SUPPORTING INFO

Ru and Rh binding sites in the structure of human serum transferrin with Fe^{3+} bound at the C-lobe

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Table S1. Data collection statistics

	Rh/Fe$_C$-hTF	**Ru/Fe$_C$-hTF**
Crystallization condition	15% (w/v) PEG 3350, 16% (v/v) glycerol, 8 mM disodium malonate, 150 mM Na-PIPES pH 6.5	15% (w/v) PEG 3350, 16% (v/v) glycerol, 8 mM disodium malonate, 150 mM Na-PIPES pH 6.5
Soaked compound	1.9 mM dirhodium tetraacetate dissolved in DMSO (final DMSO concentration <10%)	5 mM diruthenium tetraacetate dissolved in DMSO (final DMSO concentration <10%)
Soaking time	2 h	72 h
Space group	$C222_1$	$C222_1$
a (Å)	137.776	136.936
b (Å)	157.085	156.712
c (Å)	107.559	107.145
Resolution range (Å)	103.580-2.368 (2.604-2.368)	103.116-2.262 (2.502-2.262)
Observations	451990 (19327)	388150 (20473)
Unique reflections	33787 (1689)	30700 (1535)
Completeness (%)	92.8 (58.1)	93.9 (76.1)
Redundancy	13.4 (11.4)	12.6 (13.3)
Rmerge (%)	0.205 (2.088)	0.208 (2.047)
Average I/σ(I)	10.3 (1.5)	9.8 (1.6)
$CC_{1/2}$	0.996 (0.581)	0.997 (0.734)
Anom. completeness (%)	92.9 (58.9)	93.9 (76.5)
Anom. Multiplicity	7.0 (5.8)	6.6 (6.9)

Table S2. Refinement statistics.

	Rh/Fe$_C$-hTF	**Ru/Fe$_C$-hTF**
PDB code	28MS	28MR
Crystallization conditions	15% (w/v) PEG 3350 16% (v/v) glycerol 8 mM disodium malonate 150 mM Na-PIPES pH 6.5	15% (w/v) PEG 3350 16% (v/v) glycerol 8 mM disodium malonate 150 mM Na-PIPES pH 6.5
Soaking conditions	1.9 mM dirhodium tetraacetate dissolved in DMSO (final DMSO concentration <10%)	5 mM diruthenium tetraacetate dissolved in DMSO (final DMSO concentration <10%)
Soaking time	2 h	72 h
Space Group	$C222_1$	$C222_1$
Resolution (Å)	2.37	2.26
Reflections	32061	29172
R-factor/R$_{free}$	0.186/0.244	0.182/0.234
Non-H atoms in the refinement	5643	5656
Overall B-factor (Å^2)	44.06	44.34
Estimated occupancy of Rh atoms close to His14	0.50/0.50	-
Estimated occupancy of Rh atoms close to His273	0.40/0.40	-
Estimated occupancy of Rh atoms close to His289	0.50/0.50	-
Estimated occupancy of Rh atoms close to His300	0.40/0.40	-
Estimated occupancy of Rh atoms close to His349	0.50/0.50	-
Estimated occupancy of Rh atoms close to His350	0.35/0.35	-
Estimated occupancy of Rh atoms close to His578	0.50/0.50	-
Estimated occupancy of Rh atoms close to His642	0.50/0.50	-
Estimated occupancy of Rh atoms close to Met256	0.30/0.30	-
Estimated occupancy of the Ru atom close to His349 and His350	-	0.70
B-factor of Rh atoms close to His14 (Å^2)	75.78/85.03	-
B-factor of Rh atoms close to His273 (Å^2)	71.10/75.15	-
B-factor of Rh atoms close to His289 (Å^2)	74.13/87.58	-
B-factor of Rh atoms close to His300 (Å^2)	87.41/79.73	-
B-factor of Rh atoms close to His349 (Å^2)	88.35/74.89	-

B-factor of Rh atoms close to His350 (Å^2)	80.92/79.77	-
B-factor of Rh atoms close to His578 (Å^2)	69.92/85.54	-
B-factor of Rh atoms close to His642 (Å^2)	83.86/80.08	-
B-factor of Rh atoms close to Met256 (Å^2)	86.32/87.09	-
B-factor of the Ru atom close to His349-His350 (Å^2)	-	122.47
NE2(His14)-Rh distance (Å)	2.48	-
NE2(His273)-Rh distance (Å)	2.67	-
NE2(His289)-Rh distance (Å)	2.66	
NE2(His300)-Rh distance (Å)	2.49	-
ND1(His349)-Rh distance (Å)	2.30	-
ND1(His350)-Rh distance (Å)	2.37	-
NE2(His578)-Rh distance (Å)	2.31	-
ND1(His642)-Rh distance (Å)	2.25	-
SD(Met256)-Rh distance (Å)	3.10	-
NE2(His349)-Ru distance (Å)	-	2.28
NE2(His350)-Ru distance (Å)	-	2.81
In favoured regions	590 (91.33%)	576 (89.16%)
Outliers	13 (2.01%)	19 (2.94%)
R.m.s.d. bonds (Å)	0.007	0.006
R.m.s.d. angles (°)	1.781	1.487