Electronic Supplementary Information for

Quantifying the Binding Strength of Salicylaldoxime-Uranyl Complexes Relative to Competing Salicylaldoxime-Transition Metal Ion Complexes in Aqueous Solution: A Combined Experimental and Computational Study

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Table S1. Acid dissociation and formation constants of the ligands and complexes discussed in this manuscript. The ligands ($L^{(\ )}$) tabulated correspond to the ligands illustrated in **Figure 2**. The constants were obtained in aqueous solution at 25 °C and, unless otherwise noted, ionic strength I = 0.0 M.

Equilibrium	**log β**	**References**
$H_2O \leftrightarrows H^+ + OH^-$	14.00	28
$UO_2^{2+} + OH^- \leftrightarrows UO_2(OH)^+$	8.75	51
$UO_2^{2+} + 2\ OH^- \leftrightarrows UO_2(OH)_2$	15.85	51
$UO_2^{2+} + 3\ OH^- \leftrightarrows UO_2(OH)_3^-$	21.8	51
$UO_2^{2+} + 4\ OH^- \leftrightarrows UO_2(OH)_4^{2-}$	23.6	51
$2\ UO_2^{2+} + OH^- \leftrightarrows (UO_2)_2(OH)^{3+}$	11.3	51
$2\ UO_2^{2+} + 2\ OH^- \leftrightarrows (UO_2)_2(OH)_2^{2+}$	22.4	51
$3\ UO_2^{2+} + 5\ OH^- \leftrightarrows (UO_2)_3(OH)_5^+$	54.4	51
$UO_2^{2+} + CO_3^{2-} \leftrightarrows (UO_2)(CO_3)$	9.94	53
$UO_2^{2+} + 2\ CO_3^{2-} \leftrightarrows (UO_2)(CO_3)_2^{2-}$	16.61	53
$UO_2^{2+} + 3\ CO_3^{2-} \leftrightarrows (UO_2)(CO_3)_3^{4-}$	21.84	53
$L^{(I)}H_2 \leftrightarrows H^+ + L^{(I)}H^-$	8.551, 8.07	44[b] and this work
$L^{(I)}H_2 \leftrightarrows 2\ H^+ + L^{(I)2-}$	20.279, 19.35	44[b] and this work
$UO_2^{2+} + L^{(I)2-} \leftrightarrows UO_2\ L^{(I)}$	16.1	This Work
$UO_2^{2+} + 2\ L^{(I)2-} \leftrightarrows UO_2\ L_2^{(I)2-}$	25.5	This Work
$Cu^{2+} + HL^{(I)-} \leftrightarrows Cu(HL^{(I)})^+$	10.12	59
$Cu^{2+} + 2\ HL^{(I)-} \leftrightarrows Cu(HL^{(I)})_2$	15.78	59
$Fe^{3+} + HL^{(I)-} \leftrightarrows Fe(HL^{(I)})^{2+}$	9.38	60
$Fe^{3+} + 2\ HL^{(I)-} \leftrightarrows Fe(HL^{(I)})_2^+$	16.73	60
$L^{(II)}H_2 \leftrightarrows H^+ + L^{(II)}H^-$	2.97	28
$L^{(II)}H_2 \leftrightarrows 2\ H^+ + L^{(II)2-}$	16.7	28
$UO_2^{2+} + L^{(II)2-} \leftrightarrows UO_2\ L^{(II)}$	13.1	28
$UO_2^{2+} + 2\ L^{(II)2-} \leftrightarrows UO_2\ L_2^{(II)2-}$	21.8	28
$Cu^{2+} + L^{(II)2-} \leftrightarrows CuL^{(II)}$	10.60	28
$Cu^{2+} + 2\ L^{(II)2-} \leftrightarrows CuL_2^{(II)2-}$	18.45	28
$Fe^{3+} + L^{(II)2-} \leftrightarrows FeL^{(II)+}$	11.90	28
$Fe^{3+} + 2\ L^{(II)2-} \leftrightarrows FeL^{(II)}{}_2^-$	28.25	28
$L^{(III)}H \leftrightarrows H^+ + L^{(III)-}$	11.30	28
$L^{(IV)}H \leftrightarrows H^+ + L^{(IV)-}$	10.0	28
$UO_2^{2+} + L^{(IV)-} \leftrightarrows UO_2\ L^{(IV)+}$	5.9	28
$L^{(V)}H \leftrightarrows H^+ + L^{(V)-}$	4.20	28
$UO_2^{2+} + L^{(V)-} \leftrightarrows UO_2\ L^{(V)+}$	2.68	28
$L^{(VI)}H \leftrightarrows H^+ + L^{(VI)-}$	12.36	48[a]
$UO_2^{2+} + L^{(VI)-} \leftrightarrows UO_2\ L^{(VI)+}$	12.4	29
$UO_2^{2+} + 2\ L^{(VI)-} \leftrightarrows UO_2\ L^{(VI)}$	22.3	29
$L^{(VII)}H \leftrightarrows H^+ + L^{(VII)-}$	13.21	48[a]
$UO_2^{2+} + L^{(VII)-} \leftrightarrows UO_2\ L^{(VII)+}$	13.6	29
$UO_2^{2+} + 2\ L^{(VII)-} \leftrightarrows UO_2\ L^{(VII)}$	23.7	29
$L^{(VIII)}H_2 \leftrightarrows H^+ + L^{(VIII)}H^-$	12.06	50[b]
$L^{(VIII)}H_2 \leftrightarrows 2\ H^+ + L^{(VIII)2-}$	24.19	50[b]
$UO_2^{2+} + L^{(VIII)2-} \leftrightarrows UO_2\ L^{(VIII)}$	17.3	50[b]
$UO_2^{2+} + 2\ L^{(VIII)2-} \leftrightarrows UO_2\ L_2^{(VIII)2-}$	26.1	50[b]
$L^{(IX)}H_2 \leftrightarrows H^+ + L^{(IX)}H^-$	10.70	49[b]
$L^{(IX)}H_2 \leftrightarrows 2\ H^+ + L^{(IX)2-}$	22.76	49[b]
$UO_2^{2+} + L^{(IX)2-} \leftrightarrows UO_2\ L^{(IX)}$	17.8	49[b]
$UO_2\ L^{(IX)} + 2\ L^{(IX)2-} \leftrightarrows UO_2\ L_2^{(IX)2-}$	27.5	49[b]
$Cu^{2+} + L^{(IX)2-} \leftrightarrows CuL^{(IX)}$	18.94	15[b]
$Cu^{2+} + 2\ L^{(IX)2-} \leftrightarrows CuL_2^{(IX)2-}$	24.45	15[b]
$Fe^{3+} + HL^{(IX)-} \leftrightarrows Fe(HL^{(IX)})^{2+}$	25.66	15[b]
$Fe^{3+} + HL^{(IX)-} + L^{(IX)2-} \leftrightarrows Fe(L^{(IX)})(HL^{(IX)})$	43.94	15[b]

