

Supporting Information

Carbazole-based molecular tweezers as platforms for the discrimination of heavy metal ions

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Table S1. Normalized fluorescence intensities used in chemometric analyses of compound **1-8** upon additions of metal ions (5 eq.) (Total 5 trials).

	1	2	3	4	5	6	7	8
Ag ⁺	0.000	0.939	0.936	0.054	0.000	0.334	0.291	0.002
As ³⁺	0.916	0.945	0.067	0.001	0.935	0.944	0.058	0.000
Au ³⁺	0.875	0.743	0.455	0.075	0.743	0.637	0.608	0.129
Cd ²⁺	0.949	0.679	0.664	0.823	0.972	0.956	0.949	0.944
Co ²⁺	0.945	0.013	0.031	0.901	0.950	0.405	0.406	0.838
Cr ³⁺	0.933	0.937	0.746	0.913	0.942	0.932	0.641	0.683
Cu ²⁺	0.930	0.000	0.005	0.898	0.863	0.007	0.005	0.827
Fe ²⁺	0.921	0.390	0.296	0.926	0.936	0.947	0.911	0.979
Fe ³⁺	0.186	0.018	0.000	0.000	0.038	0.028	0.003	0.000
Hg ²⁺	0.000	0.282	0.283	0.003	0.000	0.002	0.001	0.001
Mn ²⁺	0.919	0.933	0.922	0.906	0.919	0.935	0.937	0.865
Ni ²⁺	0.923	0.001	0.006	0.897	0.938	0.798	0.140	0.953
Pb ²⁺	0.917	0.919	0.920	0.938	0.949	0.946	0.947	0.979
Pd ²⁺	0.789	0.517	0.003	0.001	0.727	0.392	0.001	0.001
Pt ²⁺	0.915	0.913	0.923	0.883	0.918	0.922	0.932	0.856
Ru ³⁺	0.666	0.641	0.595	0.448	0.480	0.413	0.342	0.383
Se ⁴⁺	0.906	0.903	0.038	0.002	0.906	0.900	0.030	0.000
Sn ²⁺	0.935	0.916	0.914	0.943	0.933	0.943	0.977	0.788
Zn ²⁺	0.927	0.820	0.756	0.932	0.949	0.394	0.472	0.967

	1	2	3	4	5	6	7	8
Ag ⁺	0.000	0.955	0.952	0.057	0.000	0.326	0.304	0.002
As ³⁺	0.937	0.954	0.062	0.001	0.949	0.944	0.036	0.001
Au ³⁺	0.785	0.738	0.418	0.001	0.739	0.565	0.583	0.139
Cd ²⁺	0.936	0.655	0.728	0.792	0.980	0.970	0.968	0.960
Co ²⁺	0.932	0.027	0.087	0.866	0.975	0.431	0.396	0.844
Cr ³⁺	0.940	0.944	0.766	0.867	0.961	0.940	0.657	0.602
Cu ²⁺	0.920	0.000	0.005	0.858	0.897	0.004	0.004	0.828
Fe ²⁺	0.924	0.394	0.376	0.895	0.974	0.951	0.951	0.962
Fe ³⁺	0.150	0.023	0.000	0.001	0.033	0.000	0.000	0.000
Hg ²⁺	0.000	0.309	0.309	0.000	0.000	0.001	0.001	0.001
Mn ²⁺	0.930	0.938	0.954	0.873	0.958	0.946	0.972	0.888
Ni ²⁺	0.926	0.001	0.006	0.860	0.977	0.845	0.188	0.933
Pb ²⁺	0.931	0.934	0.943	0.936	0.972	0.955	0.986	0.961
Pd ²⁺	0.829	0.515	0.003	0.000	0.807	0.367	0.001	0.000
Pt ²⁺	0.934	0.929	0.939	0.850	0.948	0.923	0.951	0.883
Ru ³⁺	0.664	0.633	0.597	0.435	0.483	0.370	0.339	0.394
Se ⁴⁺	0.919	0.910	0.054	0.000	0.934	0.914	0.022	0.000
Sn ²⁺	0.946	0.931	0.943	0.891	0.972	0.949	0.995	0.778
Zn ²⁺	0.940	0.826	0.757	0.907	0.966	0.346	0.305	0.986

