Supporting Information

An Octadentate Bis(semicarbazone) Macrocycle: A Potential Chelator for Lead and Bismuth Radiopharmaceuticals

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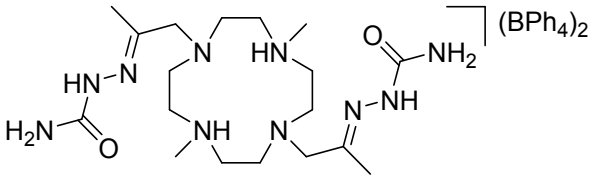

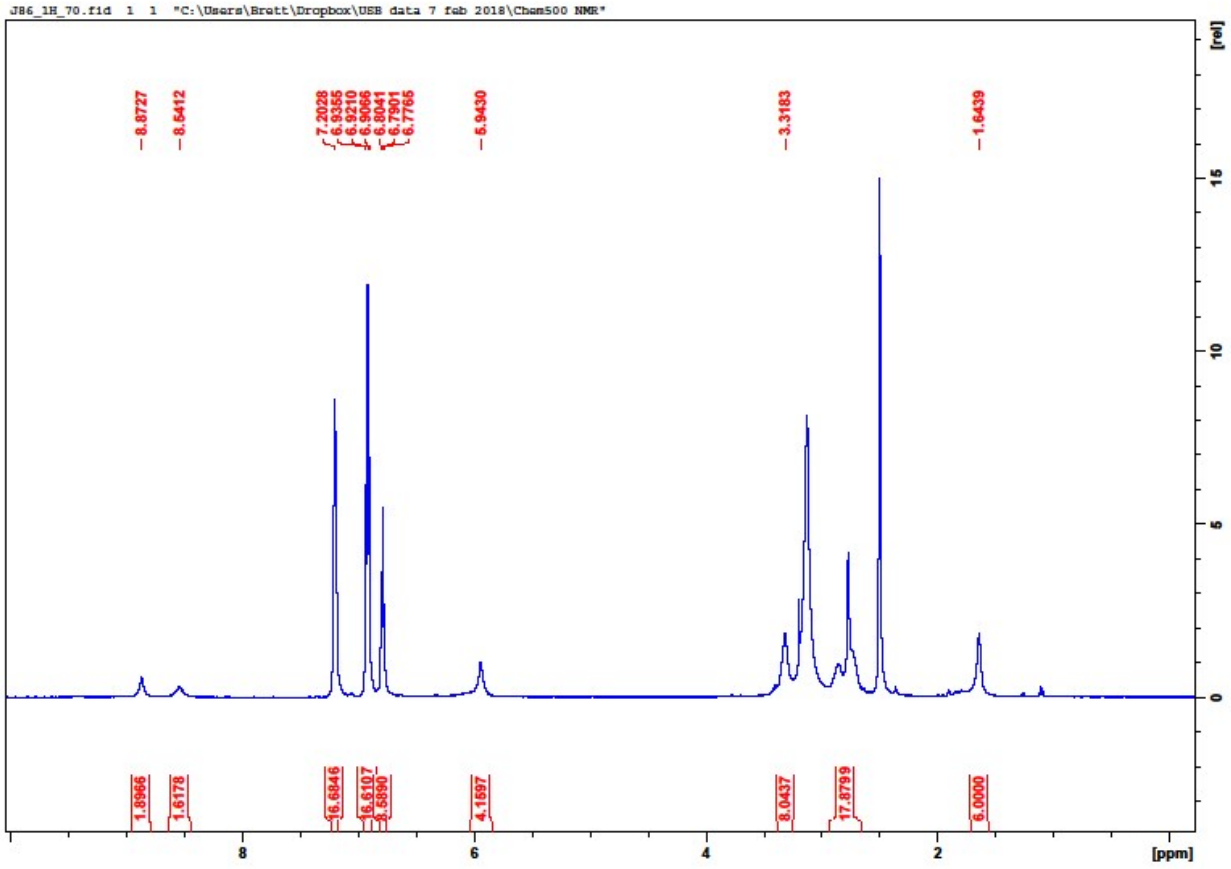

Figure S1. ^{1}H NMR of $[H_2\mathbf{L}](BPh_4)_2$; 400 MHz, $[D_6]$DMSO, 70 °C.

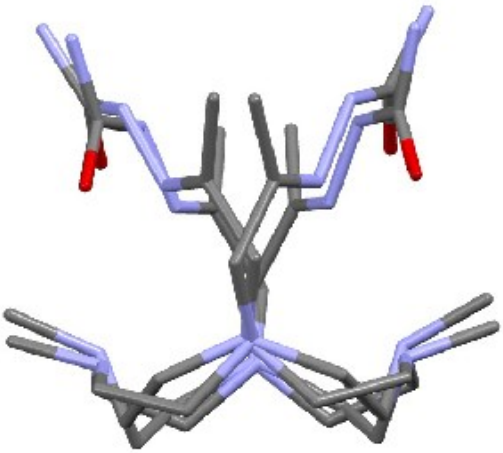

Figure S2. Overlay of the two non-superimposable enantiomers of $[H_2\mathbf{L^1}](BPh_4)_2$.

