

Electronic Supplementary Information (ESI) for

Synthesis and Characterization of the Copper(II) Complexes of New N₂S₂-donor Macrocyclic Ligands: Synthesis and In Vivo Evaluation of the ⁶⁴Cu Complexes

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Biodistribution in male, Lewis rats were injected with either complex **5** or **6** (~40 μ Ci in 150 μ L)
Rats were examined at 3 time points

Tissue	[⁶⁴ Cu(NEC-SE)] (7), %ID/g		
	1 hour	4 hour	24 hour
blood	0.8504 $\pm$ 0.0510	0.8968 $\pm$ 0.0795	0.7682 $\pm$ 0.0402
lung	0.8379 $\pm$ 0.0652	0.7684 $\pm$ 0.0445	0.7232 $\pm$ 0.0355
liver	3.9192 $\pm$ 0.3631	3.9045 $\pm$ 0.5402	3.3138 $\pm$ 0.4755
spleen	0.5595 $\pm$ 0.0251	0.7305 $\pm$ 0.1742	1.0456 $\pm$ 0.1056
kidney	8.6624 $\pm$ 0.5512	7.8487 $\pm$ 1.0991	4.9062 $\pm$ 0.2107
muscle	0.3804 $\pm$ 0.0318	0.3436 $\pm$ 0.0122	0.3091 $\pm$ 0.0262
fat	0.3341 $\pm$ 0.0541	0.2662 $\pm$ 0.0676	0.1630 $\pm$ 0.0256
heart	0.6723 $\pm$ 0.0860	0.7739 $\pm$ 0.0964	1.0412 $\pm$ 0.0704
brain	0.0657 $\pm$ 0.0057	0.0867 $\pm$ 0.0077	0.1184 $\pm$ 0.0092
pituitary	1.9725 $\pm$ 0.4205	2.5130 $\pm$ 0.5310	1.8935 $\pm$ 0.2981
bone	1.1308 $\pm$ 0.0720	1.2740 $\pm$ 0.0818	0.9840 $\pm$ 0.0756
marrow	1.1998 $\pm$ 0.0866	1.7506 $\pm$ 0.1976	1.8567 $\pm$ 0.1073
adrenals	0.8236 $\pm$ 0.1082	0.7201 $\pm$ 0.0038	0.8125 $\pm$ 0.0413
pancreas	0.9588 $\pm$ 0.1101	0.8789 $\pm$ 0.0557	0.5753 $\pm$ 0.0298
stomach	1.7355 $\pm$ 0.3881	1.0373 $\pm$ 0.3447	0.6244 $\pm$ 0.1113
sm int	2.3124 $\pm$ 0.1486	2.2358 $\pm$ 0.2385	1.8489 $\pm$ 0.2293
u lg int	1.7819 $\pm$ 0.3146	1.6331 $\pm$ 0.2672	1.2160 $\pm$ 0.1536
l lg int	0.6423 $\pm$ 0.0679	1.1553 $\pm$ 0.1475	1.2616 $\pm$ 0.1638

Tissue	[⁶⁴ Cu(NEC-SE)] (7), %ID/organ		
	1 hour	4 hour	24 hour
blood	5.1534 $\pm$ 0.3561	5.4724 $\pm$ 0.5594	4.7033 $\pm$ 0.2089
lung	0.4694 $\pm$ 0.0442	0.4378 $\pm$ 0.0397	0.4208 $\pm$ 0.0148
liver	15.3573 $\pm$ 1.0388	13.1702 $\pm$ 1.7796	14.9870 $\pm$ 1.2475
spleen	0.1485 $\pm$ 0.0086	0.1841 $\pm$ 0.0538	0.2951 $\pm$ 0.0230
kidney	4.3418 $\pm$ 0.1435	3.8251 $\pm$ 0.3763	2.5616 $\pm$ 0.1046
muscle	13.4720 $\pm$ 0.6191	12.2713 $\pm$ 0.4962	11.0724 $\pm$ 0.6845
fat	4.0217 $\pm$ 0.7255	3.2042 $\pm$ 0.8501	1.9697 $\pm$ 0.3209
heart	0.2803 $\pm$ 0.0401	0.2943 $\pm$ 0.0559	0.4430 $\pm$ 0.0386
brain	0.1012 $\pm$ 0.0131	0.1311 $\pm$ 0.0136	0.1820 $\pm$ 0.0133
pituitary	0.0073 $\pm$ 0.0012	0.0079 $\pm$ 0.0012	0.0060 $\pm$ 0.0006
bone	10.6703 $\pm$ 0.7474	12.1058 $\pm$ 1.0076	9.3739 $\pm$ 0.5135
marrow	0.0544 $\pm$ 0.0062	0.0851 $\pm$ 0.0200	0.0879 $\pm$ 0.0139
adrenals	0.0296 $\pm$ 0.0028	0.0256 $\pm$ 0.0034	0.0318 $\pm$ 0.0031
pancreas	0.8063 $\pm$ 0.0981	0.7154 $\pm$ 0.0357	0.5036 $\pm$ 0.0262
stomach	3.1488 $\pm$ 2.7473	1.5791 $\pm$ 0.1204	1.1546 $\pm$ 0.1309
sm int	4.4501 $\pm$ 0.2827	4.2208 $\pm$ 0.4785	3.8251 $\pm$ 0.3618
u lg int	3.8146 $\pm$ 0.5804	3.7430 $\pm$ 0.5009	3.6785 $\pm$ 0.1930
l lg int	2.7884 $\pm$ 0.2751	5.0148 $\pm$ 0.2899	5.8678 $\pm$ 1.7170

