

Electronic Supplementary document (ESI)

New Triazole-based Coordination Complexes as Antitumor Agents against Triple Negative Breast Cancer MDA-MB-468 Cell Line

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Content:

Table S1. Summary of crystallographic data and refinement for 5-11	3
Table S2. Selected bond lengths [Å] and angles [°] for 5-11	4
¹H NMR LM	5
¹³C NMR LM	6
Figure S1. Diffuse reflectance spectroscopic comparison of LM and 5-11	7
Figure S2. SQUID measurement on 9 carried out over the temperature range (300-5 K) over three consecutive runs.....	8
Figure S3. Mössbauer spectrum in transmission mode of 9 recorded at room temperature.....	9
HRMS of LM	10
HRMS of 5	11
HRMS of 6	12
HRMS of 7	13
HRMS of 8	14
HRMS of 10	15

Table S1. Summary of crystallographic data and refinement for **5-11**.

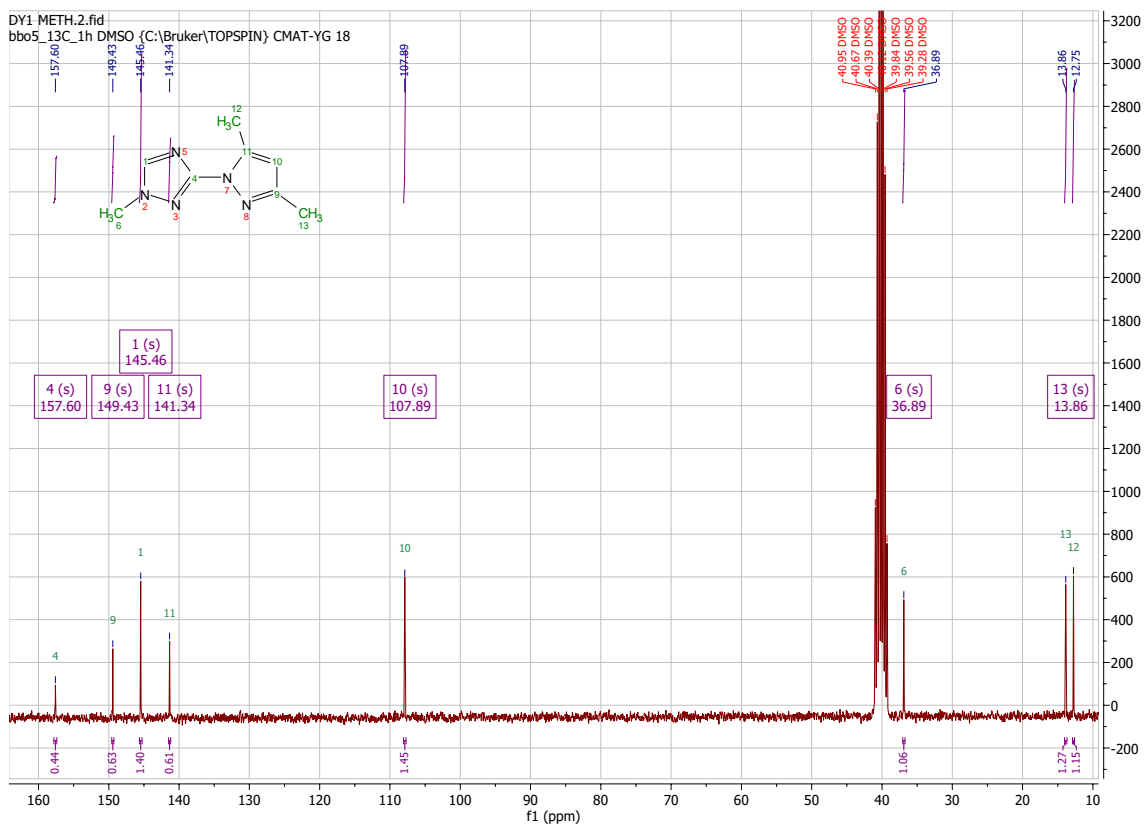
Compounds	(5)	(6)	(7)	(8)	(9)	(10)	(11)
Empirical formula	C ₂₆ H ₃₉ Cl ₂ N ₁₅ NiOS	C ₅₂ H ₇₆ Cl ₄ Co ₂ N ₃₀ O ₁₇	C ₁₆ H ₂₂ CdCl ₂ N ₁₀	C ₁₆ H ₂₂ CuN ₁₂ O ₆	C ₂₄ H ₃₃ B ₂ F ₈ Fe N ₁₅	C ₂₄ H ₃₃ B ₂ F ₈ Zn N ₁₅	C ₁₆ H ₂₂ N ₁₂ ZnO ₆
Formula weight	867.39	1653.08	537.73	541.99	761.12	770.64	543.82
Crystal size (mm)	0.30 x 0.20 x 0.10	0.30 x 0.14 x 0.10	0.60 x 0.40 x 0.30	0.50 x 0.30 x 0.25	0.40 x 0.35 x 0.15	0.50 x 0.47 x 0.20	0.20 x 0.18 x 0.15
Crystal system	Triclinic	triclinic	monoclinic	Monoclinic	triclinic	Triclinic	monoclinic
Space group	<i>P</i> -1 (#2)	<i>P</i> -1 (#2)	<i>P</i> 2 ₁ / <i>c</i> (#14)	<i>C</i> 2/ <i>c</i> (#15)	<i>P</i> -1 (#2)	<i>P</i> -1 (#2)	<i>C</i> 2/ <i>c</i> (#15)
