Electronic Supplementary Material (ESI) for Metallomics.

Intracellular distribution and stability of a luminescent rhenium(I) tricarbonyl tetrazolato complex using confocal fluorescence microscopy in conjunction with XFM imaging.

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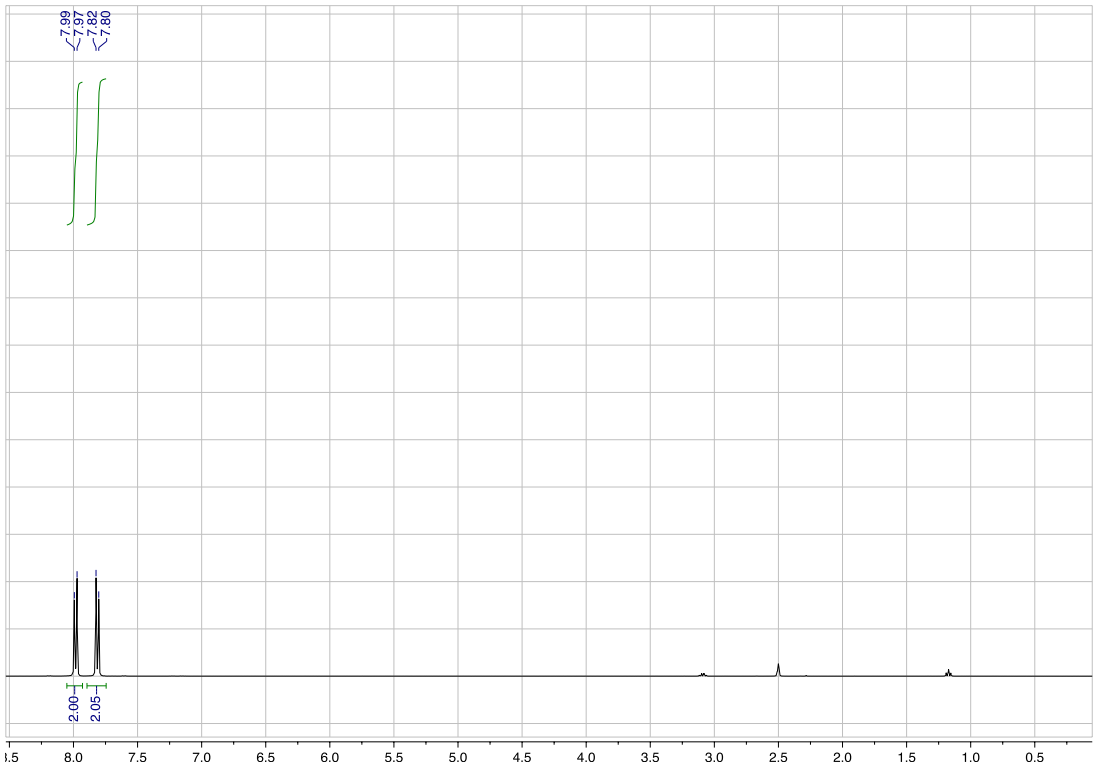
Supplementary information

NMR Spectra

Figure S1. ^{1}H- (top) and ^{13}C- (bottom) NMR spectra of 1H-5-(4-iodophenyl)tetrazole.



