Electronic Supplementary Information

Rational Design, Synthesis and Evaluation of Tetrahydroxamic Acid Chelators for Stable Complexation of Zr^{IV}

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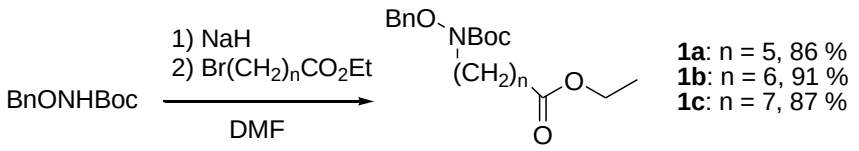
1. Syntheses

All reagents and solvents were obtained commercially and used without further purification unless otherwise noted. *N*-Boc-*O*-benzylhydroxylamine was prepared as previously reported.[1] ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Advance 300 MHz instrument, and chemical shifts are reported in ppm on the δ scale relative to TMS. Electrospray ionization-mass spectra (ESI-MS) were acquired using an Agilent LC/MS system equipped with a multimode ion. Elemental analyses were performed by Galbraith Lab. Inc. (Knoxville, TN) using combustion analysis methods for C, H, and N and inductively coupled plasma-atomic emission spectroscopy (ICP-OES) method for Zr. FT-IR spectra were recorded on a MIRacle™ Single Reflection ATR spectrometer (PIKE technologies, Madisson, WI).

_N_-alkylated-_N_-Boc-_O_-benzylhydroxylamines 1a-c.



1a: n = 5, 86 %
1b: n = 6, 91 %
1c: n = 7, 87 %

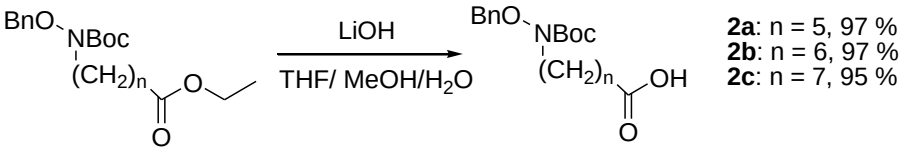
[1] A. Safavy, D. C. Smith, A. Bazooband, D. J. Buchsbaum, *Bioconjugate Chem.* **2002**, *13*, 327–332.

N-Boc-*O*-benzylhydroxylamine (5.00 g, 22.4 mmol) under nitrogen atmosphere was dissolved in dry DMF (100 mL) and cooled in an ice bath. 60% sodium hydride (887 mg, 22.2 mmol) was added and the mixture was stirred until end of hydrogen evolution (~ 30 min). Ethyl-6-bromohexanoate (6.19 g, 28 mmol) was added and the mixture was heated for 14 h at 65 °C. The DMF was then evaporated in vacuo, the residue was dissolved in AcOEt and washed twice with water. After drying the organic layer with $MgSO_4$, the oil obtained after filtration and concentration was purified by flash chromatography using hexane/acetone (9/1), affording **1a** as a colorless oil (7.04 g, 86%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.24 (t, 3H, J = 7.2 Hz), 1.31 (m, 2H), 1.50 (s, 9H), 1.61 (m, 4H), 2.28 (t, 2H, J = 7.5 Hz), 3.40 (t, 2H, J = 7.2 Hz), 4.11 (q, 2H, J = 7.2 Hz), 4.82 (s, 2H), 7.36 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 14.4, 24.8, 26.5, 26.9, 28.5, 34.4, 49.6, 60.4, 77.1, 81.4, 128.6(2), 129.5, 135.9, 156.8, 173.8. ESI-MS: m/z = 266.2 $[M+H]^+$.

The same alkylation procedure using ethyl-7-bromoheptanoate provided **1b** as a colorless oil (91%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.24 (t, 3H, J = 7.2), 1.31 (m, 4H), 1.50 (s, 9H), 1.60 (m, 4H), 2.27 (t, 2H, J = 7,5 Hz), 3.40 (t, 2H, J = 6.9 Hz), 4,11 (q, 2H, J = 6.9 H), 4.82 (s, 2H), 7.33 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 14.3, 24.9, 26.5, 26.9, 28.4, 28.8, 34.3, 49.6, 60.2, 76.9, 81.1, 128.4, 128.5, 129.4, 135.8, 156.6, 173.7. ESI-MS: m/z = 402.2 $[M+Na]^+$.

The same alkylation procedure using ethyl-8-bromooctanoate provided **1c** as a colorless oil (87%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.24 (t, 3H, J = 7.2 Hz), 1.30 (m, 6H), 1.50 (s, 9H), 1.61 (m, 4H), 2.27 (t, 2H, J = 7.2 Hz), 3.39 (t, 2H, J = 7.2 Hz), 4.11 (q, 2H, J = 7.2 Hz), 4.82 (s, 2H), 7.33 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 14.3, 24.9, 26.6, 27.1, 28.4, 29.0, 29.1, 34.4, 49.6, 60.2, 76.9, 81.1, 128.4, 128.5, 129.4, 135.8, 156.7, 173.8. ESI-MS: m/z = 416.2 $[M+Na]^+$, 294.2 $[M\text{-Boc}+2H]^+$.

Carboxylic acid building blocks 2a-c.

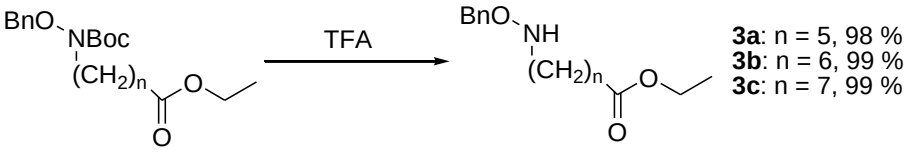


Compound **1a** (2.215 g, 6.06 mmol) was dissolved in 18 ml THF + 6 mL MeOH, and 6 mL of 2M LiOH (12 mmol) was added dropwise, and the mixture was stirred for 4 h at room temperature. After removal of the solvents in vacuo, the residue was dissolved in Et_2O and washed with 1M HCl. The organic layer was dried over $MgSO_4$, filtered, and evaporated to afford **2a** as a colorless oil (1.93 g, 97%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.33 (m, 2H), 1.50 (s, 9H), 1.62 (m, 4H), 2.34 (t, 2H, J = 7.2 Hz), 3.41 (t, 2H, J = 7.2 Hz), 4.82 (s, 2H), 7.35 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.5, 26.4, 26.9, 28.5, 34.0, 49.5, 77.1, 81.5, 128.6, 128.7, 129.6, 135.8, 156.8, 179.6. ESI-MS: m/z = 360.1 $[M+Na]^+$, 238.1 $[M\text{-Boc}+2H]^+$.

The same procedure starting with compound **1b** afforded **2b** as a colorless oil (97%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.32 (m, 4H), 1.50 (s, 9H), 1.60 (m, 4H), 2.33 (t, 2H, J = 7.5 Hz), 3.40 (t, 2H, J = 7.2 Hz), 4,82 (s, 2H), 7, 35 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.7, 26.6, 27.0, 28.5, 28.9, 34.1, 49.7, 77.1, 81.4, 128.6, 128.7, 129.6, 135.9, 156.8, 179.8. ESI-MS: m/z = 374.2 $[M+Na]^+$.

The same procedure starting with compound **1c** afforded **2c** as a colorless oil (95%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.34 (m, 6H), 1.50 (s, 9H), 1.60 (m, 4H), 2.33 (t, 2H, J = 7.5 Hz), 3.40 (t, 2H, J = 7.2 Hz), 4,82 (s, 2H), 7, 35 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.9, 26.9, 27.3, 28.9, 29.2, 29.3, 34.4, 49.9, 77.9, 81.5, 128.7, 128.8, 129.7, 136.0, 157.0, 180.3. ESI-MS: m/z = 388.2 $[M+Na]^+$.

_O_-benzylhydroxylamine building blocks 3a-c.

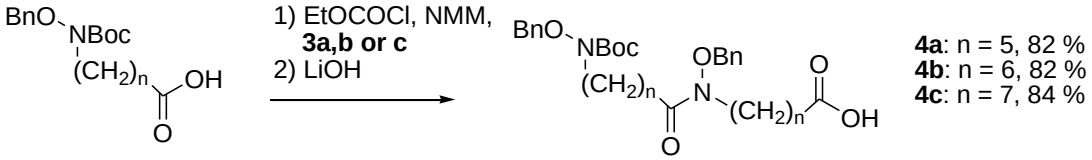


To compound **1a** (2.544 g, 6.96 mmol) cooled in an ice bath, was added dropwise trifluoroacetic acid (3.22 mL, 41.8 mmol). The mixture was stirred at room temperature for 3h. CH_2Cl_2 (50 mL) and water (50 mL) were then added and the solution was raised to pH 10-11 by addition of solid Na_2CO_3. After drying the organic layer over $MgSO_4$ and filtration, the solution was concentrated in vacuo to afford **3a** as a colorless liquid (1.81 g, 98%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.30 (t, 3H, J = 6.6 Hz), 1.37 (m, 2H), 1.53 (m, 2H), 1.63 (m, 2H), 2.29 (t, 2H, J = 7.5 Hz), 2.93 (t, 2H, J = 7.2 Hz), 4.12 (q, 2H, J = 7.2 Hz), 4,70 (s, 2H), 5.54 (s, 1H), 7.34 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): 14.4, 25.0, 26.9, 27.2, 34.4, 52.1, 60.4, 76.4, 128.0, 128.6(2), 138.2, 173.9. ESI-MS: m/z = 266.2 $[M+H]^+$.

The same procedure starting with compound **1b** afforded **3b** as a colorless liquid (99%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.24 (t, 3H, J = 7.2 Hz), 1.32 (m, 4H), 1.51 (m, 2H), 1.62 (m, 2H), 2.28 (t, 2H, J = 7.2 Hz), 2.91 (t, 2H, J = 6.9 Hz), 4.11 (q, 2H, J = 7.2 Hz), 4.69 (s, 2H), 5.53 (s, 1H) 7.31 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 14.4, 25.0, 26.9, 27.3, 29.1, 34.4, 52.2, 60.3, 76.3, 127.8, 128.4, 138.1, 173.8. ESI-MS: m/z = 280.1 $[M+H]^+$; 302.1 $[M+Na]^+$.

The same procedure starting with compound **1c** afforded **3c** as a colorless liquid (99%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.25 (t, 3H, J = 7.2 Hz), 1.31 (m, 6H), 1.48 (m, 2H), 1.61 (m, 2H), 2.28 (t, 2H, J = 7.5 Hz), 2.92 (t, 2H, J = 7.2 Hz), 4.12 (q, 2H, J = 7.2 Hz), 4.70 (s, 2H), 5.53 (s, 1H), 7.35 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 14.5, 25.1, 27.2, 27.5, 29.2, 29.3, 34.5, 52.3, 60.4, 76.4, 128.0, 128.5, 128.6, 138.2, 174.0. ESI-MS: m/z = 294.2 $[M+H]^+$.

_O_-benzyl monohydroxamates 4a-c.



