Luminescent Protein Staining with Re(I) Tetrazolato Complexes
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ESI – Electronic Supplementary Information
Table S1. Stretching frequencies (cm$^{-1}$) of the CO bands of all the Re(I) complexes reported in this work. Values are relative to solution state (dichloromethane as the solvent) IR spectra recorded at room temperature.

<table>
<thead>
<tr>
<th>Complex</th>
<th>CO A’(1)</th>
<th>CO A’(2)/A''</th>
</tr>
</thead>
<tbody>
<tr>
<td>fac-[Re(CO)$_3$(BCS)(Tph)]$^{2-}$</td>
<td>2029</td>
<td>1918</td>
</tr>
<tr>
<td>fac-[Re(CO)$_3$(BPS)(Tph)]$^{2-}$</td>
<td>2026</td>
<td>1914</td>
</tr>
<tr>
<td>fac-[Re(CO)$_3$(BC)(Tph)]</td>
<td>2022</td>
<td>1918</td>
</tr>
<tr>
<td>fac-[Re(CO)$_3$(BC)(Tph-Me)]$^{+}$</td>
<td>2037</td>
<td>1934</td>
</tr>
</tbody>
</table>
**Figure S1**: ESI-MS of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^{2-}$; negative region ions, CH$_3$OH.

**Figure S2**: ESI-MS of $\text{fac-}[\text{Re(CO)}_3(\text{BPS})(\text{Tph})]^{2-}$; negative region ions, CH$_3$OH.
Figure S3: ESI-MS of \textit{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph})], positive region ions, CH$_3$CN.

Figure S4: ESI-MS of \textit{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^+$, positive region ions, CH$_3$CN.
Figure S5: $^1$H NMR of $\textit{fac-}[\text{Re(CO)\textsubscript{3}(BCS)(Tph)}]^{2-}$, CD\textsubscript{3}OD, 400 MHz, 298K.

Figure S6: $^{13}$C NMR of $\textit{fac-}[\text{Re(CO)\textsubscript{3}(BCS)(Tph)}]^{2-}$, CD\textsubscript{3}OD, 100 MHz, 298K.
Figure S7: $^1$H NMR of \textit{fac}-[Re(CO)$_3$(BPS)(Tph)]$^2^-$, CD$_3$OD, 400 MHz, 298K.

Figure S8: $^{13}$C NMR of \textit{fac}-[Re(CO)$_3$(BPS)(Tph)]$^2^-$, CD$_3$OD, 100 MHz, 298K.
**Figure S9:** $^1$H NMR of $\text{fac-[Re(CO)}_3\text{(BC)(Tph)]]}$, Acetone $d^6$, 400 MHz, 298K.

**Figure S10:** $^{13}$C NMR of $\text{fac-[Re(CO)}_3\text{(BC)(Tph)]]}$, Acetone $d^6$, 100 MHz, 298K.
Figure S11: $^1$H-$^1$H COSY NMR of $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph})]$, Acetone $d^6$, 600 MHz, 298K.
Figure S12: $^1$H NMR of $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^{+}$, Acetone $d^6$, 400 MHz, 298K.

Figure S13: $^{13}$C NMR of $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^{+}$, Acetone $d^6$, 100 MHz, 298K.
Figure S14: $^1$H-$^1$H COSY NMR of fac-[Re(CO)$_3$(BC)(Tph-Me)]$^+$, Acetone $d^6$, 600 MHz, 298K.

Figure S15: $^1$H NMR and NOESY (overlay, 3.22 and 3.55 ppm) NMR of fac-[Re(CO)$_3$(BC)(Tph-Me)]$^+$, Acetone $d^6$, 400 MHz, 298K.
Figure S16: Absorption Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^{2-}$ in CH$_3$OH (red line) and H$_2$O (blue line), $10^{-5}$M, 298K.

![Absorption Profile](image)

Figure S17: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^{2-}$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}$M, CH$_3$OH, 298K.

![Emission Profile](image)

Figure S18: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^{2-}$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}$M, H$_2$O, 298K.

![Emission Profile](image)
Figure S19: Emission Map of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^2^-$, $10^{-5}$ M, H2O, 298K.

Figure S20: Excitation Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^2^-$ CH3OH (black line) H2O (blue line), $10^{-5}$ M, CH3OH, 298K.

Figure S21: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BCS})(\text{Tph})]^2^-$, $10^{-5}$ M, CH3OH, 77K.
**Figure S22**: Absorption Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BPS})(\text{Tph})]\text{^2-}$ in CH$_2$Cl$_2$ (red line) and H$_2$O (blue line), 10$^{-5}$M, 298K.

