Supplementary Material

Fluorescent Thiophene based Mercury sensors

Austin Shigemoto, Carolyn Virca, Sam Underwood, Lauren Shetterley, and Theresa McCormick

Table of Contents

1. DFT

Optimized Geometry Coordinates L1	2
Optimized Geometry Coordinates L2	2
Optimized Geometry Coordinates L3	3
Figure S1. Computed Absorption Spectrum L1	4-6
Figure S2. Computed Absorption Spectrum Hg(L1)(ClO ₄) ₂	7-11
Figure S3. Computed Structure of Hg(L1)(ClO ₄) ₂	8-9
Figure S4. Computed Absorption Spectrum L2	12-14
Figure S5. Computed Absorption Spectrum L3	15-18
Figure S6. Computed Frontier molecular orbitals L3	15

2. L1, L2, and L3 emission response to transition metal ions

Figure S7. L1 emission response to transition metals	19
Figure S8. L2 emission response to transition metals	19
Figure S9. L3 emission response to transition metals	19

3. Stern-Volmer plots of L1, L2, and L3 for the titration with Hg(ClO₄)₂

Figure S10. L1 Stern Volmer plot	20
Figure S11. L2 Stern Volmer plot (40.0 eq)	20
Figure S12. L2 Stern Volmer plot (300 eq)	20
Figure S13. L3 Stern Volmer plot	21

4. L2 Hg(II) titration past 20.0 eq

Figure S14. L2 titration past 20.0 eq	21
---------------------------------------	----

1. DFT

Optimized Geometry Coordinates L1

Charge = 0 Multiplicity = 1

C	0.24589	0.60995	0.30602
C	0.26839	1.15535	-0.94424
C	0.48544	2.56276	-0.9463
C	0.62891	3.09316	0.30239
S	0.28226	1.87728	1.53232
H	0.21508	-0.43929	0.51348
H	0.14665	0.57944	-1.83778
H	0.54244	3.14604	-1.84152
C	1.04151	4.54738	0.59665
C	1.16031	4.98198	1.9238
C	1.53472	6.30151	2.18129
C	1.78105	7.15369	1.1039
C	1.64708	6.66601	-0.20321
N	1.28506	5.39053	-0.42072
H	1.63123	6.65365	3.18707
H	0.96575	4.30836	2.73205
H	2.0695	8.16991	1.27419
H	1.83445	7.31405	-1.03378

Optimized Geometry Coordinates L2

Charge = 0 Multiplicity = 1

C	-0.38889	0.29673	0.00237
C	0.99029	0.34643	0.00078
C	1.50988	1.66409	-0.00089
C	0.53577	2.64181	-0.00163
S	-1.05716	1.91504	0.00083
H	1.59187	-0.55444	0.00104
H	2.56449	1.91159	-0.00178
C	0.74136	4.09497	-0.00348
C	-0.32683	5.01232	-0.004
C	-0.05005	6.37668	-0.00579
H	-1.3557	4.66393	-0.00309
C	2.27545	5.81681	-0.00646
H	-0.86273	7.09854	-0.00624
H	3.3273	6.09852	-0.00741
C	-1.23036	-0.90571	0.00445
C	-2.63714	-0.84708	0.00579
C	-3.3661	-2.03307	0.00781
H	-3.15144	0.10972	0.00531
C	-1.2844	-3.21123	0.00706
H	-4.45274	-2.00593	0.00889
H	-0.70793	-4.13503	0.0075
C	-2.68206	-3.24973	0.00851

H	-3.20887	-4.19931	0.01014
C	1.28029	6.79893	-0.00708
H	1.54341	7.85251	-0.00855
N	-0.57057	-2.08375	0.00505
N	2.02754	4.50559	-0.00468