To compound **2a** (4.213 g, 12.5 mmol) dissolved in dry Et_2O (100 mL) and cooled in an ice bath, was slowly added ethylchloroformate (1.43 mL, 15 mmol), followed by *N*-methylmorpholine (2.06 mL, 18.8 mol). The mixture was stirred for 15 min and the precipitate was removed by filtration. The filtrate was then poured onto compound **3a** and the mixture stirred at rt for 4 h. The solution was then washed twice with 1N HCl and twice with 1M

Na_2CO_3. After drying over $MgSO_4$ and concentration in vacuo, the oily residue was purified by flash chromatography using hexane/acetone (9/1) to afford the ester intermediate as a colorless oil (5.763 g, 83%). It was treated with LiOH with the hydrolysis procedure described above to afford **4a** as a colorless oil (5.70 g, 82% from **2a**). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.30 (m, 4H), 1.49 (s, 9H), 1.62 (m, 8H), 2.35 (m, 4H), 3.41 (t, 2H, J = 6.9 Hz), 3.64 (t, 2H, J = 6.9 Hz), 4.77 (s, 2H), 4.81 (s, 2H), 7,36 (m, 10H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.5, 26.3, 26.7, 27.0, 28.5, 31.1, 32.4, 34.0, 76.4, 77.0, 81.4, 128.5, 128.6, 128.9, 129.1, 129.3, 129.5, 134.7, 135.7, 156.8, 178.6. ESI-MS: m/z = 579.3 $[M+Na]^+$; 457.3 $[M\text{-}Boc+2H]^+$.

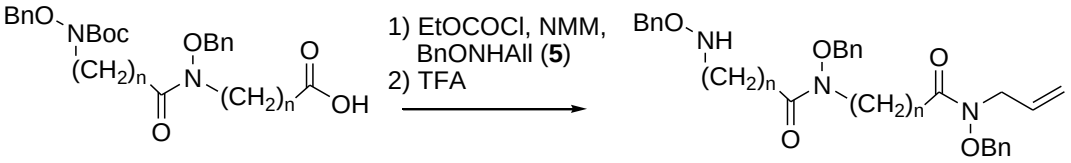
The same condensation procedure between **2b** and **3b**, followed by ester hydrolysis afforded compound **4b** as a colorless oil (82%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.30 (m, 8H), 1.49 (s, 9H), 1.60 (m, 8H), 2.32 (m, 4H), 3.39 (t, 2H, J = 7.2 Hz), 3.61 (t, 2H, J = 6.9 Hz), 4.79 (s, 2H), 4.81 (s, 2H), 7,34 (m, 10H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.7, 25.7, 26.5, 26.7, 26.8, 27.11, 28.5, 28.8, 29.3, 32.5, 34.1, 49.7, 53.6, 76.4, 77.0, 81.3, 128.5, 128.6, 128.9, 129.1, 129.2 129.5, 134.7, 135.8, 156.8, 179.1. ESI-MS: m/z = 607.3 $[M+Na]^+$; 485.3 $[M\text{-}Boc+2H]^+$.

The same condensation procedure between **2c** and **3c**, followed by ester hydrolysis afforded compound **4c** as a colorless oil (82%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.30 (m, 12H), 1.49 (s, 9H), 1.60 (m, 8H), 2.34 (m, 4H), 3.39 (t, 2H, J = 7.2 Hz), 3.62 (t, 2H, J = 6.9 Hz), 4.79 (s, 2H), 4.81 (s, 2H), 7,34 (m, 10H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.8, 26.7, 26.8, 27.0, 27.2, 28.5, 29.0, 29.1, 29.3, 29.5, 32.6, 34.1, 49.8, 76.5, 77.1, 81.4, 128.6, 128.7, 128.9, 129.1, 129.3, 129.6, 134.1, 135.9, 156.8, 178.9. ESI-MS: m/z = 635.3 $[M+Na]^+$; 513.3 $[M\text{-}Boc+2H]^+$.

***N*-allyl-*O*-benzylhydroxylamine 5**.

N-Boc-*O*-benzylhydroxylamine (2.203 g, 9.87 mmol) was melted by heating at 60 °C and, after cooling, allyl bromide (1.7 mL, 19.74 mmol) was added, followed by potassium *tert*-butoxide (1.383 g, 12.34 mmol). After heating at 60 °C for 4 h, the mixture was cooled to rt, water was added and the product was extracted by CH_2Cl_2, dried over $MgSO_4$, filtered and concentrated in vacuo resulting in an oily residue. Purification by flash chromatography using hexane/acetone (95/5) afforded a colorless oil (2.554 g). To this oil was added TFA (4.53 mL, 59.2 mmol) and the mixture was stirred at rt for 4 h. It was then diluted with CH_2Cl_2 (150 mL) and water (75 mL). Solid Na_2CO_3 was added until pH = 10-11. The organic layer was dried over $MgSO_4$, filtered and concentrated in vacuo to afford compound **5** as a colorless liquid (2.09 g, 95%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 3.55 (d, 2H, J = 6.3 Hz), 4.72 (s, 2H), 5.20 (m, 2H), 5.55 (s, 1H), 5.94 (m, 1H), 7.35 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 55.2, 76.4, 118.1, 128.0, 128.6(2), 134.5, 138.1. ESI-MS: m/z = 164.0 $[M+H]^+$.

***O*-benzylated dihydroxamates 6a-c.**



4a: n = 5
4b: n = 6
4c: n = 7

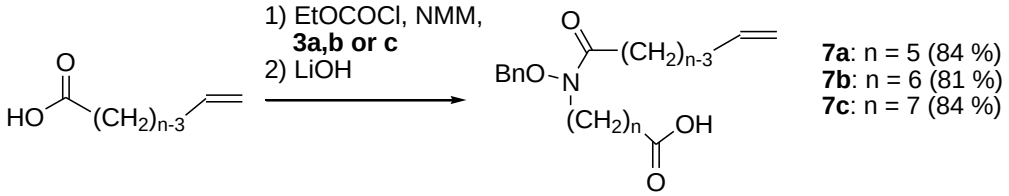
6a: n = 5 (86 %)
6b: n = 6 (84 %)
6c: n = 7 (85 %)

The condensation of **4a** with compound **5** was performed following the procedure described above. The oily residue was purified by flash chromatography with hexane/acetone (4/1) to afford a colorless oil. The Boc protection was then removed in the presence of TFA as described above to form **6a** as a colorless oil (3.45 g, 86%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.33 (m, 4H), 1.53 (m, 2H), 1.60 (m, 6H), 2.38 (m, 4H), 2.91 (t, 2H, J = 7.2 Hz), 3.61 (t, 2H, J = 6.9 Hz), 4.23 (d, 2H, J = 5.7 Hz), 4.69 (s, 2H), 4.78 (s, 2H), 4.82 (s, 2H), 5.21 (m, 2H), 5.51 (s, 1H), 5.84 (m, 1H), 7.36 (m, 15H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.4, 24.7, 26.8, 27.0, 27.2, 27.4, 32.4, 52.2, 76.4, 76.5, 77.0, 118.5, 127.9, 128.5, 128.6, 128.8, 128.9, 129.1, 129.3, 129.4, 132.6, 134.8, 138.2, 140.3. ESI-MS: m/z = 602.4 $[M+H]^+$; 624.3 $[M+Na]^+$.

The same condensation reaction between **4b** and **5** followed by Boc removal afforded **6b** as a colorless oil (84%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.30 (m, 8H), 1.47 (m, 2H), 1.61 (m, 6H), 2.37 (m, 4H), 2.93 (t, 2H, J = 6.9 Hz), 3.60 (t, 2H, J = 7.2 Hz), 4.23 (d, 2H, J = 6.0 Hz), 4.69 (s, 2H), 4.78 (s, 2H), 4.82 (s, 2H), 5.22 (m, 2H), 5.52 (s, 1H), 5.84 (m, 1H), 7.36 (m, 15H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.5, 24.7, 26.8, 27.0, 27.2, 27.4, 29.2, 29.5, 32.5, 52.3, 76.3, 76.4, 77.0, 118.4, 127.9, 128.5(2), 128.9, 129.0, 129.1, 129.2, 129.3, 132.6, 134.7, 134.8, 138.2, 174.9. ESI-MS: m/z = 630.4 $[M+H]^+$.

The same condensation reaction between **4c** and **5** followed by Boc removal afforded **6c** as a colorless oil (85%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.29 (m, 12H), 1.47 (m, 2H), 1.58 (m, 6H), 2.37 (m, 4H), 2.91 (t, 2H, J = 6.9 Hz), 3.60 (t, 2H, J = 6.9 Hz), 4.24 (d, 2H, J = 5.7 Hz), 4.70 (s, 2H), 4.80 (s, 2H), 4.83 (s, 2H), 5.22 (m, 2H), 5.53 (s, 1H), 5.86 (m, 1H), 7.36 (m, 15H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.6, 24.7, 26.8, 27.1, 27.2, 27.5, 29.2, 29.4, 29.5, 32.5, 52.3, 76.3, 76.4, 77.0, 77.4, 118.4, 127.9, 128.5(2), 128.8, 128.9, 129.0, 129.1, 129.2, 129.3, 132.6, 134.8, 138.2. ESI-MS: m/z = 658.4 $[M+H]^+$; 680.4 $[M+Na]^+$.

***O*-benzyl monohydroxamates 7a-c.**



7a: n = 5 (84 %)
7b: n = 6 (81 %)
7c: n = 7 (84 %)

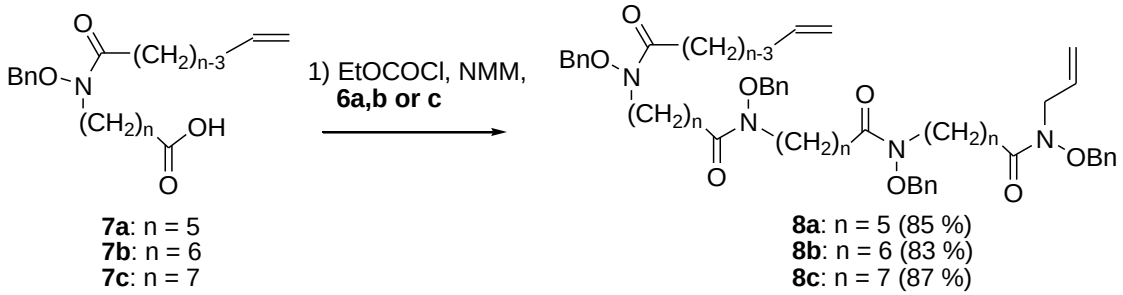
Condensation of 4-pentenoic acid with **3a** using the method described above afforded the ester intermediate as a colorless oil after purification by flash chromatography with hexane/acetone (95/5). Hydrolysis of the ester using the procedure described above afforded **7a**

as a colorless oil (84%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.36 (m, 2H), 1.64 (m, 4H), 2.34 (m, 4H), 2.50 (m, 2H), 3.64 (m, 2H), 4.80 (s, 2H), 4.99 (m, 2H), 5.80 (m, 1H), 7.40 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.5, 26.4, 26.7, 28.8, 31.8, 34.0, 45.4, 76.6, 115.3, 128.9, 129.2, 129.3, 134.7, 137.6, 179.2. ESI-MS: m/z = 320.2 $[M+H]^+$; 342.2 $[M+Na]^+$.

Condensation of 5-hexenoic acid with **3b** using the method described above followed by hydrolysis afforded **7b** as a colorless oil (81%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.33 (m, 4H), 1.60 (m, 6H), 2.06 (m, 2H), 2.36 (m, 4H), 3.63 (m, 2H), 4.80 (s, 2H), 4.95 (m, 2H), 5.78 (m, 1H), 7.41 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 23.9, 24.7, 26.5, 26.9, 28.8, 31.8, 33.5, 34.1, 45.6, 76.5, 115.3, 128.9, 129.1, 129.3, 134.7, 138.3, 175.0, 179.4. ESI-MS: m/z = 348.2 $[M+H]^+$; 370.2 $[M+Na]^+$.