<i>a</i> (Å)	11.1956(13)	11.7384(12)	7.1207(3)	15.2108(11)	11.6977(19)	11.7208(8)	15.3500(5)
<i>b</i> (Å)	14.8446(14)	11.7537(11)	17.0820(8)	14.0236(9)	11.7249(9)	11.7347(10)	13.6196(4)
<i>c</i> (Å)	14.8844(18)	15.3103(9)	8.8551(4)	11.5087(9)	15.229(2)	15.1727(9)	11.4186(3)
α (°)	119.056(11)	80.114(7)	90	90	79.371(9)	79.553(6)	90
β (°)	92.646(10)	78.156(8)	94.076(2)	108.678(9)	79.491(12)	79.334(6)	109.496(3)
γ (°)	110.233(10)	73.278(9)	90	90	73.371(10)	73.196(7)	90
Volume (Å ³)	1958.6(4)	1965.6(3)	1074.37(8)	2325.6(3)	1948.3(5)	1945.0(3)	2250.31(12)
<i>Z</i>	2	1	2	4	2	2	4
ρ_{calc} (g/cm ³)	1.471	1.397	1.662	1.548	1.297	1.316	1.605
F(000)	900	856	540.00	1116	780	788	1120
$\mu_{\text{MoK}\alpha}$ (cm ⁻¹)	0.752	0.637	1.291	0.999	0.463	0.707	1.153
T (K)	293(2)	293(2)	293	293(2)	293(2)	297(2)	150(2)
θ min/max	3.157/26.158	3.035/26.203	3.106/ 27.500	3.455/26.040	2.873/26.165	3.096/26.157	2.454/53.701
Refl. collected/unique	30651/7776	27103/7827	4681/2316	7610/2272	20213/ 7758	15416/7190	17389/7841
Data/restraints/parameters	7776/156/ 555	7827/50/551	2316/0/133	2272/62/194	7758/60/522	7190/110/506	7841/1/178
Goodness of fit on <i>F</i> ²	1.046	1.068	1.065	1.078	1.068	1.030	1.056
Final <i>R</i> indices [<i>I</i> >2 σ (<i>I</i>)]	R ₁ = 0.0514, wR ₂ =0.1412	R ₁ =0.0478, wR ₂ =0.1397	R ₁ = 0.0469, wR ₂ = 0.1278	R ₁ =0.0452, wR ₂ =0.1284	R ₁ =0.0554, wR ₂ =0.1499	R ₁ =0.0456, wR ₂ =0.1268	R ₁ =0.0587, wR ₂ =0.1700
<i>R</i> indices (all data)	R ₁ = 0.0584, wR ₂ =0.1462	R ₁ = 0.0558, wR ₂ =0.1458	R ₁ = 0.0489, wR ₂ = 0.1312	R ₁ = 0.0472, wR ₂ =0.1299	R ₁ =0.0723, wR ₂ =0.1635	R ₁ =0.0506, wR ₂ =0.1304	R ₁ =0.0990, wR ₂ =0.1894

