Novel Copper(II) Complexes with Dipinodiazafluorene Ligands: Synthesis, Structure, Magnetic and Catalytic Properties

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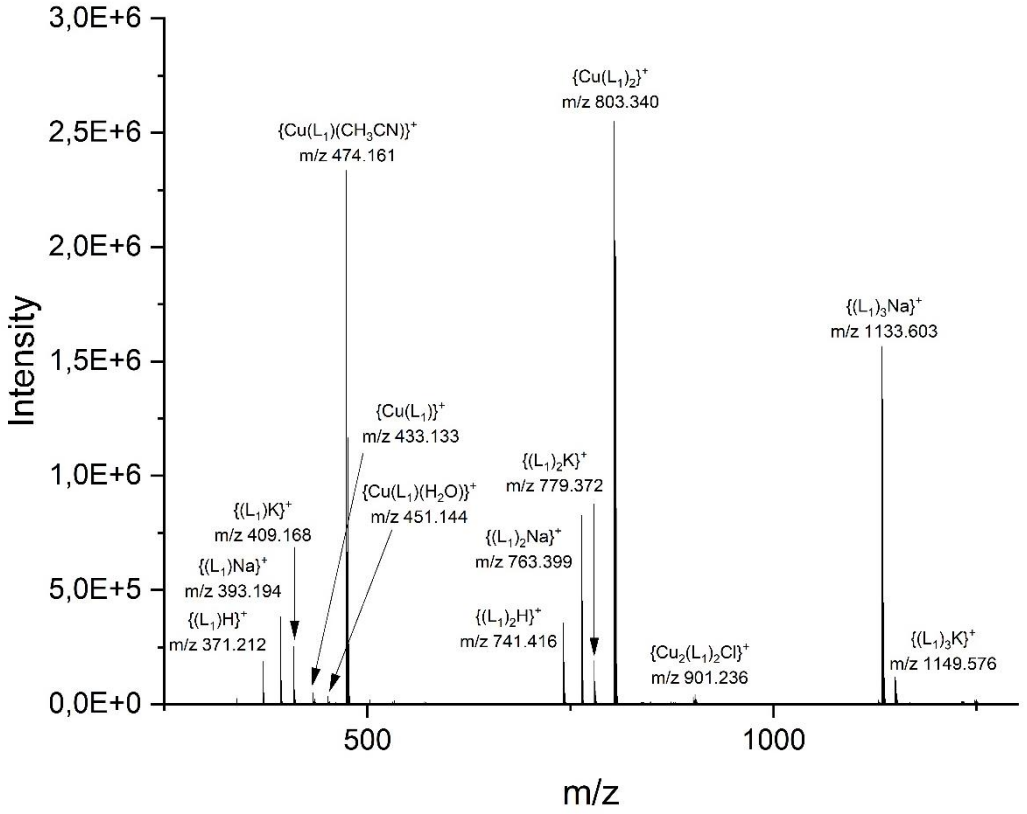

