Electronic Supplementary Information

Luminescence of a Novel Eu(diketonato) – Epoxiphenanthroline Complex and Covalent Coupling to Peptides via the Epoxigroup

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Supporting information contained in this document:

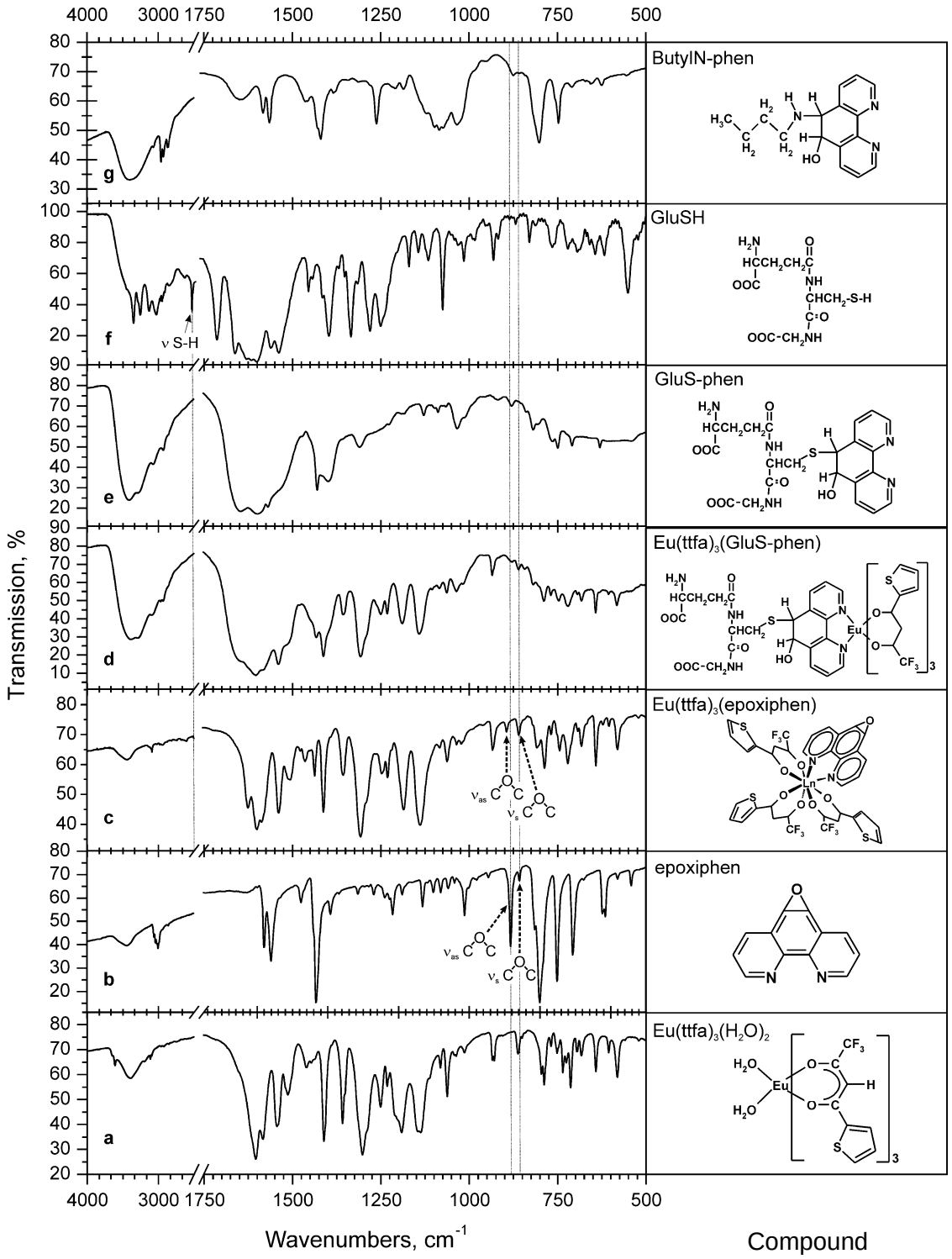


Fig. S1 FTIR spectra and principle structures of compounds used in the investigation. The disappearance of both, ν(S-H) and ν_{as}(COC) in the reaction of GluSH and epoxiphen evidence linkage via sulfur. The product obtained from a coupling reaction between butyamine and epoxiphen at a pH of 10 (g) shows that coupling with amines is possible in principle also. However, with Mel and Trigly (not shown), no pure materials could be obtained.