Optimized Geometry Coordinates L3

Charge = 0 Multiplicity = 1

C	-2.85017	0.2089	0.00756
C	-1.44277	0.21865	0.00594
C	-0.78639	1.44595	0.00653
C	-1.52991	2.62253	0.00867
C	-2.93431	2.5305	0.01018
N	-3.56821	1.34516	0.00963
H	0.29981	1.48535	0.00533
H	-0.87706	-0.708	0.00428
H	-1.03255	3.58762	0.00915
C	-3.79877	3.72058	0.01257
C	-5.17639	3.75049	0.01425
S	-3.15569	5.35163	0.01363
C	-5.71583	5.06828	0.01648
H	-5.76764	2.84302	0.01385
C	-4.7462	6.03807	0.0165
H	-6.7785	5.28734	0.01805
H	-4.86977	7.11337	0.01788
C	-3.62563	-1.04098	0.00701
C	-4.99742	-1.17212	0.00833
S	-2.86449	-2.62058	0.00439
C	-5.4385	-2.52595	0.00731
H	-5.65397	-0.3107	0.01008
C	-4.40027	-3.42185	0.00522
H	-6.48219	-2.82257	0.00814
H	-4.44471	-4.50331	0.00419

L1

Figure S1: Calculated absorbance spectrum of **L1** (0.3 eV FVHM) as determined by TD-DFT calculations using B3LYP/6-311+G(d) basis set

Excitation Energies and oscillator strengths of 18 lowest energy transitions

42 is the HOMO

Excited State 1: Singlet 3.6651 eV 338.29 nm $f=0.4881$ $\langle S^2 \rangle=0.000$
42 -> 43 0.69918

Excited State 2: Singlet 4.2431 eV 292.20 nm $f=0.0010$ $\langle S^2 \rangle=0.000$
40 -> 43 -0.70101

Excited State 3: Singlet 4.2725 eV 290.19 nm $f=0.0139$ $\langle S^2 \rangle=0.000$
38 -> 43 -0.13987
39 -> 43 0.10422
42 -> 44 0.67583

Excited State 4: Singlet 4.7396 eV 261.59 nm $f=0.0321$ $\langle S^2 \rangle=0.000$
41 -> 43 -0.66657
42 -> 47 0.16939

Excited State 5: Singlet 4.8045 eV 258.06 nm $f=0.0008$ $\langle S^2 \rangle=0.000$
42 -> 45 -0.68417
42 -> 48 0.12461

Excited State 6: Singlet 5.1540 eV 240.56 nm $f=0.0023$ $\langle S^2 \rangle=0.000$
40 -> 44 -0.67713
42 -> 46 0.15578

Excited State 7: Singlet 5.1699 eV 239.82 nm $f=0.0003$ $\langle S^2 \rangle=0.000$

40 -> 44	-0.16215
42 -> 46	-0.67100
Excited State 8: Singlet 5.1756 eV 239.55 nm f=0.0075 <S**2>=0.000	
39 -> 43	0.55042
41 -> 43	0.14501
42 -> 47	0.38838
Excited State 9: Singlet 5.5199 eV 224.61 nm f=0.0086 <S**2>=0.000	
42 -> 45	-0.11785
42 -> 46	0.11279
42 -> 48	-0.67459
Excited State 10: Singlet 5.5721 eV 222.51 nm f=0.0530 <S**2>=0.000	
38 -> 43	-0.51473
38 -> 44	-0.17442
39 -> 43	0.21329
39 -> 44	-0.16445
42 -> 44	-0.13300
42 -> 47	-0.30212
Excited State 11: Singlet 5.7405 eV 215.98 nm f=0.0425 <S**2>=0.000	
38 -> 43	-0.15112
41 -> 44	-0.67616
Excited State 12: Singlet 5.7489 eV 215.67 nm f=0.0034 <S**2>=0.000	
42 -> 49	-0.69370
Excited State 13: Singlet 5.8528 eV 211.84 nm f=0.0514 <S**2>=0.000	
38 -> 43	-0.36955
38 -> 44	0.15349
39 -> 43	-0.29230
39 -> 44	-0.10830
41 -> 44	0.15343
42 -> 47	0.44342
Excited State 14: Singlet 5.9355 eV 208.88 nm f=0.0021 <S**2>=0.000	
41 -> 45	-0.17831
42 -> 50	-0.66256
Excited State 15: Singlet 6.0024 eV 206.56 nm f=0.0018 <S**2>=0.000	
41 -> 45	0.62222
41 -> 48	-0.15543
42 -> 50	-0.19102

