

**Supplementary Material for**  
**Molecular Form and Molecular Mimicry in Mercury**  
**Toxicology**

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**Table S1. Computed Cartesian coordinates for Methionine**

<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
S	4.5372	8.7570	9.7583
N	8.3621	13.2569	1.7363
H	9.9763	13.8638	2.6107
H	8.7739	13.1790	-0.1486
O	9.3358	6.6232	1.4516
H	10.8929	5.6230	1.4318
O	12.1375	9.4001	3.1359
C	9.9851	8.9078	2.4767
C	7.7401	10.7212	2.6699
C	6.8390	10.9173	5.4400
H	8.4276	11.6134	6.5833
H	5.3634	12.3736	5.4895
C	5.8195	8.4521	6.5496
H	7.2465	6.9445	6.5619
H	4.2182	7.7565	5.4261
C	7.4410	9.1129	11.5927
H	6.8620	9.1645	13.5805
H	8.4348	10.8747	11.1479
H	8.7022	7.4934	11.3050
H	6.1925	9.9688	1.51103

**Table S2. Computed Cartesian coordinates for L-cysteinato(methyl)mercury(II).**

<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-5.1816	6.3154	4.2386
C	-6.0565	3.6887	4.5069
C	-8.7588	3.2314	3.5489
C	-12.9484	10.3330	0.1757
Hg	-10.2139	9.3881	2.8875
N	-6.1680	2.7590	7.2433
O	-10.2895	1.7366	4.5353
O	-9.1821	4.3520	1.3171
S	-6.9768	8.7002	5.8562
H	-5.1516	-6.8034	2.1405
H	-3.1724	6.4841	4.9972
H	-4.7178	2.4089	3.4065
H	-13.6664	9.3174	-1.5832
H	-13.6664	12.3641	0.1757
H	-10.7941	10.3330	0.1757
H	-7.8933	1.5978	7.5175
H	-6.2209	4.4068	8.5400
H	-10.1514	1.8715	6.6240

**Table S3. Computed Cartesian coordinates for Cystine**

<b>Atom</b>	<b><i>x</i></b>	<b><i>y</i></b>	<b><i>z</i></b>
C	2.2715	-1.066	-2.8629
C	4.9504	-2.0619	-3.3406
C	4.8580	-4.3238	-5.1823
N	6.3031	-2.8077	-0.9614
O	6.1984	-6.3720	-4.3930
O	3.7263	-4.2716	-7.1929
S	-0.0411	-3.5519	-1.9252
H	1.4823	-0.1995	-4.5734
H	2.2813	0.3626	-1.3648
H	6.0784	-0.5957	-4.2762
H	4.9753	-3.5617	0.2236
H	6.9634	-1.2431	-0.0595
H	6.7362	-5.9708	-2.6623
S	-0.0185	-3.5565	1.9684
C	-2.3143	-1.0606	2.9079
C	-5.0474	-2.0038	3.3049
C	-5.0791	-4.3409	5.0850
N	-6.4144	-2.6695	0.9674
O	-5.9474	-6.3788	4.5702
O	-3.8771	-3.9593	7.3829
H	-2.2804	0.4010	1.4417
H	-1.5056	-0.2067	4.6268
H	-6.1585	-0.4789	4.1861
H	-5.2222	-3.6296	-0.1972
H	-6.8839	-1.0325	0.0721
H	-3.7084	-2.1637	7.7066

**Table S4. Computed Cartesian coordinates for Mercury(II) bis-L-cysteinate**

<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Hg	1.4392	1.7065	48.8216
S	-1.9068	1.8746	45.7669
C	-0.9229	3.9232	43.2102
H	0.8776	3.1468	42.3183
H	-0.5389	5.8937	43.9913
C	-3.0059	4.0909	41.1864
H	-4.8077	4.8727	42.0707
C	-2.1075	5.8751	39.0711
O	-3.5768	6.0512	36.6320
O	0.3146	7.3495	39.3877
H	-2.5105	7.2246	35.2587
S	4.8084	1.5532	51.8520
C	4.2895	3.9047	54.2806
H	2.4626	3.4636	55.3330
H	4.1453	5.8554	53.3781
C	6.5148	3.8713	56.1538
H	6.6729	1.9226	57.0588
N	8.9305	4.4745	54.7594
H	10.5319	4.4619	56.1140
H	8.7733	6.3716	53.8784
C	6.0683	5.8696	58.2193
O	8.2119	7.5630	59.0439
O	3.4318	6.3239	59.2073
H	9.0228	6.8378	60.8372
N	-3.5134	1.5021	40.0983
H	-4.1668	0.2108	41.6162
H	-1.7503	0.7480	39.2481