[a]Ionic strength 0.3 M $NaClO_4$. [b]Ionic strength 0.5 M NaCl.

Table S2. Comparison of experimental, calculated, and predicted stability constant (log β) values for UO_2^{2+}-ligand complexes

ligand	*exp log β*[a]	*calc log β*[b]	*pred log β*[c]	*abs. error*
1 acetate	3.1	9.9	5.3	2.2
2 acetylacetonate	7.7	15.6	8.5	0.8
3 phenolate	6.4	13.6	7.4	1.0
4 OH^-	8.8	18.4	10.1	1.3
5 NO_3^-	0.0	1.0	0.2	0.2
6 ClO_3^-	0.5	-1.9	-1.4	1.9
7 $H_2PO_4^-$	3.3	6.3	3.2	0.1
8 acetamidoxime	13.6	24.3	13.4	0.2
9 benzamidoxime	12.4	22.1	12.2	0.2
10 2acetamidoxime	23.7	41.2	23.1	0.6
11 2benzamidoxime	22.3	37.7	21.1	1.2
12 glutarimidedioxime (HL^-)	11.3	23.4	12.9	1.6
13 oxalate	7.3	11.7	6.3	1.0
14 phthalate	5.6	9.4	5.0	0.6
15 salicylate	13.0	20.2	11.1	1.9
16 catecholate	16.8	24.7	13.7	3.1
17 glutarimidedioxime (L^{2-})	19.1	35.2	19.6	0.5
18 CO_3^{2-}	9.7	17.5	9.6	0.1
19 SO_4^{2-}	3.0	5.2	2.6	0.4
20 HPO_4^{2-}	7.2	14.7	8.0	0.8
21 phthalimidedioxime	16.8	25.5	14.1	2.7

[a]Corrected to zero ionic strength with the Davies equation. [b]Calculated using the methodology described in ref 41. [c]Predicted from the correlation [pred log β = 0.5692 × calc log β] shown in **Figure 8**.