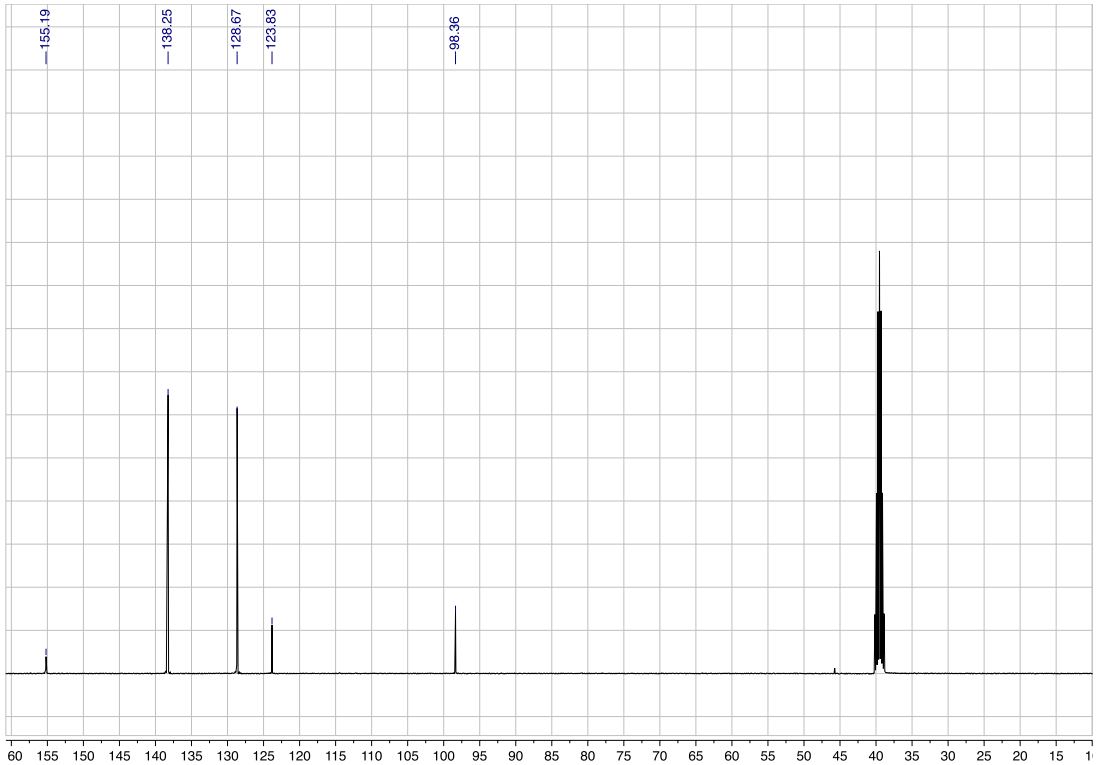
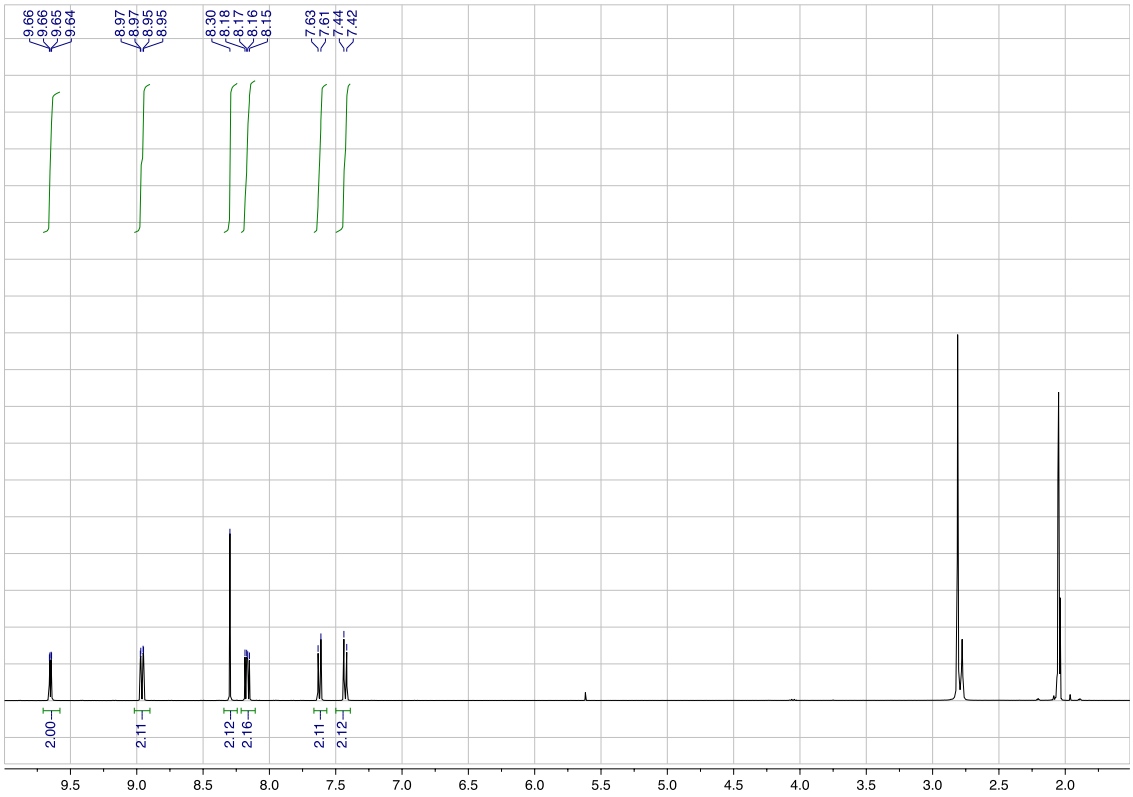