42 -> 51 0.14945
42 -> 52 0.11389

Excited State 16: Singlet 6.0593 eV 204.62 nm f=0.0000 <S**2>=0.000

41 -> 45 0.19182
42 -> 51 -0.59014
42 -> 52 -0.32010

Excited State 17: Singlet 6.2158 eV 199.46 nm f=0.0001 <S**2>=0.000

42 -> 51 -0.33014
42 -> 52 0.60495

Excited State 18: Singlet 6.3805 eV 194.32 nm f=0.0607 <S**2>=0.000

41 -> 47 0.20528
42 -> 53 0.64793
42 -> 55 -0.13993

Figure S2: a) Calculated absorbance spectrum of Hg(L1)(ClO₄)₂ (0.3 eV FWHM) including electronic transitions indicated by line as determined by TD-DFT calculations using B3LYP/6-311+G(d) basis set for all atoms but Hg, which was run with a LanL2DZ basis set with proposed molecular structure depicted in spectrum b) Orbitals involved in electronic transitions of Hg(L1)(ClO₄)₂ and energy diagram with transitions indicated by colored lines corresponding to those in calculated absorbance spectrum.

Optimized Geometry Coordinates Hg(L1)(ClO₄)₂

Figure S3: Optimized structure Hg(L1)(ClO₄)₂ from DFT calculations using B3LYP/6-311G+(d) /LanL2DZ basis set

Charge = 0 Multiplicity = 1

Hg	-0.42265	-0.44562	0.0377
S	1.46991	0.87771	2.06589
N	0.05926	1.83223	-0.59213
O	-3.99282	1.2636	0.79772
C	2.13757	1.63394	0.62228
O	-2.30961	-0.38225	1.54743
Cl	-3.44769	-0.07546	0.5397
O	-2.71684	-0.08602	-0.82334
Cl	1.51137	-2.58908	-1.02223
O	1.14057	-3.82485	-1.71039
O	2.95366	-2.48066	-0.77169
O	1.00754	-1.35763	-1.79287
O	0.74081	-2.48766	0.33324
O	-4.46084	-1.12753	0.58689
C	3.01587	0.21134	2.4838
H	3.10982	-0.39815	3.37019
C	3.98168	0.58454	1.59805
H	5.01488	0.27297	1.68207
C	3.48298	1.3963	0.53757
H	4.092	1.7424	-0.28855
C	1.27081	2.36382	-0.30578
C	1.6677	3.57632	-0.87842
H	2.6289	4.00049	-0.61571
C	0.80696	4.2333	-1.74943
H	1.10403	5.17396	-2.20045

C	-0.44412	3.68432	-2.01675
H	-1.14922	4.17089	-2.67933
C	-0.7806	2.47942	-1.41431
H	-1.73678	1.99931	-1.58861

Excitation energies and oscillator strengths of 20 lowest energy transitions

97 is the HOMO:

Excited State 1: Singlet-A 3.5560 eV 348.66 nm $f=0.0237$ $\langle S^2 \rangle=0.000$
 97 -> 98 0.69941

Excited State 2: Singlet-A 4.0853 eV 303.49 nm $f=0.0475$ $\langle S^2 \rangle=0.000$
 96 -> 98 0.46730
 97 -> 99 0.51470

Excited State 3: Singlet-A 4.2959 eV 288.61 nm $f=0.0839$ $\langle S^2 \rangle=0.000$
 91 -> 98 -0.11334
 92 -> 98 0.37356
 94 -> 98 -0.15615
 96 -> 98 0.39967
 97 -> 99 -0.34615
 97 -> 100 -0.13551