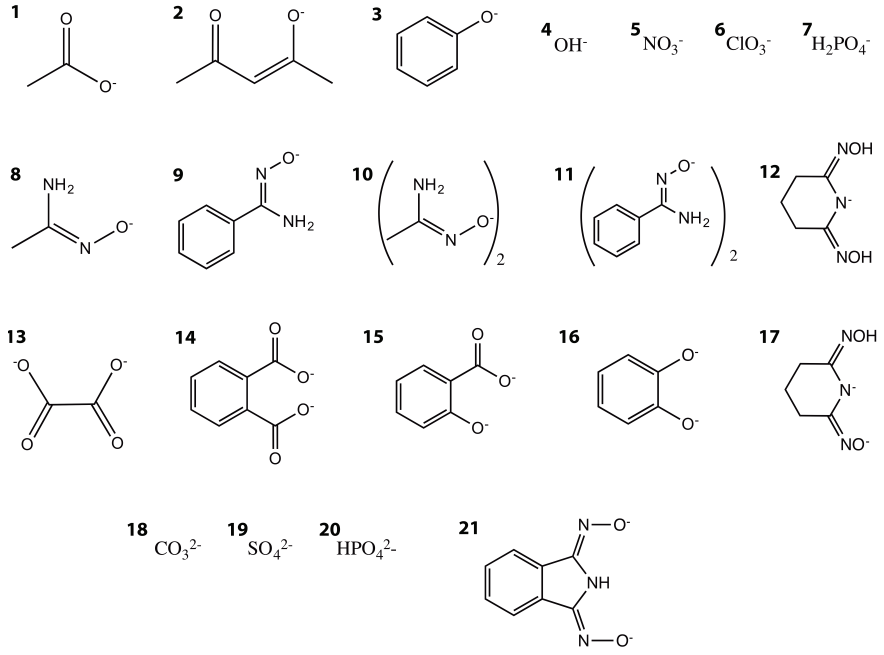

Table S3. Full chemical name of the CSD crystal structures depicted in Figures 1, S5, and S6 by CSD reference code.

Figure	Ref. Code	Full Chemical Name
1	ACOXNI10	bis(2,2'-Imino-bis(Acetamidoxime)) copper(II) chloride
1	AICOCU10	bis(4-Aminoimidazole-5-carboxamidoxime) copper(II) perchlorate
1	YOHFEI	bis(Acetato-O)-bis(N'-hydroxypyridine-2-carboximidamide) cadmium(II) ethanol solvate
1	CUHJUK	Disodium bis(adenine-N^1-oxide) copper(II) octahydrate
1	ORUTIF	(N'-(oxy)-N-methylbenzenecarboximidamidato)-(N-(oxy)-N'-methylbenzenecarboximidamide) oxo-technetium(IV)
1	CIMMIW	tris(N'^{1}, N'^{2} –dihydroxyethanediimidamide) nickel(II) ditetrafluoroborate
1	WOBHUS	Aqua-(N'^{1}, N'^{2} –dihydroxyethanediimidamide)-oxolato copper(II)
1	TEKYUD	bis(N-(2,6-Dimethylphenyl)aminoglyoximato-N,N') nickel(II)
1	RASBIW	Oxo-(2-thienylamidoximato-N,O)-(2-thienylamidoximato-N',O)-acetylacetonato molybdenum(VI)
1	FOWJAC	bis(Acetylacetonato-O,O')-(acetamidoximato-N,O)-nitrosyl molybdenum(VI)
S6	GIQBUE	bis(Triethylammonium) bis(m2-2-oxybenzoato)-bis(nitrato-O,O')-tetraoxo-di-uranium(VI)
S6	BIDVUF	bis(2-Amino-2-methyl-1-propanol)-copper(II) bis(salicylato)-copper(II) 2-propanol solvate
S6	PIMSUB	bis(Oxonium) chloride diaqua-bis(2-oxy-5-nitrobenzoato) iron(III)
S6	TEVWAU	dioxo-bis(2,6-bis(N-oxidoiminio)piperidinato) uranium(VI) monohydrate
S6	Ref. 15	Glutarimidedioxime iron(III) dichloride
S7	BOCCOL	tetrakis((μ_3-Salicylidenealdoximato)-(salicylidenealdoxime) iron(III)) salicylidenealdoxime xylene solvate
S7	CSALCU	bis(5-Chlorosalicylaldoximato) copper(II)

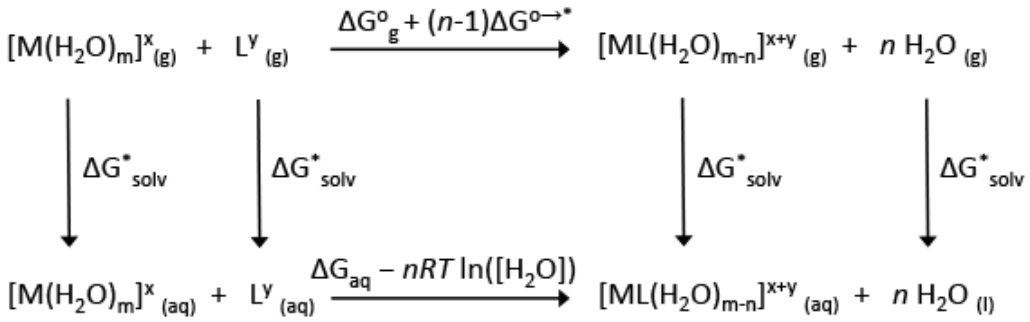

Figure S1. Thermodynamic cycle used to calculate ΔG_{aq}.

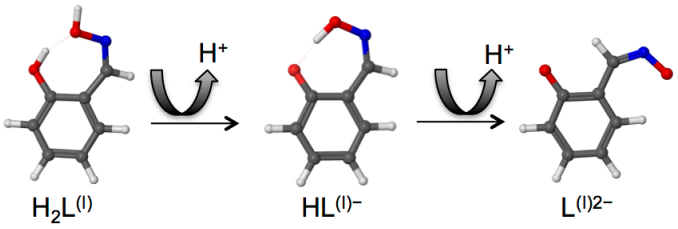

Figure S2. Stepwise dissociation of salicylaldoxime used to fit UV/Vis titration data. Color legend: O, red; N, blue; C, grey; H, white.