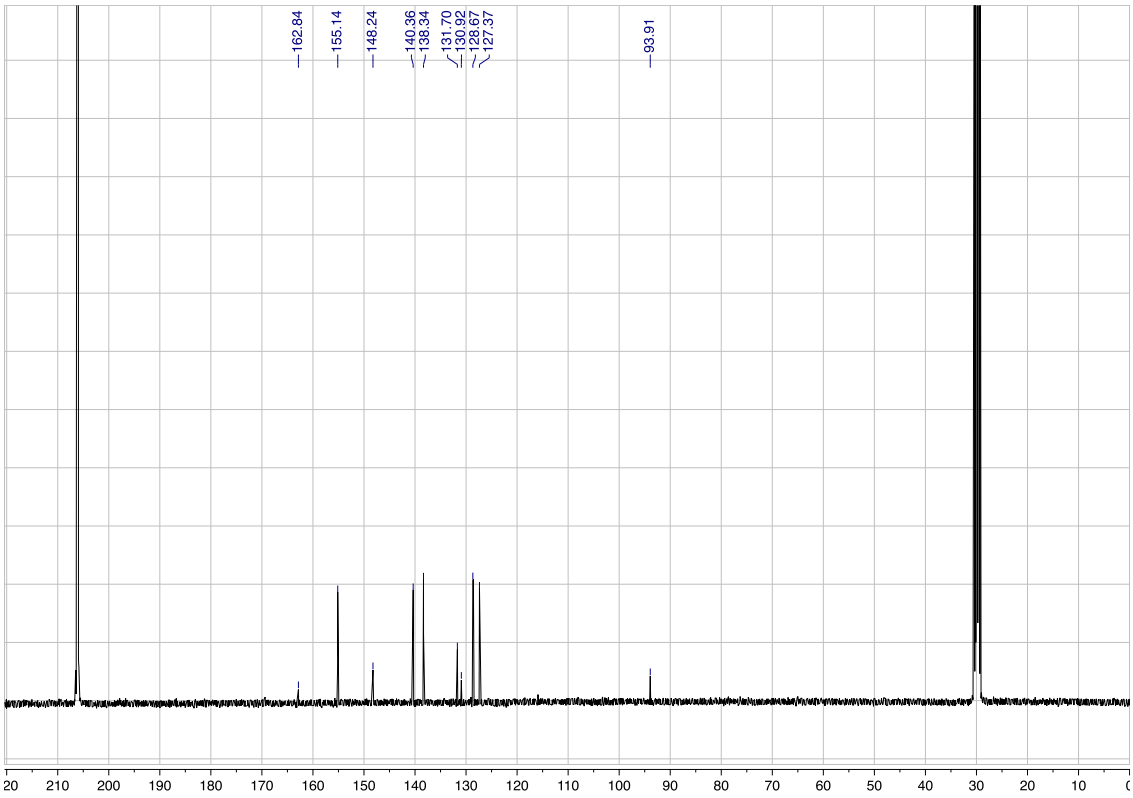


