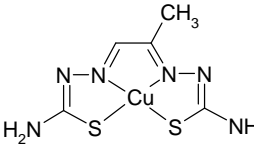
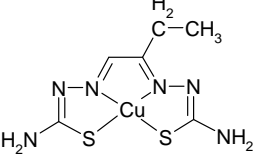
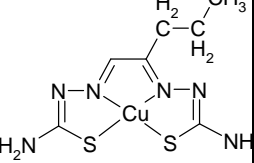
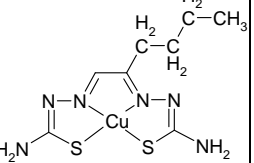
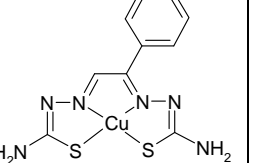
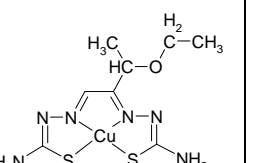


Common bis-thiosemicarbazone (BTS) family compounds [1]

Ligand	H ₂ PTSM	H ₂ ETSM	H ₂ nPrTSM	H ₂ nBuTSM	H ₂ PhTSM	H ₂ KTSM
Molecular Formula #	C ₇ H ₁₂ CuN ₆ S ₂	C ₈ H ₁₄ CuN ₆ S ₂	C ₉ H ₁₆ CuN ₆ S ₂	C ₁₀ H ₁₈ CuN ₆ S ₂	C ₁₂ H ₁₄ CuN ₆ S ₂	C ₁₀ H ₁₈ CuN ₆ OS ₂
Molecular Weight #	308	322	336	350	370	366
Structure						
Log P	1.92	2.65	2.86	3.16	3.06	2.64
Brain Uptake (% , rat) *	3.0%	2.8%	3.1%	2.4%	1.8%	2.5%
Heart Uptake (% , rat) *	2.7%	2.6%	2.4%	1.7%	1.8%	2.1%
Lung Uptake (% , rat) *	8.2%	4.7%	7.1%	2.4%	4.9%	15.0%
Liver Uptake (% , rat) *	12.5%	9.9%	10.0%	13.3%	24.6%	10.1%
Kidney Uptake (% , rat) *	3.7%	2.3%	2.4%	2.0%	2.7%	2.6%
Blood Uptake (% , rat) *	9.3%	7.3%	7.7%	5.8%	12.8%	7.5%