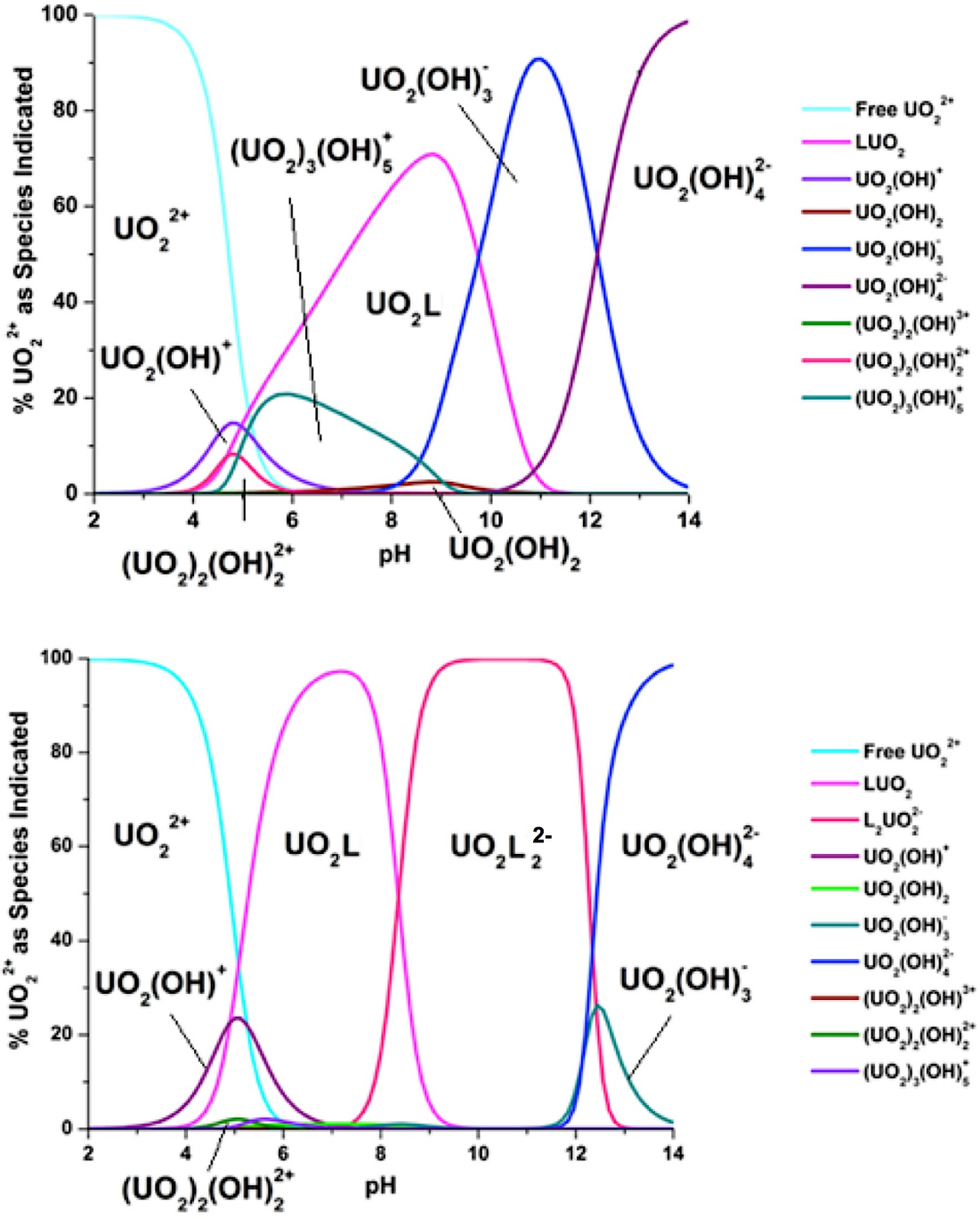

Figure S3. Species distribution diagrams of the 1:1 *(left)* and the 10:1 salicylaldoxime (L) to uranyl titration solutions as a function of pH. Distribution diagrams were generated with the HYSS[52] software using the uranyl hydrolysis constants in ref. 51 and the uranyl-salicylaldoxime formation constants from this work.