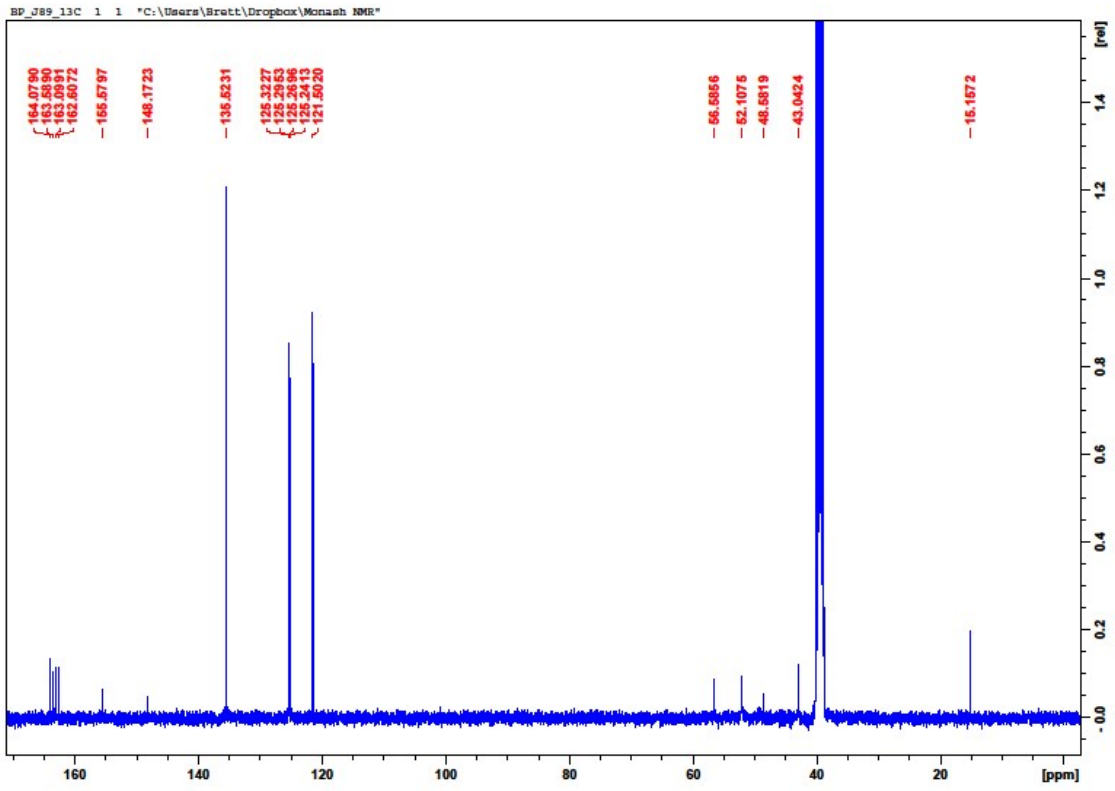

Figure S3. ^{13}C NMR of $[H_2\mathbf{L}](BPh_4)_2$; 100 MHz, $[D_6]$DMSO, 25 °C.

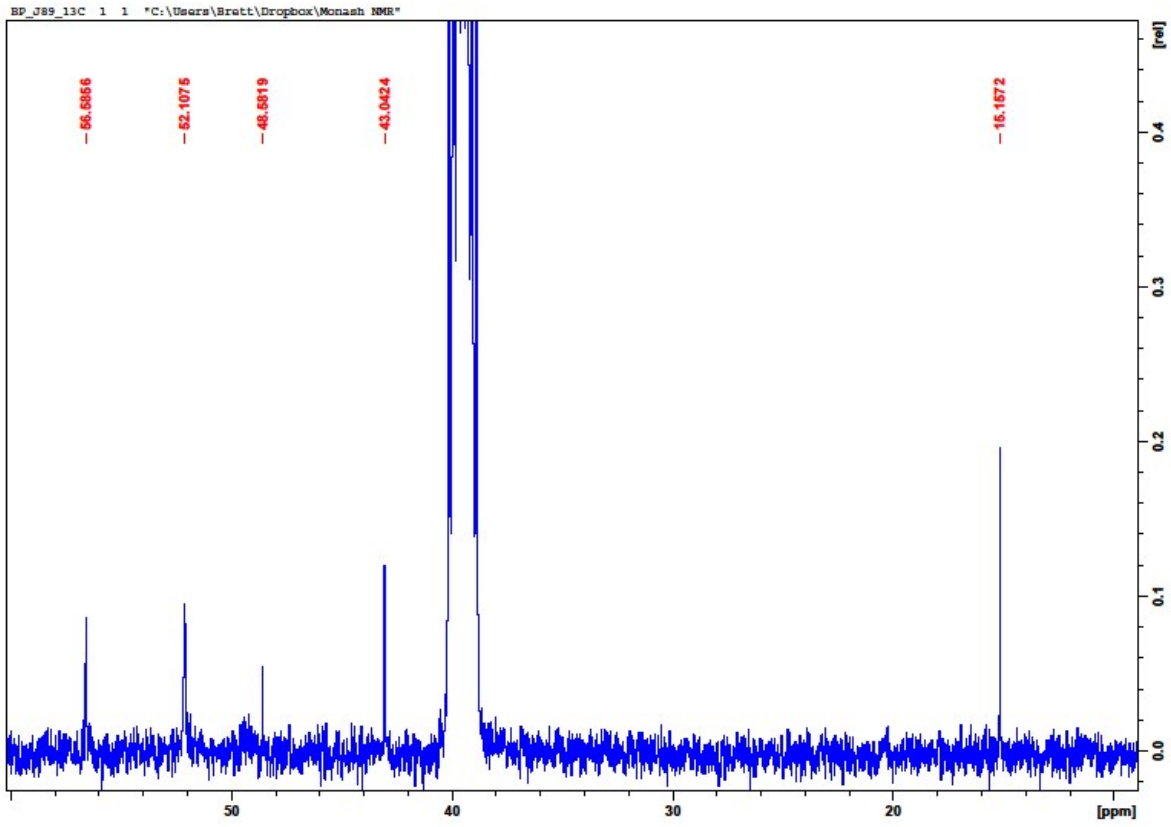

Figure S4. Partial spectrum: ^{13}C NMR of $[H_2\mathbf{L}](BPh_4)_2$; 100 MHz, $[D_6]$DMSO, 25 °C.