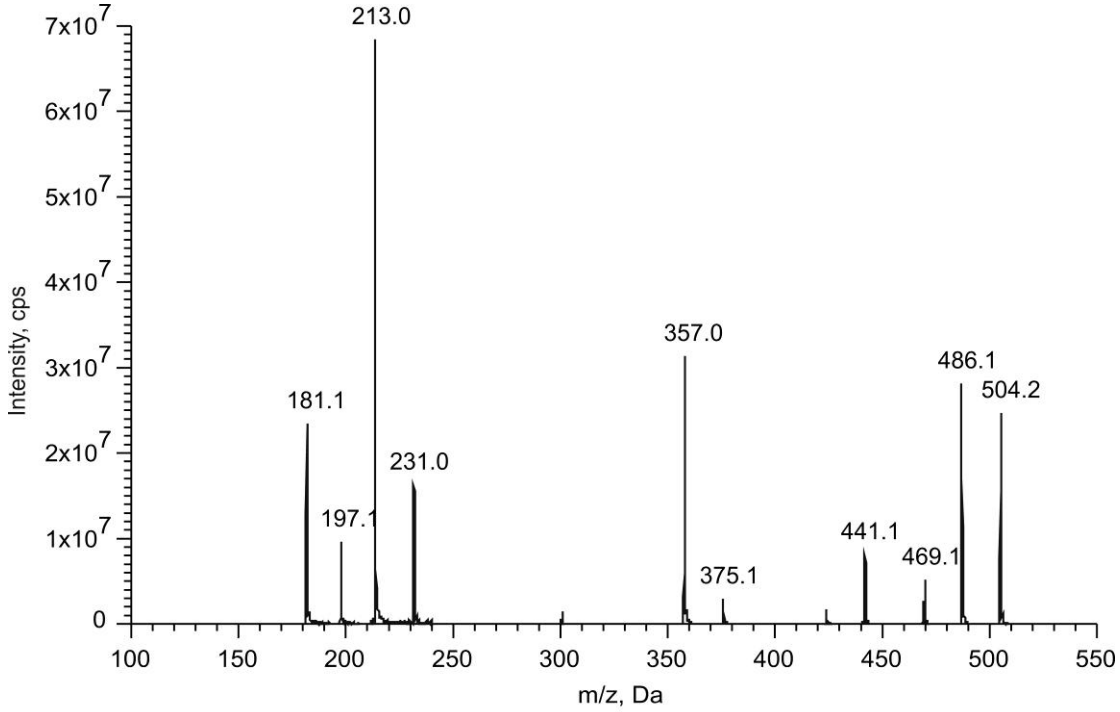
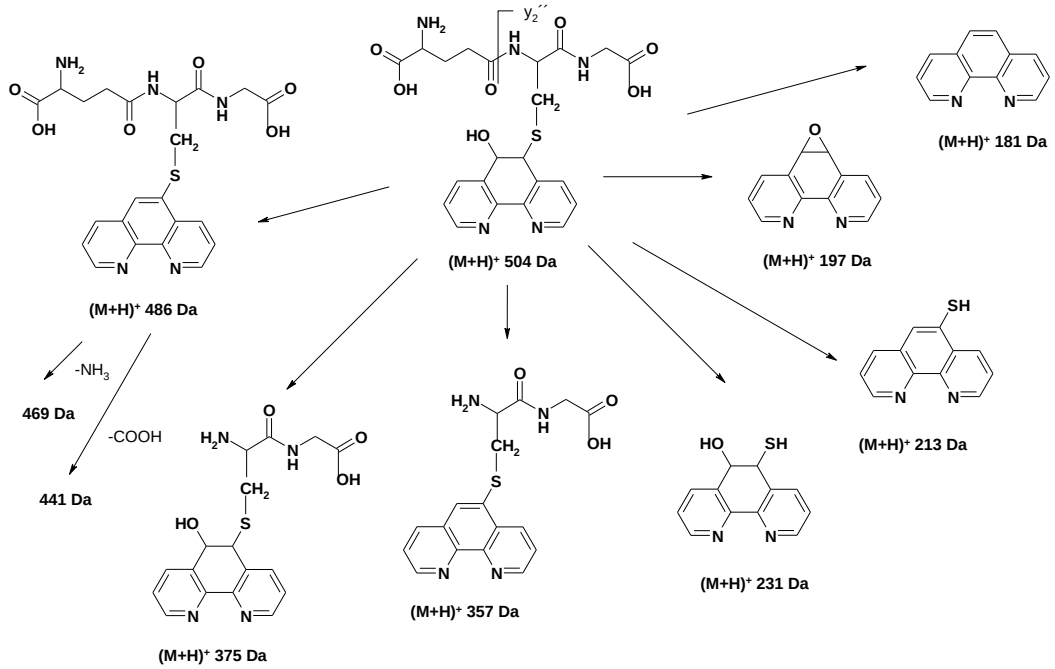