	1	2	3	4	5	6	7	8
Ag ⁺	0.000	0.955	0.952	0.057	0.000	0.326	0.304	0.002
As ³⁺	0.937	0.954	0.062	0.001	0.949	0.944	0.036	0.001
Au ³⁺	0.785	0.738	0.418	0.001	0.739	0.565	0.583	0.139
Cd ²⁺	0.936	0.655	0.728	0.792	0.980	0.970	0.968	0.960
Co ²⁺	0.932	0.027	0.087	0.866	0.975	0.431	0.396	0.844
Cr ³⁺	0.940	0.944	0.766	0.867	0.961	0.940	0.657	0.602
Cu ²⁺	0.920	0.000	0.005	0.858	0.897	0.004	0.004	0.828
Fe ²⁺	0.924	0.394	0.376	0.895	0.974	0.951	0.951	0.962
Fe ³⁺	0.150	0.023	0.000	0.001	0.033	0.000	0.000	0.000
Hg ²⁺	0.000	0.309	0.309	0.000	0.000	0.001	0.001	0.001
Mn ²⁺	0.930	0.938	0.954	0.873	0.958	0.946	0.972	0.888
Ni ²⁺	0.926	0.001	0.006	0.860	0.977	0.845	0.188	0.933
Pb ²⁺	0.931	0.934	0.943	0.936	0.972	0.955	0.986	0.961
Pd ²⁺	0.829	0.515	0.003	0.000	0.807	0.367	0.001	0.000
Pt ²⁺	0.934	0.929	0.939	0.850	0.948	0.923	0.951	0.883
Ru ³⁺	0.664	0.633	0.597	0.435	0.483	0.370	0.339	0.394
Se ⁴⁺	0.919	0.910	0.054	0.000	0.934	0.914	0.022	0.000
Sn ²⁺	0.946	0.931	0.943	0.891	0.972	0.949	0.995	0.778
Zn ²⁺	0.940	0.826	0.757	0.907	0.966	0.346	0.305	0.986

	1	2	3	4	5	6	7	8
Ag ⁺	0.003	0.943	0.950	0.080	0.000	0.420	0.256	0.002
As ³⁺	0.942	0.955	0.064	0.001	0.951	0.949	0.038	0.000
Au ³⁺	0.819	0.743	0.426	0.053	0.707	0.562	0.546	0.001
Cd ²⁺	0.946	0.693	0.526	0.818	0.986	0.937	0.924	0.916
Co ²⁺	0.940	0.019	0.039	0.882	0.990	0.500	0.519	0.805
Cr ³⁺	0.950	0.947	0.792	0.892	0.978	0.910	0.712	0.574
Cu ²⁺	0.935	0.000	0.005	0.868	0.932	0.007	0.006	0.790
Fe ²⁺	0.932	0.449	0.333	0.901	0.981	0.932	0.888	0.918
Fe ³⁺	0.205	0.020	0.000	0.000	0.025	0.000	0.000	0.000
Hg ²⁺	0.004	0.301	0.317	0.002	0.000	0.001	0.001	0.001
Mn ²⁺	0.938	0.924	0.941	0.901	0.944	0.938	0.951	0.847
Ni ²⁺	0.930	0.001	0.006	0.834	0.987	0.803	0.174	0.890
Pb ²⁺	0.932	0.923	0.934	0.929	0.986	0.921	0.950	0.949
Pd ²⁺	0.828	0.572	0.003	0.001	0.813	0.405	0.001	0.000
Pt ²⁺	0.918	0.917	0.926	0.845	0.969	0.905	0.923	0.843
Ru ³⁺	0.658	0.632	0.556	0.467	0.478	0.383	0.332	0.376
Se ⁴⁺	0.911	0.908	0.056	0.001	0.943	0.904	0.029	0.000
Sn ²⁺	0.937	0.932	0.937	0.903	0.980	0.928	0.964	0.742
Zn ²⁺	0.939	0.828	0.739	0.906	0.988	0.343	0.328	0.940