Condensation of 6-heptenoic acid with **3c** using the method described above followed by hydrolysis afforded **7c** as a colorless oil (81%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.31 (m, 8H), 1.61 (m, 6H), 2.04 (m, 2H), 2.35 (m, 4H), 3.62 (m, 2H), 4.80 (s, 2H), 4.95 (m, 2H), 5.78 (m, 1H), 7.37 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.4, 24.8, 26.7, 27.0, 28.8, 29.0, 29.1, 32.4, 34.1, 76.5, 114.7, 128.9, 129.1, 129.3, 134.8, 138.8, 179.3. ESI-MS: m/z = 376.3 $[M+H]^+$; 398.3 $[M+Na]^+$.

Acyclic *O*-benzylated tetrahydroxamates 8a-c.



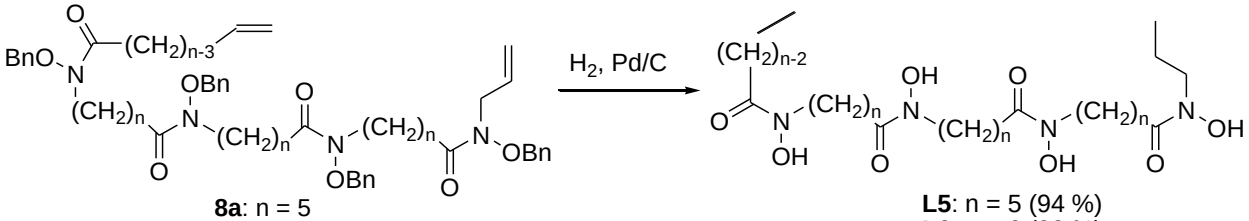
The condensation reaction between **7a** and **6a** was performed as described above. Purification by flash chromatography using hexane/acetone (7/3) afforded **8a** as a colorless oil (87%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.29 (m, 6H), 1.61 (m, 12H), 2.36 (m, 8H), 2.47 (m, 2H), 3.60 (m, 6H), 4.77 (d, 2H, J = 5.7 Hz), 4.77 (s, 4H), 4.79 (s, 2H), 4.81 (s, 2H), 4.99 (m, 2H), 5.21 (m, 2H), 5.83 (m, 2H), 7.35 (m, 20H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.3, 24.4, 26.7(2), 26.9, 28.7, 31.0, 21.8, 32.3, 76.4, 76.8, 115.2, 118.4, 128.8(2), 129.0(2), 129.2, 129.3, 132.5, 134.7, 137.6, 174.7. ESI-MS: m/z = 903.5 $[M+H]^+$; 925.5 $[M+Na]^+$.

The condensation reaction between **7b** and **6b** as described above afforded **8b** as a colorless oil (83%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.29 (m, 12H), 1,60 (m, 14H), 2.05 (m, 2H), 2.37 (m, 4H), 3.60 (m, 6H), 4.23 (d, 2H, J = 6.0 Hz), 4.78 (s, 6H), 4.82 (s, 2H), 4.97 (m, 2H), 5.22 (m, 2H), 5.80 (m, 2H), 7.36 (m, 20H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 23.8, 24.4, 24.6, 26.7, 26.9, 29.1, 31.0, 31.8, 32.4, 33.4, 45.5, 76.3, 76.9, 115.2, 118.4, 128.8, 128.9, 129.0, 129.2(2), 129.3, 132.5, 134.7, 138.3, 174.9. ESI-MS: m/z = 959.5 $[M+H]^+$; 971.5 $[M+Na]^+$.

The condensation reaction between **7c** and **6c** as described above afforded **8c** as a colorless oil (87%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.28 (m, 18H), 1.38 (m, 2H), 1.59 (m, 14H), 2.06 (m, 2H), 2.37 (m, 8H), 3.60 (m, 6H), 4.24 (d, 2H, J = 6.0 Hz), 4.79 (s, 6H), 4.83 (s, 2H), 4.94 (m, 2H), 5.22 (m, 2H), 5.84 (m, 2H), 7.37 (m, 20H). ^{13}C NMR ($CDCl_3$, 75 MHz,

ppm): δ 24.3, 24.6, 24.7, 26.8, 27.1, 28.8, 29.3, 29.4, 29.5, 32.4, 32.5, 33.7, 45.6, 76.4, 76.9, 114.6, 118.4, 128.8, 129.0(2), 129.2, 129.3, 132.6, 134.8, 138.8, 175.1. ESI-MS: m/z = 1015.5 $[M+H]^+$; 1037.5 $[M+Na]^+$.

Acyclic tetrahydroxamic acid chelators L5-7.



8a: n = 5
8b: n = 6
8c: n = 7

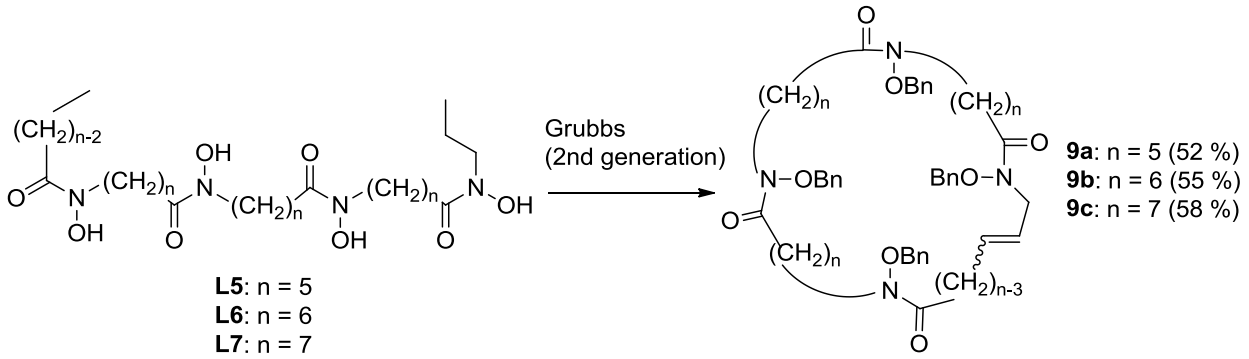
L5: n = 5 (94 %)
L6: n = 6 (92 %)
L7: n = 7 (92 %)

Compound **8a** (276 mg, 221 µmol) was dissolved in MeOH (20 mL) and hydrogenated in a Paar apparatus at 30 psi H_2 in the presence of 10% Pd/C (20 mg) for 48 h. Pd/C was then removed by centrifugation at 8500 rpm. The supernatant was then centrifugated a second time and the solvent evaporated. The oily residue was dissolved in the minimum amount of MeOH, Et_2O was added until the solution became cloudy and placed in the fridge at 4 °C. **L5** precipitated as a white solid that was filtered and washed with Et_2O (187 mg, 94%). ^{1}H NMR (DMSO, 300 MHz, ppm): δ 0.87 (m, 6H), 1.23 (m, 8H), 1.51 (m, 16H), 2.33 (m, 8H), 3.46 (m, 8H), 9.54 (s, 4H). ^{13}C NMR (DMSO, 75 MHz, ppm): δ 11.1, 13.8, 21.9, 23.9, 25.9, 26.2, 31.4, 31.6, 47.0, 172.5. ESI-MS: m/z = 547.3 $[M+H]^+$; 569.2 $[M+Na]^+$; 545.2 $[M-H]^-$; 581.2 $[M+Cl]^-$. Elemental analyses: Calculated for $C_{26}H_{50}N_4O_8$: C, 57.12; H, 9.22; N, 10.25%. Found: C, 56.14; H, 8.74; N, 9.85. Mp: 117 °C.

Compound **8b** was hydrogenated using the same procedure. A white precipitate formed. It was dissolved in hot isopropyl alcohol. Pd/C was then removed by centrifugation at 8500 rpm. The supernatant was centrifugated a second time and the solvent evaporated to form **L6** as a white solid (92 %). ^{1}H NMR (DMSO, 300 MHz, ppm): δ 0.84 (m, 6H), 1.24 (m, 16H), 1.48 (m, 16H), 2.32 (m, 8H), 3.44 (m, 8H), 9.53 (s, 4H). ^{13}C NMR (DMSO, 75 MHz, ppm): δ 11.1, 13.9, 19.6, 21.9, 23.9, 24.2, 26.0, 26.2, 28.5, 31.0, 31.6, 47.0, 172.6. ESI-MS: m/z = 603.2 $[M+H]^+$; 625.3 $[M+Na]^+$; 601.3 $[M-H]^-$; 637.3 $[M+Cl]^-$. Elemental analyses: Calculated for $C_{30}H_{58}N_4O_8$: C, 59.77; H, 9.70; N, 9.29%. Found: C, 59.82; H, 9.43; N, 8.99. Mp: 139 °C.

Compound **8c** was hydrogenated using the same procedure. A white precipitate formed. It was dissolved in hot isopropyl alcohol. Pd/C was then removed by centrifugation at 8500 rpm. The supernatant was centrifugated a second time and the solvent evaporated to form **L7** as a white solid (92%). ^{1}H NMR (DMSO, 300 MHz, ppm): δ 0.83 (m, 6H), 1.24 (m, 24H), 1.47 (m, 16H), 2.31 (m, 8H), 3.45 (m, 8H), 9.54 (ms, 4H). ^{13}C NMR (DMSO, 75 MHz, ppm): δ 11.1, 13.9, 19.6, 22.0, 24.2, 26.0, 26.3, 28.5, 28.6, 28.8, 31.1, 31.7, 47.0, 172.6. ESI-MS: m/z = 659.4 $[M+H]^+$; 681.4 $[M+Na]^+$; 657.4$[M-H]^-$; 693.3 $[M+Cl]^-$. Elemental analyses: Calculated for $C_{34}H_{66}N_4O_8$: C, 61.98; H, 10.10; N, 8.50%. Found: C, 61.69; H, 9.79; N, 8.27. Mp: 122 °C.

Macrocyclic *O*-benzylated tetrahydroxamates 9a-c.

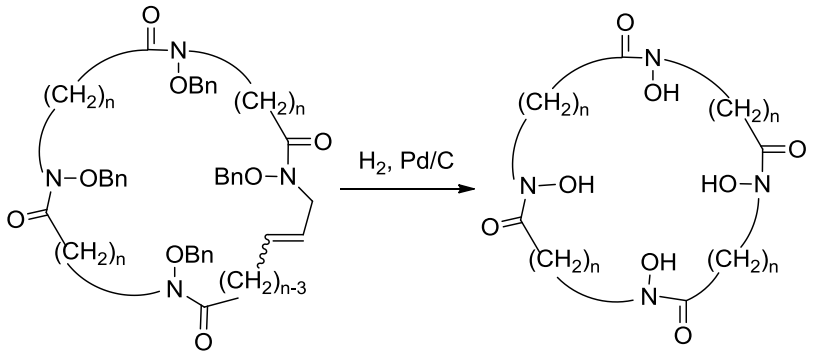


Compound **8a** (990 mg, 1.10 mmol) was dissolved in CH_2Cl_2 (1000 mL) and degassed by bubbling nitrogen in the solution for 20 minutes. Grubbs catalyst, 2nd generation (279 mg, 329 µmol) was then added and the mixture was refluxed for 15 h. The solvent volume was then reduced to ~ 200 mL in vacuo, cysteine (2.0 g, 16.5 mmol) and sodium hydroxide (2.63 g, 66 mmol) in water (100 mL) were added and the biphasic mixture was stirred for 20 h at 50 °C. The organic layer was dried over $MgSO_4$, filtered and evaporated. The dark residue obtained was extracted with boiling hexane (3 times). Evaporation of the hexane afforded a lightly red oil which was purified by flash chromatography using hexane/acetone (7/3 followed by 6/4) to afford a golden oil of **9a** as a 85/15 mixture of Z/E isomers (502 mg, 52%). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.25 (m, 6H), 1.57 (m, 12H), 2.32 (m, 8H), 2.42 (m, 2H), 3.58 (m, 6H), 4.10 (d, 1.7H, J = 5.4 Hz), 4.24 (d, 0.3H, J = 5.4), 4.75 (s, 6H), 4.77 (s, 2H), 5.47 (m, 1H), 5.65 (m, 1H), 7.34 (m, 20H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.3, 24.4, 24.5, 26.4, 26.5, 26.8, 27.2, 31.8, 32.3, 45.1, 76.2, 76.3, 124.8, 128.7, 128.8, 128.9(2), 129.3, 129.4, 174.8. ESI-MS: m/z = 875.4 $[M+H]^+$; 697.3 $[M+Na]^+$.