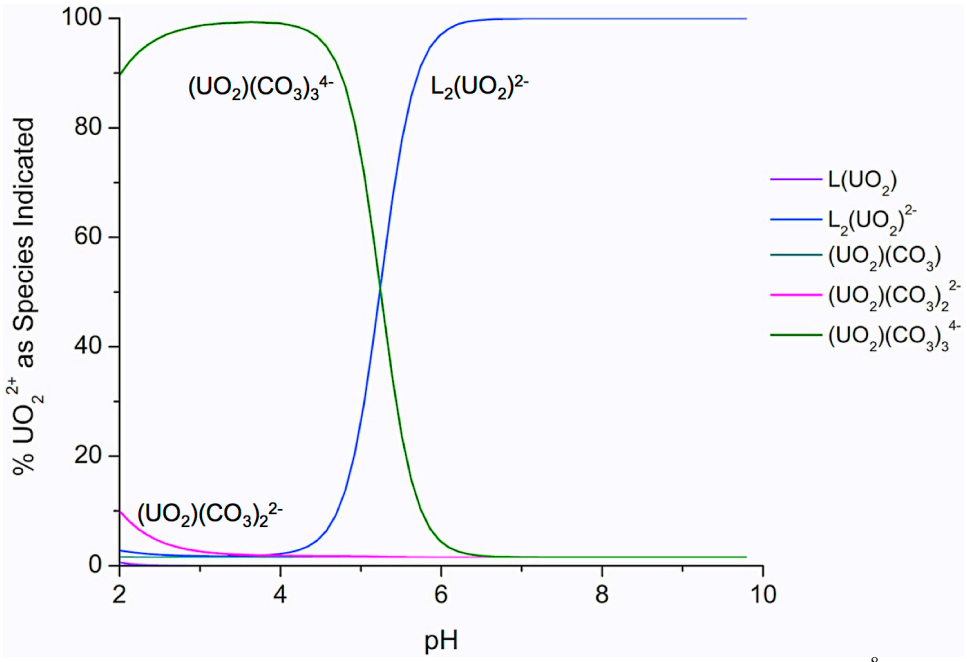

Figure S4. Species distribution diagrams of 0.001 M salicylaldoxime, 1.3 x 10^{-8} M uranyl, and 0.0025 M carbonate calculated using the HYSS[52] software. The uranyl carbonate constants were taken from ref. 53 and the uranyl-salicylaldoxime formation constants from this work.

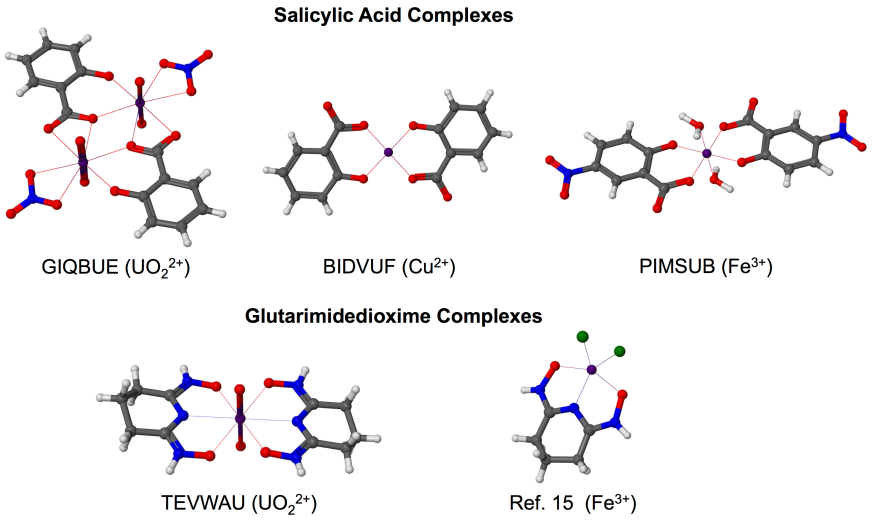

Figure S5. Crystal structures of salicylic acid and glutarimidedioxime complexes. GIQBUE[59] ($C_{30}H_{32}Cu_2N_4O_{10}$•2($H_3BO_3$•4($H_2O$)): phenolate-$UO_2^{2+}$ bond = 2.23(1) Å and carboxylate-UO_2^{2+} bond = 2.42(1) Å. BIDVUF[60] ($C_{14}H_8CuO_6^{2-}$•$C_8H_{22}CuN_2O_2^{2+}$•4(C_3H_8O)): phenolate-Cu^{2+} bond = 1.900 Å and carboxylate-Cu^{2+} bond = 1.903 Å. PIMSUB[61] ($C_{14}H_{10}FeN_2O_{12}^-$•2($H_3O^+$)•$Cl^-$): phenolate-$Fe^{3+}$ bond = 1.973 Å and carboxylate-Fe^{3+} bond = 1.944 Å. TEVWAU[49] ($C_{10}H_{16}N_6O_6U$•H_2O): oximate-UO_2^{2+} bond 1 = 2.430 Å, oximate-UO_2^{2+} bond 2 = 2.535 Å, and piperidine-UO_2^{2+} bond = 2.563 Å. Ref. 15 ($C_{10}H_{16}N_6O_6FeCl_2^+$): oximate-$UO_2^{2+}$ bond 1 = 2.019(7) Å, oximate-UO_2^{2+} bond 1 = 2.027(7) Å, and piperidine-UO_2^{2+} bond = 2.009(8) Å. Color legend: O, red; N, blue; C, grey; H, white; S, yellow; metal ion, purple.

