Electronic Supplementary Information for Dalton Transactions

SUPPLEMENTARY INFORMATION

For

Synthesis, characterization and potent superoxide dismutase like activity of new bis(pyrazole) – 2,2′-bipyridyl mixed ligand copper(II) complexes

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Running title: **SOD like activity of new bipy ligand copper complexes**

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Supplementary Table S1. Atomic coordinates for density functional theory (DFT)-optimized structures of Cu(II) complexes.

Atom	X (Å)	Y (Å)	Z (Å)
Complex [Cu(L2)($O_2NO)_2$] (**2**)			
Cu	0.000008	-0.974169	-0.000001
N	1.920185	1.441232	-0.146099
N	1.590451	0.239305	0.406909
C	2.642674	-0.138323	1.151671
C	3.647526	0.841868	1.077141
C	3.159988	1.838498	0.247371
C	3.791518	3.118402	-0.202121
C	0.933875	2.200658	-0.901638
C	0.000017	3.026915	-0.000076
N	-1.920151	1.441221	0.145978
N	-1.590409	0.239263	-0.406958
C	-2.642647	-0.138440	-1.151660
C	-3.647497	0.841757	-1.077210
C	-3.159950	1.838460	-0.247532
C	-3.791478	3.118401	0.201856
C	-0.933865	2.200697	0.901500
C	2.659486	-1.433929	1.900922
C	-2.659464	-1.434114	-1.900793
H	4.614739	0.818620	1.558181
H	3.218137	3.999225	0.111750
H	4.791746	3.202273	0.229473
H	3.894733	3.159667	-1.293204
H	1.480912	2.866438	-1.573827
H	0.381704	1.492812	-1.522213
H	-0.601849	3.680915	-0.644006
H	0.601904	3.680905	0.643844
H	-4.614715	0.818466	-1.558238
H	-3.218091	3.999197	-0.112078
H	-4.791703	3.202242	-0.229750
H	-3.894698	3.159748	1.292936
H	-1.480929	2.866508	1.573636
H	-0.381709	1.492889	1.522129
H	3.522218	-1.469171	2.571570
H	1.748278	-1.550224	2.496443
H	2.718686	-2.279504	1.207797
H	-3.522202	-1.469417	-2.571431
H	-1.748263	-1.550466	-2.496312
H	-2.718659	-2.279626	-1.207589
N	1.398048	-1.911193	-1.978100
O	0.747596	-0.890749	-2.331569
O	1.177981	-2.337791	-0.757818
O	2.190325	-2.500034	-2.689284
N	-1.398085	-1.910850	1.978293
O	-0.747798	-0.890252	2.331597
O	-1.177927	-2.337647	0.758092
O	-2.190409	-2.499598	2.689505

Complex [Cu(L3)($O_2NO)_2$] (**3**)			
Cu	-0.000399	-0.387838	0.044330
O	-0.001936	2.075905	-0.238001
N	2.016457	-0.117750	0.089029
N	2.680376	0.876580	-0.552401
N	-2.682735	0.975292	0.338823
N	-2.017510	-0.137847	-0.060602
C	2.928094	-0.766490	0.817905
C	4.197939	-0.191759	0.650837
C	3.998056	0.852398	-0.232324
C	2.011186	1.762491	-1.499747
C	1.067301	2.773157	-0.854328
C	-1.071559	2.893588	0.205499
C	-2.015138	2.053474	1.061697
C	-4.000069	0.878337	0.031500
C	-4.198639	-0.339051	-0.591868
C	-2.928435	-0.935950	-0.623315
H	2.615840	-1.608718	1.418435
H	5.128119	-0.499385	1.103763
H	4.683760	1.568693	-0.661797
H	2.796646	2.304507	-2.033234
H	1.462020	1.141586	-2.211634
H	1.594579	3.390932	-0.110881
H	0.687790	3.435852	-1.647835
H	-0.692613	3.717982	0.829655
H	-1.598957	3.328121	-0.657915
H	-1.466410	1.611223	1.896681
H	-2.801806	2.701104	1.458090
H	-4.686635	1.672600	0.287506
H	-5.128425	-0.742280	-0.963246
H	-2.615677	-1.892560	-1.016471
O	-0.098090	-0.063709	1.979214
O	-0.039128	-1.266797	3.802670
O	0.361132	-2.188668	1.853764
N	0.076200	-1.218344	2.588992
O	-0.349269	-2.558809	-1.306317
O	0.096368	-0.515287	-1.913120
O	0.041651	-2.101668	-3.414993
N	-0.070626	-1.779537	-2.243492
Complex [Cu(L4)($O_2NO)_2$] (**4**)			
Cu	0.000145	-0.441631	0.000110
O	0.000072	2.115789	-0.000573
N	-1.999463	-0.077168	-0.282754
N	-2.680308	0.991007	0.230838
N	2.680326	0.990887	-0.231448
N	1.999481	-0.077023	0.282705
C	-2.866167	-0.745720	-1.053176
C	-4.115182	-0.096201	-1.034385
C	-3.969997	1.003603	-0.208661
C	-2.051678	1.899193	1.181170