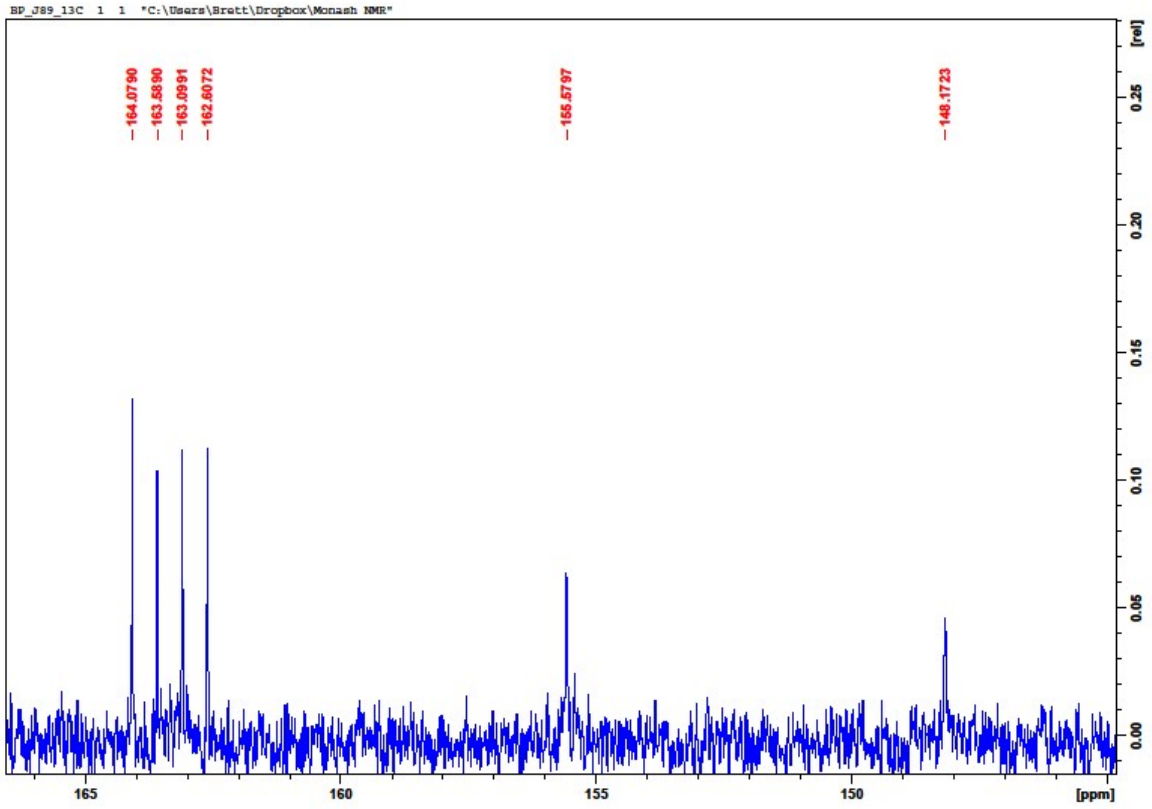

Figure S5. Partial spectrum: ^{13}C NMR of $[H_2\mathbf{L}](BPh_4)_2$; 100 MHz, $[D_6]DMSO$, 25 °C.