Compound **8b** was treated using the same procedure and afforded a colorless oil of **9b** (55%) as a mixture of the Z/E isomers (92/8). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.25 (m, 12H), 1.57 (m, 12H), 1.67 (m, 2H), 2.03 (m, 2H), 2.31 (m, 8H), 3.59 (m, 6H), 4.12 (d, 1.85H, J = 4.8 Hz), 4.23 (d, 0.15H, J = 6.0 Hz), 4.73 (s, 2H), 4.76 (s, 6H), 5.47 (m, 1H), 5.58 (m, 1H), 7.35 (m, 20H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 23.9, 24.4, 24.5, 26.4, 26.5, 26.8, 29.0, 29.3, 31.0, 31.6, 31.7, 32.3, 45.2, 124.7, 128.7, 128.7, 128.8, 129.2(2), 134.2, 134.8, 174.8. ESI-MS: m/z = 931.4 $[M+H]^+$; 953.4 $[M+Na]^+$.

Compound **8c** was treated using the same procedure and afforded a colorless oil of **9c** (58%) as a mixture of the Z/E isomers (88/12). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 1.26 (m, 18H), 1.37 (m, 2H), 2.04 (m, 2H), 2.34 (m, 8H), 3.59 (m, 6H), 4.13 (d, 1.76H, J = 5.7 Hz), 4.23 (d, 0.24H, J = 6.6 Hz), 4.77 (s, 6H), 4.79 (s, 2H), 5.46 (m, 1H), 5.60 (m, 1H), 7.36 (m, 20H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 24.3, 24.6, 24.7, 26.6, 27.0, 28.7, 29.1(2), 29.2, 29.3, 29.4, 29.8, 32.1, 32.3, 32.5, 45.5, 76.3, 124.3, 128.7, 128.8, 128.9, 129.0, 129.2, 129.3, 134.7, 134.9, 175.0. ESI-MS: m/z = 988.4 $[M+H]^+$.

Macrocyclic tetrahydroxamic acid chelators C5-7.



Compound **9a** (494 mg, 575 µmol) was dissolved in MeOH (50 mL) and hydrogenated in a Paar apparatus at 30 psi H_2 in the presence of 10% Pd/C (25 mg) for 48 h. Pd/C was removed by centrifugation at 8500 rpm. The supernatant was then centrifugated a second time and the solvent evaporated. The oily residue was dissolved in the minimum amount of MeOH, Et_2O was added until the solution became cloudy and placed in the fridge at 4 °C. **C5** precipitated as a white solid that was filtered and washed with Et_2O (268 mg, 92%). ^{1}H NMR (DMSO, 300 MHz, ppm): δ 1.20 (m, 8H), 1.49 (m, 16H), 2.32 (m, 8H), 3.47 (t, 8H, J = 6.6 Hz), 9.50 (s, 4H). ^{13}C NMR (DMSO, 75 MHz, ppm): δ 23.9, 25.7, 26.1, 31.5, 46.8, 172.5. ESI-MS: m/z = 517.2 $[M+H]^+$; 539.2 $[M+Na]^+$; 515.2 $[M-H]^-$. Elemental analyses: Calculated for $C_{24}H_{44}N_4O_8$: C, 55.80; H, 8.58; N, 10.84%. Found: C, 55.74; H, 8.80; N, 9.64. Mp: 150 °C.

Compound **9b** was hydrogenated using the same procedure. A white precipitate formed that was dissolved in hot isopropyl alcohol. The Pd/C was then removed by centrifugation at 8500 rpm. The supernatant was centrifugated a second time and the solvent evaporated to leave **C6** as a white solid (92%). ^{1}H NMR (DMSO, 300 MHz, ppm): δ 1.23 (m, 16H), 1.49 (m, 16H), 2.31 (t, 8H, J = 7.2 Hz), 3.46 (t, 8H, J = 6.6 Hz), 9.52 (s, 4H). ^{13}C NMR (DMSO, 75 MHz, ppm): δ 24.2, 25.8, 26.1, 28.4, 31.6, 48.9, 172.6. ESI-MS: m/z = 573.3 $[M+H]^+$; 595.3 $[M+Na]^+$; 571.3 $[M-H]^-$; 607.2 $[M+Cl]^-$. Elemental analyses: Calculated for $C_{28}H_{52}N_4O_8$: C, 58.72; H, 9.15; N, 9.78%. Found: C, 58.08; H, 8.93; N, 9.37. Mp: 167 °C.

Compound **9c** was hydrogenated using the same procedure. A white precipitate formed that was dissolved in hot isopropyl alcohol. The Pd/C was then removed by centrifugation at 8500 rpm. The supernatant was centrifugated a second time and the solvent evaporated to leave **C7** as a white solid (95%). ^{1}H NMR (DMSO, 300 MHz, ppm): δ 1.24 (m, 24H), 1.48 (m, 16H), 2.32 (t, 8H, J = 7.2 Hz), 3.47 (t, 8H, J = 6.6 Hz), 9.51 (s, 4H). ^{13}C NMR (DMSO, 75 MHz, ppm): δ 24.2, 25.9, 26.2, 28.4, 28.7, 31.6, 46.8, 172.6. ESI-MS: m/z = 629.3 $[M+H]^+$; 651.3 $[M+Na]^+$; 627.2 $[M-H]^-$; 663.2 $[M+Cl]^-$. Elemental analyses: Calculated for $C_{32}H_{60}N_4O_8$: C, 61.12; H, 9.62; N, 8.91%. Found: C, 60.96; H, 9.98; N, 8.60. Mp: 172 °C.

2. Examples of TLC obtained with ^{89}Zr complexes

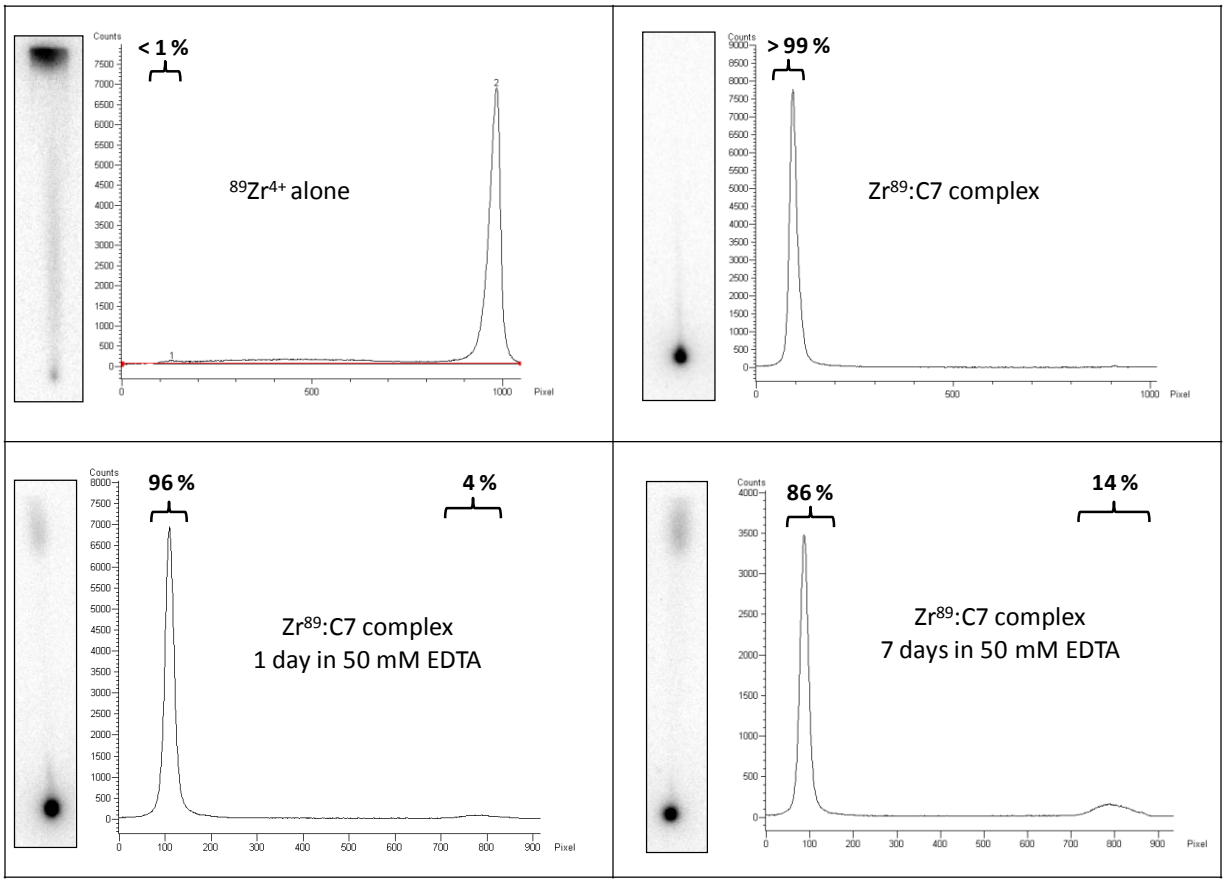


Figure S1 : Representative radio-TLCs and corresponding chromatograms of Free ^{89}Zr in water at pH 7 and its C7 complex at various times of incubation in 50 mM EDTA at 37 °C.

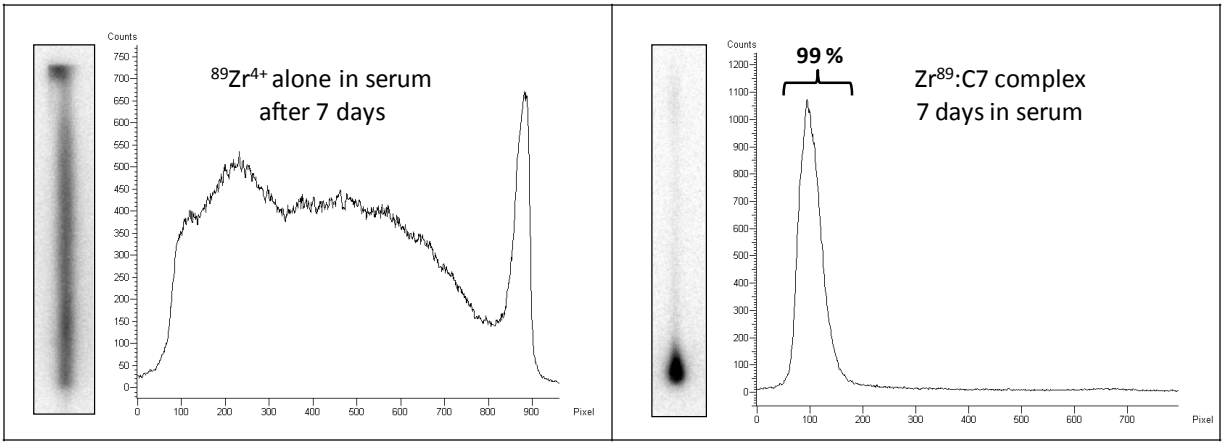


Figure S2 : Representative radio-TLCs and corresponding chromatograms of free ^{89}Zr and its C7 complex after 7 days incubation in serum at 37 °C.