Excited State 4: Singlet-A 4.3429 eV 285.49 nm $f=0.0253$ $\langle S^2 \rangle=0.000$
 92 -> 98 0.37320
 93 -> 98 0.20516
 94 -> 98 0.13151
 95 -> 98 0.45173
 96 -> 98 -0.21605
 97 -> 99 0.14040

Excited State 5: Singlet-A 4.3500 eV 285.02 nm $f=0.0024$ $\langle S^2 \rangle=0.000$
 92 -> 98 0.32061
 93 -> 98 -0.17476
 94 -> 98 0.47056
 95 -> 98 -0.34003

Excited State 6: Singlet-A 4.3705 eV 283.68 nm $f=0.0021$ $\langle S^2 \rangle=0.000$
 91 -> 98 0.51377
 91 -> 99 0.11529
 93 -> 98 -0.37864
 94 -> 98 -0.13741
 95 -> 98 0.19142

Excited State 7: Singlet-A 4.3957 eV 282.06 nm f=0.0255 <S**2>=0.000
 92 -> 98 -0.28325
 93 -> 98 -0.12263
 94 -> 98 0.42492
 95 -> 98 0.33640
 96 -> 98 0.18786
 97 -> 99 -0.17292
 97 ->100 -0.13511

Excited State 8: Singlet-A 4.4339 eV 279.63 nm f=0.0059 <S**2>=0.000
 91 -> 98 0.43189
 93 -> 98 0.49268
 94 -> 98 0.11180

Excited State 9: Singlet-A 4.6602 eV 266.05 nm f=0.1072 <S**2>=0.000
 90 -> 98 0.21039
 96 -> 98 0.10186
 97 -> 99 -0.14695
 97 ->100 0.62587

Excited State 10: Singlet-A 4.7134 eV 263.05 nm f=0.0323 <S**2>=0.000
 90 -> 98 0.62882
 90 -> 99 0.10748
 96 -> 98 -0.10689
 96 -> 99 0.18444
 97 ->100 -0.16312

Excited State 11: Singlet-A 4.8099 eV 257.77 nm f=0.0232 <S**2>=0.000
 90 -> 98 -0.16372
 96 -> 99 0.65856

Excited State 12: Singlet-A 5.0413 eV 245.94 nm f=0.0151 <S**2>=0.000
 89 -> 98 0.68609

Excited State 13: Singlet-A 5.0779 eV 244.16 nm f=0.0008 <S**2>=0.000
 92 -> 99 -0.10531
 93 -> 99 0.20799
 94 -> 99 -0.34262
 95 -> 99 0.54058

Excited State 14: Singlet-A 5.1211 eV 242.11 nm f=0.0007 <S**2>=0.000
 91 -> 99 -0.11592
 92 -> 99 0.12541
 93 -> 99 0.20957

94 -> 99	0.55535	
95 -> 99	0.30375	
Excited State 15:	Singlet-A	5.1473 eV 240.87 nm f=0.0000 <S**2>=0.000
92 -> 99	-0.34291	
93 -> 98	-0.10706	
93 -> 99	0.51586	
95 -> 99	-0.27149	
Excited State 16:	Singlet-A	5.1659 eV 240.01 nm f=0.0002 <S**2>=0.000
91 -> 99	0.30726	
92 -> 98	-0.10693	
92 -> 99	0.49782	
93 -> 99	0.32261	
95 -> 99	-0.12807	
Excited State 17:	Singlet-A	5.1746 eV 239.60 nm f=0.0001 <S**2>=0.000
91 -> 98	-0.12945	
91 -> 99	0.59305	
92 -> 99	-0.25827	
94 -> 99	0.20343	
Excited State 18:	Singlet-A	5.2639 eV 235.53 nm f=0.0132 <S**2>=0.000
96 ->100	0.67265	
Excited State 19:	Singlet-A	5.4080 eV 229.26 nm f=0.0057 <S**2>=0.000
87 -> 98	-0.15000	
89 -> 99	-0.14047	
90 -> 98	-0.11061	
90 -> 99	0.61787	
97 ->101	0.18254	
Excited State 20:	Singlet-A	5.4582 eV 227.15 nm f=0.0304 <S**2>=0.000
89 -> 99	-0.42687	
90 -> 99	-0.23269	
97 ->101	0.45268	
97 ->102	0.13861	