C	-1.066287	2.871487	0.540609
C	1.066318	2.871196	-0.542372
C	2.051725	1.898516	-1.182339
C	3.969980	1.003772	0.208125
C	4.115150	-0.095557	1.034485
C	2.866161	-0.745103	1.053587
C	4.969875	2.039498	-0.200956
C	2.485576	-1.985021	1.799753
C	-2.485564	-1.986038	-1.798677
C	-4.969913	2.039517	0.199896
H	-5.014091	-0.400968	-1.550669
H	-2.846681	2.467038	1.669709
H	-1.537237	1.297942	1.934955
H	-1.550896	3.467831	-0.248890
H	-0.698342	3.561070	1.317155
H	0.698258	3.560193	-1.319386
H	1.550937	3.468147	0.246662
H	1.537289	1.296817	-1.935767
H	2.846747	2.466057	-1.671198
H	5.014037	-0.399987	1.551005
H	5.917409	1.848680	0.308713
H	5.165055	2.019679	-1.280487
H	4.649172	3.054761	0.061975
H	2.043099	-1.735521	2.770522
H	1.759020	-2.576642	1.237942
H	3.372330	-2.600578	1.977474
H	-2.043160	-1.737058	-2.769614
H	-1.758940	-2.577303	-1.236577
H	-3.372291	-2.601750	-1.975994
H	-5.165005	2.020324	1.279454
H	-4.649292	3.054646	-0.063659
H	-5.917478	1.848347	-0.309584
O	0.248341	-0.471997	-1.932472
O	1.233924	-1.774792	-3.385552
O	0.955433	-2.443259	-1.317926
N	0.845694	-1.612299	-2.238587
O	-0.955665	-2.441978	1.319519
O	-0.248224	-0.470426	1.932684
O	-1.234292	-1.771908	3.386611
N	-0.845853	-1.610363	2.239587
Complex [Cu(L2)(bipy)(O_2NO)]NO_3 (**9**)			
C	-4.142063	-0.829139	-2.175867
C	-5.036561	-0.562757	-1.142370
C	-4.539116	-0.201406	0.108352
C	-3.156717	-0.117565	0.289599
N	-2.296662	-0.377013	-0.718859
C	-2.777088	-0.722492	-1.919664
C	-2.512261	0.218962	1.579218
C	-3.220802	0.596354	2.723900
C	-2.529550	0.848617	3.905116
C	-1.143345	0.704535	3.920550

C	-0.505449	0.333894	2.741572
N	-1.162276	0.111049	1.594217
H	-4.485045	-1.116993	-3.163515
H	-6.107752	-0.637666	-1.301823
H	-5.221900	-0.001565	0.925418
H	-2.040084	-0.905078	-2.690333
H	-4.299335	0.693460	2.696658
H	-3.067692	1.143713	4.800536
H	-0.564492	0.871121	4.822322
H	0.567032	0.183032	2.710515
C	1.584133	3.799542	-0.423325
C	0.587834	3.966403	-1.367172
C	-0.085204	2.734871	-1.449446
N	0.454845	1.847131	-0.597419
C	1.203001	-2.491779	1.249991
N	1.284661	-1.348246	0.541513
N	2.598795	-1.229173	0.165938
C	3.337716	-2.267698	0.639819
C	2.469171	-3.085495	1.344197
C	2.616536	4.764958	0.068813
C	-1.232173	2.399290	-2.352213
C	-0.087120	-3.025630	1.793481
C	4.799623	-2.430035	0.367501
C	2.425871	1.826551	0.887555
N	1.472930	2.518265	0.030241
C	3.070651	-0.128787	-0.675657
C	3.538922	1.095925	0.121969
H	0.372742	4.864953	-1.927434
H	2.716157	-4.013980	1.838209
H	2.537869	4.935911	1.149302
H	2.479912	5.727576	-0.428965
H	3.637793	4.425709	-0.141656
H	-1.376165	3.201325	-3.080869
H	-2.170056	2.284121	-1.797377
H	-1.038330	1.471732	-2.898042
H	-0.889263	-2.941341	1.055420
H	-0.397622	-2.508896	2.708783
H	0.030874	-4.084276	2.038455
H	5.385845	-1.568704	0.707409
H	4.997707	-2.569391	-0.702062
H	5.170966	-3.314076	0.890490
H	2.863765	2.575903	1.551486
H	1.873810	1.125209	1.513325
H	2.270461	0.118108	-1.373893
H	3.902587	-0.517765	-1.267444
H	4.305343	0.793784	0.846709
H	4.018808	1.792874	-0.575588
Cu	-0.290600	-0.259389	-0.229055
N	0.280449	-1.981762	-2.295787
O	0.935592	-2.348350	-3.254873
O	-0.392081	-2.714129	-1.555899
O	0.272516	-0.668896	-2.028962