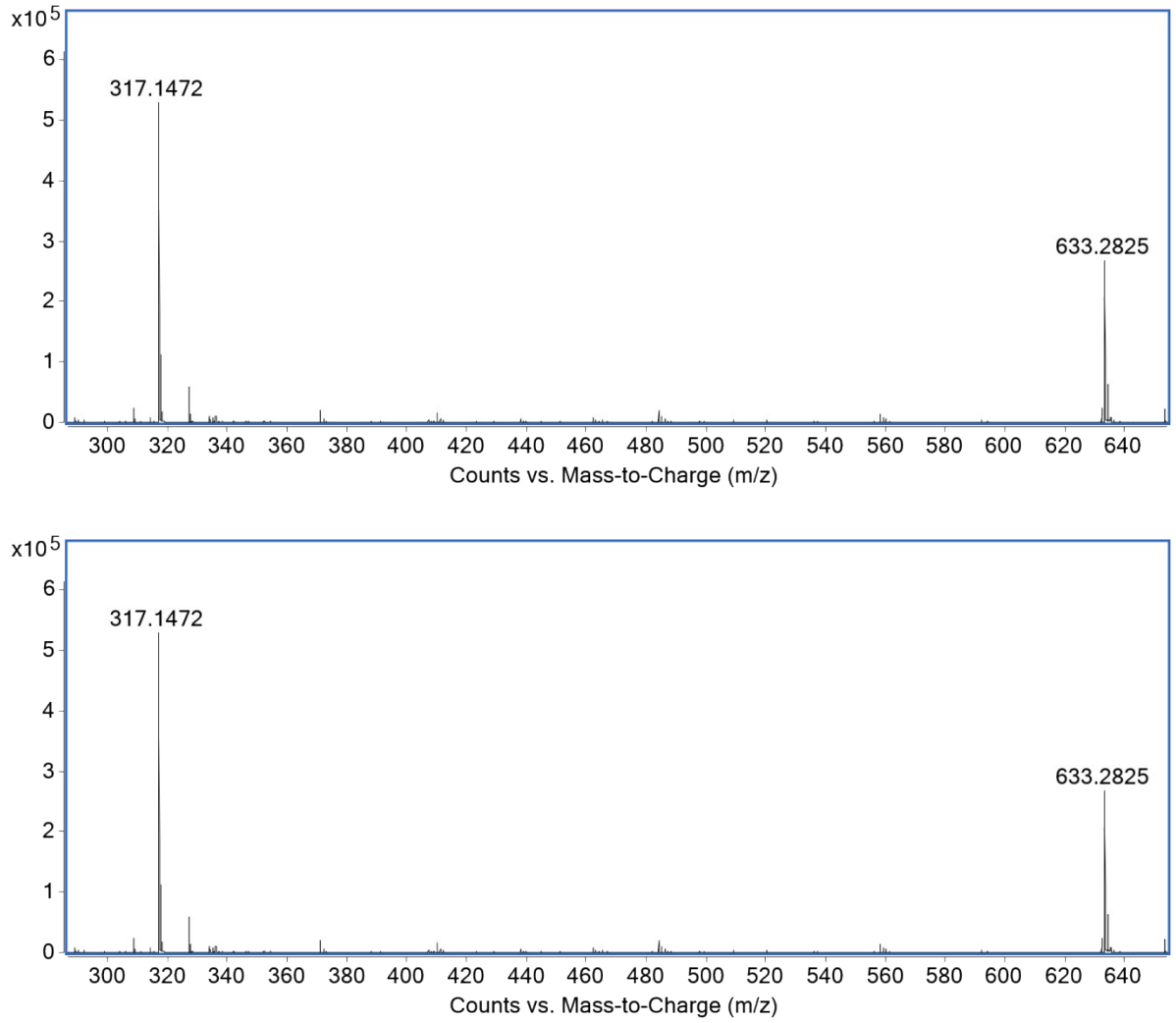

Figure S6. High resolution mass spectrometry showing an isotopic distribution for [Bi(**L** – H^+)]$^{2+}$ and Bi(**L** – H^+)]$^+$ at *m/z* 100% = 317.1472 and 633.2823, respectively.

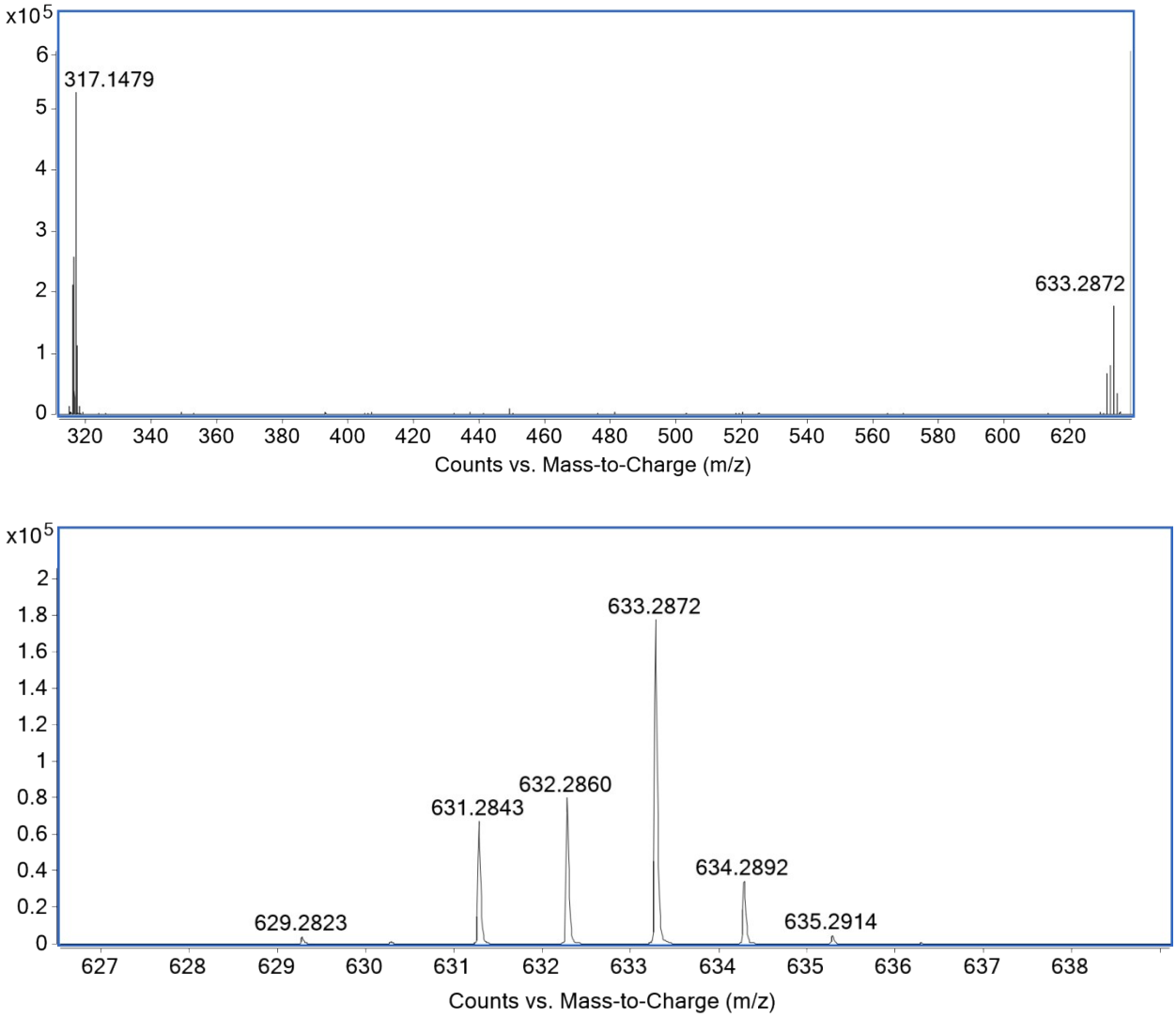

Figure S7. High resolution mass spectrometry showing an isotopic distribution for $[Pb(\mathbf{L^1})]^{2+}$ and $Pb(\mathbf{L^1} - H^+)]^+$ at *m/z* 100% = 317.1479 and 633.2872, respectively.