Table S2. Selected bond lengths [Å] and angles [°] for **5-11**.

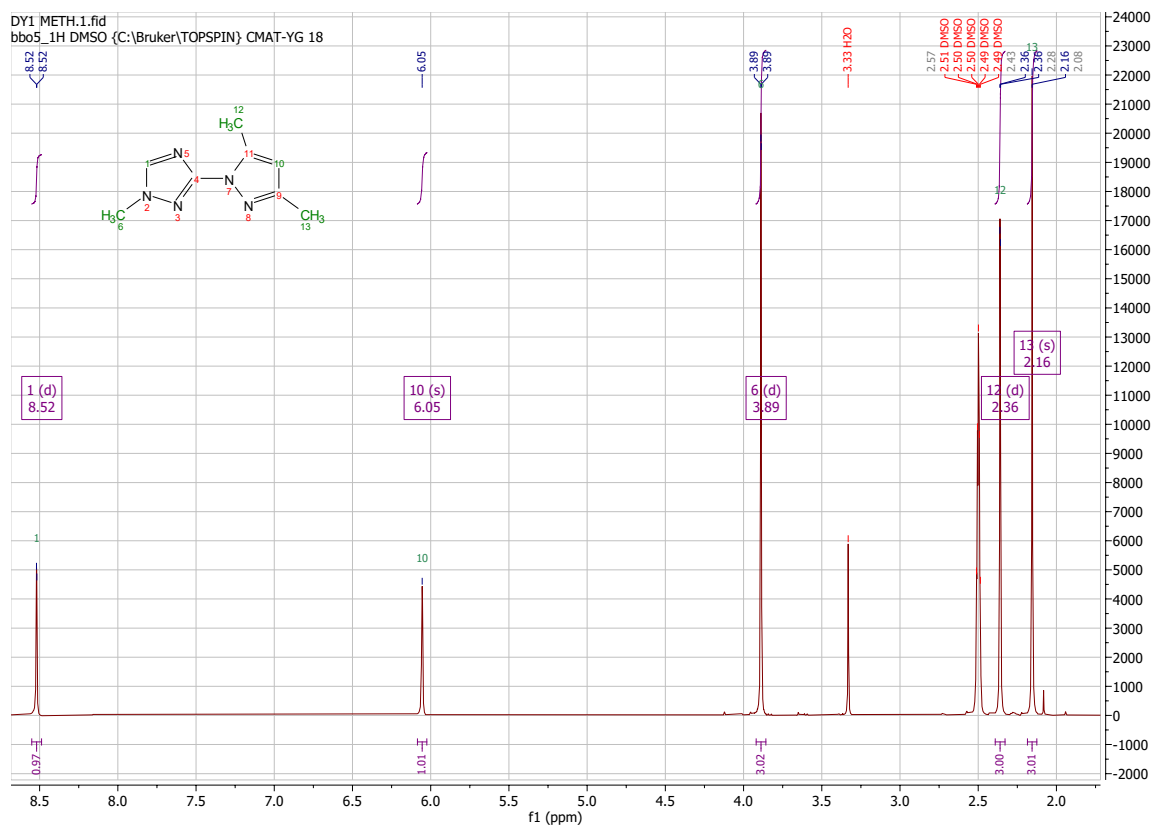
Compound	Bond lengths, Å		Bond angles, °	
5	Ni(1)-N(30)	2.072(2)	N(30)-Ni(1)-N(2)	91.94(9)
	Ni(1)-N(10)	2.073(2)	N(30)-Ni(1)-N(22)	77.68(8)
	Ni(1)-N(50)	2.080(2)	N(50)-Ni(1)-N(22)	93.84(9)
	Ni(1)-N(2)	2.136(2)	N(2)-Ni(1)-N(22)	98.81(8)
	Ni(1)-N(22)	2.138(2)	N(50)-Ni(1)-N(42)	77.18(9)
	Ni(1)-N(42)	2.142(2)	N(2)-Ni(1)-N(42)	100.49(9)
6	Co(1)-N(10)	2.100(2)	N(10)-Co(1)-N(2)	77.14(8)
	Co(1)-N(50)	2.116(2)	N(50)-Co(1)-N(2)	95.50(8)
	Co(1)-N(30)	2.125(2)	N(30)-Co(1)-N(22)	75.84(8)
	Co(1)-N(2)	2.170(2)	N(2)-Co(1)-N(22)	89.40(9)
	Co(1)-N(22)	2.170(2)	N(10)-Co(1)-N(42)	93.70(8)
	Co(1)-N(42)	2.173(2)	N(22)-Co(1)-N(42)	101.25(8)
7	Cd(1)-N(3)#1	2.411(3)	N(1)#1-Cd(1)-N(1)	180.0
	Cd(1)-N(3)	2.411(3)	N(3)#1-Cd(1)-Cl(1)	89.24(8)
	Cd(1)-N(1)#1	2.414(2)	N(3)-Cd(1)-Cl(1)	90.76(8)
	Cd(1)-N(1)	2.414(2)	N(1)#1-Cd(1)-Cl(1)	89.24(6)
	Cd(1)-Cl(1)	2.5426(9)	N(3)#1-Cd(1)-Cl(1)#1	90.76(8)
	Cd(1)-Cl(1)#1	2.5426(9)	Cl(1)-Cd(1)-Cl(1)#1	180.0
8	Cu(1)-O(23)	2.018(5)	O(23)-Cu(1)-N(2)	86.42(17)
	Cu(1)-N(2)	2.042(2)	N(2)#1-Cu(1)-N(10)#1	79.22(9)
	Cu(1)-N(2)#1	2.042(2)	O(23)-Cu(1)-N(10)	100.97(14)
	Cu(1)-N(10)#1	2.112(2)	N(2)-Cu(1)-N(10)	79.22(9)
	Cu(1)-N(10)	2.112(2)	N(2)#1-Cu(1)-N(10)	97.82(10)
			N(10)#1-Cu(1)-N(10)	104.36(13)
9	Fe(1)-N(30)	2.152(2)	N(10)-Fe(1)-N(50)	87.89(9)
	Fe(1)-N(10)	2.161(2)	N(30)-Fe(1)-N(42)	102.94(8)
	Fe(1)-N(50)	2.186(2)	N(50)-Fe(1)-N(42)	74.03(8)
	Fe(1)-N(42)	2.196(2)	N(30)-Fe(1)-N(22)	75.53(8)
	Fe(1)-N(22)	2.201(2)	N(42)-Fe(1)-N(22)	92.11(9)
	Fe(1)-N(2)	2.216(2)	N(30)-Fe(1)-N(2)	94.02(8)
10	Zn(1)-N(30)	2.1104(18)	N(10)-Zn(1)-N(22)	95.60(8)
	Zn(1)-N(10)	2.1411(19)	N(30)-Zn(1)-N(42)	101.03(7)
	Zn(1)-N(50)	2.1512(19)	N(50)-Zn(1)-N(42)	75.16(7)
	Zn(1)-N(22)	2.191(2)	N(22)-Zn(1)-N(42)	91.87(8)
	Zn(1)-N(42)	2.191(2)	N(30)-Zn(1)-N(2)	94.04(7)
	Zn(1)-N(2)	2.211(2)	N(42)-Zn(1)-N(2)	99.48(8)
11	N(6)-Zn(1)	2.1884(14)	N(11)-Zn(1)-N(11)#1	105.08(8)