Complex $[Cu(L3)(bipy)(O_2NO)]NO_3$ (**10**)			
C	0.935648	-4.034467	0.590564
C	0.167776	-2.911232	0.264016
N	0.796638	-1.774060	0.593805
N	1.994236	-2.160219	1.116541
C	2.091949	-3.512923	1.135116
C	-0.843314	4.075423	-1.164175
C	-1.103540	2.759497	-0.766939
N	0.032779	2.085147	-0.539138
N	1.035574	2.963730	-0.796503
C	0.536917	4.166320	-1.167220
C	2.448610	2.635632	-0.610191
C	2.927643	-1.255378	1.785627
C	2.790741	2.316313	0.847038
C	3.333687	-0.012756	1.004962
O	2.372330	1.016880	1.258956
H	0.694968	-5.074050	0.429455
H	-0.793322	-2.867706	-0.224504
H	2.971483	-3.996692	1.535381
H	-1.553446	4.847366	-1.418630
H	-2.056272	2.266533	-0.643818
H	1.196589	4.988772	-1.403941
H	3.006450	3.521312	-0.925915
H	2.705346	1.803632	-1.268317
H	2.514857	-0.950661	2.754321
H	3.819556	-1.856107	1.978343
H	2.292100	3.028219	1.512459
H	3.875479	2.419391	0.988122
H	4.312737	0.315485	1.381706
H	3.418251	-0.227524	-0.065963
C	0.143665	0.042890	-0.187881
O	0.816869	-1.839343	-2.578801
O	1.494953	-0.011823	-1.548123
N	1.756988	-1.101634	-2.268878
O	2.927422	-1.278169	-2.577898
C	-1.449210	0.775767	3.722262
C	-2.798229	0.447941	3.597268
C	-3.286017	0.038755	2.359220
C	-2.415559	-0.036767	1.266382
N	-1.106936	0.274593	1.406285
C	-0.637089	0.671457	2.597648
C	-2.844786	-0.442283	-0.099049
C	-4.178761	-0.669656	-0.450723
C	-4.478293	-1.034610	-1.763123
C	-3.443312	-1.164155	-2.685602
C	-2.136979	-0.921589	-2.259185
N	-1.846561	-0.566493	-1.000690
H	-1.030731	1.102636	4.667904
H	-3.465204	0.508567	4.451757
H	-4.331204	-0.224768	2.251124
H	0.421271	0.909767	2.629993

H	-4.976749	-0.559786	0.274155
H	-5.508486	-1.213751	-2.055549
H	-3.634216	-1.449415	-3.714540
H	-1.284645	-1.030570	-2.921410
Complex [Cu(L4)(bipy)(O_2NO)]NO_3 (**11**)			
C	2.821011	-3.206032	0.397610
C	1.522383	-2.686008	0.324817
N	1.555650	-1.339729	0.240515
N	2.891001	-1.015591	0.241255
C	3.676253	-2.122699	0.340105
C	-2.270572	3.824251	-0.347238
C	-2.200439	2.435248	-0.169983
N	-0.914970	2.025352	-0.131219
N	-0.176029	3.169876	-0.295573
C	-0.965489	4.270632	-0.421457
C	1.276186	3.185384	-0.213634
C	1.807975	3.054665	1.221654
O	1.906724	1.712998	1.694430
C	3.375338	0.356094	0.211138
C	3.186242	1.107807	1.536290
C	-3.395527	1.539736	-0.056670
C	-0.441638	5.660337	-0.609503
C	0.272628	-3.508685	0.301786
C	5.172514	-2.089154	0.357773
H	3.099831	-4.247683	0.461463
H	-3.165894	4.424159	-0.422394
H	1.596002	4.148519	-0.617642
H	1.660672	2.411654	-0.876230
H	1.134459	3.579077	1.907655
H	2.792493	3.538235	1.282860
H	4.443253	0.293826	-0.006799
H	2.913193	0.872564	-0.629020
H	3.967660	1.874976	1.626082
H	3.305887	0.409421	2.370929
H	-3.460287	0.833278	-0.888652
H	-3.400142	0.972954	0.878369
H	-4.301205	2.151504	-0.073205
H	0.175956	5.992750	0.233146
H	0.157785	5.752791	-1.522885
H	-1.282255	6.352650	-0.695225
H	-0.389803	-3.280668	1.141890
H	-0.281401	-3.364274	-0.629399
H	0.538777	-4.566418	0.370903
H	5.581656	-1.661617	-0.565239
H	5.569320	-1.513691	1.202317
H	5.552878	-3.109306	0.445632
C	-0.111091	-0.048074	-0.268510
O	0.954027	-1.361245	-2.829646
O	0.818297	0.588504	-1.803311
N	1.466328	-0.262302	-2.607083
O	2.527637	0.133271	-3.069944