Figure S1. Mass spectrum of **1** in CH_3CN

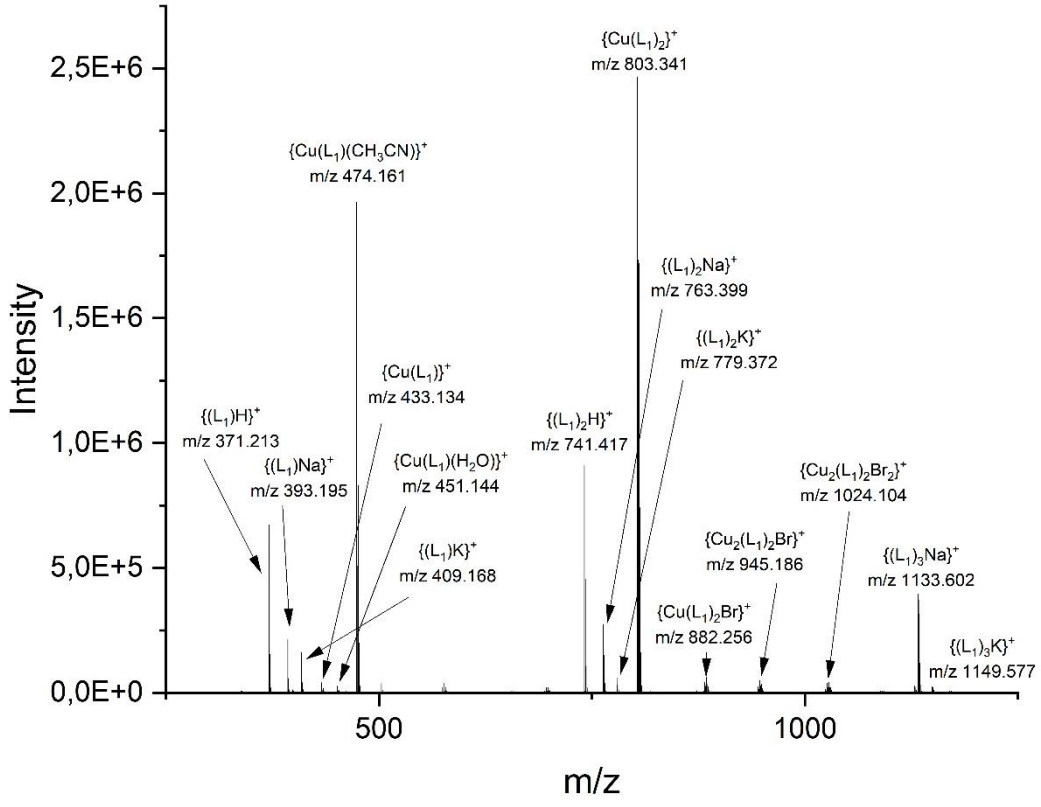

Figure S2. Mass spectrum of **2** in CH_3CN

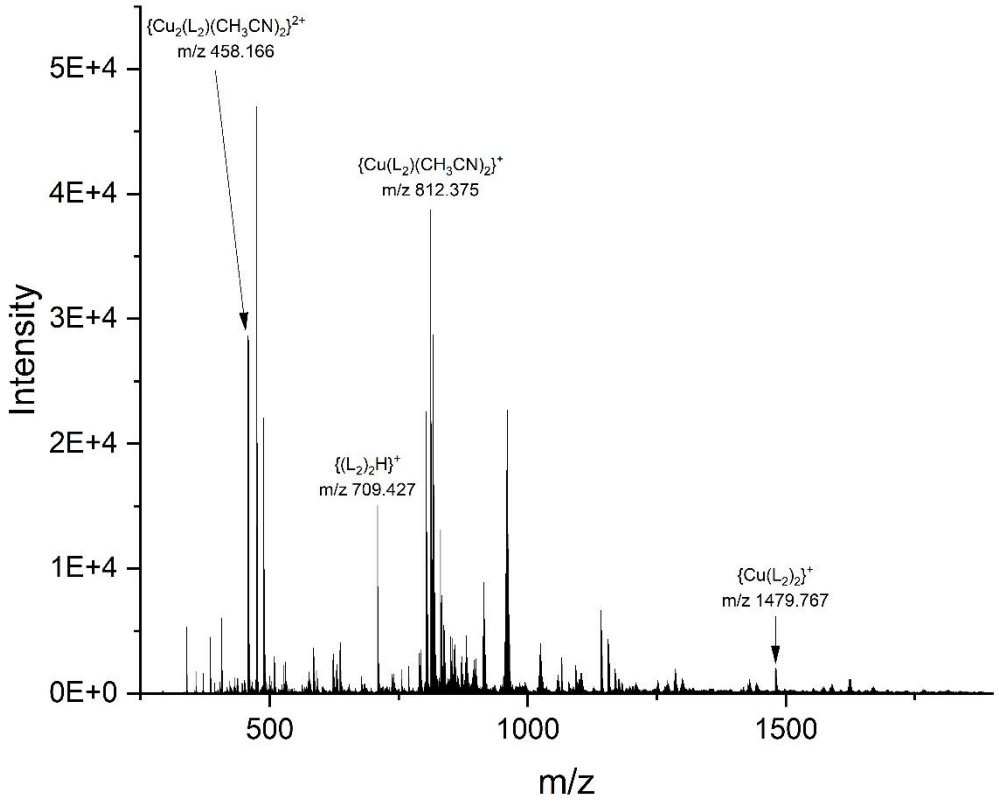

Figure S3. Mass spectrum of **3** in CH_3CN

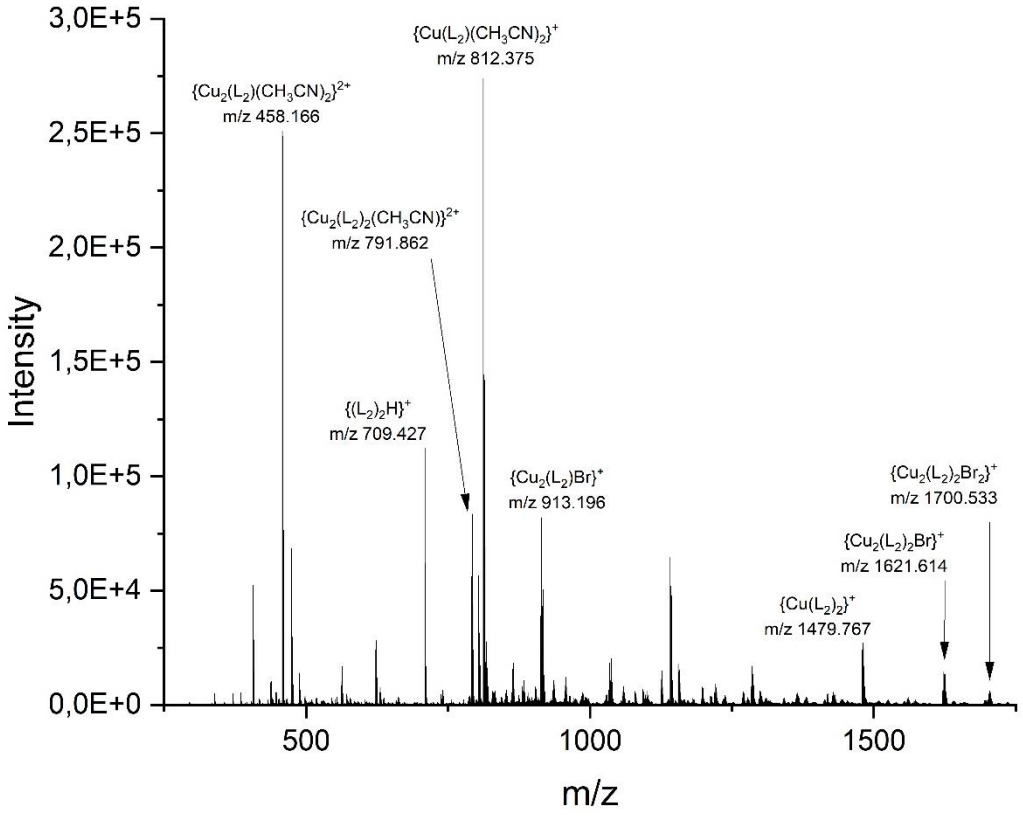

Figure S4. Mass spectrum of **4** in CH_3CN

Table S1. Identified signals in the mass spectra of complexes **1-4** in acetonitrile

$[CuCl_2L_1]_2$ (1)			
Identified chemical formula	**Measured m/z**	**Calculated m/z**	**Fragment**
$C_{25}H_{26}N_2O + H$	371.212	371.212	$L_1 + H$
$C_{25}H_{26}N_2O + Na$	393.194	393.194	$L_1 + Na$
$C_{25}H_{26}N_2O + K$	409.168	409.168	$L_1 + K$
$C_{25}H_{26}N_2O + Cu$	433.133	433.134	$L_1 + Cu$
$C_{25}H_{26}N_2O + Cu + H_2O$	451.144	451.145	$Cu(L_1)(H_2O)$