Fig. S2 ESI MS spectra of epoxiphenanthroline coupled glutathione ("GluS-phen").



Scheme S2 MS fragmentation scheme for epoxiphenanthroline coupled glutathione ("GluS-phen") in ESI MS.

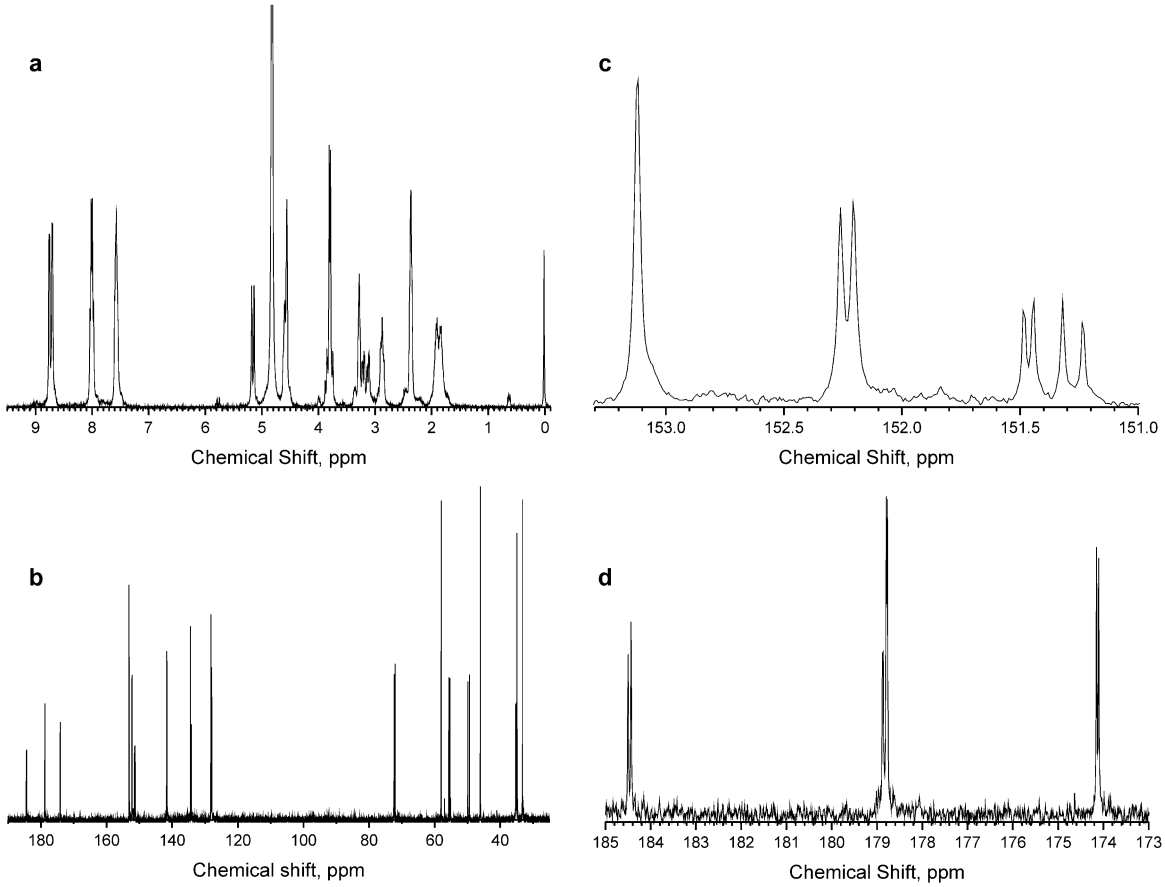


Fig S3 NMR-spectra of epoxiphenanthroline coupled glutathione ("GluS-phen"): (a) ^{1}H NMR; (b), (c), (d) ^{13}C NMR. (c) and (d) serve to illustrate the subtle splittings indicated in table S1.