Table S1. Crystallographic data

Crystal identification	[Pb(**L**)]$(ClO_4)_2$.2.5(H_2O)	[Bi(**L**)]$(ClO_4)_3$·18H_2O	([H_2**L**]$(BPh_4)_2)_2$
Chemical formula	$C_{18}H_{37}Cl_2N_{10}O_{12.5}Pb$	$C_{18}H_{38}BiCl_3N_{10}O_{14}$	$C_{66}H_{80}B_2N_{10}O2$
M	871.66	933.91	1067.02
Crystal System	Triclinic	Monoclinic	Triclinic
Temperature / K	130.01(10)	130.01(10)	130.00(10)
Space group	P 1	I 2/a	P -1
a / Å	12.2202(3)	15.2422(6)	13.3950(7)
b / Å	15.0117(3)	16.9179(6)	20.6036(12)
c / Å	18.5855(6)	27.1280(16)	26.8080(14)
α / °	95.581(2)	90.00	95.435(4)
β / °	108.641(2)	99.245(4)	101.326(4)
γ / °	99.640(2)	90.00	102.064(5)
V / Å^3	3143.75(15)	6904.5(6)	7022.8(7)
Z	4	8	4
ρ_{calcd} / g/cm^3	1.842	1.797	1.009
μ / mm^{-1}	5.610	5.413	0.479
λ / Å	0.71073	0.71073	1.54184
F(000)	1724	3696	2288
$2\theta_{max}$	50.000	71.206	134.998
Independent Reflections	15154	6054	25002
R_{int}	0.0365	0.0508	0.0946
R (I > 2σ(I))	0.0314	0.0424	0.0758
wR (all data)	0.0717	0.1116	0.2275
GOF	1.024	1.030	0.93
Flack parameter	0.049(6)		