Figure S2. ^{1}H- (top) and ^{13}C- (bottom) NMR spectra of **Re-I**.





Crystallography

The crystal data for **Re-I** are summarized below with the structure depicted in Fig. S3, where ellipsoids have been drawn at the 50% probability level. Selected coordination geometries are given in Table S1. Crystallographic data for the structures were collected at 100(2) K on an Oxford Diffraction Xcalibur diffractometer using Mo Kα radiation. Following analytical absorption corrections and solution by direct methods, the structure was refined against F^2 with full-matrix least-squares using the program SHELXL-97[1]. Anisotropic displacement parameters were employed for the non-hydrogen atoms. All hydrogen atoms were added at calculated positions and refined by use of a riding model with isotropic displacement parameters based on those of the parent atom.

Crystal data. Empirical formula $C_{22}H_{12}IN_6O_3Re$. *MW* = 721.48. Monoclinic, space group $P2_1/n$, a = 7.0191(3), b = 18.0476(8), c = 16.9652(6) Å, β = 99.850(3)°, Volume = 2117.44(15) Å^3, Z = 4, ρ_c = 2.263 g cm^{-3}, μ = 7.236 mm^{-1}. Reflections collected = 21406, unique reflections = 6157 [R(int) = 0.0448]. Max. and min. transmission = 0.855 and 0.219. No. parameters = 298. GoF = 1.129. Final R indices [$I>2\sigma(I)$] $R1$ = 0.0372, $wR2$ = 0.0787, R indices (all data) $R1$ = 0.0448, $wR2$ = 0.0815. Largest diff. peak and hole = 2.204 and -0.802 e Å^{-3}.CCDC 1510599.

Figure S3. X-ray crystal structure of **Re-I**.

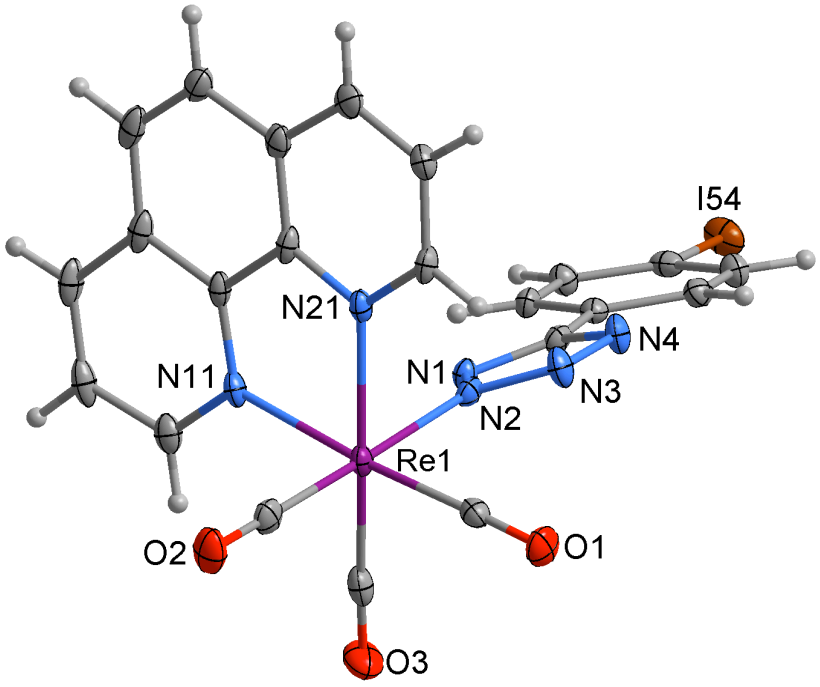
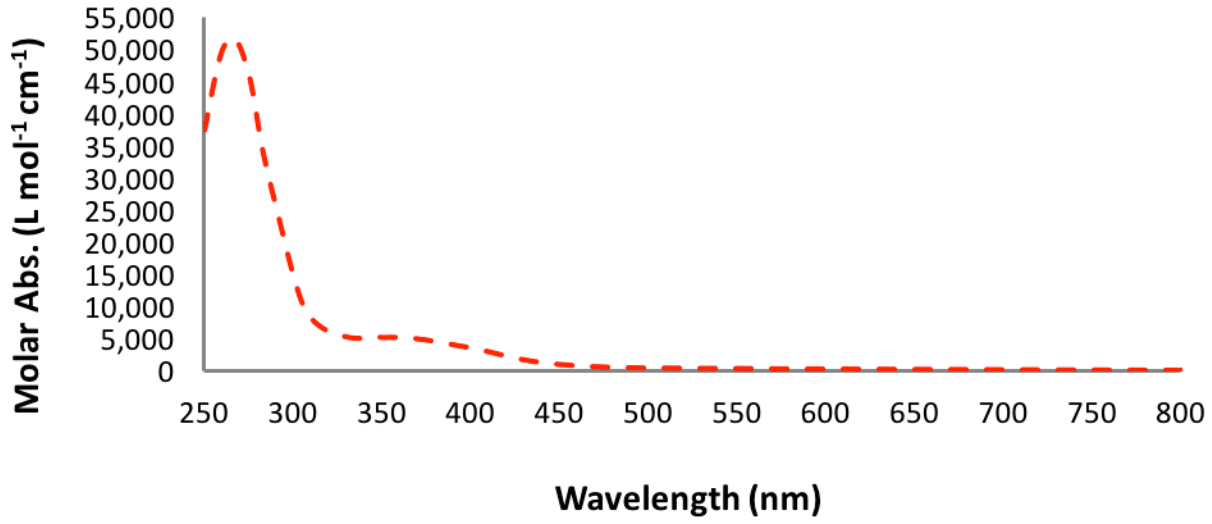