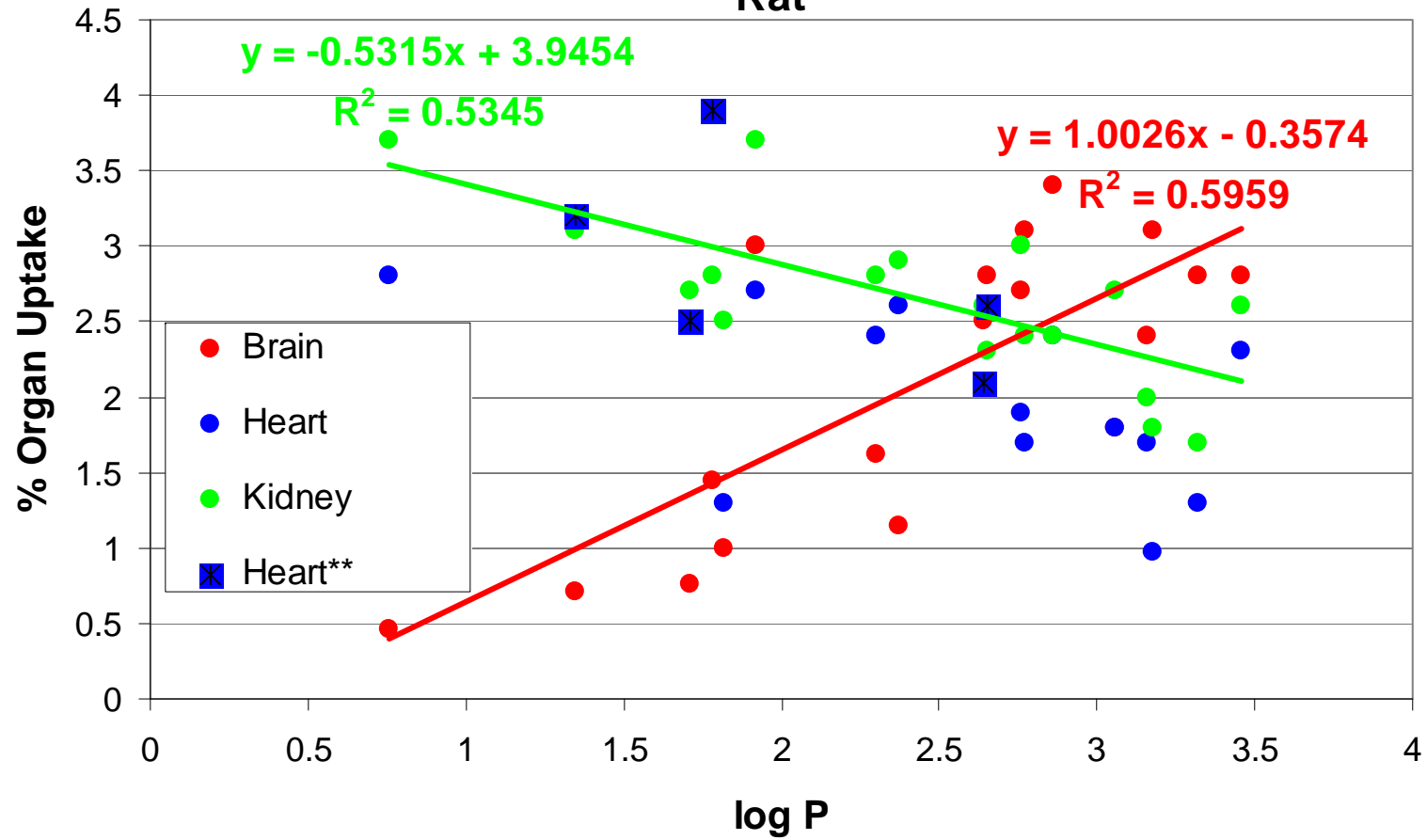
Ligand	H ₂ PTS	H ₂ ETS	H ₂ nPrTS	H ₂ nBuTS	H ₂ PhTS	H ₂ KTS
Molecular Formula #	C ₅ H ₈ CuN ₆ S ₂	C ₆ H ₁₀ CuN ₆ S ₂	C ₇ H ₁₂ CuN ₆ S ₂	C ₈ H ₁₄ CuN ₆ S ₂	C ₁₀ H ₁₀ CuN ₆ S ₂	C ₈ H ₁₄ CuN ₆ OS ₂
Molecular Weight #	280	294	308	322	342	338
Structure						
Log P	0.76	1.35	1.78	2.30	2.37	1.71
Brain Uptake (% rat) *	0.46%	0.71%	1.45%	1.62%	1.15%	0.76%
Heart Uptake (% rat) *	2.8%	3.2%	3.9%	2.4%	2.6%	2.5%
Lung Uptake (% rat) *	15%	12.8%	13.1%	12.2%	11.1%	15.1%
Liver Uptake (% rat) *	7.8%	11.7%	11.5%	10.0%	12.6%	9.7%
Kidney Uptake (% rat) *	3.7%	3.1%	2.8%	2.8%	2.9%	2.7%
Blood Uptake (% rat) *	18%	13.4%	15.2%	8.4%	13.4%	15.8%

1. Elizabeth K. John and Mark A. Green, "Structure- Activity Relationships for Metal-Labeled Blood Flow Tracers: Comparison of Keto Aldehyde Bis(thiosemicarbazone)copper (II) Derivatives, *J. Med. Chem.* 1990, 33, P1764-1770