3. Quantum Chemical Study: coordinates of free ligands and their ^{89}Zr complexes

Table S1-A: N-methyl acetohydroxamic acid (Me-AHA)

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-0.624	0.393	0.987
C	0.316	-0.779	0.982
O	-0.753	1.167	1.943
N	-1.339	0.622	-0.148
O	-2.286	1.649	-0.049
C	-1.656	-0.278	-1.219
H	-2.085	1.994	0.856
H	-0.231	-1.727	1.049
H	0.938	-0.817	0.081
H	0.966	-0.697	1.855
H	-2.622	-0.773	-1.049
H	-1.705	0.278	-2.161
H	-0.869	-1.031	-1.294

Table S1-B: $Zr(Me\text{-}AHA)_4$

	Coordinates (Angstroms)		
	X	Y	Z
ZR	15.76	1.878	2.587
C	15.177	4.54	6.123
H	14.497	3.891	6.678
H	14.613	5.426	5.804
H	15.974	4.873	6.797
O	15.173	2.667	4.619
N	16.701	4.242	4.216
C	15.69	3.775	4.944
O	17.126	3.486	3.174
C	17.355	5.518	4.324
H	18.438	5.366	4.387
H	17.005	6.053	5.209
H	17.139	6.115	3.428
C	17.54	-1.77	4.115
H	17.639	-1.621	5.197
H	18.412	-2.307	3.735
H	16.636	-2.365	3.928
O	16.388	0.265	3.929
N	17.414	-0.492	3.468
C	18.109	-0.024	2.435
O	17.77	1.086	1.931
C	19.269	-0.791	1.881
H	19.803	-0.142	1.185
H	18.929	-1.675	1.327
H	19.968	-1.127	2.655
C	14.082	-2.066	1.093
H	13.144	-2.119	0.528
H	14.029	-2.814	1.893
H	14.902	-2.334	0.425
O	15.413	-0.073	1.346
C	14.349	-0.691	1.631
N	13.463	-0.098	2.426
O	13.742	1.156	2.854
C	12.204	-0.61	2.9
H	11.394	0.052	2.573
H	12.213	-0.637	3.995
H	12.035	-1.617	2.51
O	15.962	2.604	0.563
C	15.961	4.374	-0.971
H	15.569	5.382	-1.125
H	15.606	3.714	-1.772
H	17.056	4.398	-0.999
N	15.528	3.86	0.301
C	14.765	4.452	1.214
O	14.513	3.832	2.286
C	14.221	5.829	0.968
H	13.626	5.886	0.05
H	15.021	6.576	0.89
H	13.581	6.097	1.811

Table S2-A: C5

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.804	-3.314	-1.348
O	-0.453	-3.59	-1.902

O	0.837	-1.476	-2.631	H	-3.744	3.649	0.473
C	1.395	-2.167	-1.774	C	-4.857	1.84	0.888
C	1.162	-4.317	-0.37	H	-5.845	2.137	0.508
C	2.726	-1.775	-1.164	C	-4.74	0.31	0.906
H	3.526	-2.371	-1.632	C	-3.701	-1.693	-0.303
C	2.98	-0.288	-1.385	C	-4.495	-0.386	-0.436
H	2.201	0.28	-0.858	H	-3.924	-2.195	0.645
H	2.821	-0.068	-2.447	C	-1.31	-1.471	0.595
H	2.745	-2.011	-0.092	H	5.109	-0.381	-1.593
H	2.215	-4.155	-0.109	H	4.5	1.231	-1.278
H	1.098	-5.292	-0.873	C	4.769	0.02	0.482
C	0.265	-4.29	0.871	H	5.862	0.084	0.577
C	0.705	-3.242	1.896	H	4.492	-0.975	0.853
C	-0.401	-2.549	2.701	C	4.204	1.073	1.428
H	1.271	-2.47	1.368	H	4.587	0.9	2.447
H	1.413	-3.696	2.605	H	4.521	2.074	1.117
H	0.245	-5.294	1.319	H	-2.177	4.114	-1.427
H	-0.757	-4.105	0.513	H	-1.043	3.407	-2.584
N	2.759	1.091	1.47	H	-0.153	5.2	-0.856
N	-1.665	2.158	-1.043	H	-0.252	3.896	0.328
N	-2.266	-1.485	-0.369	H	1.248	2.52	-1.294
O	2.236	-0.183	1.698	H	1.473	3.993	-2.205
O	0.653	1.824	1.341	H	-4.826	2.18	1.931
O	-0.575	1.27	-1.097	H	-5.448	-0.6	-0.939
O	-2.098	1.198	0.973	H	-3.937	0.257	-1.132
O	-1.896	-1.067	-1.649	H	-3.925	0.042	1.587
O	-0.187	-1	0.363	H	-5.658	-0.092	1.359
C	1.866	2.095	1.33	H	-3.956	-2.389	-1.114
C	2.345	3.519	1.165	C	-1.647	-2.116	1.919
H	3.301	3.696	1.673	H	0.04	-1.67	3.189
H	1.597	4.119	1.697	H	-0.746	-3.202	3.515
C	2.442	3.997	-0.293	H	-2.307	-2.978	1.751
H	3.363	3.594	-0.741	H	-2.226	-1.404	2.527
H	2.573	5.09	-0.273	C	1.272	3.61	-1.193
C	-0.104	4.106	-0.741	C	4.378	0.175	-0.986
C	-1.279	3.489	-1.514	H	-0.755	-2.697	-2.202
C	-2.447	1.974	0.094	H	1.287	-0.118	1.412
C	-3.811	2.626	0.074	H	-1.23	-0.339	-1.511
H	-4.13	2.732	-0.971	H	-0.311	1.116	-0.152

Table S2-B: Zr-**C5**

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	-0.231	0.039	-0.187
N	1.626	-1.928	-1.356
O	0.288	-1.732	-1.285
O	1.745	0.304	-1.336
C	2.351	-0.812	-1.435
C	2.013	-3.345	-1.37
C	3.824	-0.842	-1.713
H	3.933	-0.694	-2.798
C	4.607	0.249	-0.971
H	3.934	1.101	-0.803
H	5.409	0.616	-1.625
H	4.244	-1.837	-1.508
H	2.979	-3.439	-0.855
H	2.155	-3.673	-2.411
C	0.943	-4.204	-0.692
C	0.761	-3.884	0.792
C	-0.55	-4.318	1.467
H	0.887	-2.807	0.945
H	1.578	-4.359	1.358
H	1.235	-5.256	-0.834
H	0.004	-4.061	-1.239
N	2.228	0.717	1.441
N	-1.888	2.412	-0.978
N	-2.537	-1.884	-0.511
O	1.422	-0.371	1.265
O	0.426	1.88	0.896
O	-0.834	1.642	-1.409
O	-2.031	1.052	0.839
O	-2.09	-0.724	-1.047
O	-1.003	-1.592	1.112
C	1.636	1.901	1.259
C	2.244	3.261	1.406
H	3.287	3.233	1.744
H	1.671	3.747	2.21
C	2.153	4.13	0.121
H	3.046	3.917	-0.484
H	2.261	5.177	0.443
C	-0.442	4.367	-0.304
C	-1.621	3.844	-1.152
C	-2.544	1.943	0.13
C	-3.994	2.313	0.337
H	-4.443	2.473	-0.651
H	-4.082	3.277	0.861
C	-4.796	1.265	1.141
H	-5.858	1.517	0.995
C	-4.579	-0.239	0.895
C	-3.962	-2.09	-0.772
C	-4.726	-0.775	-0.53
H	-4.313	-2.897	-0.115
C	-1.862	-2.344	0.558
H	5.93	-1.045	0.108
H	5.874	0.592	0.73
C	4.291	-0.68	1.436
H	4.885	-1.175	2.215
H	3.585	-1.44	1.068
C	3.476	0.414	2.12
H	3.211	0.089	3.137
H	4.05	1.346	2.205
H	-2.544	4.373	-0.882
H	-1.441	4.01	-2.223
H	-0.532	5.465	-0.266
H	-0.578	4.005	0.723
H	0.922	2.963	-1.209
H	1.175	4.619	-1.7
H	-4.599	1.431	2.209
H	-5.782	-0.95	-0.784
H	-4.342	-0.049	-1.256
H	-3.581	-0.491	1.265
H	-5.286	-0.769	1.552
H	-4.092	-2.409	-1.815
C	-1.906	-3.802	0.929
H	-0.471	-4.011	2.517
H	-0.619	-5.417	1.48
H	-2.226	-4.377	0.049
H	-2.664	-3.991	1.705
C	0.952	3.985	-0.827
C	5.24	-0.218	0.335

Table S3-A: L5

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.112	1.521	-2.031
O	-1.487	0.366	-2.292
O	1.119	0.85	-2.341
N	0.198	1.83	-1.962
C	0.849	3.101	-1.746
C	-2.094	2.653	-1.792
H	-2.008	3.365	-2.627
C	-3.531	2.163	-1.67
H	-3.768	1.538	-2.539
H	-4.202	3.035	-1.711
H	-1.801	3.21	-0.893
H	1.681	2.913	-1.054
H	0.14	3.749	-1.218
C	1.337	3.756	-3.032
C	1.387	0.778	3.474
C	1.718	2.254	3.643
H	0.481	3.928	-3.702
H	2.001	3.056	-3.554
N	-1.898	0.774	1.794
N	-0.881	-3.171	-1.735
N	3.398	-0.106	0.409
O	-1.018	1.657	1.163
O	-0.537	-0.962	1.306
O	-1.574	-2.354	-2.628
O	0.816	-1.686	-1.667
O	3.535	0.364	-0.896
O	1.606	1.218	0.675
C	-1.611	-0.554	1.769
C	-2.645	-1.493	2.358
H	-3.107	-1.073	3.26
H	-2.086	-2.379	2.681
C	-3.732	-1.891	1.352
H	-4.379	-1.023	1.152
H	-4.377	-2.649	1.822
C	-2.392	-3.699	0.166
C	-1.741	-4.172	-1.129
C	0.329	-2.76	-1.292
C	1.072	-3.723	-0.382
H	1.311	-4.629	-0.962
H	0.404	-4.05	0.426
C	2.335	-3.126	0.223
H	2.721	-3.83	0.979
C	4.438	-1.039	0.793
C	4.68	-2.157	-0.217
H	5.378	-0.492	0.975
C	2.42	0.426	1.176
H	-4.774	0.887	-0.451
H	-3.056	0.55	-0.359
C	-3.686	2.209	0.88
H	-4.664	2.629	1.155
H	-3.028	3.07	0.713
C	-3.148	1.447	2.088
H	-2.988	2.139	2.929
H	-3.856	0.682	2.42
H	-1.146	-5.077	-0.959
H	-2.491	-4.418	-1.889
H	-3.038	-4.507	0.547
H	-1.601	-3.554	0.917
H	-2.551	-1.637	-0.429
H	-4.018	-2.558	-0.681
H	2.038	-2.219	0.763
H	5.303	-2.904	0.3
H	5.288	-1.771	-1.044
C	3.423	-2.798	-0.794
H	3.003	-2.122	-1.543
H	3.711	-3.716	-1.329
H	4.123	-1.465	1.75
C	2.378	-0.008	2.63
H	1.81	2.718	2.652
H	2.702	2.358	4.129
C	0.658	2.981	4.451
H	-0.318	2.913	3.952
H	0.894	4.044	4.577
H	0.384	0.678	3.043
H	1.335	0.302	4.465
H	3.385	0.083	3.065
H	2.125	-1.078	2.666
C	-3.188	-2.409	0.026
C	-3.787	1.369	-0.393
C	2.059	5.062	-2.75
H	2.416	5.532	-3.673
H	2.93	4.901	-2.103