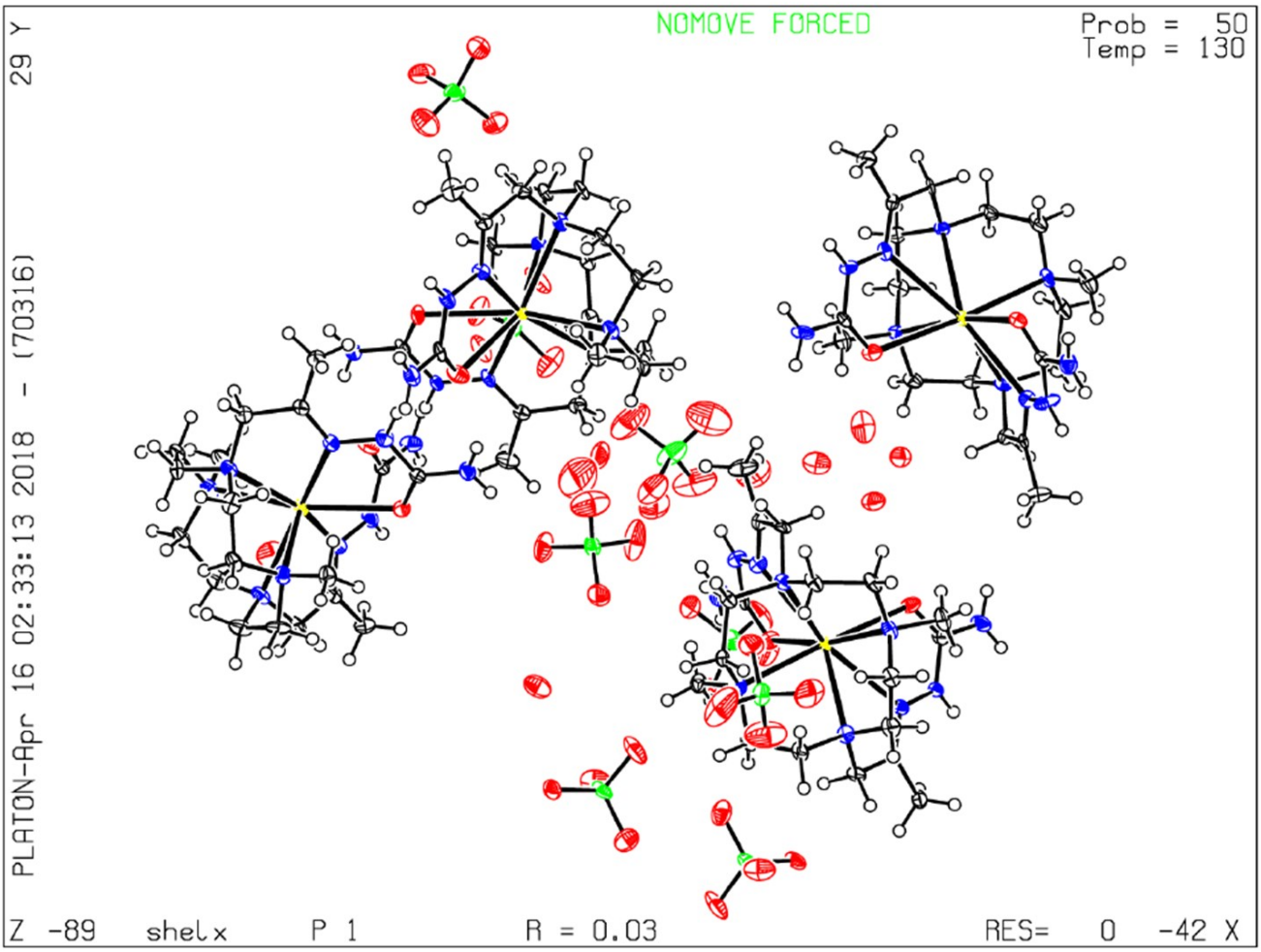

Figure S8. Ellipsoid plot of [Pb(**L**)]$(ClO_4)_2 \cdot 2.5H_2O$

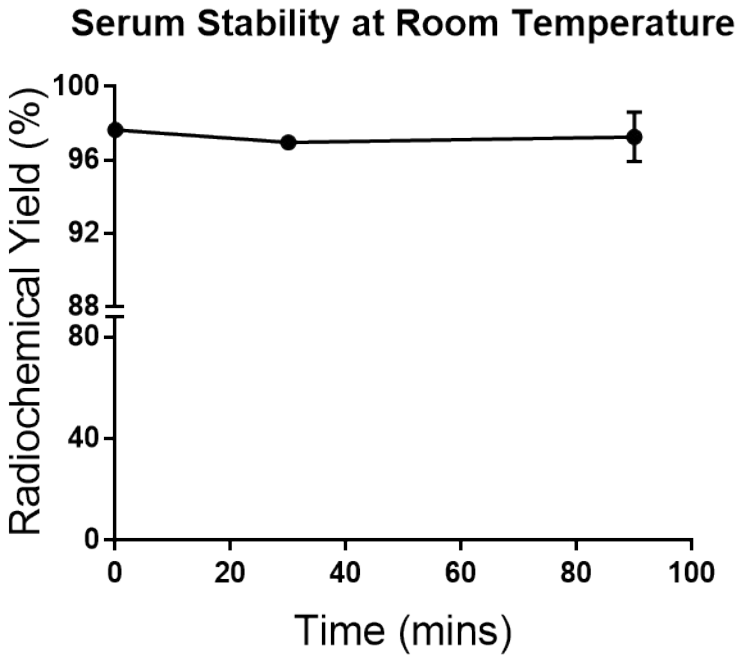

Figure S9. [^{213}Bi(**L**)]$^{3+}$ stability (% intact complex remaining) measured at t = 0, 30 and 90 mins by TLC after challenging with human serum at room temperature.

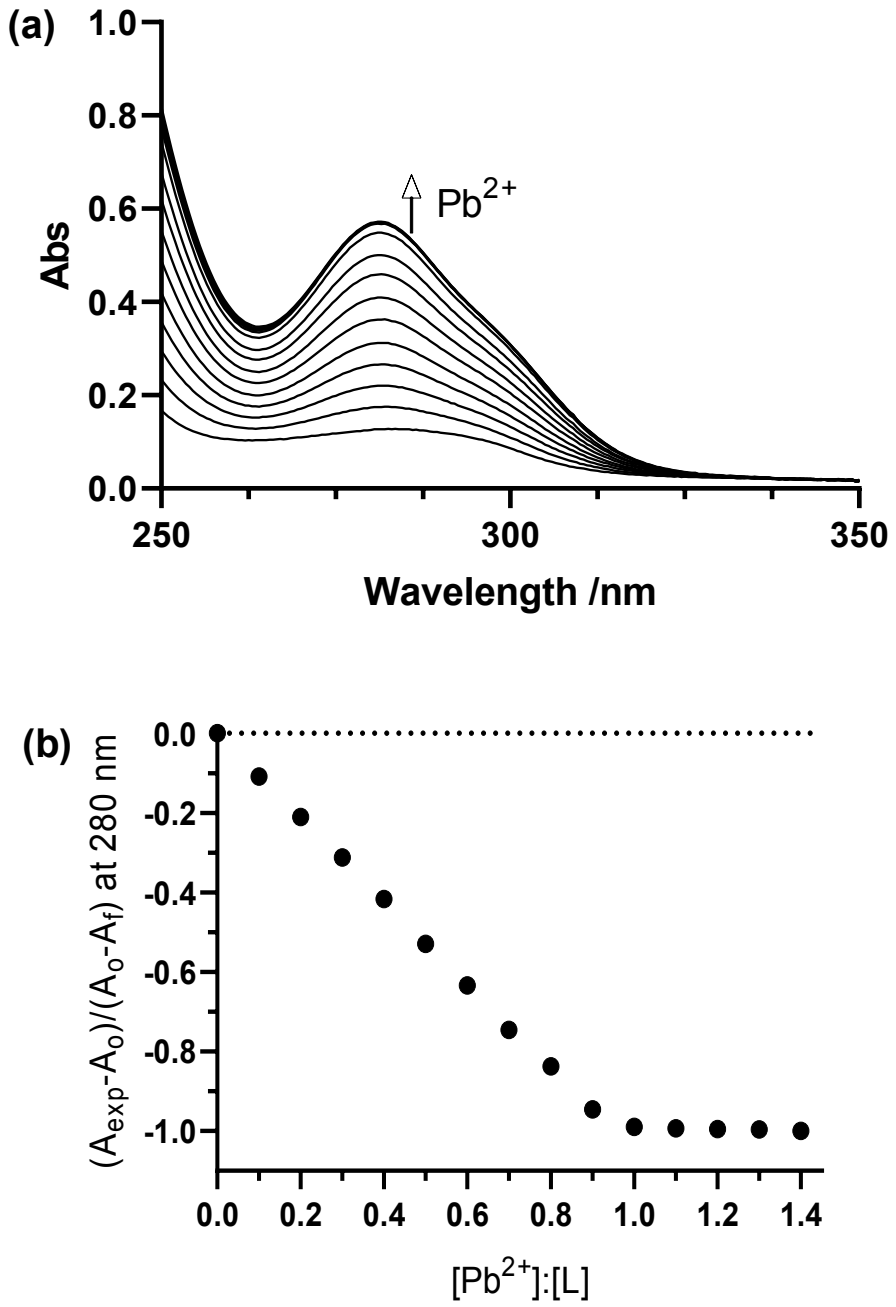

Figure S10. (a) Change in the UV absorption spectrum of a solution containing **L** (100 μM) in MOPS (20 mM, pH 7.4) upon titration with Pb^{2+} (9.8 mM). (b) A plot of $(A_{exp}-A_0)/(A_0-A_f)$ at 280 nm vs $[Pb^{2+}]/[\mathbf{L}]$.

