

Electronic Supplementary Information

^{99m}Tc(CO)₃-Labeled Pamidronate and Alendronate for Bone Imaging*

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Fig. S1. RP-HPLC analytical chromatograms of **2** ($t_R = 11.9$ min; UV/Vis-detection – 254 nm) and **2a** ($t_R = 12.0$ min γ -detection).

Table S1: Crystallographic data of *fac*-[Re(CO)₃(k³-p_z-COOH)]⁺·CF₃COO⁻·H₂O.

Empirical formula	C ₁₈ H ₂₆ F ₃ N ₄ O ₈ Re
M [g mol ⁻¹]	669.63
Diffractometer	Bruker-AXS APEX
Wavelength	0.7107 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
Unit cell dimensions	a = 68.7619(2) Å b = 20.2966(5) Å c = 39.1115(8) Å β = 95.4290(10)°
Volume [Å ³]	6924.3(3)
Z	12
Density _{calcd.} [Mg m ⁻³]	1.927
Absorption coefficient [mm ⁻¹]	5.341
F(000)	3936
Crystal size	0.24 x 0.08 x 0.03 mm ³
θ range	2.80 to 25.68°
Index ranges	-10 ≤ h ≤ 10, -24 ≤ k ≤ 24, -43 ≤ l ≤ 47
Reflections collected	53647
Independent reflections	13125 [R(int) = 0.0823]
Completeness to θ	99.8 % (25.68°)
Max. and min. transmission	0.8562 and 0.3605
Data / restraints / parameters	13125 / 0 / 928
Goodness-of-fit on F ²	0.969
Final R indices [I > 2σ(I)]	R ₁ = 0.0389, wR ₂ = 0.0680
R indices (all data)	R ₁ = 0.0665, wR ₂ = 0.0738
Largest diff. peak and hole	0.885 and -0.853 e. Å ⁻³