**Figure S23**: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BPS})(\text{Tph})]\text{^2-}$ air-equilibrated (black line) and deoxygenated solution (blue line), 10$^{-5}$M, CH$_2$Cl$_2$, 298K.

**Figure S24**: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BPS})(\text{Tph})]\text{^2-}$, 10$^{-5}$M, H$_2$O, 298K.
Figure S25: Excitation Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BPS})(\text{Tph})]^2-$ CH$_2$Cl$_2$ (black line) H$_2$O (blue line), 10$^{-5}$M, CH$_3$OH, 298K.

Figure S26: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BPS})(\text{Tph})]^2-$, 10$^{-5}$M, CH$_2$Cl$_2$, 77K.
Figure S27: Absorption Profile of $\text{fac-}[\text{Re(CO)}_3\text{(BC)(Tph)}]$ $10^{-5}$M, CH$_2$Cl$_2$, 298K.

Figure S28: Emission Profile of $\text{fac-}[\text{Re(CO)}_3\text{(BC)(Tph)}]$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}$M, CH$_2$Cl$_2$, 298K.

Figure S29: Excitation Profile of $\text{fac-}[\text{Re(CO)}_3\text{(BC)(Tph)}]$ $10^{-5}$M, CH$_2$Cl$_2$, 298K.
Figure S30: Emission Profile of $\text{fac-[Re(CO)\textsubscript{3}(BC)(Tph)]}$, $\lambda_{\text{exc}} = 370$ nm, $10^{-5}$M, CH\textsubscript{2}Cl\textsubscript{2}, 298K.

Figure S31: Emission Profile of $\text{fac-[Re(CO)\textsubscript{3}(BC)(Tph)]}$, $\lambda_{\text{exc}} = 302$ nm, $10^{-5}$M, CH\textsubscript{2}Cl\textsubscript{2}, 298K.

Figure S32: Emission Profile of $\text{fac-[Re(CO)\textsubscript{3}(BC)(Tph)]}$, $10^{-5}$M, CH\textsubscript{2}Cl\textsubscript{2}, 77K.
Figure S33: Absorption Profile of $\textit{fac-}[\text{Re(CO)}_3\text{BC}(\text{Tph-Me})]^+$ $10^{-5}$M, CH$_2$Cl$_2$, 298K.

Figure S34: Emission Profile of $\textit{fac-}[\text{Re(CO)}_3\text{BC}(\text{Tph-Me})]^+$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}$M, CH$_2$Cl$_2$, 298K.

Figure S35: Excitation Profile of $\textit{fac-}[\text{Re(CO)}_3\text{BC}(\text{Tph-Me})]^+$ $10^{-5}$M, CH$_2$Cl$_2$, 298K.
**Figure S36**: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^+$, $\lambda_{\text{exc}} = 370$ nm, $10^{-5}$M, CH$_2$Cl$_2$, 298K.

**Figure S37**: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^+$, $\lambda_{\text{exc}} = 302$ nm, $10^{-5}$M, CH$_2$Cl$_2$, 298K.

**Figure S38**: Emission Profile of $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^+$ ($\lambda_{\text{exc}} = 370$ nm blue line) and $\text{fac-}[\text{Re(CO)}_3(\text{BC})(\text{Tph-Me})]^+$ ($\lambda_{\text{exc}} = 302$ nm black line), $10^{-5}$M, CH$_2$Cl$_2$, 298K.
Figure S39: Emission Profile of \( \text{fac-[Re(CO)}_3\text{(BC)(Tph-Me)}]^+ \), \( 10^{-5} \text{M}, \text{CH}_2\text{Cl}_2, 77\text{K} \).

Figure S40: Excitation Profile of \( \text{fac-[Re(CO)}_3\text{(BC)(Tph)}] \) (black line) and \( \text{fac-[Re(CO)}_3\text{(BC)(Tph-Me)}]^+ \) (blue line), \( 10^{-5} \text{M}, \text{CH}_2\text{Cl}_2, 298\text{K} \).

Figure S41: Normalized Emission Profile of \( \text{fac-[Re(CO)}_3\text{(BC)(Tph)}] \) (black line) and \( \text{fac-[Re(CO)}_3\text{(BC)(Tph-Me)}]^+ \) (blue line), \( 10^{-5} \text{M}, \text{CH}_2\text{Cl}_2, 298\text{K} \).
**Table S2** - Crystal data and collection details for *fac-[Re(CO)₃(BC)(Tph)]*.

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<th><strong>Formula</strong></th>
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<td><strong>Dc, g cm⁻³</strong></td>
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<td><strong>wR₂ (all data)</strong></td>
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<td><strong>Largest diff. peak and hole, e Å⁻³</strong></td>
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