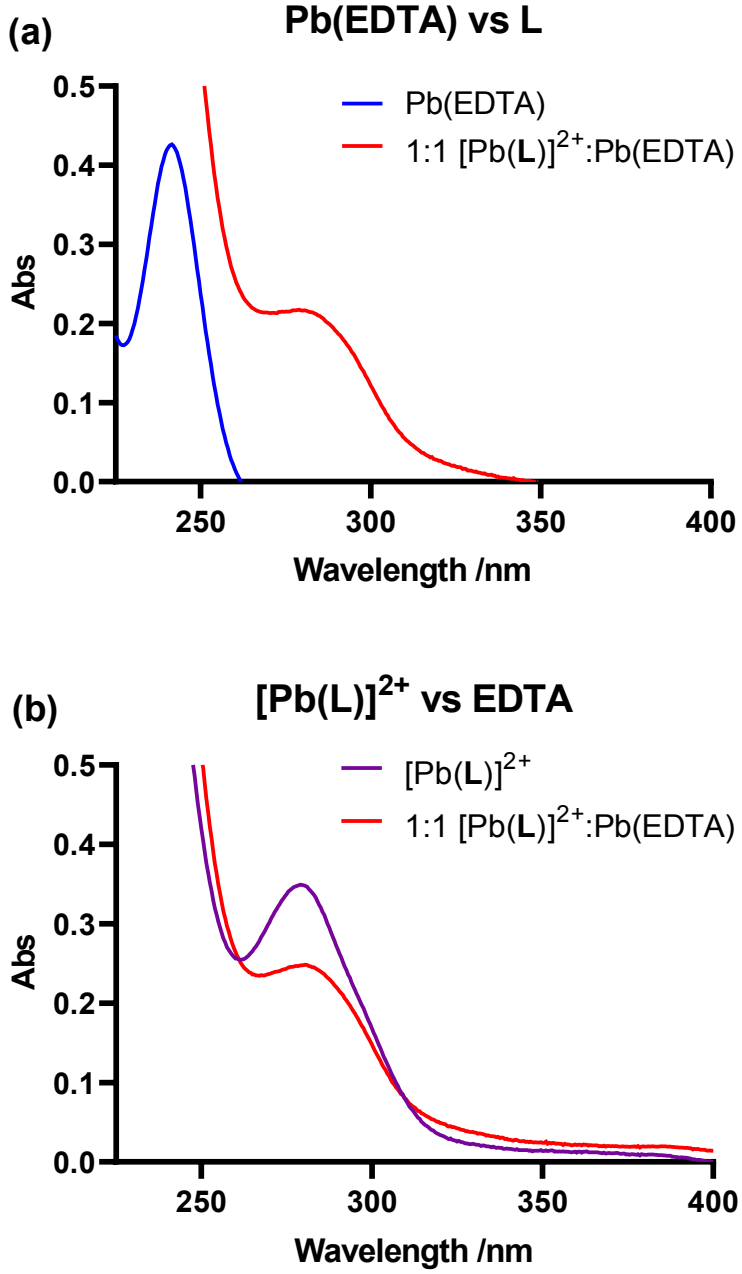

Figure S11. (a) Change in the UV absorption spectrum of a solution containing $[Pb(EDTA)]^{2-}$ (0.05 mM) in MOPS (0.02 M, pH 7.4, 0.1 M KCl) upon 2 week incubation at 50 °C with **L** (0.1 mM) and EDTA (0.05 mM). (b) Change in the UV absorption spectrum of a solution containing $[Pb(\mathbf{L})]^{2+}$ (0.05 mM) in MOPS (0.02 M, pH 7.4, 0.1 M KCl) upon 2-week incubation at 50 °C with EDTA (0.1 mM) and **L** (0.05 mM).

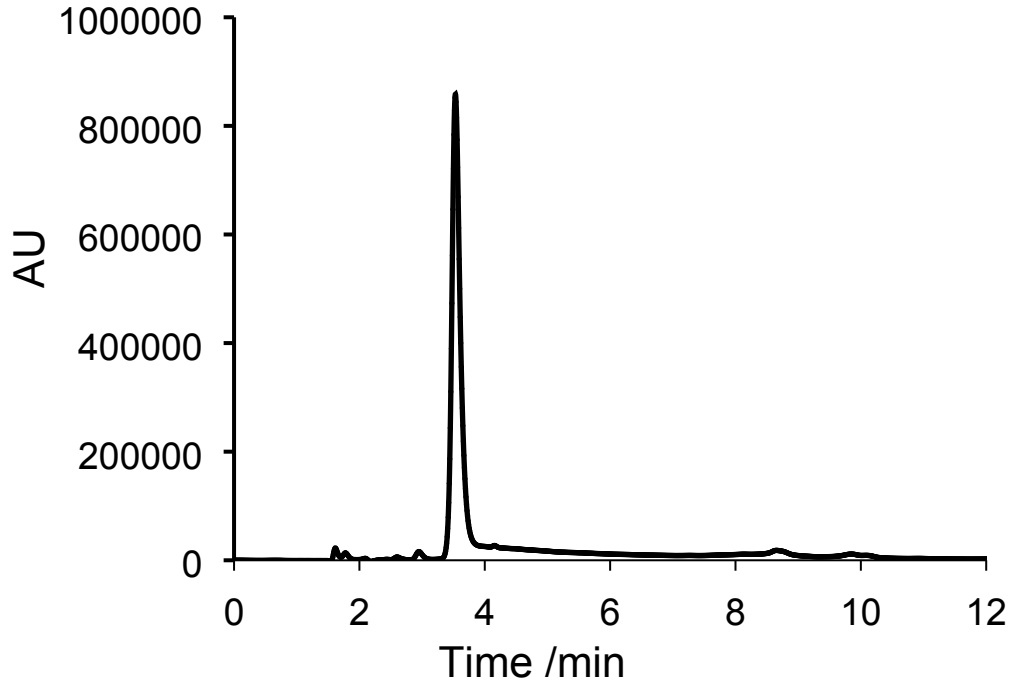

Figure S12. HPLC chromatogram of **L**: R_T = 3.5 min.