	1	2	3	4	5	6	7	8
Ag ⁺	0.001	0.952	0.925	0.037	0.000	0.361	0.217	0.002
As ³⁺	0.946	0.953	0.046	0.000	0.946	0.996	0.050	0.000
Au ³⁺	0.822	0.743	0.416	0.076	0.747	0.563	0.594	0.112
Cd ²⁺	0.953	0.739	0.698	0.706	0.975	0.959	0.936	0.922
Co ²⁺	0.953	0.025	0.045	0.803	0.971	0.556	0.410	0.798
Cr ³⁺	0.946	0.947	0.744	0.815	0.961	0.938	0.660	0.684
Cu ²⁺	0.941	0.000	0.005	0.793	0.913	0.009	0.008	0.869
Fe ²⁺	0.947	0.433	0.338	0.858	0.962	0.953	0.894	0.901
Fe ³⁺	0.145	0.024	0.000	0.001	0.030	0.030	0.005	0.000
Hg ²⁺	0.000	0.385	0.368	0.001	0.000	0.001	0.001	0.001
Mn ²⁺	0.933	0.951	0.926	0.846	0.954	0.946	0.943	0.930
Ni ²⁺	0.939	0.001	0.006	0.877	0.960	0.862	0.132	0.869
Pb ²⁺	0.937	0.954	0.926	0.900	0.956	0.944	0.971	0.956
Pd ²⁺	0.844	0.615	0.003	0.000	0.805	0.298	0.000	0.000
Pt ²⁺	0.919	0.936	0.912	0.805	0.935	0.924	0.938	0.876
Ru ³⁺	0.646	0.643	0.477	0.421	0.447	0.388	0.331	0.347
Se ⁴⁺	0.917	0.940	0.050	0.000	0.930	0.888	0.052	0.002
Sn ²⁺	0.931	0.954	0.930	0.850	0.961	0.957	0.981	0.966
Zn ²⁺	0.944	0.880	0.777	0.860	0.960	0.477	0.458	0.980

Table S2. Normalized fluorescence intensities used in chemometric analyses of compound **1-8** upon additions of metal ions (10 eq.) (Total 5 trials).

	1	2	3	4	5	6	7	8
Ag ⁺	0.001	0.927	0.933	0.021	0.000	0.063	0.046	0.000
As ³⁺	0.932	0.926	0.090	0.001	0.928	0.949	0.048	0.001
Au ³⁺	0.619	0.285	0.010	0.009	0.552	0.005	0.000	0.000
Cd ²⁺	0.918	0.680	0.642	0.748	0.957	0.948	0.933	0.898
Co ²⁺	0.921	0.001	0.005	0.860	0.957	0.517	0.413	0.709
Cr ³⁺	0.919	0.936	0.443	0.797	0.950	0.944	0.385	0.247
Cu ²⁺	0.927	0.000	0.005	0.953	0.845	0.002	0.002	0.826
Fe ²⁺	0.917	0.418	0.470	0.892	0.910	0.906	0.885	0.904
Fe ³⁺	0.000	0.000	0.000	0.002	0.000	0.000	0.000	0.000
Hg ²⁺	0.000	0.182	0.217	0.002	0.001	0.001	0.001	0.001
Mn ²⁺	0.903	0.939	0.943	0.913	0.950	0.882	0.912	0.867
Ni ²⁺	0.916	0.000	0.004	0.925	0.962	0.763	0.128	0.956
Pb ²⁺	0.908	0.921	0.938	0.936	0.949	0.902	0.964	0.931
Pd ²⁺	0.774	0.246	0.003	0.002	0.694	0.248	0.001	0.000
Pt ²⁺	0.891	0.880	0.907	0.960	0.922	0.920	0.953	0.977
Ru ³⁺	0.416	0.446	0.312	0.255	0.239	0.124	0.054	0.020
Se ⁴⁺	0.875	0.875	0.008	0.001	0.883	0.873	0.005	0.001
Sn ²⁺	0.907	0.925	0.904	0.791	0.950	0.920	0.920	0.295
Zn ²⁺	0.910	0.869	0.729	0.925	0.954	0.220	0.250	0.935

