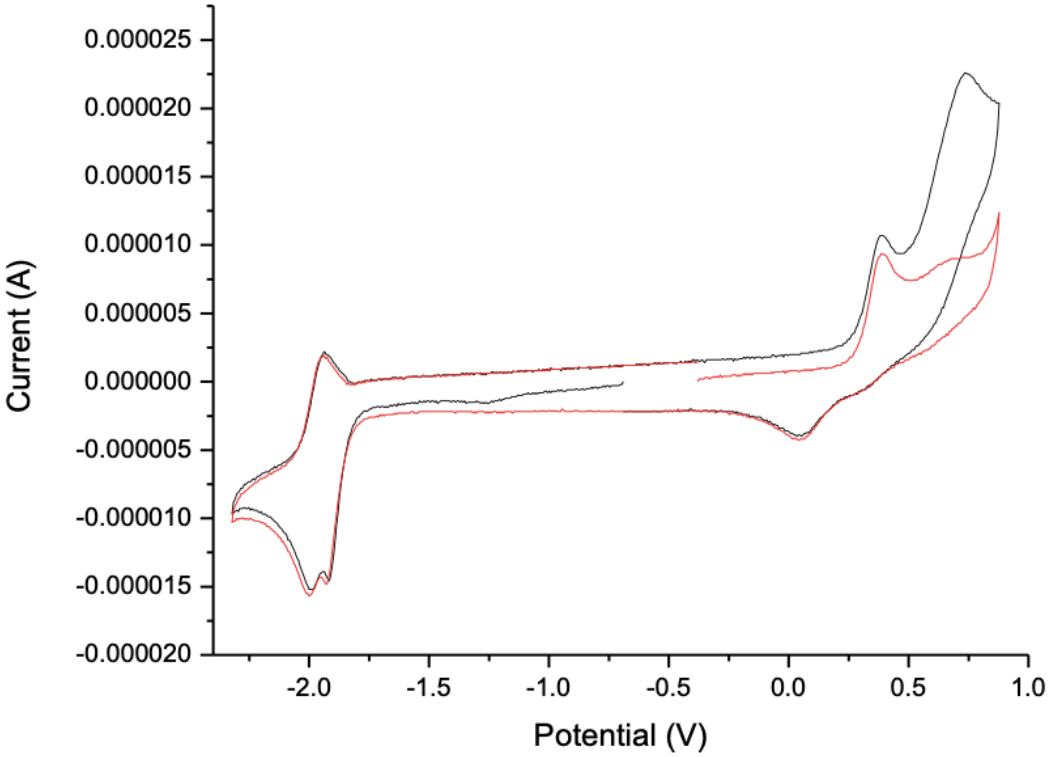


Figure S45. Voltammogram of NiBr*salen* 1 mM in DMSO at 100 mV.

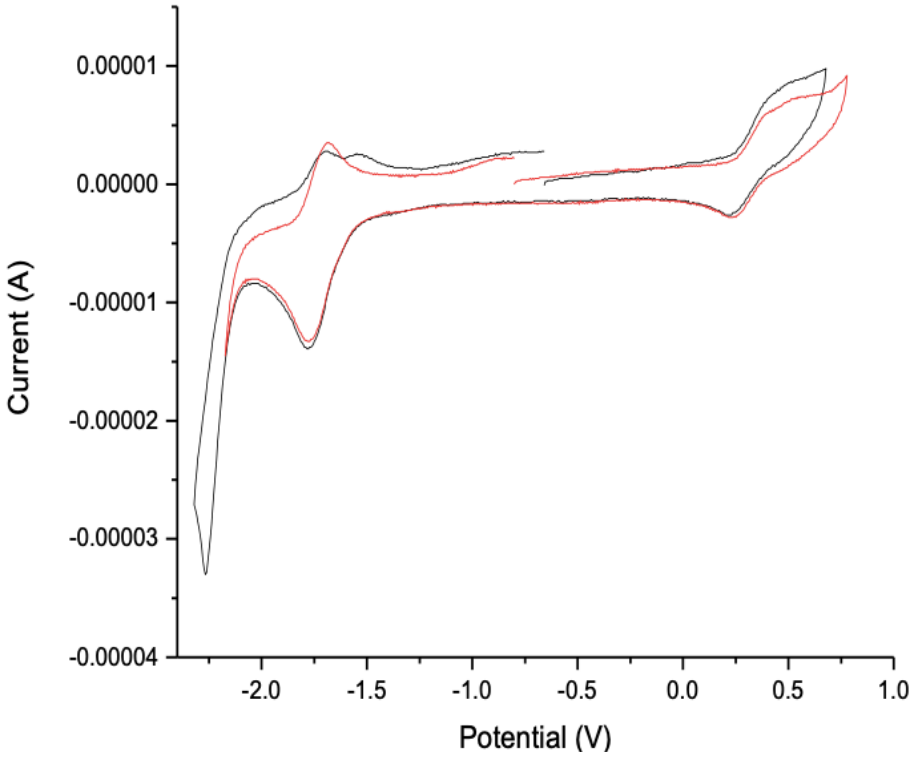


Figure S46. Voltammogram of $NiNO_2$*salen* 1 mM in DMSO at 100 mV.