L2

Figure S4: Computed absorbance spectrum of **L2** calculated by TD-DFT using a B3LYP/6-311+G(d) basis set displayed with 0.3 eV FWHM gaussians

Excitation energies and oscillator strengths of 20 lowest energy transitions

62 is HOMO:

Excited State 1: Singlet 3.4942 eV 354.83 nm $f=0.8651$ $\langle S^2 \rangle=0.000$
62 -> 63 0.70425

Excited State 2: Singlet- 4.1302 eV 300.19 nm $f=0.0038$ $\langle S^2 \rangle=0.000$
61 -> 63 0.18067
62 -> 64 0.66859

Excited State 3: Singlet- 4.2548 eV 291.40 nm $f=0.0000$ $\langle S^2 \rangle=0.000$
59 -> 64 0.13672
59 -> 66 0.10862
60 -> 63 0.68354

Excited State 4: Singlet- 4.2848 eV 289.36 nm $f=0.0003$ $\langle S^2 \rangle=0.000$
57 -> 63 0.12454
62 -> 65 0.68794

Excited State 5: Singlet- 4.3166 eV 287.23 nm $f=0.0018$ $\langle S^2 \rangle=0.000$
59 -> 63 0.67812
60 -> 64 0.15415
60 -> 66 0.11667

Excited State 6: Singlet- 4.4655 eV 277.65 nm $f=0.0049$ $\langle S^2 \rangle=0.000$
58 -> 63 0.12068
61 -> 63 0.60608
62 -> 64 -0.14444
62 -> 66 0.29181

Excited State 7: Singlet- 4.6469 eV 266.81 nm f=0.0084 $\langle S^2 \rangle = 0.000$
 58 -> 63 0.45078
 61 -> 63 -0.28192
 62 -> 66 0.44440

Excited State 8: Singlet- 4.9981 eV 248.06 nm f=0.0042 $\langle S^2 \rangle = 0.000$
 59 -> 63 -0.10314
 59 -> 65 0.45069
 60 -> 64 0.49279
 60 -> 66 -0.19302

Excited State 9: Singlet- 5.0026 eV 247.84 nm f=0.0000 $\langle S^2 \rangle = 0.000$
 59 -> 64 0.46389
 59 -> 66 -0.18666
 60 -> 65 0.48810

Excited State 10: Singlet- 5.1015 eV 243.03 nm f=0.1045 $\langle S^2 \rangle = 0.000$
 58 -> 63 0.49446
 61 -> 65 0.16760
 62 -> 66 -0.43316

Excited State 11: Singlet- 5.1343 eV 241.48 nm f=0.0005 $\langle S^2 \rangle = 0.000$
 62 -> 68 0.58386
 62 -> 69 -0.36595
 62 -> 73 -0.13225

Excited State 12: Singlet- 5.1761 eV 239.53 nm f=0.0000 $\langle S^2 \rangle = 0.000$
 62 -> 67 0.69533

Excited State 13: Singlet- 5.2609 eV 235.67 nm f=0.0165 $\langle S^2 \rangle = 0.000$
 57 -> 63 0.52141
 58 -> 64 -0.20457
 61 -> 64 0.38007
 62 -> 65 -0.11325

Excited State 14: Singlet- 5.3625 eV 231.21 nm f=0.0979 $\langle S^2 \rangle = 0.000$
 57 -> 63 -0.32636
 58 -> 64 0.15269
 61 -> 64 0.59266