	1	2	3	4	5	6	7	8
Ag ⁺	0.001	0.938	0.960	0.004	0.000	0.039	0.058	0.002
As ³⁺	0.937	0.925	0.081	0.002	0.924	0.917	0.089	0.001
Au ³⁺	0.684	0.254	0.029	0.001	0.561	0.030	0.024	0.009
Cd ²⁺	0.934	0.676	0.644	0.705	0.982	0.974	0.876	0.917
Co ²⁺	0.906	0.001	0.005	0.724	0.984	0.476	0.393	0.631
Cr ³⁺	0.918	0.943	0.472	0.814	0.957	0.949	0.336	0.233
Cu ²⁺	0.922	0.000	0.005	0.880	0.837	0.003	0.003	0.842
Fe ²⁺	0.921	0.438	0.464	0.826	0.975	0.956	0.874	0.974
Fe ³⁺	0.001	0.000	0.000	0.001	0.000	0.001	0.000	0.000
Hg ²⁺	0.000	0.140	0.259	0.002	0.000	0.000	0.001	0.001
Mn ²⁺	0.916	0.935	0.951	0.928	0.976	0.966	0.903	0.829
Ni ²⁺	0.922	0.001	0.004	0.849	0.985	0.772	0.124	0.871
Pb ²⁺	0.910	0.919	0.958	0.874	0.984	0.969	0.903	0.931
Pd ²⁺	0.776	0.267	0.003	0.001	0.758	0.267	0.001	0.000
Pt ²⁺	0.891	0.885	0.912	0.931	0.929	0.933	0.949	0.969
Ru ³⁺	0.433	0.446	0.353	0.095	0.229	0.132	0.065	0.050
Se ⁴⁺	0.874	0.858	0.009	0.001	0.871	0.871	0.003	0.001
Sn ²⁺	0.912	0.904	0.903	0.677	0.977	0.981	0.902	0.343
Zn ²⁺	0.921	0.850	0.714	0.831	0.985	0.251	0.252	0.899

	1	2	3	4	5	6	7	8
Ag ⁺	0.001	0.952	0.953	0.028	0.000	0.032	0.022	0.001
As ³⁺	0.901	0.951	0.055	0.001	0.923	0.933	0.126	0.001
Au ³⁺	0.716	0.319	0.095	0.001	0.654	0.104	0.031	0.001
Cd ²⁺	0.950	0.678	0.663	0.713	0.979	0.949	0.907	0.840
Co ²⁺	0.937	0.001	0.005	0.816	0.947	0.495	0.392	0.639
Cr ³⁺	0.932	0.965	0.472	0.814	0.967	0.954	0.357	0.297
Cu ²⁺	0.923	0.000	0.005	0.948	0.816	0.003	0.002	0.815
Fe ²⁺	0.940	0.508	0.426	0.862	0.968	0.947	0.902	0.876
Fe ³⁺	0.039	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hg ²⁺	0.000	0.168	0.256	0.003	0.000	0.002	0.001	0.001
Mn ²⁺	0.929	0.978	0.954	0.908	0.960	0.941	0.935	0.826
Ni ²⁺	0.941	0.001	0.003	0.880	0.963	0.760	0.101	0.964
Pb ²⁺	0.943	0.967	0.958	0.895	0.971	0.940	0.958	0.925
Pd ²⁺	0.805	0.233	0.003	0.001	0.767	0.237	0.001	0.000
Pt ²⁺	0.886	0.953	0.915	0.960	0.921	0.927	0.939	0.985
Ru ³⁺	0.414	0.501	0.346	0.119	0.221	0.103	0.058	0.061
Se ⁴⁺	0.878	0.924	0.009	0.000	0.881	0.872	0.004	0.001
Sn ²⁺	0.943	0.960	0.923	0.785	0.966	0.950	0.940	0.334
Zn ²⁺	0.938	0.848	0.715	0.999	0.977	0.249	0.249	0.891