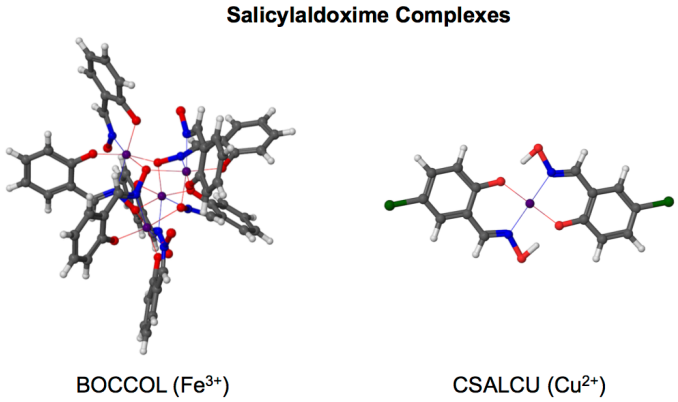

Figure S6. Crystal structures of salicylaldoxime-Fe^{3+} and –Cu^{2+} complexes. BOCCOL[65] ($C_{56}H_{44}Fe_4N_8O_{16}$•$C_7H_7NO_2$•$C_8H_{10}$•$C_8H_{10}$): phenolate-$Fe^{3+}$ bond = 1.889(8) Å and oximate-Fe^{3+} bond = 2.14(1) Å. CSALCU[64] ($C_{14}H_{10}Cl_2CuN_2O_4$): phenolate-Cu^{2+} bond = 1.9082 Å and oximate-Cu^{2+} bond = 1.9579 Å. Color legend: O, red; N, blue; C, grey; H, white; S, yellow; metal ion, purple.

Optimized geometries of salicylaldoxime ligands, UO_2^{2+}, and Cu^{2+} complexes discussed in the main text and their total energies at the M06/SSC/6-311++G** level of theory

Salicylaldoxime:

1) $H_2L^{(I)}$; total energy: - 475.9163087 Hartrees

symmetry c1

N	2.457273000	-1.030157000	0.023359000
C	1.246482000	-1.286549000	-0.286277000
C	-2.594349000	0.507900000	0.118076000
C	-2.420764000	-0.872432000	0.183089000
C	-1.150571000	-1.389886000	0.047146000
C	-0.022129000	-0.572103000	-0.122601000
C	-0.217849000	0.820702000	-0.197748000
C	-1.509067000	1.337221000	-0.074011000
H	-3.586918000	0.938229000	0.210625000
H	-3.269822000	-1.531693000	0.326187000
H	-1.001650000	-2.466701000	0.077200000
O	0.752779000	1.709894000	-0.453666000
H	-1.622779000	2.414158000	-0.143087000
O	2.606182000	0.207013000	0.664980000
H	1.162998000	-2.279580000	-0.730274000
H	3.549636000	0.252571000	0.848890000
H	1.613867000	1.351606000	-0.174843000

2) $HL^{(I)-}$; total energy: -475.376987 Hartrees

symmetry c1

N	2.464990000	-0.948622000	0.070220000
C	1.238101000	-1.255691000	-0.158932000
C	-2.645004000	0.495463000	0.073156000
C	-2.469543000	-0.892308000	0.104222000
C	-1.178271000	-1.383386000	0.016686000
C	-0.050342000	-0.560425000	-0.082050000
C	-0.219194000	0.869909000	-0.156224000
C	-1.565277000	1.340329000	-0.046852000
H	-3.648537000	0.915267000	0.137965000
H	-3.318565000	-1.564566000	0.189052000
H	-1.016838000	-2.462218000	0.032265000
O	0.744772000	1.679510000	-0.332066000
H	-1.698748000	2.419161000	-0.089150000
O	2.764083000	0.319869000	0.485292000
H	1.149906000	-2.312491000	-0.432036000
H	2.022018000	0.943274000	0.197891000

3) $L^{(I)2-}$; total energy: -474.658113 Hartrees

symmetry c1

N	1.622994000	-2.512728000	-0.155315000
C	1.203245000	-1.263496000	-0.161247000
C	-2.682090000	0.535910000	0.057551000
C	-2.573980000	-0.851588000	0.078304000
C	-1.298495000	-1.429761000	0.005822000
C	-0.125178000	-0.674239000	-0.087036000
C	-0.213452000	0.792587000	-0.112849000
C	-1.542199000	1.326410000	-0.034267000
H	-3.666768000	1.011513000	0.113376000
H	-3.461656000	-1.481496000	0.150637000
H	-1.162631000	-2.507947000	0.020552000
O	0.798465000	1.552335000	-0.197643000
H	-1.619989000	2.415834000	-0.052217000
O	0.761835000	-3.494371000	-0.070777000
H	2.012689000	-0.537448000	-0.234415000

Uranyl complexes with salicylaldoxime:

1) $[UO_2(HL^{(I)})(H_2O)_3]^+$; total energy: -1331.951756 Hartrees

symmetry c1

N	1.620771000	1.495598000	1.914273000
C	0.398930000	1.205690000	1.611566000
C	-1.110834000	-2.570435000	0.547856000
C	-1.924970000	-1.438528000	0.464480000
C	-1.399042000	-0.213799000	0.801037000
C	-0.056005000	-0.084763000	1.198792000