$C_{25}H_{26}N_2O + Cu + CH_3CN$	474.161	474.161	$Cu(L_1)(CH_3CN)$
$(C_{25}H_{26}N_2O)_2 + H$	741.416	741.417	$(L_1)_2 + H$
$(C_{25}H_{26}N_2O)_2 + Na$	763.399	763.399	$(L_1)_2 + Na$
$(C_{25}H_{26}N_2O)_2 + K$	779.372	779.373	$(L_1)_2 + K$
$(C_{25}H_{26}N_2O)_2 + Cu$	803.340	803.339	$(L_1)_2 + Cu$
$C_{50}H_{52}Cu_2N_4O_2Cl$	901.236	901.237	$Cu_2(L_1)_2Cl$
$C_{50}H_{52}Cu_2N_4O_2Cl_2$	936.205	936.206	$Cu_2(L_1)_2Cl_2$
$C_{50}H_{52}Cu_3N_4O_2Cl_2$	999.133	999.136	$Cu_3(L_1)_2Cl_2$
$(C_{25}H_{26}N_2O)_3 + Na$	1133.603	1133.603	$(L_1)_3 + Na$
$(C_{25}H_{26}N_2O)_3 + K$	1149.576	1149.577	$(L_1)_3 + K$
$[CuBr_2L_1]_2$ (2)			
$C_{25}H_{26}N_2O + H$	371.213	371.212	$L_1 + H$
$C_{25}H_{26}N_2O + Na$	393.195	393.194	$L_1 + Na$