Tissue	[⁶⁴ Cu(NEC-SP)] (8), %ID/g		
	1 hour	4 hour	24 hour
blood	0.8204 ± 0.0461	0.8348 ± 0.0206	0.7740 ± 0.0307
lung	0.7762 ± 0.0891	0.7365 ± 0.0086	0.7707 ± 0.0613
liver	3.1507 ± 0.2856	3.4176 ± 0.3705	3.1821 ± 0.1876
spleen	0.4826 ± 0.0538	0.7043 ± 0.0141	1.0777 ± 0.0990
kidney	9.4382 ± 1.0190	7.8182 ± 0.6632	5.0696 ± 0.5182
muscle	0.3931 ± 0.0546	0.3524 ± 0.0165	0.3187 ± 0.0305
fat	0.3182 ± 0.0738	0.2137 ± 0.0235	0.1530 ± 0.0189
heart	0.6570 ± 0.0253	0.7359 ± 0.0482	1.0130 ± 0.0775
brain	0.0708 ± 0.0073	0.0865 ± 0.0108	0.1206 ± 0.0074
pituitary	2.3166 ± 0.5941	2.1296 ± 0.1239	1.5167 ± 0.2158
bone	1.0986 ± 0.0977	1.2549 ± 0.0402	0.9986 ± 0.0647
marrow	1.1274 ± 0.0404	1.6730 ± 0.0385	1.8999 ± 0.0503
adrenals	0.7995 ± 0.2038	0.7159 ± 0.0142	0.7352 ± 0.0868
pancreas	0.8859 ± 0.0708	0.8686 ± 0.0189	0.5714 ± 0.0434
stomach	1.1381 ± 0.1548	1.1291 ± 0.2482	0.5979 ± 0.1881
sm int	2.1204 ± 0.2397	2.2102 ± 0.1866	1.8591 ± 0.1783
u lg int	1.5406 ± 0.2163	1.5746 ± 0.1370	1.2246 ± 0.1285
l lg int	0.6184 ± 0.0745	1.1438 ± 0.0344	1.2009 ± 0.0909

Tissue	⁶⁴ Cu(NEC-SP)] (8), %ID/organ		
	1 hour	4 hour	24 hour
blood	5.0815 ± 0.2045	5.4621 ± 0.1852	4.6416 ± 0.1062
lung	0.4004 ± 0.0591	0.4249 ± 0.0229	0.4466 ± 0.0469
liver	12.1934 ± 0.9247	13.3691 ± 0.5757	14.5346 ± 0.3398
spleen	0.1201 ± 0.0256	0.1950 ± 0.0180	0.2886 ± 0.0271
kidney	4.9000 ± 0.6496	4.1334 ± 0.2921	2.5881 ± 0.1932
muscle	14.2360 ± 1.6459	13.4920 ± 0.1519	11.1814 ± 0.7838
fat	3.8721 ± 0.8096	2.7506 ± 0.2269	1.8088 ± 0.2138
heart	0.2838 ± 0.0140	0.3171 ± 0.0354	0.4086 ± 0.0334
brain	0.1115 ± 0.0101	0.1331 ± 0.0171	0.1844 ± 0.0140
pituitary	0.0083 ± 0.0014	0.0075 ± 0.0010	0.0053 ± 0.0007
bone	10.5819 ± 0.6005	12.7803 ± 0.2140	9.3194 ± 0.3564
marrow	0.0458 ± 0.0083	0.0758 ± 0.0101	0.0813 ± 0.0160
adrenals	0.0272 ± 0.0101	0.0294 ± 0.0043	0.0266 ± 0.0048
pancreas	0.7401 ± 0.0402	0.7799 ± 0.0648	0.4986 ± 0.0382
stomach	1.7949 ± 0.0561	1.7978 ± 0.0947	1.3370 ± 0.2653
sm int	4.4502 ± 0.2188	4.5194 ± 0.4399	3.8927 ± 0.4469
u lg int	3.7927 ± 0.3612	4.0661 ± 0.2241	3.5477 ± 0.1964
l lg int	2.9545 ± 0.1889	5.4550 ± 0.1347	6.5743 ± 0.3327