C	0.768383000	-1.239713000	1.271542000
C	0.206265000	-2.478752000	0.952691000
H	-1.519852000	-3.543690000	0.294532000
H	-2.958565000	-1.527251000	0.151622000
H	-2.020056000	0.677526000	0.763106000
O	2.021806000	-1.148893000	1.658024000
H	0.830669000	-3.362957000	1.025457000
O	1.763847000	2.841490000	2.339092000
U	3.735671000	0.204816000	1.409351000
O	4.142083000	0.451781000	3.091157000
O	3.515355000	0.107103000	-0.318795000
O	4.089110000	2.677959000	0.993729000
H	3.371993000	3.169314000	1.440093000
H	4.194959000	3.052327000	0.113961000
O	4.700672000	-2.155052000	1.554024000
H	4.015820000	-2.828691000	1.635535000
H	5.482308000	-2.475505000	2.013669000
H	-0.342171000	2.004006000	1.704791000
H	1.875786000	2.794633000	3.299725000
O	6.245778000	0.409819000	0.947830000
H	6.680021000	0.278296000	0.098556000
H	6.882899000	0.823674000	1.539662000

2) $[UO_2(HL^{(I)})_2(H_2O)]$; total energy: -1654.6585449 Hartrees
symmetry c1

N	-1.149985000	1.238379000	0.668627000
C	-2.334548000	1.714920000	0.545601000
H	-2.466642000	2.768579000	0.808107000
C	-5.859978000	-0.221589000	-0.757961000
C	-5.877839000	1.130234000	-0.416689000
C	-4.705918000	1.724127000	0.004935000
C	-3.507487000	1.004196000	0.096161000
C	-3.495660000	-0.371890000	-0.247708000
C	-4.695482000	-0.958908000	-0.675514000
H	-6.773179000	-0.705002000	-1.093892000
H	-6.794905000	1.705211000	-0.481468000
H	-4.697497000	2.777735000	0.275456000
O	-2.401183000	-1.076829000	-0.165699000
H	-4.676259000	-2.011211000	-0.941438000
O	-0.254557000	2.176931000	1.136003000
U	-0.217138000	-1.135117000	0.253976000
O	-0.497203000	-1.558171000	1.937894000
O	0.180649000	-0.812511000	-1.419824000
O	1.611825000	0.229001000	0.752901000
N	1.973456000	-2.484599000	0.602892000
O	1.875116000	-3.852016000	0.968716000

C	3.173676000	-2.156769000	0.281363000
C	3.588499000	-0.828349000	-0.067667000
C	2.792424000	0.320880000	0.210618000
C	3.348934000	1.579552000	-0.085178000
C	4.603112000	1.695635000	-0.641466000
C	5.384665000	0.567487000	-0.911872000
C	4.876342000	-0.673129000	-0.610153000
H	3.934599000	-2.942585000	0.298251000
H	5.470106000	-1.565553000	-0.795495000
H	6.374258000	0.671376000	-1.342117000
H	4.991673000	2.684341000	-0.869127000
H	2.749634000	2.460487000	0.126639000
H	0.596974000	1.692400000	1.135841000
H	1.488634000	-3.814272000	1.854991000
O	-0.501032000	-3.606141000	-0.416615000
H	-1.335878000	-4.073646000	-0.340278000
H	0.213532000	-4.166145000	-0.072927000

3) $[UO_2(L^{(I)})(H_2O)_2]$; total energy: -1255.1180818 Hartrees
symmetry c1

N	1.418780000	1.472192000	0.833286000
C	0.198387000	1.387873000	0.462221000
H	-0.455528000	2.262199000	0.498521000
C	-1.353103000	-2.297229000	-0.934728000
C	-2.169511000	-1.170077000	-0.875476000
C	-1.631999000	0.015328000	-0.413942000
C	-0.297377000	0.111719000	-0.007974000
C	0.541085000	-1.041055000	-0.068256000
C	-0.030358000	-2.233106000	-0.540310000
H	-1.756513000	-3.239741000	-1.294653000
H	-3.207756000	-1.221112000	-1.185086000
H	-2.251608000	0.908265000	-0.359302000
O	1.802747000	-1.026433000	0.293746000
H	0.609186000	-3.109821000	-0.585268000
O	2.129057000	2.464426000	1.286400000
U	3.369900000	0.386249000	1.102404000
O	3.053655000	-0.041416000	2.785887000
O	3.983463000	0.798953000	-0.501098000
O	4.722505000	-1.812573000	0.942540000
O	4.919492000	2.260433000	1.997405000
H	4.732408000	-2.170098000	0.048520000
H	4.357762000	-2.501357000	1.507951000
H	4.927724000	2.945786000	1.319582000
H	4.446802000	2.648697000	2.742830000