Table S1 Assignment of ^{1}H and ^{13}C NMR signals for GluS-phen (see scheme 1, eqn. 1b)[a]

Assignment of atoms	Atom	Chemical shift, ppm	
		^{1}H	^{13}C {H}
	Glu -COO-	-	184.22, 184.25[b]
	Glu α -CH-	3.28 (s, 1H)	55.1, 55.7[b]
	Glu β -CH_2-	1.88 (d, 2H)	33.2
	Glu γ -CH_2-	2.37 (s, 2H)	34.91
	Glu -CONH-	-	178.77, 178.80[b]
	Cys α -CH-	4.56 (s, 1H)	58
	Cys β -CH_2-	2.87 (s, 1H); 3.17 (d, 1 H)	35.20, 35.30[b]
	Cys -CONH-	-	174.11, 174.15[b]
	Gly α-CH_2-	3.80 (s, 2H)	46.06
	Gly -COO-	-	178.9
	Phen C(2), C(9)	8.70 (s, 1H), 8.75 (s, 1H)	152.18, 152.27[b] ; 153.1
	Phen C(1a), C(10a)	-	151.22, 151.23[b]; 151.45, 151.48[b]
	Phen C(4), C(7)	8.00 (d, 2H)	141.55; 141.65
	Phen C(3), C(8)	7.57 (s, 2H)	127.95, 128.00[b]; 128.20
	Phen C(4a), Phen C(6a	-	134.15, 134.27[b]; 134.41
	Phen C(5)-S-	4.60 (d, 1H)	49.37, 49.88[b]
	Phen C(6)-OH	5.18 (d, 1H)	72.07, 72.35[b]

[a] for assignment compare references [19,20]. [b] Signals resolving into doublets under higher magnification, see Fig. S3 (c), (d) for examples.

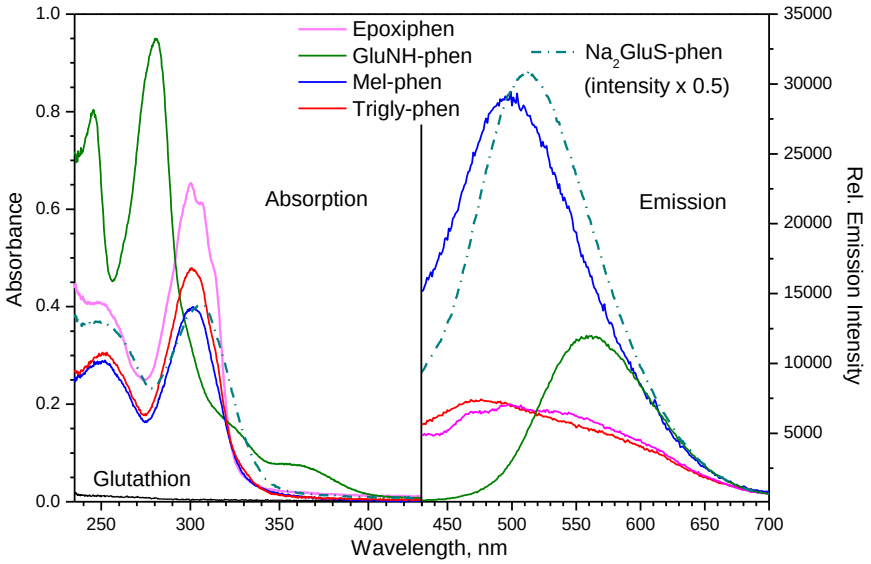


Fig. S4 Absorption and emission spectra (at $5 \cdot 10^{-3}$ Mol/L) of epoxiphen coupling products with glutathione at pH = 4, melanostatin and triglycine at pH = 10; for comparison glutathion and epoxiphen coupled to glutathion at pH = 10 (yielding Na_2GluS-phen) is also included. Note that the emission intensity of Na_2GluS-phen is approximately three times that of Mel-phen and six times that of Trigly-phen (coupled via $-NH_2$, see scheme 1, eqn.1a).