Excited State 15: Singlet- 5.4199 eV 228.76 nm f=0.0118 $\langle S^2 \rangle = 0.000$
 56 -> 63 0.52132
 58 -> 65 0.23150

61 -> 65 -0.37249

Excited State 16: Singlet- 5.5078 eV 225.11 nm f=0.0053 <S**2>=0.000
62 -> 68 0.38483
62 -> 69 0.56846
62 -> 73 0.13207

Excited State 17: Singlet- 5.5440 eV 223.64 nm f=0.0064 <S**2>=0.000
56 -> 63 0.30463
58 -> 63 -0.14081
58 -> 65 0.19112
61 -> 65 0.57071

Excited State 18: Singlet- 5.6537 eV 219.30 nm f=0.0001 <S**2>=0.000
59 -> 63 -0.16219
59 -> 65 -0.27167
59 -> 72 -0.11231
60 -> 64 0.40615
60 -> 66 0.47025

Excited State 19: Singlet- 5.6892 eV 217.93 nm f=0.0000 <S**2>=0.000
59 -> 64 0.45037
59 -> 66 0.42413
60 -> 63 -0.14751
60 -> 65 -0.28460
60 -> 72 -0.11386

Excited State 20: Singlet- 5.7067 eV 217.26 nm f=0.0255 <S**2>=0.000
55 -> 63 0.44878
57 -> 63 0.13217
58 -> 64 0.39126
62 -> 72 0.32560

L3

Figure S5: Computed absorbance spectrum of **L3** calculated by TD-DFT using a B3LYP/6-311+G(d) basis set displayed with a) 0.3 eV FWHM Gaussians functions and b) 0.15 eV FWHM Gaussian functions.

Figure S6: Computed frontier molecular orbitals of **L3** using a B3LYP/6-311+G(d) basis set

Excitation energies and oscillator strengths of 17 lowest energy transitions
63 is HOMO:

Excited State 1: Singlet- 3.7323 eV 332.20 nm $f=0.1915$ $\langle S^2 \rangle=0.000$
62 -> 64 -0.19217
63 -> 65 0.67264

Excited State 2: Singlet- 3.9514 eV 313.77 nm $f=0.1061$ $\langle S^2 \rangle=0.000$
62 -> 65 -0.12210
63 -> 64 0.69051

Excited State 3: Singlet- 4.2805 eV 289.65 nm $f=0.6077$ $\langle S^2 \rangle=0.000$
62 -> 64 0.67409
63 -> 65 0.18951

Excited State 4: Singlet- 4.4313 eV 279.79 nm $f=0.0424$ $\langle S^2 \rangle=0.000$
60 -> 64 -0.14920
62 -> 65 0.67017
63 -> 64 0.10779

Excited State 5: Singlet- 4.5594 eV 271.93 nm $f=0.0018$ $\langle S^2 \rangle=0.000$
59 -> 65 0.70079

Excited State 6: Singlet- 4.5676 eV 271.44 nm $f=0.0000$ $\langle S^2 \rangle=0.000$
59 -> 64 0.70157

Excited State 7: Singlet- 4.8280 eV 256.80 nm $f=0.0016$ $\langle S^2 \rangle=0.000$
61 -> 64 0.67265
63 -> 66 0.16188

Excited State 8: Singlet- 4.8748 eV 254.34 nm $f=0.0953$ $\langle S^2 \rangle=0.000$
60 -> 64 0.65802
61 -> 65 -0.14362
62 -> 65 0.13756

Excited State 9: Singlet- 4.9267 eV 251.66 nm $f=0.0263$ $\langle S^2 \rangle=0.000$
60 -> 65 0.67352
63 -> 66 -0.15124

Excited State 10: Singlet- 4.9328 eV 251.35 nm $f=0.0001$ $\langle S^2 \rangle=0.000$
60 -> 64 0.15568
61 -> 65 0.67557

Excited State 11: Singlet- 5.0717 eV 244.46 nm $f=0.0182$ $\langle S^2 \rangle=0.000$
58 -> 64 -0.14807
60 -> 65 0.16496
61 -> 64 -0.14212