C	-1.250411	-0.487608	3.817091
C	-2.382276	-1.297054	3.742467
C	-2.842484	-1.710900	2.494245
C	-2.158043	-1.309373	1.343382
N	-1.054636	-0.529682	1.434105
C	-0.612153	-0.125905	2.634016
C	-2.570093	-1.676504	-0.035763
C	-3.703408	-2.437398	-0.329277
C	-4.007967	-2.708144	-1.663479
C	-3.172811	-2.218700	-2.664416
C	-2.052783	-1.474071	-2.292849
N	-1.764026	-1.207837	-1.013282
H	-0.864072	-0.140676	4.769157
H	-2.905354	-1.603311	4.643214
H	-3.722636	-2.338534	2.422791
H	0.270363	0.506584	2.623963
H	-4.345662	-2.813384	0.458427
H	-4.886294	-3.296004	-1.911986
H	-3.372201	-2.410677	-3.713063
H	-1.344653	-1.098877	-3.022151
Complex [Cu(L6)(O_2NO)$_2$] (**16**)			
C	-1.786317	-2.272464	2.417331
C	-0.526032	-1.733898	2.101202
N	-0.560236	-1.115757	0.921008
N	-1.830073	-1.243843	0.465782
C	-2.595120	-1.934208	1.349187
C	-2.569157	2.942583	-0.823045
C	-1.186055	2.692563	-0.699456
N	-0.929971	1.386969	-0.688134
N	-2.138194	0.783327	-0.800039
C	-3.149003	1.691490	-0.879362
C	-2.189701	-0.663676	-0.819917
H	-2.064404	-2.831847	3.297604
H	0.397358	-1.756152	2.662344
H	-3.637112	-2.136216	1.146131
H	-3.069779	3.898077	-0.870548
H	-0.366172	3.393881	-0.626209
H	-4.178992	1.380197	-0.981730
H	-1.481080	-1.026918	-1.568106
H	-3.203342	-0.979074	-1.066109
Cu	0.813141	0.049878	-0.007510
O	1.455336	0.884941	1.659472
N	2.234101	1.713217	1.026681
O	2.183946	1.575112	-0.247600
O	2.918584	2.527790	1.595071
O	2.187512	-1.882506	-0.469135
N	1.581812	-1.858104	-1.564822
O	0.734427	-0.853367	-1.728326
O	1.711280	-2.674895	-2.456303
Complex [Cu(L6)(bipy)(O_2NO)]NO_3 (**17**)			

C	3.592775	-2.308513	1.211917
C	4.570013	-1.391340	0.833111
C	4.183189	-0.179137	0.262587
C	2.823996	0.081913	0.083401
N	1.885307	-0.821942	0.443225
C	2.254959	-1.984869	0.995376
C	2.281915	1.337136	-0.487097
C	3.069246	2.432136	-0.850408
C	2.455927	3.580419	-1.345760
C	1.067410	3.613565	-1.458831
C	0.345504	2.485730	-1.080691
N	0.932729	1.372754	-0.617073
H	3.852320	-3.261136	1.660230
H	5.622962	-1.612656	0.977050
H	4.933643	0.541777	-0.039341
H	1.446819	-2.660658	1.252550
H	4.146796	2.395807	-0.744690
H	3.056405	4.437880	-1.633226
H	0.548703	4.490052	-1.831121
H	-0.735769	2.458004	-1.151557
N	-2.408142	0.396857	1.847144
C	-2.932469	1.186069	2.822537
C	-1.875185	1.821916	3.441712
C	-0.732410	1.357059	2.763508
N	-1.054200	0.491385	1.800357
C	-2.031901	0.273111	-2.350634
N	-1.778002	0.028285	-1.061397
N	-2.990434	-0.039729	-0.452159
C	-3.994224	0.150273	-1.346065
C	-3.414199	0.364157	-2.581830
C	-3.085300	-0.493978	0.930121
H	-3.997161	1.222216	3.005249
H	-1.921704	2.513743	4.269217
H	0.305651	1.607364	2.936043
H	-1.213312	0.357771	-3.051360
H	-5.029965	0.110875	-1.039816
H	-3.917867	0.550000	-3.518289
H	-2.632968	-1.486107	0.998367
H	-4.140138	-0.538163	1.199086
Cu	-0.014881	-0.329095	-0.050670
N	-0.434073	-2.795722	-0.901750
O	-0.820845	-3.942615	-0.993674
O	0.132689	-2.143380	-1.800833
O	-0.616925	-2.159018	0.258867