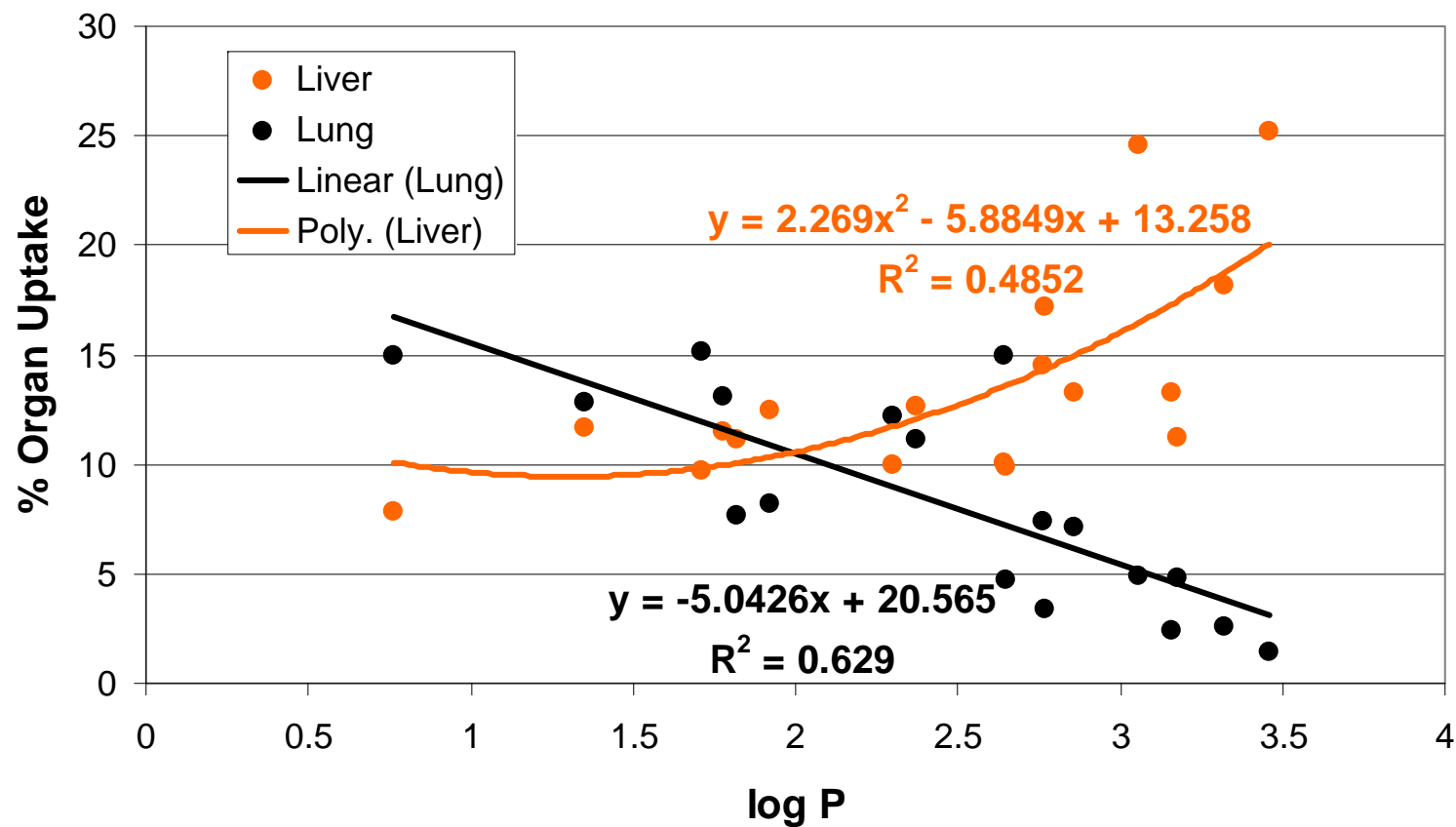
Molecular formula and weight for the copper complexes * Measured at 1 min post injection