N(11)-Zn(1)	2.0637(14)	N(11)#1-Zn(1)-O(30)#1	97.75(5)
O(30)-Zn(1)	2.1682(14)	O(30)#1-Zn(1)-O(30)	59.80(7)
		N(11)-Zn(1)-N(6)	77.57(5)
		O(30)#1-Zn(1)-N(6)	95.53(5)
		O(30)-Zn(1)-N(6)	89.40(5)

¹H NMR LM



¹³C NMR LM:



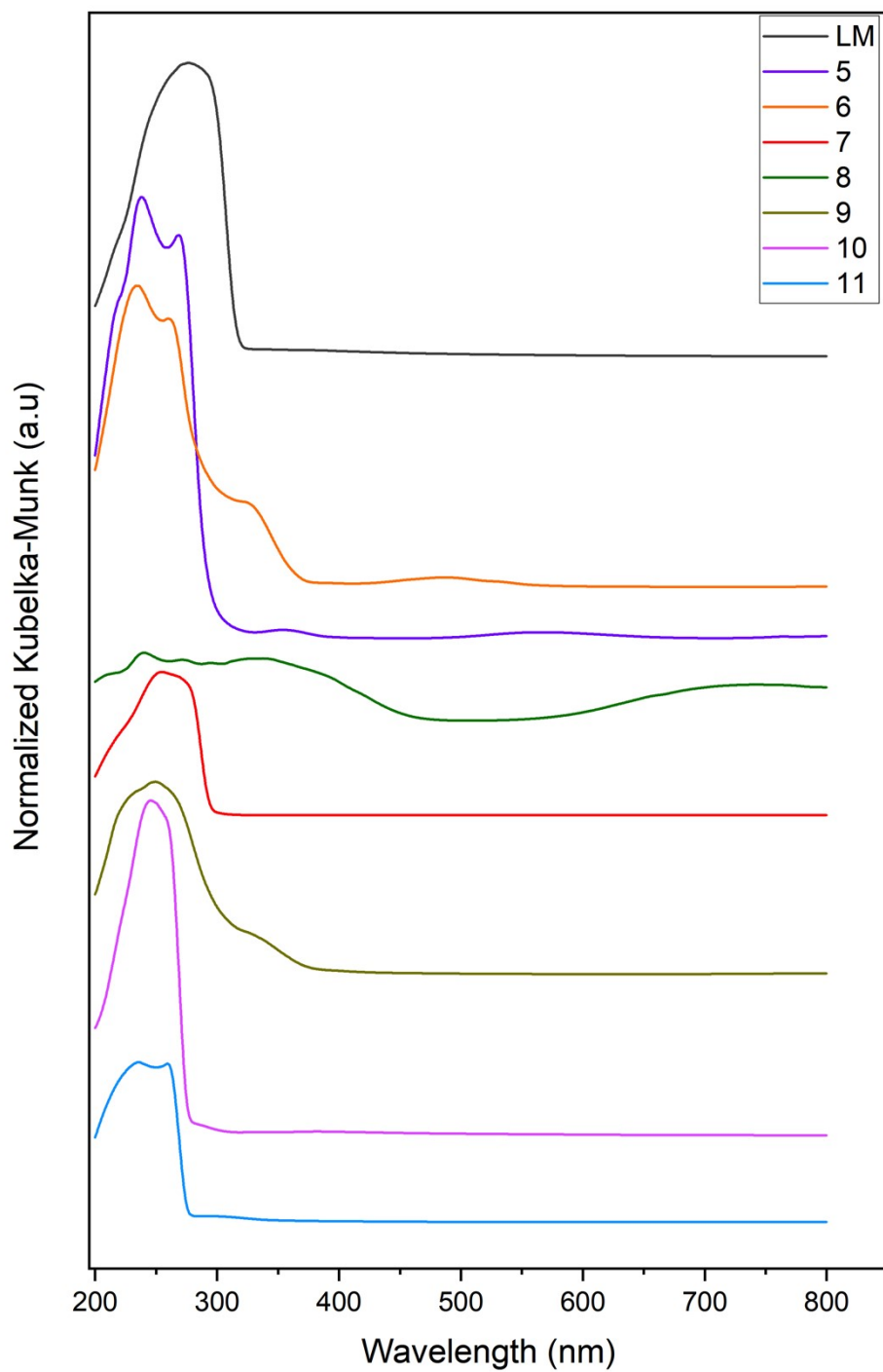


Figure S1. Diffuse reflectance spectroscopic comparison of **LM** and **5-11**.

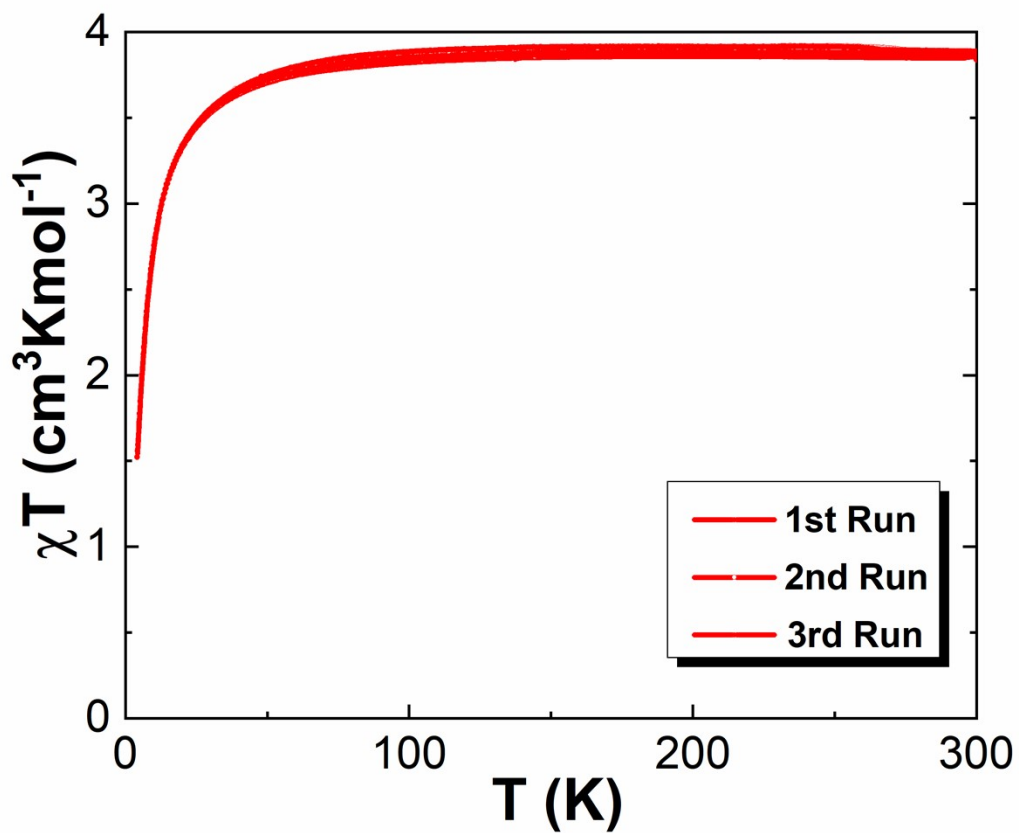


Figure S2. SQUID measurement on **9** carried out over the temperature range (300-5 K) over three consecutive runs.