Table S1. Selected bond lengths [Å] and angles [°] for **Re-I**.

Re(1)-C(2)	1.914(5)
Re(1)-C(3)	1.918(5)
Re(1)-C(1)	1.923(4)
Re(1)-N(2)	2.173(4)
Re(1)-N(11)	2.178(3)
Re(1)-N(21)	2.179(4)
C(2)-Re(1)-C(3)	89.76(19)
C(2)-Re(1)-C(1)	90.71(18)
C(3)-Re(1)-C(1)	87.73(18)
C(2)-Re(1)-N(2)	177.78(17)
C(3)-Re(1)-N(2)	92.40(16)
C(1)-Re(1)-N(2)	88.87(15)
C(2)-Re(1)-N(11)	89.59(16)
C(3)-Re(1)-N(11)	97.23(16)
C(1)-Re(1)-N(11)	175.03(16)
N(2)-Re(1)-N(11)	90.64(13)
C(2)-Re(1)-N(21)	97.32(17)
C(3)-Re(1)-N(21)	170.14(16)
C(1)-Re(1)-N(21)	98.98(15)
N(2)-Re(1)-N(21)	80.59(13)
N(11)-Re(1)-N(21)	76.06(13)

Figure S4. Absorption (top) and excitation/emission (bottom) spectra of **Re-I** from diluted (*ca* 10^{-4} M) dichloromethane solution.



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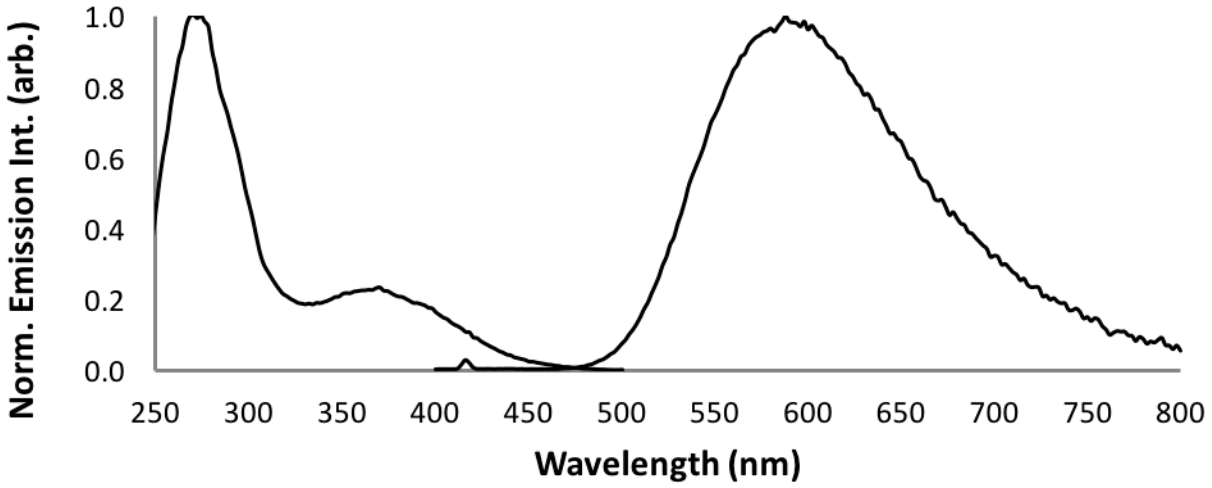

References

1. Sheldrick, G.M. (2015). *Acta Cryst*. C71, 3-8.