	1	2	3	4	5	6	7	8
Ag ⁺	0.039	0.950	0.932	0.023	0.000	0.028	0.023	0.001
As ³⁺	0.888	0.949	0.051	0.001	0.920	0.931	0.031	0.001
Au ³⁺	0.789	0.285	0.019	0.002	0.563	0.009	0.001	0.001
Cd ²⁺	0.926	0.664	0.655	0.698	0.968	0.978	0.900	0.788
Co ²⁺	0.949	0.001	0.004	0.817	0.971	0.456	0.366	0.660
Cr ³⁺	0.938	0.920	0.492	0.849	0.948	0.963	0.390	0.320
Cu ²⁺	0.882	0.000	0.005	0.872	0.872	0.002	0.002	0.813
Fe ²⁺	0.952	0.477	0.556	0.812	0.949	0.961	0.831	0.878
Fe ³⁺	0.043	0.000	0.000	0.002	0.000	0.000	0.000	0.000
Hg ²⁺	0.004	0.148	0.234	0.005	0.001	0.001	0.001	0.001
Mn ²⁺	0.949	0.922	0.955	0.902	0.952	0.960	0.950	0.812
Ni ²⁺	0.941	0.001	0.005	0.852	0.970	0.757	0.129	0.922
Pb ²⁺	0.947	0.920	0.940	0.894	0.966	0.960	0.950	0.934
Pd ²⁺	0.798	0.267	0.003	0.002	0.670	0.196	0.001	0.000
Pt ²⁺	0.869	0.891	0.918	0.960	0.920	0.925	0.943	0.980
Ru ³⁺	0.465	0.458	0.366	0.091	0.195	0.071	0.041	0.021
Se ⁴⁺	0.871	0.868	0.007	0.002	0.866	0.867	0.005	0.001
Sn ²⁺	0.958	0.909	0.917	0.676	0.960	0.965	0.973	0.382
Zn ²⁺	0.952	0.827	0.757	0.928	0.977	0.227	0.220	0.821

	1	2	3	4	5	6	7	8
Ag ⁺	0.003	0.950	0.856	0.032	0.042	0.073	0.062	0.001
As ³⁺	0.897	0.930	0.092	0.000	0.911	0.937	0.032	0.001
Au ³⁺	0.661	0.262	0.051	0.004	0.551	0.057	0.003	0.008
Cd ²⁺	0.974	0.651	0.665	0.696	0.996	0.952	0.978	0.815
Co ²⁺	0.914	0.001	0.038	0.796	0.942	0.507	0.391	0.628
Cr ³⁺	0.937	0.939	0.452	0.831	0.969	0.961	0.395	0.297
Cu ²⁺	0.927	0.000	0.040	0.895	0.819	0.004	0.052	0.804
Fe ²⁺	0.821	0.458	0.426	0.800	0.974	0.977	0.854	0.835
Fe ³⁺	0.077	0.000	0.003	0.006	0.001	0.005	0.000	0.009
Hg ²⁺	0.000	0.160	0.202	0.022	0.003	0.002	0.003	0.009
Mn ²⁺	0.877	0.934	0.878	0.918	0.948	0.982	0.991	0.909
Ni ²⁺	0.993	0.001	0.004	0.820	0.961	0.773	0.112	0.898
Pb ²⁺	0.871	0.946	0.843	0.948	0.917	0.923	0.973	0.907
Pd ²⁺	0.734	0.279	0.000	0.004	0.663	0.230	0.000	0.004
Pt ²⁺	0.888	0.914	0.917	0.998	0.918	0.927	0.939	0.945
Ru ³⁺	0.372	0.473	0.338	0.346	0.181	0.122	0.064	0.066
Se ⁴⁺	0.874	0.897	0.013	0.001	0.876	0.879	0.005	0.001
Sn ²⁺	0.831	0.926	0.849	0.828	0.990	0.942	0.912	0.305
Zn ²⁺	0.840	0.807	0.693	0.938	0.962	0.248	0.205	0.899