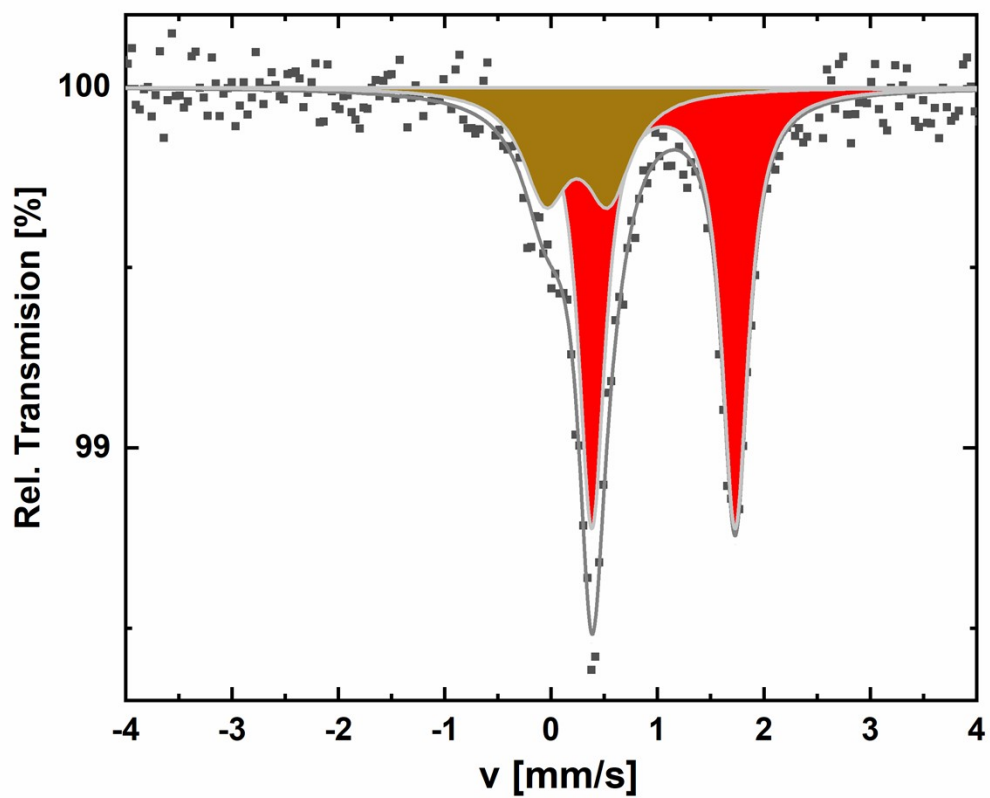
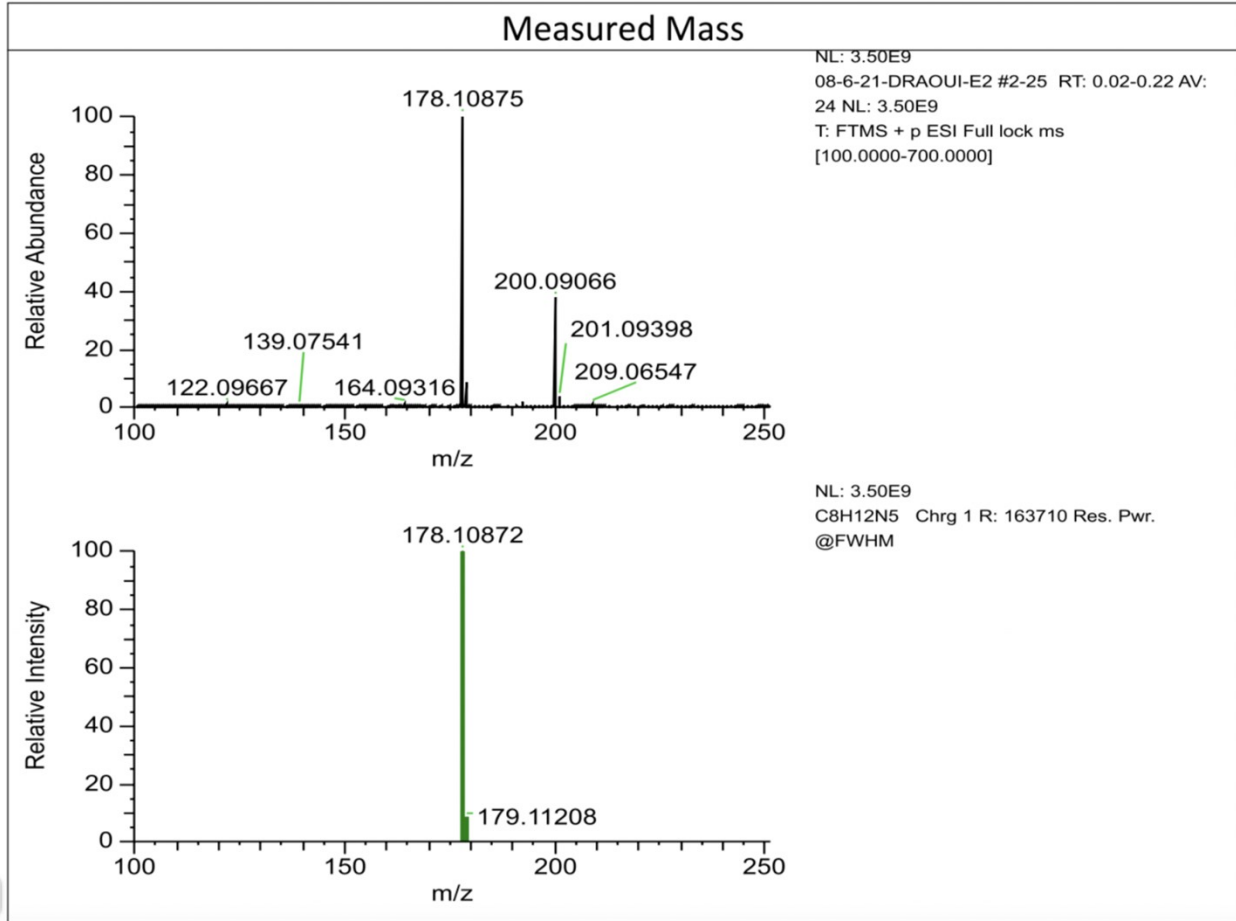


Figure S3. Mössbauer spectrum in transmission mode of **9** recorded at room temperature.