H	1.405	5.784	-2.244
H	0.547	2.545	5.454
H	-0.153	1.174	1.051
H	2.609	0.556	-1.196
H	-1.29	-1.425	-2.44
H	0.673	-0.019	-2.163

Table S3-B: Zr-**L5**

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	0.11	0.052	-0.127
C	-2.572	1.155	-1.138
O	-2.056	0.01	-0.97
O	-0.442	1.966	-0.944
N	-1.768	2.216	-1.086
C	-2.058	3.601	-1.404
C	-4.051	1.333	-1.37
H	-4.235	1.447	-2.449
C	-4.915	0.192	-0.829
H	-4.862	-0.663	-1.516
H	-5.959	0.538	-0.854
H	-4.374	2.279	-0.918
H	-1.562	4.208	-0.635
H	-3.138	3.767	-1.311
C	-1.564	3.989	-2.79
C	3.649	1.765	2.945
C	3.174	3.209	2.858
H	-2.087	3.379	-3.542
H	-0.502	3.723	-2.858
N	-1.97	-0.223	2.095
N	0.636	-2.734	-1.266
N	2.977	0.835	-0.615
O	-1.237	0.768	1.522
O	-0.442	-1.614	1.283
O	-0.185	-1.649	-1.401
O	1.863	-1.475	0.134
O	1.848	0.729	-1.357
O	1.653	0.958	1.188
C	-1.522	-1.466	1.935
C	-2.198	-2.712	2.425
H	-2.894	-2.526	3.252
H	-1.388	-3.332	2.833
C	-2.929	-3.49	1.306
H	-3.934	-3.061	1.187
H	-3.085	-4.519	1.667
C	-0.944	-4.295	-0.13
C	-0.065	-4.01	-1.356
C	1.737	-2.543	-0.509
C	2.961	-3.393	-0.715
H	2.782	-4.173	-1.467
H	3.268	-3.886	0.217
C	4.063	-2.415	-1.181
H	4.982	-2.976	-1.402
C	4.257	0.727	-1.312
C	4.253	-0.187	-2.535
H	4.584	1.731	-1.628
C	2.83	0.99	0.696
H	-5.358	-0.923	0.963
H	-3.679	-0.969	0.446
C	-4.16	0.764	1.592
H	-5.047	1.198	2.075
H	-3.623	1.596	1.119
C	-3.231	0.213	2.669
H	-3.001	0.982	3.418
H	-3.681	-0.644	3.184
H	0.7	-4.791	-1.459
H	-0.655	-3.99	-2.282
H	-1.167	-5.373	-0.117
H	-0.338	-4.091	0.765
H	-2.08	-2.476	-0.406
H	-2.963	-3.937	-0.789
H	4.288	-1.762	-0.328
H	5.306	-0.265	-2.846
H	3.73	0.325	-3.352
C	3.622	-1.57	-2.383
H	2.54	-1.405	-2.343
H	3.801	-2.131	-3.312
H	4.988	0.369	-0.578
C	4.023	1.172	1.594
H	2.309	3.26	2.183
H	3.964	3.824	2.398
C	2.8	3.781	4.214
H	1.984	3.206	4.67

H	2.467	4.823	4.14
H	2.862	1.149	3.4
H	4.524	1.704	3.609
H	4.779	1.804	1.105
H	4.495	0.185	1.732
C	-2.254	-3.504	-0.067
C	-4.539	-0.302	0.568
C	-1.772	5.466	-3.068
H	-1.413	5.741	-4.066
H	-1.233	6.088	-2.342
H	-2.833	5.745	-3.013
H	3.649	3.753	4.91
ZR	0.11	0.052	-0.127
C	-2.572	1.155	-1.138
O	-2.056	0.01	-0.97
O	-0.442	1.966	-0.944
N	-1.768	2.216	-1.086
C	-2.058	3.601	-1.404
C	-4.051	1.333	-1.37

Table S4-A: C6

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-3.335	-0.237	-2.194
O	-2.389	0.63	-2.736
O	-1.737	-1.823	-1.964
C	-2.91	-1.476	-1.822
C	-4.601	0.434	-1.979
C	-3.955	-2.423	-1.245
H	-4.448	-2.934	-2.086
C	-3.304	-3.438	-0.317
C	-2.699	-2.793	0.921
H	-3.49	-2.319	1.526
H	-2.032	-1.979	0.604
H	-2.511	-3.96	-0.871
H	-4.045	-4.198	-0.027
H	-4.746	-1.883	-0.709
H	-5.384	-0.328	-1.895
H	-4.809	1.006	-2.892
C	-4.597	1.351	-0.759
C	-4.545	0.581	0.553
C	-2.94	1.713	2.263
C	-4.375	1.43	1.814
H	-3.725	-0.149	0.508
H	-5.476	-0.003	0.637
H	-5.502	1.977	-0.789
H	-3.747	2.042	-0.858
N	0.352	-1.783	1.312
N	4.055	0.352	-0.911
N	-0.771	2.842	-0.626
O	0.041	-0.513	1.806
O	1.133	-0.795	-0.562
O	3.493	-0.375	-1.964
O	2.426	1.884	-1.246
O	-0.222	2.264	-1.762
O	-1.534	0.807	-0.005
C	0.925	-1.836	0.078
C	1.242	-3.198	-0.493
H	0.562	-3.334	-1.345
H	1.017	-4.005	0.212
C	2.702	-3.268	-0.949
H	2.816	-2.716	-1.89
H	2.959	-4.312	-1.176
C	3.668	-2.68	0.073
C	5.762	-1.235	0.081
C	5.461	0.009	-0.748
C	3.432	1.531	-0.622
C	3.887	2.289	0.599
H	3.862	3.359	0.35
H	4.916	2.048	0.89
C	2.961	2.005	1.793
H	3.397	2.498	2.675
C	1.512	2.457	1.631
C	-0.415	4.241	-0.439
C	1.022	4.466	0.025
H	-1.124	4.671	0.278
C	-1.461	2.028	0.205
H	-2.636	-4.485	2.25
H	-1.28	-4.396	1.144
C	-1.076	-3.114	2.869
H	-0.952	-3.783	3.733
H	-1.578	-2.212	3.248
C	0.324	-2.744	2.399
H	0.9	-2.301	3.225

H	0.866	-3.637	2.074
H	5.97	0.879	-0.321
H	5.856	-0.12	-1.767
H	6.857	-1.341	0.081
H	5.473	-1.058	1.129
H	5.115	-2.513	-1.526
H	5.711	-3.386	-0.125
H	3.296	-1.687	0.362
H	3.653	-3.278	0.999
H	2.974	0.924	2.001
H	1.194	5.551	-0.025
H	1.706	4.006	-0.7
C	1.337	3.976	1.441
H	2.254	4.481	1.783
H	0.55	4.348	2.117
H	1.069	1.894	0.802
H	0.969	2.126	2.527
H	-0.583	4.736	-1.404
C	-2.128	2.678	1.404
H	-4.916	2.384	1.698
H	-4.871	0.915	2.649
H	-2.393	0.763	2.354
H	-2.986	2.138	3.275
H	-2.763	3.51	1.063
H	-1.342	3.143	2.016
C	5.106	-2.52	-0.426
C	-1.929	-3.779	1.79
H	0.676	1.934	-1.509
H	2.552	-0.507	-1.671
H	-1.631	0.614	-2.106
H	-0.456	-0.08	1.067

Table S4-B: Zr-**C6**

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	-0.062	0.073	-0.508
N	-2.59	1.282	-1.626
O	-1.316	1.652	-1.34
O	-1.756	-0.781	-1.766
C	-2.767	-0.013	-1.862
C	-3.626	2.324	-1.513
C	-4.126	-0.6	-2.096
H	-4.115	-1.133	-3.056
C	-4.452	-1.574	-0.955
C	-4.393	-0.889	0.403
H	-5.198	-0.14	0.482
H	-3.453	-0.323	0.463
H	-3.71	-2.386	-0.979
H	-5.435	-2.034	-1.134
H	-4.891	0.183	-2.168
H	-4.365	1.996	-0.766
H	-4.146	2.408	-2.478
C	-3.031	3.664	-1.117
C	-2.453	3.717	0.303
C	-0.405	4.445	1.687
C	-1.209	4.598	0.383
H	-2.17	2.707	0.628
H	-3.217	4.073	1.012
H	-3.82	4.417	-1.247
H	-2.246	3.912	-1.842
N	-1.52	-1.527	1.696
N	2.483	-1.315	-1.216
N	1.769	2.536	-0.452
O	-1.346	-0.251	1.241
O	-0.286	-2.162	-0.033
O	1.261	-1.08	-1.771
O	1.757	-0.479	0.75
O	1.511	1.436	-1.2
O	0.151	1.831	0.912
C	-0.901	-2.49	1.011
C	-0.847	-3.929	1.463
H	-1.862	-4.331	1.598
H	-0.371	-3.978	2.456
C	-0.072	-4.777	0.453
H	-0.588	-4.698	-0.514
H	-0.154	-5.829	0.757
C	1.406	-4.384	0.262
C	3.218	-3.693	-1.431
C	3.308	-2.26	-1.962
C	2.699	-0.959	0.052
C	4.095	-1.046	0.616
H	4.818	-0.737	-0.153
H	4.343	-2.095	0.843
C	4.273	-0.215	1.885

H	5.313	-0.351	2.221
C	3.968	1.281	1.795
C	3.033	3.165	-0.802
C	4.226	2.219	-0.641
H	3.157	4.066	-0.189
C	1.011	2.717	0.628
H	-5.49	-2.06	1.868
H	-3.98	-2.785	1.35
C	-3.724	-1.223	2.823
H	-4.211	-1.508	3.765
H	-3.767	-0.126	2.773
C	-2.263	-1.659	2.932
H	-1.744	-1.079	3.708
H	-2.212	-2.718	3.214
H	4.35	-1.909	-1.954
H	2.944	-2.194	-2.992
H	3.764	-4.333	-2.139
H	3.782	-3.762	-0.487
H	1.068	-3.498	-1.652
H	1.643	-5.162	-1.731
H	1.615	-3.444	0.793
H	2.062	-5.142	0.72
H	3.636	-0.643	2.67
H	5.025	2.605	-1.291
H	3.931	1.249	-1.064
C	4.788	2.082	0.776
H	5.798	1.645	0.71
H	4.946	3.1	1.169
H	2.895	1.408	1.618
H	4.157	1.697	2.796
H	2.948	3.476	-1.852
C	1.038	3.984	1.437
H	-0.568	4.326	-0.471
H	-1.484	5.651	0.217
H	-0.891	3.702	2.331
H	-0.377	5.383	2.255
H	1.6	4.769	0.915
H	1.55	3.802	2.394
C	1.783	-4.204	-1.209
C	-4.448	-1.822	1.613

Table S5-A: L6

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	2.624	-2.369	0.522
O	1.553	-2.791	0.056
O	1.451	-1.107	2.1
N	2.67	-1.488	1.547
C	3.844	-0.923	2.208
C	3.936	-2.791	-0.109
H	4.154	-3.824	0.195
C	3.823	-2.695	-1.635
C	3.28	-1.33	-2.099
H	3.998	-0.825	-2.764
H	3.184	-0.667	-1.222
H	3.152	-3.49	-1.985
H	4.809	-2.906	-2.069
H	4.774	-2.178	0.244
H	3.474	-0.04	2.738
H	4.542	-0.554	1.445
C	4.518	-1.891	3.169
C	6.579	2.186	-1.737
C	3.572	2.483	-1.199
C	4.645	2.619	-0.124
H	6.829	3.256	-1.755
H	7.51	1.627	-1.886
H	5.388	-1.381	3.609
H	4.921	-2.744	2.601
N	-0.741	-1.105	-1.523
N	-3.491	-0.234	1.352
N	0.232	2.408	0.55
O	-0.107	-0.713	-0.349
O	-2.028	-2.481	-0.285
O	-2.215	-0.681	1.679
O	-2.65	0.997	-0.367
O	-0.409	1.594	1.474
O	2.093	1.106	0.696
C	-1.801	-1.93	-1.373
C	-2.705	-2.18	-2.563
H	-2.177	-2.789	-3.312
H	-2.933	-1.221	-3.053
C	-3.998	-2.858	-2.115
H	-3.747	-3.813	-1.637