63 -> 66 0.64282

Excited State 12: Singlet- 5.2181 eV 237.60 nm f=0.0000 <S**2>=0.000
62 -> 69 -0.16856
63 -> 67 -0.31720
63 -> 68 0.58367

Excited State 13: Singlet- 5.3132 eV 233.35 nm f=0.0000 <S**2>=0.000
62 -> 69 0.12076
63 -> 67 0.59353
63 -> 68 0.35431

Excited State 14: Singlet- 5.3332 eV 232.47 nm f=0.0044 <S**2>=0.000
62 -> 67 0.23866
62 -> 68 -0.17308
63 -> 69 0.59996
63 -> 71 -0.18347

Excited State 15: Singlet- 5.6189 eV 220.66 nm f=0.0014 <S**2>=0.000
57 -> 64 0.13296
58 -> 65 -0.12511
62 -> 66 0.66909

Excited State 16: Singlet- 5.6606 eV 219.03 nm f=0.0049 <S**2>=0.000
62 -> 67 0.15296
62 -> 68 0.26043
62 -> 70 -0.13621
63 -> 69 0.22013
63 -> 71 0.57020

Excited State 17: Singlet- 5.7434 eV 215.87 nm f=0.0081 <S**2>=0.000
57 -> 65 0.46118
58 -> 64 0.50647

Excited State 18: Singlet- 5.7476 eV 215.72 nm f=0.0000 <S**2>=0.000
62 -> 69 0.10006
62 -> 71 -0.16537
62 -> 73 -0.11271
63 -> 68 0.12865
63 -> 70 0.64097

Excited State 19: Singlet- 5.8147 eV 213.22 nm f=0.0090 <S**2>=0.000
57 -> 64 -0.40883
61 -> 66 0.12596

62 -> 66	0.10732
63 -> 72	0.54019

Excited State 20: Singlet- 5.8959 eV 210.29 nm f=0.0016 $\langle S^2 \rangle = 0.000$

60 -> 69	0.10120
62 -> 67	0.56165
62 -> 68	-0.24198
63 -> 69	-0.26471
63 -> 73	0.10725

2. L1, L2, and L3 response to transition metal ions

Figure S7: Emission spectrum of **L1** (solid) and **L1** in the presence of 5 eq of Hg(II) (dots), Cu(II) (dots and dashes), and Fe(III) (dashes) in CH₃CN excited at 297 nm

Figure S8: Emission spectrum of **L2** (solid) and **L2** in the presence of 5 eq of Hg(II) (dots), and Fe(III) (dashes) in CH₃CN excited at 361 nm

Figure S9: Emission spectrum of **L3** (solid) and **L3** in the presence of 5 eq of Hg(II) (dots), and Fe(III) (dashes) in CH₃CN excited at 297 nm

3. Stern Volmer plots of L1, L2, and L3 for the titration of $\text{Hg}(\text{ClO}_4)_2$

Figure S10: Stern-Volmer plot of **L1** emission titration with $\text{Hg}(\text{ClO}_4)_2$ in CH_3CN .

Figure S11: Stern-Volmer plot of **L2** emission titration with $\text{Hg}(\text{ClO}_4)_2$ ending at 40.0 eq in CH_3CN .

Figure S12: Stern-Volmer plot of **L2** emission titration with $\text{Hg}(\text{ClO}_4)_2$ ending at 300.0 eq in CH_3CN .

Figure S13: Stern-Volmer plot of **L3** emission titration with $\text{Hg}(\text{ClO}_4)_2$ in CH_3CN .

4. L2 Titration past 20.0 eq

Figure S14: Change in emission spectrum of **L2** after 20.0 eq of $\text{Hg}(\text{ClO}_4)_2$ had been added in CH_3CN excited at 361 nm. Pictures of solution with 20.0 eq and 250 eq of $\text{Hg}(\text{ClO}_4)_2$ in solution with **L2**