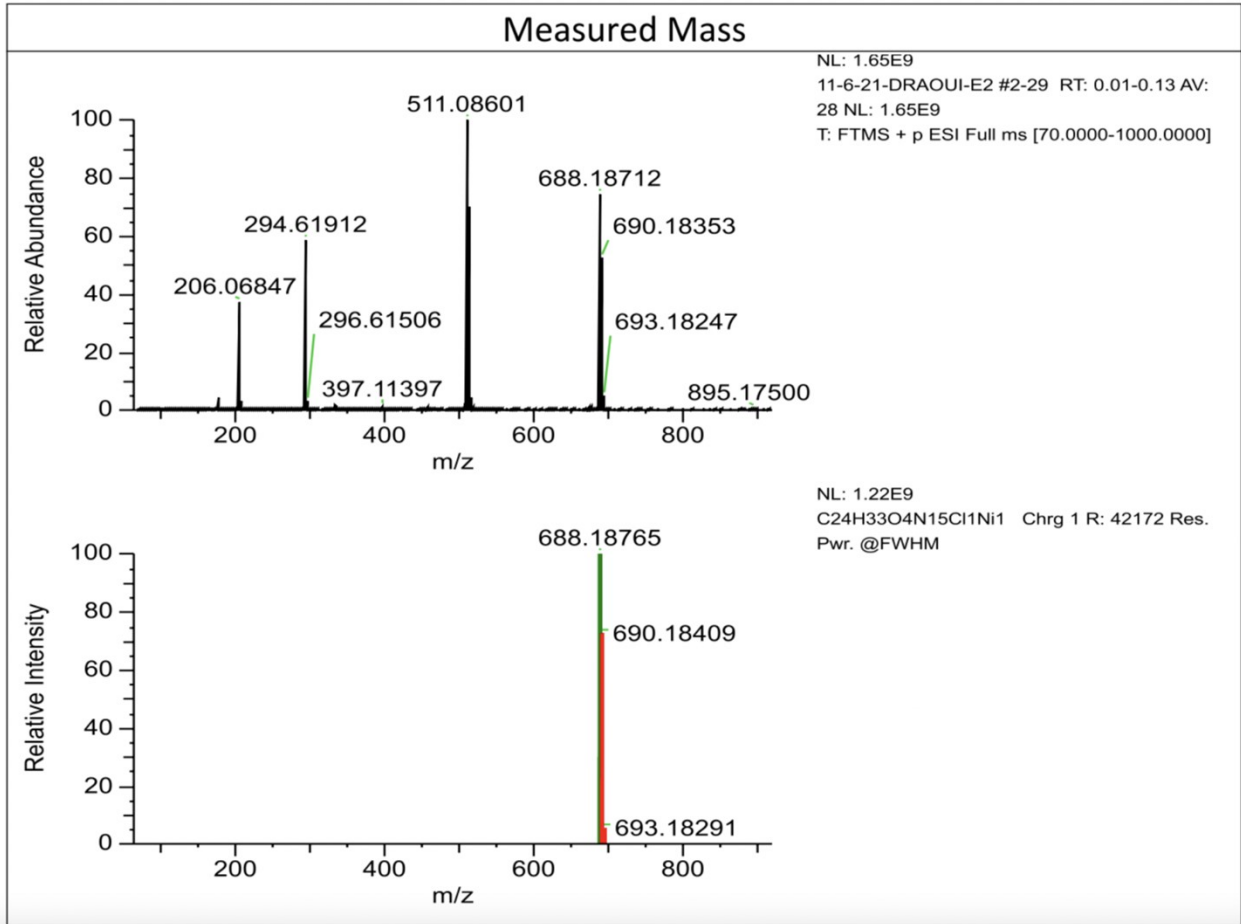
HRMS of LM:



Elemental Composition Results

Peak Mass	Display Formula	MS Cov. [%]	Delta [ppm]	Theo. mass
178.10875	C ₈ H ₁₂ N ₅	99.74	0.18	178.10872

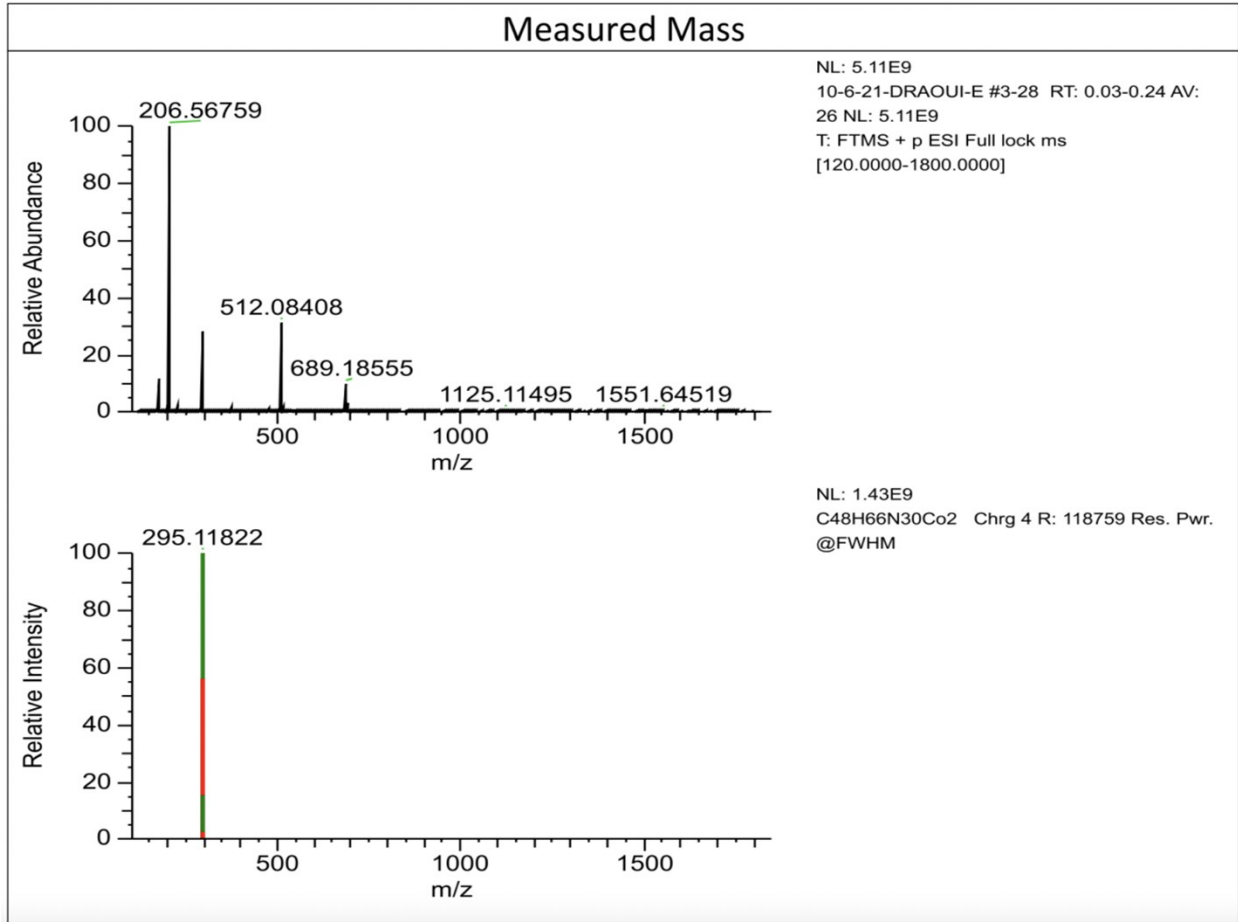
HRMS of 5:



Elemental Composition Results

Peak Mass	Display Formula	MS Cov. [%]	Delta [ppm]	Theo. mass
688.18712	C ₂₄ H ₃₃ O ₄ N ₁₅ ³⁵ Cl ⁶⁸ Ni	99.94	-0.76	688.18765

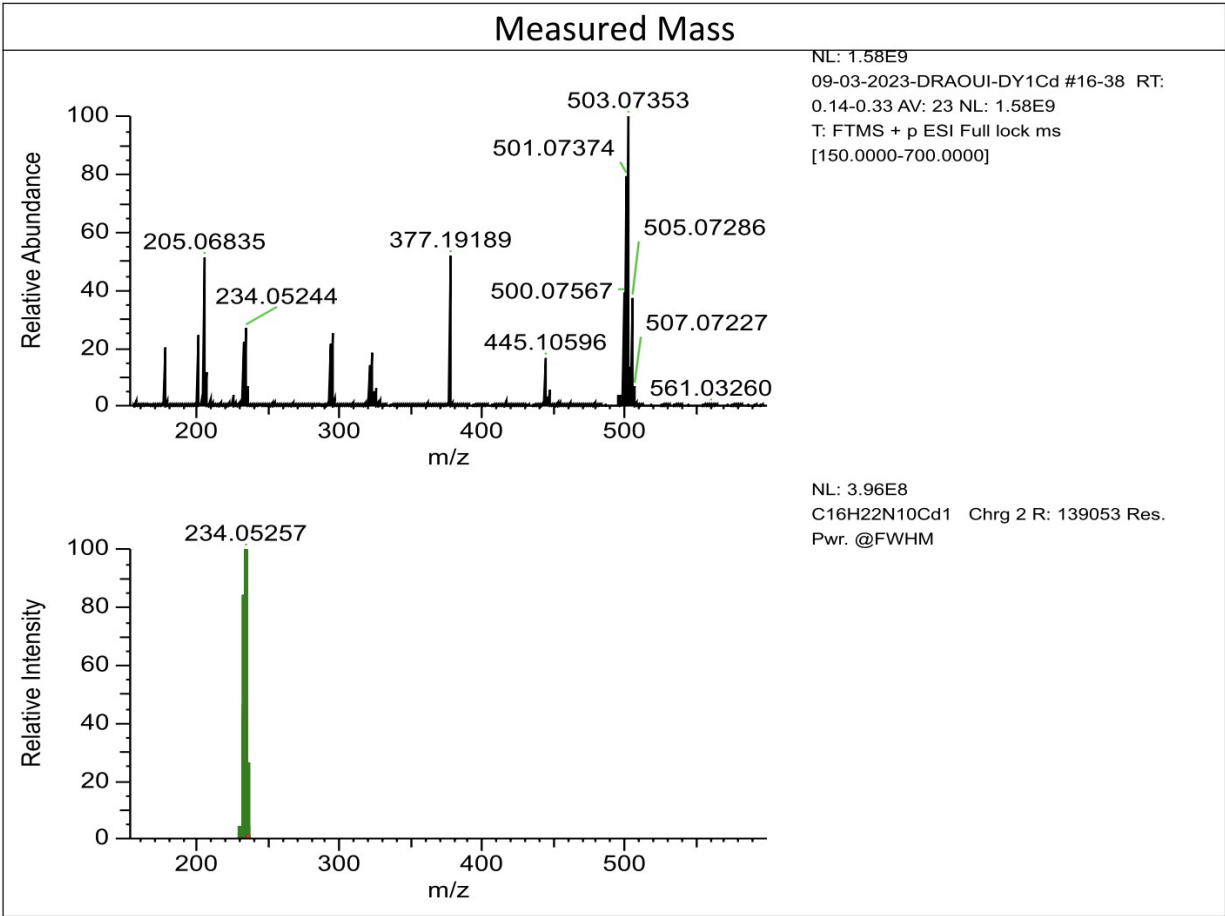
HRMS of 6:



Elemental Composition Results

Peak Mass	Display Formula	MS Cov. [%]	Delta [ppm]	Theo. mass
295.11811	C ₄₈ H ₆₆ N ₃₀ ⁵⁹ Co ₂	78.07	-0.37	295.11822
295.11811	C ₂₄ H ₃₃ N ₁₅ ⁵⁹ Co	99.21	-0.37	295.11822

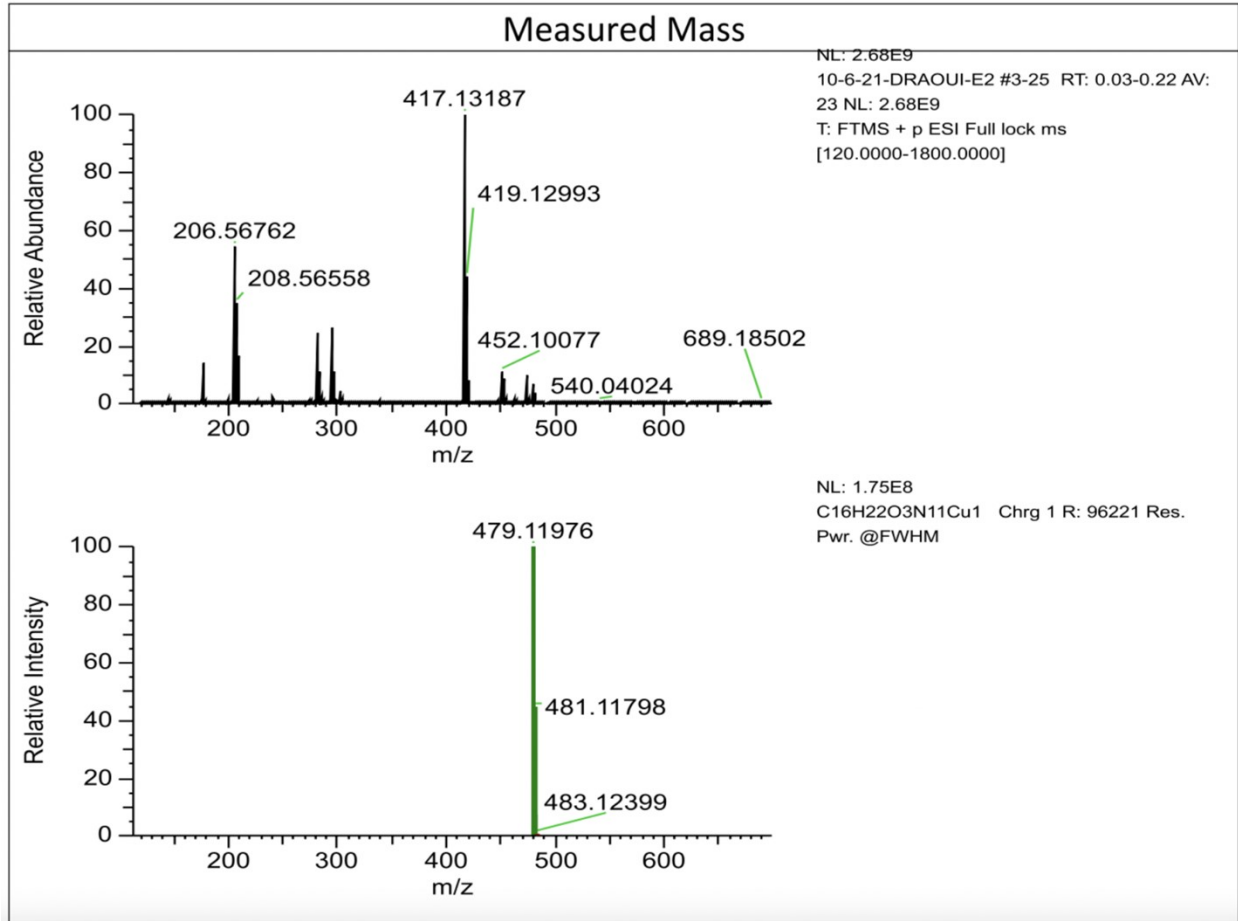
HRMS of 7:



Elemental Composition Results

Peak Mass	Display Formula	MS Cov. [%]	Delta [ppm]	Theo. mass
230.05410	C ₁₆ H ₂₂ N ₁₀ ¹⁰⁸ Cd	99.53	-0.11	230.05413

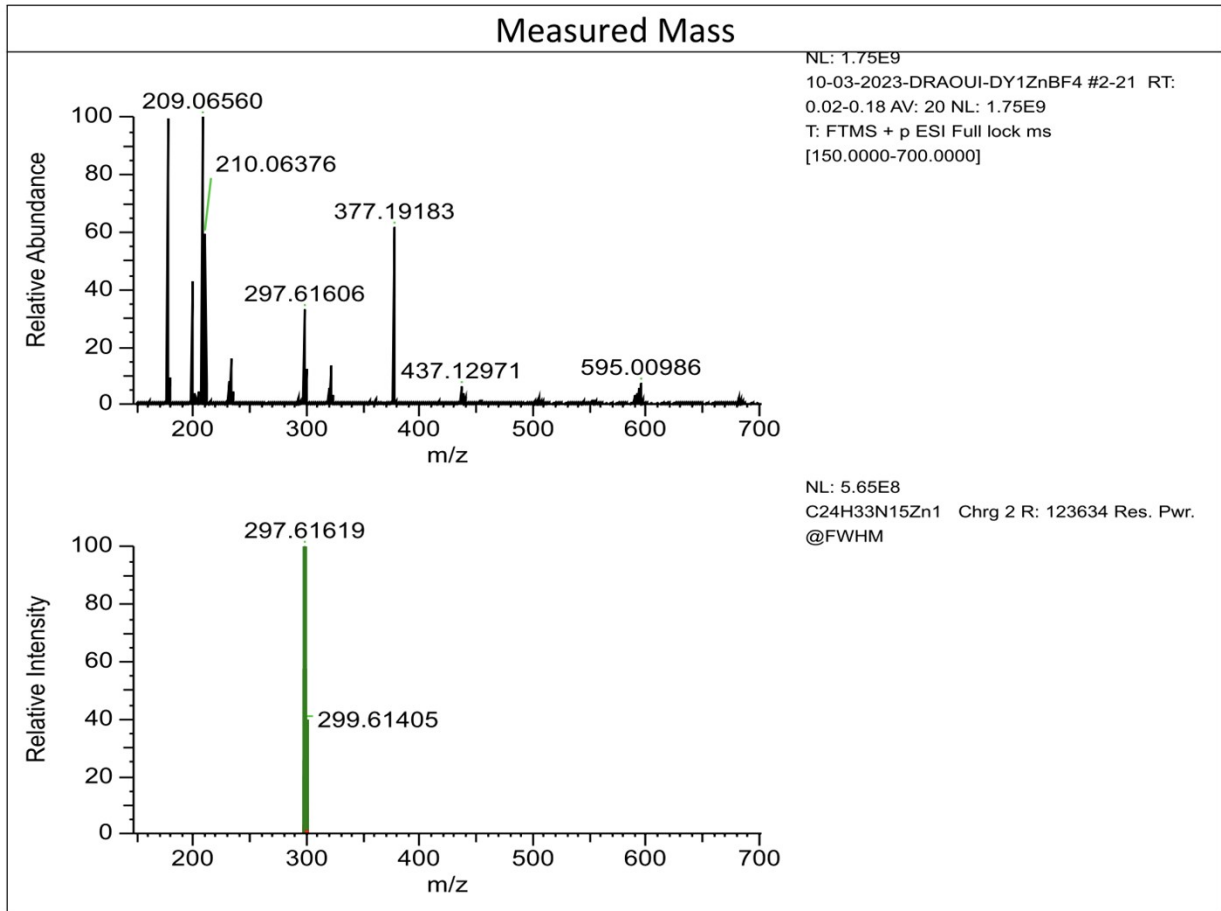
HRMS of 8:



Elemental Composition Results

Peak Mass	Display Formula	MS Cov. [%]	Delta [ppm]	Theo. mass
479.11979	C ₁₆ H ₂₂ O ₃ N ₁₁ ⁶³ Cu	99.23	0.06	479.11976

HRMS of 10:



Elemental Composition Results

Peak Mass	Display Formula	MS Cov. [%]	Delta [ppm]	Theo. mass
297.61606	C ₂₄ H ₃₃ N ₁₅ ⁶⁺ Zn	99.02	-0.46	297.61619