$C_{25}H_{26}N_2O + K$	409.168	409.168	$L_1 + K$
$C_{25}H_{26}N_2O + Cu$	433.134	433.134	$L_1 + Cu$
$C_{25}H_{26}N_2O + Cu + H_2O$	451.144	451.145	$Cu(L_1)(H_2O)$
$C_{25}H_{26}N_2O + Cu + CH_3CN$	474.161	474.161	$Cu(L_1)(CH_3CN)$
$C_{25}H_{26}N_2OCuBr$	512.052	512.052	$Cu(L_1)Br$
$C_{25}H_{26}N_2OCu_2Br$	574.981	574.981	$Cu_2(L_1)Br$
$C_{25}H_{26}N_2OCu_2Br_2$	653.900	653.900	$Cu_2(L_1)Br_2$
$C_{25}H_{26}N_2OCu_2Br_2 + CH_3CN$	694.926	694.926	$Cu_2(L_1)Br_2(CH_3CN)$
$(C_{25}H_{26}N_2O)_2 + H$	741.417	741.417	$(L_1)_2 + H$
$(C_{25}H_{26}N_2O)_2 + Na$	763.399	763.399	$(L_1)_2 + Na$
$(C_{25}H_{26}N_2O)_2 + K$	779.372	779.373	$(L_1)_2 + K$
$(C_{25}H_{26}N_2O)_2 + Cu$	803.341	803.339	$(L_1)_2Cu$
$C_{50}H_{52}CuN_4O_2Br$	882.256	882.257	$Cu(L_1)_2Br$
$C_{50}H_{52}N_4O_2Cu_2Br$	945.186	945.187	$Cu_2(L_1)_2Br$
$C_{50}H_{52}N_4O_2Cu_2Br_2$	1024.104	1024.105	$Cu_2(L_1)_2Br_2$
$C_{50}H_{52}N_4O_2Cu_3Br_2$	1087.034	1087.034	$Cu_3(L_1)_2Br_2$
$(C_{25}H_{26}N_2O)_3 + Na$	1133.602	1133.603	$(L_1)_3 + Na$
$(C_{25}H_{26}N_2O)_3 + K$	1149.577	1149.577	$(L_1)_3 + K$
$C_{50}H_{52}N_4O_2Cu_3Br_3$	1165.952	1165.952	$Cu_3(L_1)_2Br_3$
$[(CuCl_2)_2L_2]_n$ (3)			
$(C_{50}H_{52}N_4)Cu_2(CH_3CN)_2^{2+}$	458.166	458.166	$Cu_2(L_2)(CH_3CN)_2$
$C_{50}H_{52}N_4 + H$	709.427	709.427	$L_2 + H$

$C_{50}H_{52}N_4$ + Na	731.408	731.409	L_2 + Na
$C_{50}H_{52}N_4Cu(CH_3CN)$	812.375	812.375	$Cu(L_2)(CH_3CN)$
$(C_{50}H_{52}N_4)_2Cu$	1479.767	1479.767	$Cu(L_2)_2$
$[(CuBr_2)_2L_2]_n$ (4)			
$(C_{50}H_{52}N_4)Cu_2(CH_3CN)_2^{2+}$	458.166	458.166	$Cu_2(L_2)(CH_3CN)_2$
$C_{50}H_{52}N_4$ + H	709.427	709.427	L_2+ H
$(C_{50}H_{52}N_4)_2Cu_2(CH_3CN)^{2+}$	791.862	791.862	$Cu_2(L_2)_2(CH_3CN)$
$C_{50}H_{52}N_4Cu(CH_3CN)$	812.375	812.375	$Cu(L_2)(CH_3CN)$
$(C_{50}H_{52}N_4)Cu_2Br$	913.196	913.197	$Cu_2(L_2)Br$
$(C_{50}H_{52}N_4)Cu_3Br_2$	1055.043	1055.044	$Cu_3(L_2)Br_2$
$(C_{50}H_{52}N_4)_2Cu$	1479.767	1479.767	$Cu(L_2)_2$
$(C_{50}H_{52}N_4)_2Cu_2Br$	1621.614	1621.615	$Cu_2(L_2)_2Br$
$(C_{50}H_{52}N_4)_2Cu_2Br_2$	1700.533	1700.534	$Cu_2(L_2)_2Br_2$