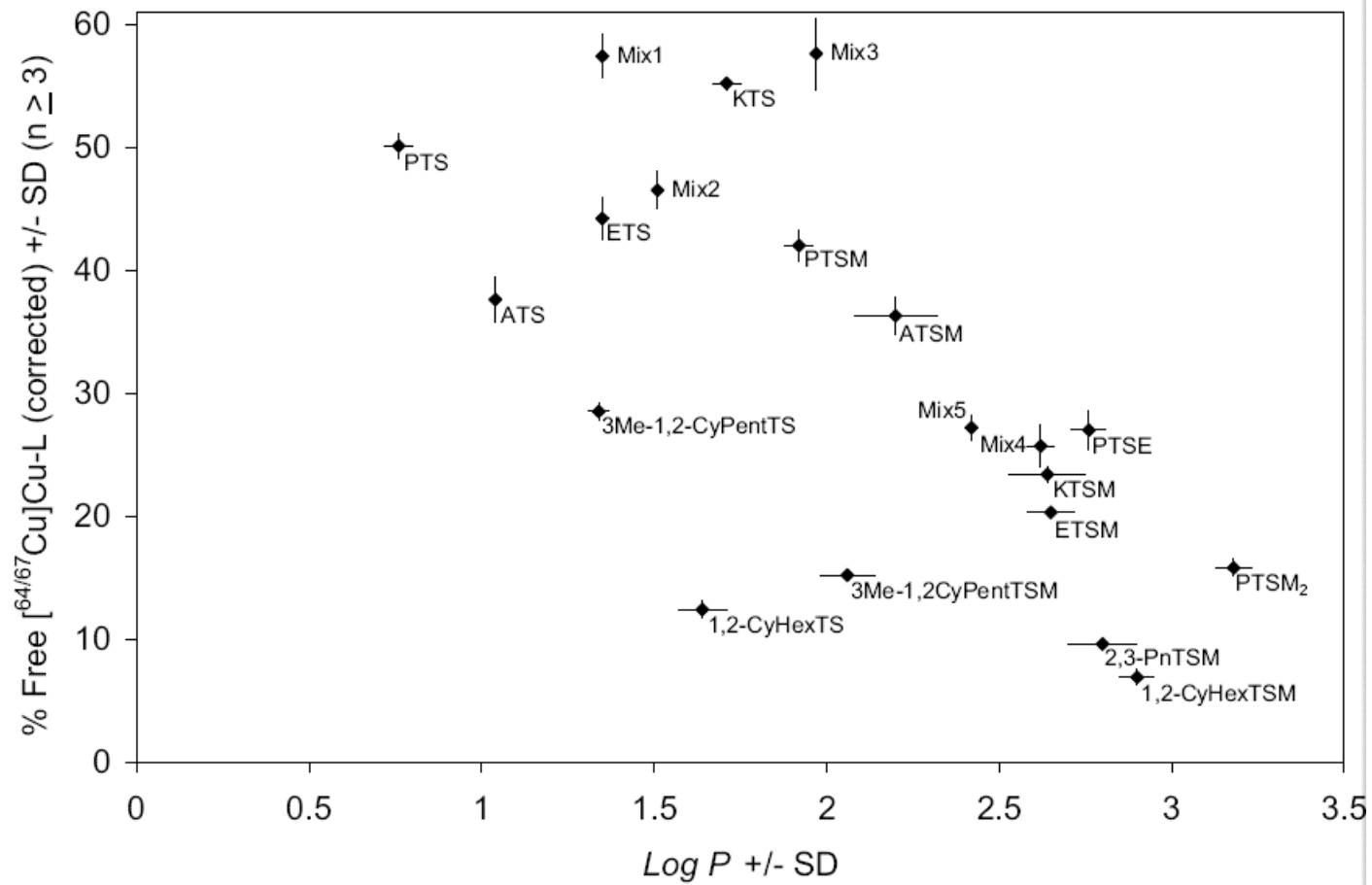
CuBTS Organ Uptake vs log P

Rat

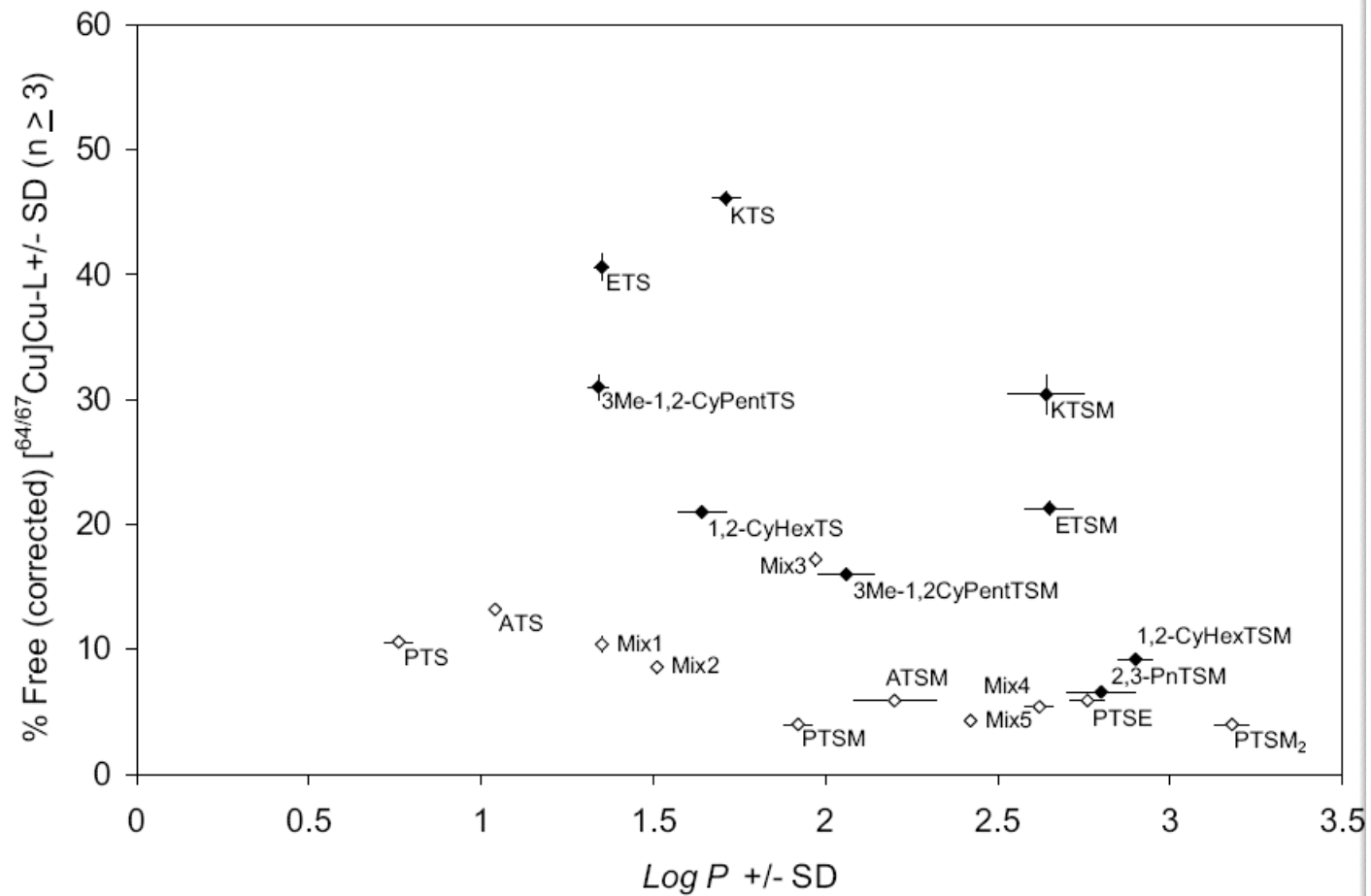


CuBTS Organ Uptake vs log P Rat

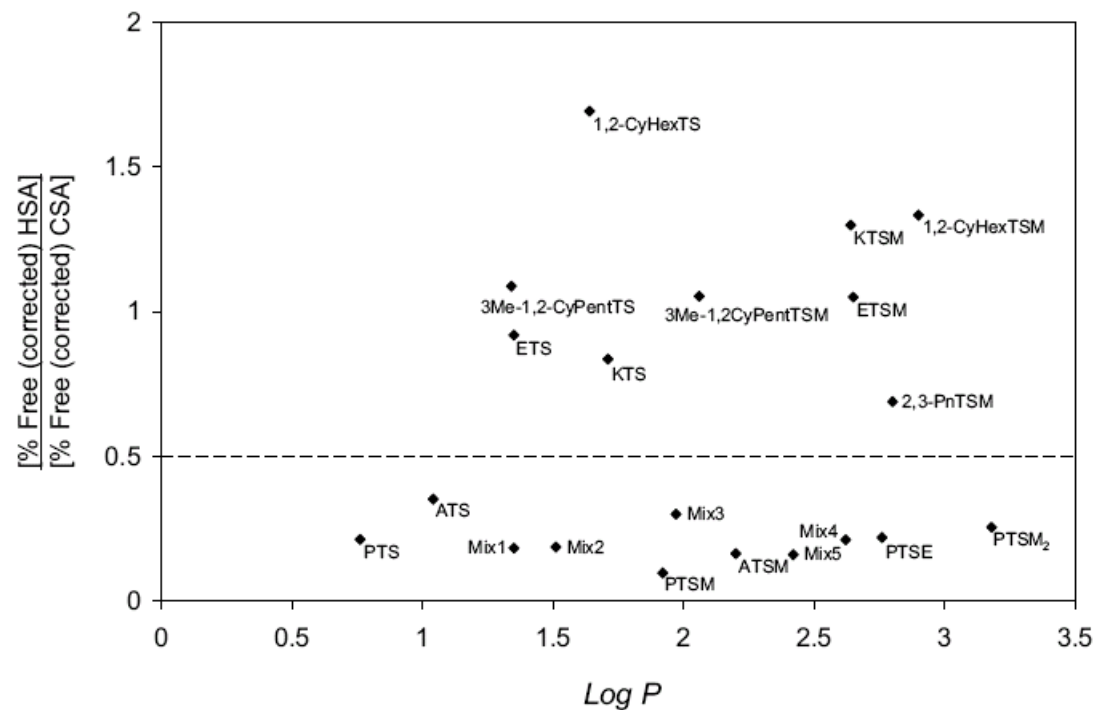




. Effect of Chelate Lipophilicity on CSA Binding



Effect of Chelate Lipophilicity on HSA Binding. In this figure, the eleven chelates believed to bind in the IIA site of HSA are shown as open symbols.



Ratio of HSA Binding to CSA Binding. The dashed line in this figure is a hypothetical threshold, above which, binding to HSA is believed to be entirely non-specific, and therefore, largely approximated by the binding to CSA. Chelates below the dashed line all have one or two (-CH₃) groups at the diimine backbone, and are all believed to bind with high affinity to the IIA site of HSA.