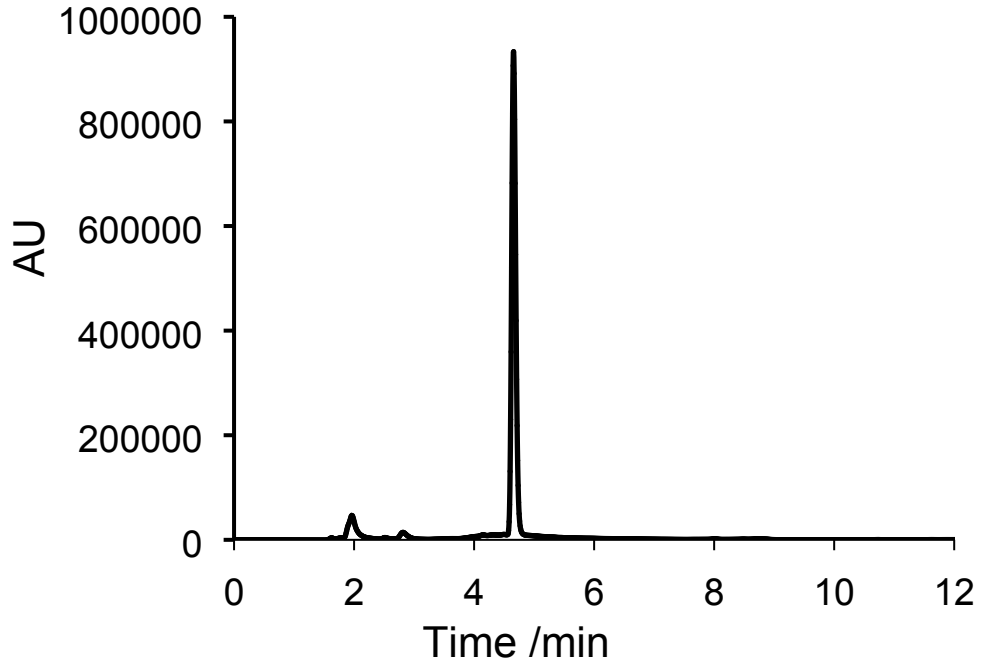

Figure S13. HPLC chromatogram of [Pb**L**]$^{2+}$: R_T = 4.6 min.

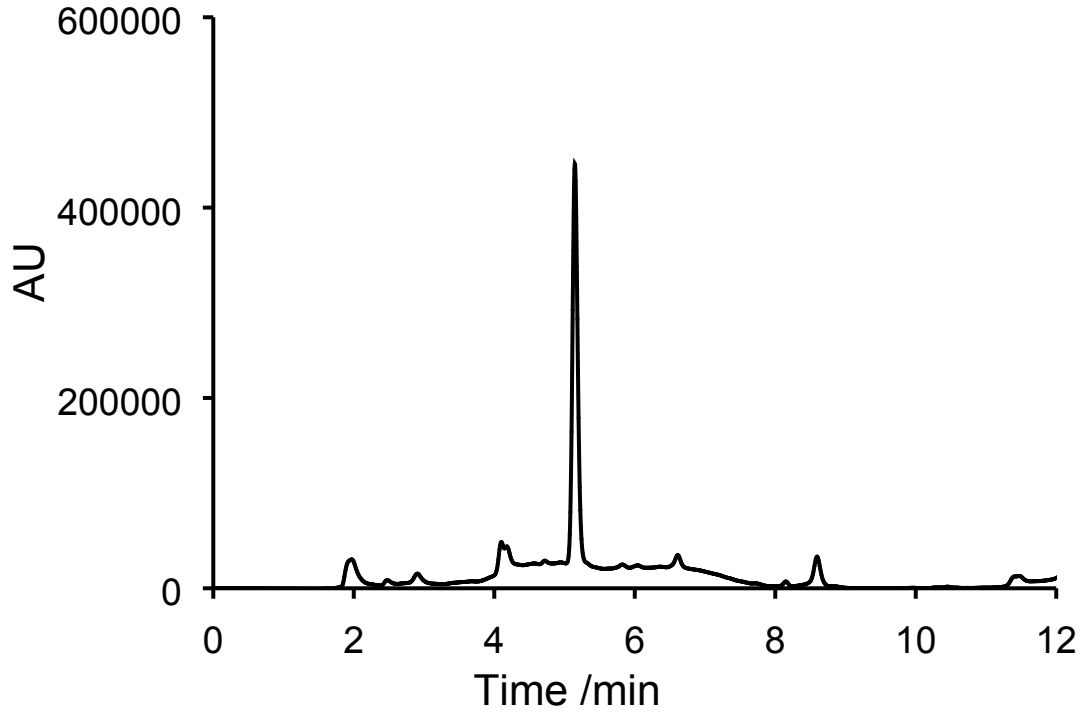

Figure S14. HPLC chromatogram of [Bi**L**]$^{3+}$: R_T = 5.1 min.