⁶⁴Cu(NEC-SB)] (9), %ID/g

	1 hr.			4 hr.			24 hr.		
<i>blood</i>	0.8738	+/-	0.1398	0.8793	+/-	0.1117	0.6925	+/-	0.1509
<i>lung</i>	1.6730	+/-	0.2253	0.9489	+/-	0.1087	0.7464	+/-	0.1430
<i>liver</i>	4.1054	+/-	0.4646	3.8664	+/-	0.6354	3.2960	+/-	0.7279
<i>spleen</i>	0.6976	+/-	0.1679	0.8151	+/-	0.1366	0.9235	+/-	0.2070
<i>kidney</i>	8.8945	+/-	0.6124	7.0956	+/-	1.0588	4.7376	+/-	0.6171
<i>muscle</i>	0.4111	+/-	0.0557	0.3299	+/-	0.0500	0.3016	+/-	0.0330
<i>fat</i>	0.3709	+/-	0.0731	0.2183	+/-	0.0371	0.1360	+/-	0.0350
<i>heart</i>	0.8394	+/-	0.2282	0.7522	+/-	0.0594	0.9232	+/-	0.1891
<i>brain</i>	0.0792	+/-	0.0113	0.0903	+/-	0.0068	0.1086	+/-	0.0195
<i>pituitary</i>	3.1498	+/-	0.8057	2.1487	+/-	0.9642	1.9032	+/-	1.6195
<i>bone</i>	1.1426	+/-	0.1954	1.1546	+/-	0.1606	0.8548	+/-	0.1879
<i>marrow</i>	1.1164	+/-	0.1591	1.5088	+/-	0.2664	1.7238	+/-	0.3234
<i>adrenals</i>	0.8655	+/-	0.1851	0.7541	+/-	0.1404	0.9363	+/-	0.1988
<i>pancreas</i>	0.8952	+/-	0.1283	0.8456	+/-	0.1745	0.5935	+/-	0.1429
<i>stomach</i>	1.5054	+/-	0.5496	1.2625	+/-	0.4010	0.6760	+/-	0.2047
<i>sm int</i>	2.3465	+/-	0.3124	2.1002	+/-	0.2551	1.7107	+/-	0.1795
<i>u lg int</i>	1.7314	+/-	0.1940	1.5708	+/-	0.2721	1.1087	+/-	0.1641
<i>l lg int</i>	0.6986	+/-	0.1439	1.1160	+/-	0.2475	1.2342	+/-	0.1904
<i>tail</i>	2.2282	+/-	1.6246	3.0701	+/-	2.0105	1.4050	+/-	0.2416

[⁶⁴ Cu(NEC-SB)] (9), %ID/organ									
	1 hr.			4 hr.			24 hr.		
<i>blood</i>	4.6204	+/-	0.3514	5.1034	+/-	0.6410	3.8784	+/-	0.6381
<i>lung</i>	0.9193	+/-	0.1413	0.5729	+/-	0.0535	0.4637	+/-	0.0867
<i>liver</i>	12.6959	+/-	0.9281	12.3851	+/-	1.0954	13.5960	+/-	2.2414
<i>spleen</i>	0.1430	+/-	0.0183	0.1878	+/-	0.0439	0.2208	+/-	0.0410
<i>kidney</i>	3.9939	+/-	0.3514	3.5244	+/-	0.6605	2.3495	+/-	0.1922
<i>muscle</i>	12.7603	+/-	0.5338	11.1404	+/-	0.5636	9.9542	+/-	0.7406
<i>fat</i>	3.8850	+/-	0.6169	2.4763	+/-	0.1207	1.5077	+/-	0.3369
<i>heart</i>	0.2992	+/-	0.0895	0.2778	+/-	0.0335	0.3422	+/-	0.0457
<i>brain</i>	0.1185	+/-	0.0147	0.1361	+/-	0.0069	0.1694	+/-	0.0309
<i>pituitary</i>	0.0069	+/-	0.0010	0.0058	+/-	0.0011	0.0070	+/-	0.0057
<i>bone</i>	9.3966	+/-	0.7776	10.3772	+/-	0.4961	7.4533	+/-	1.2477
<i>marrow</i>	0.0483	+/-	0.0072	0.0696	+/-	0.0183	0.0732	+/-	0.0114
<i>adrenals</i>	0.0250	+/-	0.0047	0.0249	+/-	0.0022	0.0330	+/-	0.0062
<i>pancreas</i>	0.6493	+/-	0.0427	0.6852	+/-	0.1136	0.4539	+/-	0.0819
<i>stomach</i>	1.6760	+/-	0.2189	1.5921	+/-	0.1399	1.0439	+/-	0.2958
<i>sm int</i>	3.7978	+/-	0.2140	3.6529	+/-	0.2885	3.3009	+/-	0.3217
<i>u lg int</i>	3.3693	+/-	0.1347	3.8394	+/-	0.5064	3.0604	+/-	0.4085
<i>l lg int</i>	2.7473	+/-	0.2807	5.0136	+/-	1.7315	6.3314	+/-	0.6913
<i>tail</i>	4.8471	+/-	4.3162	6.6370	+/-	4.3945	3.0631	+/-	0.4170