H	-4.585	-3.102	-3.01
C	-4.82	-1.991	-1.142
C	-5.614	-1.635	1.274
C	-4.582	-0.855	2.099
C	-3.585	0.734	0.399
C	-4.896	1.498	0.418
H	-5.167	1.663	1.471
H	-5.697	0.862	0.014
C	-4.907	2.831	-0.331
H	-5.791	3.378	0.027
C	-3.657	3.712	-0.218
C	-0.577	3.468	-0.04
C	-1.466	4.226	0.95
H	0.124	4.169	-0.499
C	1.507	2.085	0.218
H	2.002	-1.801	-3.792
H	1.327	-2.172	-2.215
C	1.13	-0.101	-2.747
H	1.358	0.524	-3.623
H	1.439	0.474	-1.865
C	-0.382	-0.28	-2.665
H	-0.883	0.7	-2.578
H	-0.772	-0.782	-3.559
H	-5.093	-0.097	2.715
H	-4.073	-1.532	2.79
H	-6.224	-2.179	2.009
H	-6.314	-0.945	0.781
H	-4.086	-3.016	0.602
H	-5.718	-3.467	0.137
H	-4.315	-1.023	-1.032
H	-5.803	-1.754	-1.58
H	-5.091	2.645	-1.398
H	-1.524	5.268	0.6
H	-0.965	4.256	1.926
C	-2.89	3.689	1.103
H	-2.831	2.676	1.518
H	-3.414	4.293	1.859
H	-2.98	3.406	-1.021
H	-3.941	4.75	-0.449
H	-1.176	3.031	-0.852
C	2.196	2.989	-0.797
H	4.233	2.293	0.839
H	4.917	3.681	-0.007
C	5.896	1.802	-0.433
H	5.618	0.736	-0.47
H	6.608	1.901	0.399
H	3.486	1.425	-1.486
H	3.883	3.021	-2.106
H	2.266	4.011	-0.392
H	1.557	3.069	-1.689
C	-5.038	-2.608	0.241
C	1.905	-1.418	-2.764
C	3.586	-2.388	4.26
H	5.937	1.986	-2.605
H	4.097	-3.083	4.936
H	2.719	-2.907	3.835
H	3.198	-1.557	4.861
H	-0.877	0.893	0.953
H	-1.975	-1.366	0.995
H	1.322	-0.193	1.728
H	0.409	-1.517	-0.046

Table S5-B: Zr-**L6**

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	-0.35	-0.04	0.34
C	2.15	-1.381	1.322
O	1.118	-1.723	0.671
O	0.836	0.298	2.151
N	2.044	-0.327	2.127
C	3.064	0.227	2.998
C	3.448	-2.117	1.116
H	3.79	-2.57	2.059
C	3.31	-3.181	0.028
C	2.905	-2.633	-1.354
H	3.761	-2.674	-2.047
H	2.624	-1.574	-1.271
H	2.556	-3.908	0.36
H	4.258	-3.733	-0.031
H	4.225	-1.388	0.837
H	2.968	1.319	2.92
H	4.042	-0.052	2.585
C	2.947	-0.231	4.447
C	6.993	0.988	-1.313

C	3.98	1.74	-1.679
C	4.658	1.4	-0.357
H	7.351	1.939	-0.898
H	7.841	0.293	-1.326
H	3.802	0.194	4.994
H	3.074	-1.323	4.484
N	-0.829	-1.906	-1.997
N	-3.148	0.762	1.213
N	0.563	2.774	-0.485
O	-0.065	-0.829	-1.667
O	-1.535	-1.941	0.128
O	-1.976	0.26	1.706
O	-2.293	0.537	-0.85
O	-0.462	2.096	0.077
O	1.626	0.81	-0.521
C	-1.576	-2.445	-1.03
C	-2.556	-3.56	-1.3
H	-2.025	-4.521	-1.377
H	-3.041	-3.4	-2.274
C	-3.592	-3.625	-0.176
H	-3.061	-3.864	0.754
H	-4.264	-4.471	-0.372
C	-4.396	-2.327	0.03
C	-5.198	-0.564	1.732
C	-4.296	0.615	2.103
C	-3.233	0.933	-0.115
C	-4.382	1.723	-0.683
H	-4.808	2.355	0.109
H	-5.19	1.041	-0.99
C	-3.98	2.581	-1.895
H	-4.797	3.3	-2.061
C	-2.638	3.315	-1.811
C	0.19	4.051	-1.097
C	-0.996	4.746	-0.434
H	1.068	4.709	-1.05
C	1.63	2.041	-0.812
H	1.978	-4.422	-2.155
H	0.937	-3.4	-1.174
C	1.141	-2.711	-3.216
H	1.423	-3.258	-4.126
H	1.558	-1.701	-3.314
C	-0.384	-2.571	-3.213
H	-0.71	-1.984	-4.084
H	-0.881	-3.548	-3.257
H	-4.869	1.553	2.115
H	-3.858	0.485	3.096
H	-5.943	-0.666	2.534
H	-5.778	-0.301	0.832
H	-3.421	-1.805	1.861
H	-4.926	-2.691	2.083
H	-3.946	-1.516	-0.561
H	-5.42	-2.448	-0.357
H	-3.954	1.941	-2.786
H	-1.051	5.728	-0.927
H	-0.751	4.948	0.617
C	-2.375	4.068	-0.514
H	-2.468	3.372	0.327
H	-3.144	4.844	-0.365
H	-1.843	2.571	-1.943
H	-2.574	4.005	-2.668
H	-0.026	3.88	-2.164
C	2.788	2.677	-1.533
H	3.905	0.962	0.314
H	5.005	2.329	0.127
C	5.832	0.437	-0.5
H	5.475	-0.5	-0.958
H	6.192	0.162	0.503
H	3.646	0.811	-2.164
H	4.702	2.21	-2.362
H	3.087	3.601	-1.013
H	2.441	3.001	-2.527
C	-4.453	-1.89	1.495
C	1.71	-3.373	-1.955
C	1.644	0.166	5.119
H	6.71	1.172	-2.357
H	1.634	-0.151	6.168
H	0.782	-0.278	4.612
H	1.501	1.253	5.092

Table S6-A: C7

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-3.374	-1.178	-2.193
O	-2.245	-0.536	-2.687

O	-2.08	-2.324	-0.717	C	5.607	-0.975	-1.94
C	-3.196	-2.076	-1.198	C	4.608	0.095	-2.374
C	-4.609	-0.7	-2.799	C	3.477	0.771	-0.213
C	-4.413	-2.821	-0.672	C	4.765	1.444	0.225
H	-4.553	-3.721	-1.289	H	5.113	2.105	-0.583
C	-4.195	-3.196	0.788	H	5.554	0.688	0.335
C	-4.115	-1.968	1.694	C	4.664	2.22	1.536
C	-3.331	-2.214	2.981	H	5.641	2.701	1.687
H	-5.131	-1.611	1.923	C	3.552	3.269	1.634
H	-3.633	-1.146	1.14	C	0.344	3.076	0.538
H	-3.265	-3.773	0.859	C	0.775	4.352	-0.17
H	-5.005	-3.86	1.123	H	1.208	2.428	0.72
H	-5.328	-2.227	-0.775	C	-1.819	1.848	0.112
H	-3.653	-3.168	3.425	H	-1.317	-2.669	3.636
H	-3.577	-1.437	3.723	H	-1.572	-2.87	1.903
H	-5.373	-1.477	-2.686	C	-1.252	-0.834	2.513
H	-4.399	-0.608	-3.871	H	-1.431	-0.2	3.396
C	-5.088	0.632	-2.228	H	-1.778	-0.354	1.675
C	-5.602	0.522	-0.799	C	0.238	-0.812	2.213
C	-3.949	2.175	1.385	H	0.625	0.22	2.181
C	-4.768	2.723	0.211	H	0.793	-1.352	2.989
H	-4.833	0.026	-0.19	H	5.121	1.062	-2.489
H	-6.482	-0.143	-0.786	H	4.164	-0.148	-3.343
H	-5.88	1.02	-2.885	H	6.441	-0.954	-2.657
H	-4.257	1.349	-2.282	H	6.055	-0.669	-0.984
N	0.544	-1.441	0.937	H	3.957	-2.388	-1.78
C	5.548	-3.078	-0.519	H	5.338	-2.996	-2.68
N	3.471	0.26	-1.474	H	4.383	-1.57	0.487
N	-0.586	2.271	-0.237	H	5.52	-2.373	1.551
O	-0.02	-0.743	-0.127	H	5.413	-4.167	-0.591
O	1.996	-2.349	-0.546	H	6.633	-2.92	-0.427
O	2.244	-0.129	-2.006	H	4.548	1.508	2.364
O	2.481	0.712	0.519	H	-0.049	5.081	-0.164
O	-0.02	1.734	-1.386	H	0.967	4.105	-1.223
O	-2.432	0.971	-0.512	C	2.036	4.965	0.438
C	1.667	-2.14	0.629	H	2.238	5.911	-0.081
C	2.483	-2.724	1.768	H	1.854	5.238	1.49
H	1.843	-3.376	2.381	C	3.263	4.043	0.35
H	2.808	-1.907	2.431	H	4.156	4.624	0.074
C	3.69	-3.478	1.223	H	2.635	2.776	1.976
H	3.35	-4.113	0.396	H	3.814	3.986	2.427
H	4.078	-4.154	1.997	H	3.102	3.338	-0.482
C	4.814	-2.555	0.727	H	-0.112	3.292	1.512

C	-2.471	2.529	1.307
H	-4.123	2.821	-0.674
H	-5.107	3.742	0.448
C	-5.972	1.855	-0.15
H	-6.64	2.413	-0.824
H	-6.559	1.661	0.762
H	-4.034	1.08	1.424
H	-4.358	2.547	2.334
H	-2.331	3.618	1.239
H	-1.952	2.215	2.225
C	5.054	-2.402	-1.801
C	-1.819	-2.226	2.761
H	1.982	-0.957	-1.512
H	-2.033	0.14	-1.989
H	0.493	0.942	-1.087
H	-0.77	-1.314	-0.462