4) $[UO_2(L^{(I)})_2]^{2-}$; total energy: -1577.0735695 Hartrees

symmetry c1

N	0.921845000	1.089174000	0.748487000
C	-0.165602000	1.193887000	0.075684000
H	-0.630633000	2.179567000	-0.058286000
C	-2.072829000	-2.174767000	-1.684633000
C	-2.623279000	-0.901199000	-1.830513000
C	-1.961649000	0.166994000	-1.236211000
C	-0.781532000	0.017881000	-0.508050000
C	-0.196488000	-1.295744000	-0.348818000
C	-0.903964000	-2.362012000	-0.970246000
H	-2.566363000	-3.034986000	-2.137565000
H	-3.541832000	-0.745414000	-2.391346000
H	-2.370512000	1.174540000	-1.333878000
O	0.880241000	-1.530032000	0.297281000
H	-0.470601000	-3.352953000	-0.854069000
O	1.595177000	2.024576000	1.327738000
U	2.605789000	-0.343148000	1.572982000
O	1.674088000	-0.589665000	3.061122000
O	3.537493000	-0.096644000	0.084837000
O	4.331331000	0.843759000	2.848649000
N	4.289715000	-1.775457000	2.397556000
O	3.616402000	-2.710862000	1.818285000
C	5.377108000	-1.880170000	3.070445000
C	5.993005000	-0.704152000	3.654190000
C	5.407984000	0.609474000	3.494873000
C	6.115434000	1.675757000	4.116306000
C	7.284236000	1.488522000	4.830799000
C	7.834656000	0.214952000	4.976774000
C	7.173059000	-0.853253000	4.382455000
H	5.842119000	-2.865851000	3.204481000
H	7.581901000	-1.860801000	4.480193000
H	8.753157000	0.059175000	5.537692000
H	7.777745000	2.348753000	5.283735000
H	5.682100000	2.666701000	4.000051000

Copper complexes with salicylaldoxime:

1) $[Cu(HL^{(I)})(H_2O)_2]^+$; total energy: -825.3637068 Hartrees

symmetry c1

N	1.880590000	1.162398000	0.904042000
C	0.595168000	1.032131000	0.740641000
H	-0.024435000	1.857073000	1.098865000
C	-1.407019000	-2.092587000	-1.199477000
C	-2.115025000	-0.965400000	-0.751902000
C	-1.434135000	0.029272000	-0.107746000
C	-0.038379000	-0.063077000	0.115029000

C	0.670525000	-1.223598000	-0.320828000
C	-0.053239000	-2.219660000	-0.999404000
H	-1.939274000	-2.886097000	-1.715324000
H	-3.182217000	-0.886092000	-0.920674000
H	-1.955997000	0.917284000	0.238757000
O	1.942715000	-1.418325000	-0.106210000
H	0.488004000	-3.095914000	-1.338804000
O	2.264199000	2.294539000	1.638183000
Cu	3.140939000	-0.265296000	0.736189000
O	4.513070000	-1.707036000	0.368959000
H	5.377328000	-1.577982000	-0.035527000
H	4.057124000	-2.414428000	-0.107803000
O	4.444879000	0.700484000	1.930760000
H	3.995233000	1.464498000	2.329547000
H	4.978203000	0.259150000	2.600304000
H	2.496741000	2.969365000	0.983666000

2) $[Cu(HL^{(I)})_2]$; total energy: -1148.103999 Hartrees
symmetry c2h

N	0.819874000	1.773927000	0.000000000
C	2.074882000	2.045812000	0.000000000
H	2.346880000	3.103966000	0.000000000
C	5.306615000	-0.664251000	0.000000000
C	5.535332000	0.714568000	0.000000000
C	4.451775000	1.561168000	0.000000000
C	3.131887000	1.075882000	0.000000000
C	2.900928000	-0.326043000	0.000000000
C	4.026435000	-1.171130000	0.000000000
H	6.149213000	-1.350080000	0.000000000
H	6.545352000	1.108635000	0.000000000
H	4.602363000	2.638464000	0.000000000
O	1.709229000	-0.862301000	0.000000000
H	3.849064000	-2.242279000	0.000000000
O	-0.004559000	2.864272000	0.000000000
Cu	0.000000000	0.000000000	0.000000000
O	-1.709229000	0.862301000	0.000000000
N	-0.819874000	-1.773927000	0.000000000
O	0.004559000	-2.864272000	0.000000000
C	-2.074882000	-2.045812000	0.000000000
C	-3.131887000	-1.075882000	0.000000000
C	-2.900928000	0.326043000	0.000000000
C	-4.026435000	1.171130000	0.000000000
C	-5.306615000	0.664251000	0.000000000
C	-5.535332000	-0.714568000	0.000000000
C	-4.451775000	-1.561168000	0.000000000
H	-2.346880000	-3.103966000	0.000000000

H	-4.602363000	-2.638464000	0.000000000
H	-6.545352000	-1.108635000	0.000000000
H	-6.149213000	1.350080000	0.000000000
H	-3.849064000	2.242279000	0.000000000
H	-0.897451000	2.455605000	0.000000000
H	0.897451000	-2.455605000	0.000000000