Table S6-B: Zr-**C7**

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	-0.1	0.038	0.172
C	2.149	-1.595	1.454
O	1.226	-1.757	0.602
O	1.104	0.375	1.964
N	2.123	-0.49	2.19
C	3.053	-0.075	3.223
C	3.222	-2.641	1.635
H	3.187	-3.02	2.667
C	3.054	-3.788	0.648
C	3.359	-3.429	-0.805
C	2.791	-4.471	-1.77
H	4.448	-3.341	-0.935
H	2.935	-2.441	-1.041
H	2.023	-4.158	0.725
H	3.703	-4.621	0.958
H	4.214	-2.177	1.522
H	3.015	-5.476	-1.38
H	3.301	-4.408	-2.743
H	3.675	-0.94	3.487
H	2.45	0.192	4.1
C	3.908	1.098	2.768
C	4.915	0.715	1.692
C	4.475	1.899	-1.241
C	4.675	2.651	0.072
H	4.399	0.13	0.913
H	5.67	0.043	2.129
H	4.43	1.516	3.641
H	3.227	1.881	2.406
N	-0.817	-2.074	-1.873
C	-4.976	-2.443	1.775
N	-2.747	1.076	1.248
N	0.977	2.708	-0.923
O	-0.029	-0.973	-1.74
O	-1.455	-1.786	0.251
O	-1.542	0.599	1.671
O	-2.104	0.624	-0.851
O	-0.092	2.147	-0.314
O	1.894	0.679	-0.81
C	-1.522	-2.467	-0.813
C	-2.415	-3.684	-0.863
H	-1.786	-4.587	-0.907
H	-3.007	-3.683	-1.79
C	-3.324	-3.738	0.359
H	-2.703	-3.584	1.251
H	-3.752	-4.747	0.448
C	-4.46	-2.712	0.357
C	-4.768	0.046	2.212
C	-3.766	1.191	2.285
C	-2.974	1.095	-0.07
C	-4.191	1.789	-0.617
H	-4.615	2.455	0.146
H	-4.973	1.047	-0.84
C	-3.874	2.573	-1.897
H	-4.756	3.19	-2.129
C	-2.62	3.446	-1.845
C	0.703	4.057	-1.407
C	0.008	4.918	-0.341
H	1.654	4.499	-1.718
C	1.984	1.881	-1.206
H	0.825	-5.277	-2.247
H	0.82	-3.997	-1.034
C	0.951	-3.285	-3.061
H	1.198	-3.69	-4.053
H	1.562	-2.383	-2.922

C	-0.509	-2.846	-3.065
H	-0.72	-2.209	-3.934
H	-1.19	-3.706	-3.1
H	-4.271	2.164	2.192
H	-3.213	1.196	3.229
H	-5.592	0.24	2.917
H	-5.231	0.063	1.212
H	-3.132	-1.367	2.101
H	-4.112	-1.51	3.553
H	-4.102	-1.765	-0.08
H	-5.269	-3.066	-0.299
H	-4.929	-3.379	2.352
H	-6.039	-2.16	1.755
H	-3.765	1.863	-2.727
H	0.634	5.8	-0.148
H	-0.024	4.349	0.595
C	-1.401	5.405	-0.686
H	-1.643	6.21	0.023
H	-1.391	5.886	-1.679
C	-2.533	4.375	-0.638
H	-3.487	4.921	-0.542
H	-1.744	2.788	-1.86
H	-2.586	4.05	-2.766
H	-2.427	3.777	0.281
H	0.075	3.973	-2.307
C	3.202	2.323	-1.967
H	3.694	2.806	0.553
H	5.062	3.659	-0.138
C	5.595	1.919	1.044
H	5.939	2.607	1.831
H	6.5	1.595	0.509
H	4.412	0.818	-1.058
H	5.342	2.054	-1.898
H	3.204	3.405	-2.138
H	3.158	1.847	-2.957
C	-4.169	-1.339	2.469
C	1.283	-4.311	-1.984

Table S7-A: L7

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	3.006	-1.969	0.866
O	1.958	-2.221	0.252
O	1.793	-0.881	2.543
N	3.021	-1.27	2.022
C	4.17	-0.809	2.79
C	4.333	-2.474	0.326
H	4.554	-3.437	0.809
C	4.253	-2.63	-1.185
C	4.077	-1.286	-1.894
C	3.335	-1.391	-3.224
H	5.063	-0.822	-2.05
H	3.531	-0.598	-1.229
H	3.404	-3.287	-1.416
H	5.155	-3.139	-1.553
H	5.16	-1.803	0.598
H	3.762	-2.22	-3.809
H	3.51	-0.48	-3.82
H	3.835	0.109	3.286
H	4.972	-0.52	2.099
C	4.667	-1.826	3.808
C	6.165	1.907	-1.662
C	3.159	2.564	-1.368
C	4.238	2.986	-0.365
H	6.486	2.905	-2.001
C	7.367	0.982	-1.572
H	5.53	-1.388	4.331
H	5.053	-2.709	3.274
N	-0.684	-1.274	-1.212
C	-5.685	-3.237	-0.216
N	-3.802	0.103	1.146
N	0.197	2.19	0.905
O	-0.2	-0.679	-0.047
O	-2.161	-2.386	0.096
O	-2.548	-0.259	1.632
O	-2.904	0.644	-0.876
O	-0.134	1.348	1.965
O	2.158	1.066	0.689
C	-1.782	-2.053	-1.035
C	-2.506	-2.57	-2.265

H	-1.801	-3.136	-2.892
H	-2.834	-1.713	-2.873
C	-3.704	-3.422	-1.859
H	-3.383	-4.104	-1.062
H	-4.006	-4.051	-2.707
C	-4.904	-2.595	-1.372
C	-5.87	-1.286	1.409
C	-4.924	-0.254	2.016
C	-3.872	0.632	-0.11
C	-5.193	1.267	-0.502
H	-5.775	1.528	0.392
H	-5.793	0.523	-1.046
C	-5.014	2.497	-1.399
H	-5.993	2.995	-1.458
C	-3.943	3.493	-0.955
C	-0.934	2.956	0.405
C	-1.525	3.884	1.456
H	-0.596	3.524	-0.469
C	1.381	1.942	0.291
H	1.394	-1.926	-4.017
H	1.632	-2.394	-2.333
C	1.118	-0.324	-2.606
H	1.275	0.472	-3.352
H	1.562	0.041	-1.669
C	-0.378	-0.475	-2.391
H	-0.861	0.507	-2.261
H	-0.845	-0.964	-3.253
H	-5.475	0.658	2.291
H	-4.457	-0.631	2.93
H	-6.742	-1.37	2.073
H	-6.271	-0.879	0.47
H	-4.166	-2.621	1.166
H	-5.553	-3.36	1.951
H	-4.54	-1.61	-1.04
H	-5.568	-2.388	-2.225
H	-5.534	-4.326	-0.236
H	-6.767	-3.085	-0.346
H	-4.776	2.167	-2.418
H	-0.741	4.572	1.806
H	-1.814	3.279	2.327
C	-2.733	4.681	0.967
H	-3.034	5.355	1.78
H	-2.435	5.338	0.133
C	-3.931	3.826	0.535
H	-4.872	4.338	0.793
H	-2.964	3.098	-1.252
H	-4.071	4.426	-1.524
H	-3.928	2.899	1.133
H	-1.678	2.228	0.05
C	1.738	2.828	-0.893
H	3.805	3.026	0.643
H	4.584	4.007	-0.592
C	5.425	2.033	-0.338
H	5.056	1.037	-0.037
H	6.135	2.345	0.444
H	3.255	1.487	-1.564
H	3.31	3.062	-2.336
H	1.603	3.887	-0.625
H	1.022	2.63	-1.706
C	-5.263	-2.673	1.144
C	1.828	-1.593	-3.061
C	3.599	-2.246	4.802
H	5.473	1.537	-2.436
H	3.99	-2.972	5.524
H	2.741	-2.7	4.294
H	3.218	-1.383	5.363
H	7.07	-0.02	-1.231
H	8.105	1.361	-0.852
H	7.874	0.865	-2.536
H	1.592	-0.04	2.053
H	-0.788	0.707	1.589
H	0.582	-1.244	0.22
H	-2.256	-1.058	1.102

Table S7-B: Zr-**L7**

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	-0.355	0.101	-0.036
C	2.139	-1.002	1.365
O	1.29	-1.361	0.494
O	0.755	0.782	1.734
N	1.911	0.133	2.02
C	2.637	0.634	3.174

C	3.35	-1.852	1.656	C	-4.688	1.055	-0.782
H	3.283	-2.233	2.687	H	-5.244	1.575	0.009
C	3.463	-3.012	0.676	H	-5.308	0.192	-1.071
C	3.772	-2.602	-0.763	C	-4.515	1.971	-2.002
C	3.475	-3.737	-1.744	H	-5.499	2.416	-2.215
H	4.829	-2.301	-0.836	C	-3.458	3.069	-1.869
H	3.176	-1.718	-1.036	C	-0.266	4.313	-1.245
H	2.518	-3.572	0.7	C	-1.174	4.924	-0.166
H	4.24	-3.704	1.031	H	0.61	4.94	-1.441
H	4.261	-1.235	1.63	C	1.369	2.398	-1.176
H	3.875	-4.676	-1.333	H	1.737	-4.923	-2.304
H	4.011	-3.573	-2.691	H	1.414	-3.663	-1.114
H	2.608	1.729	3.1	C	1.5	-2.953	-3.143
H	3.683	0.32	3.072	H	1.884	-3.299	-4.114
C	2.064	0.162	4.506	H	1.899	-1.941	-2.985
C	6.492	1.411	-0.194	C	-0.017	-2.832	-3.234
C	3.847	2.474	-1.421	H	-0.308	-2.261	-4.125
C	4.142	2.407	0.076	H	-0.498	-3.817	-3.289
H	6.927	2.393	0.053	H	-4.866	1.26	2.028
C	7.43	0.303	0.252	H	-3.644	0.487	3.048
H	2.731	0.536	5.297	H	-5.786	-0.912	2.658
H	2.129	-0.936	4.55	H	-5.363	-0.962	0.958
N	-0.548	-2.134	-2.077	H	-3.039	-1.964	1.853
C	-4.62	-3.387	1.481	H	-3.984	-2.335	3.289
N	-3.148	0.532	1.069	H	-3.867	-2.53	-0.353
N	0.217	2.993	-0.864	H	-4.723	-4.051	-0.598
O	-0.031	-0.883	-1.931	H	-4.408	-4.303	2.052
O	-1.311	-1.97	0.017	H	-5.718	-3.317	1.432
O	-1.875	0.29	1.49	H	-4.259	1.352	-2.872
O	-2.419	0.315	-1.04	H	-0.758	5.899	0.119
O	-0.776	2.175	-0.449	H	-1.118	4.29	0.728
O	1.463	1.149	-0.99	C	-2.642	5.136	-0.548
C	-1.188	-2.661	-1.034	H	-3.061	5.836	0.189
C	-1.791	-4.045	-1.093	H	-2.696	5.665	-1.515
H	-0.98	-4.788	-1.114	C	-3.552	3.903	-0.596
H	-2.345	-4.178	-2.034	H	-4.594	4.246	-0.474
C	-2.696	-4.292	0.109	H	-2.467	2.604	-1.923
H	-2.143	-4.008	1.014	H	-3.55	3.735	-2.742
H	-2.899	-5.369	0.193	H	-3.334	3.269	0.279
C	-4.025	-3.533	0.077	H	-0.811	4.211	-2.197
C	-4.927	-0.915	1.969	C	2.533	3.182	-1.723
C	-4.177	0.405	2.095	H	3.199	2.237	0.617
C	-3.368	0.574	-0.249	H	4.528	3.379	0.425

C	5.113	1.296	0.442	C	0.636	0.61	4.769
H	4.661	0.336	0.142	H	6.395	1.394	-1.29
H	5.229	1.249	1.537	H	0.305	0.286	5.763
H	3.79	1.453	-1.824	H	-0.058	0.213	4.022
H	4.663	2.981	-1.955	H	0.552	1.704	4.724
H	2.541	4.197	-1.304	H	7.025	-0.685	-0.004
H	2.402	3.3	-2.81	H	7.576	0.321	1.34
C	-4.063	-2.156	2.207	H	8.419	0.384	-0.215
C	1.978	-3.883	-2.035				

Table S7-B: $Zr(OH)_4$

Atom	Coordinates (Angstroms)		
	X	Y	Z
ZR	15.949	1.757	2.34
H	18.752	2.029	2.583
O	17.899	1.914	2.157
O	15.483	1.537	4.236
H	14.94	1.81	4.979
O	15.319	0.195	1.328
H	15.538	-0.607	0.848
O	15.097	3.382	1.637
H	14.571	3.794	0.946