Supporting Information For

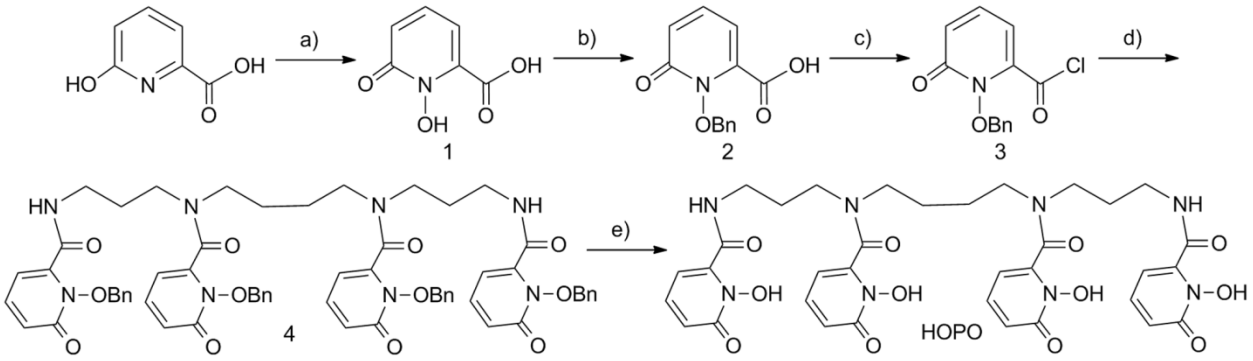
An Alternative Chelator for ^{89}Zr Radiopharmaceuticals: Radiolabeling and Evaluation of 3,4,3-(LI-1,2-HOPO)

Melissa A. Deri,[†,‡,§] Shashikanth Ponnala,[†,‡] Brian M. Zeglis,[†] Gabor Pohl,[‖] J. J. Dannenberg,*[,‖] Jason S. Lewis,*[,†] and Lynn C. Francesconi*[,‡,§]

† Department of Radiology and the Program in Molecular Pharmacology and Chemistry, Memorial Sloan-Kettering Cancer Center, 1275 York Avenue, New York, NY 10065, USA. ‡ Department of Chemistry, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065, USA. § Department of Chemistry, The Graduate Center of the City University of New York, 365 Fifth Avenue, New York, NY 10016, USA. ‖ Department of Chemistry, City University of New York - Hunter College and the Graduate School, New York, NY, USA

*Email: Joseph Dannenberg, jdannenberg@gc.cuny.edu (Hunter College); Jason S. Lewis, lewisj2@mskcc.org (MSKCC); Lynn C. Francesconi, lfrances@hunter.cuny.edu (Hunter College)

Supporting Information Contents



Scheme 1. Synthesis of 3,4,3-(LI-1,2-HOPO) (HOPO).

Reagents and conditions: a) CH_3COOOH (1.2 equiv), AcOH, TFA, 1 h, 79%; b) BnCl (1.2 equiv), K_2CO_3 (2.0 equiv), CH_3OH, 16 h, 63 ^oC, 92%; c) $(COCl)_2$ (2.2 equiv), CH_2Cl_2, 0-25 ^oC, 6 h; d) spermine (0.17 equiv), TEA (2.0 equiv), CH_2Cl_2, 0-25 ^oC, 24 h, 81% over steps c & d; e) AcOH, HCl (12 N), 18 h, 45 ^oC, 42%

6-Carboxy-1-hydroxy-2(*1H*)-pyridinone [1,2-HOPO carboxylic acid] (1). The synthetic protocol from Xu et al. was employed with slight modifications.[43] 6-Hydroxypicolinic acid (10.0 g, 71.9 mmol) and peracetic acid (21.0 g, 88.4 mmol) were added to a stirring solution of glacial acetic acid (40.0 mL) and trifluoroacetic acid (60.0 mL). This mixture was stirred under nitrogen for 1 h at room temperature before being heated to 80 ^oC for 12 h. The reaction mixture started off a red-brown color and turned orange over time. A light color precipitate formed, was collected by filtration, and washed with cold methanol. After drying, the product was obtained as a beige solid (yield 79%).

1-Benzyloxy-6-carboxy-2(*1H*)-pyridinone [1,2-HOPOBn carboxylic acid] (2). Compound 1 (3.70 g, 23.8 mmol) and potassium carbonate (6.60 g, 47.7 mmol) were added to a stirring solution of benzyl chloride (3.60 g, 28.6 mmol) in methanol (10.0 mL). The mixture was heated to 63 ^oC and left to reflux for 16 h. The reaction mixture was a dark green suspension and formed a precipitate over time. The blue-gray solid was filtered out of the reaction mixture and the filtrate was collected. The solvent was evaporated and its residue was redissolved in 12.0 mL water. The solution was acidified to pH 2 by dropwise addition of 12 N HCl. An off-white precipitate was formed and was isolated by filtration. The product was washed with cold water and dried to yield a light beige solid (yield 92%).

1-Benzyloxy-2(*1H*)-pyridinone-6-carbonyl chloride [**1,2-HOPOBn acid chloride] (3).** A suspension of **2** (1.03 g, 4.20 mmol) in anhydrous dichloromethane (25 mL) was cooled to 0 ^oC. Excess oxalyl chloride (0.715 mL, 9.40 mmol) was added while stirring followed by catalytic amount of DMF (0.1 mL). Gas bubbles evolved, and the suspension became clear. The mixture was then left at room temperature for 6 h, and the solvent was removed by rotary evaporation to leave pale brown oil. After the oil was co-evaporated twice with toluene (10 mL), the crude acid chloride (**3**) was used directly for the next reaction without any purification.

3,4,3-(LI-1,2-HOPO)Bn [benzyl-protected HOPO] (4). A solution of crude **3** (0.79 g, 3.0 mmol) in dichloromethane (15 mL) was added drop wise to a stirred solution of triethylamine (0.84 mL, 6.0 mmol), spermine (0.10 g, 0.50 mmol) and DMAP (0.0060 g, 0.050 mmol) in dry dichloromethane (10 mL) at 0 ^{o}C. The reaction mixture was warmed to room temperature and stirring was continued for 24 h. The reaction mixture was washed with 10% $NaHCO_3$ solution, followed by water. The organic phase was dried over anhydrous Na_2SO_4, filtered, and concentrated to dryness. Purification by column chromatography (SiO_2, 2-6% MeOH in CH_2Cl_2) afforded the benzyl-protected precursor 3,4,3-LI(1,2-HOPOBn) (**4**) as white foam (yield 81%).

3,4,3-(LI-1,2-HOPO) (HOPO). Compound **4** (0.20 g, 0.18 mmol) was dissolved in 1:1 mixture of acetic acid and concentrated HCl (15 mL) at room temperature and the reaction mixture was stirred at 50 ^{o}C for 18 h. The reaction progress was monitored by TLC. The crude product was dried, redissolved in water, and purified by HPLC on a semi-preparative C4 column (Jupiter 250 × 10 mm, 5 µM, Phenomenox) using a gradient of 5-28% MeCN in water (both containing 0.1% TFA) over 20 min. The product peak was collected from 7-8.92 min and the eluted solution was lyophilized to recover the product as a white solid. The purified ligand was collected in multiple small batches with an approximate combined yield of 42%.

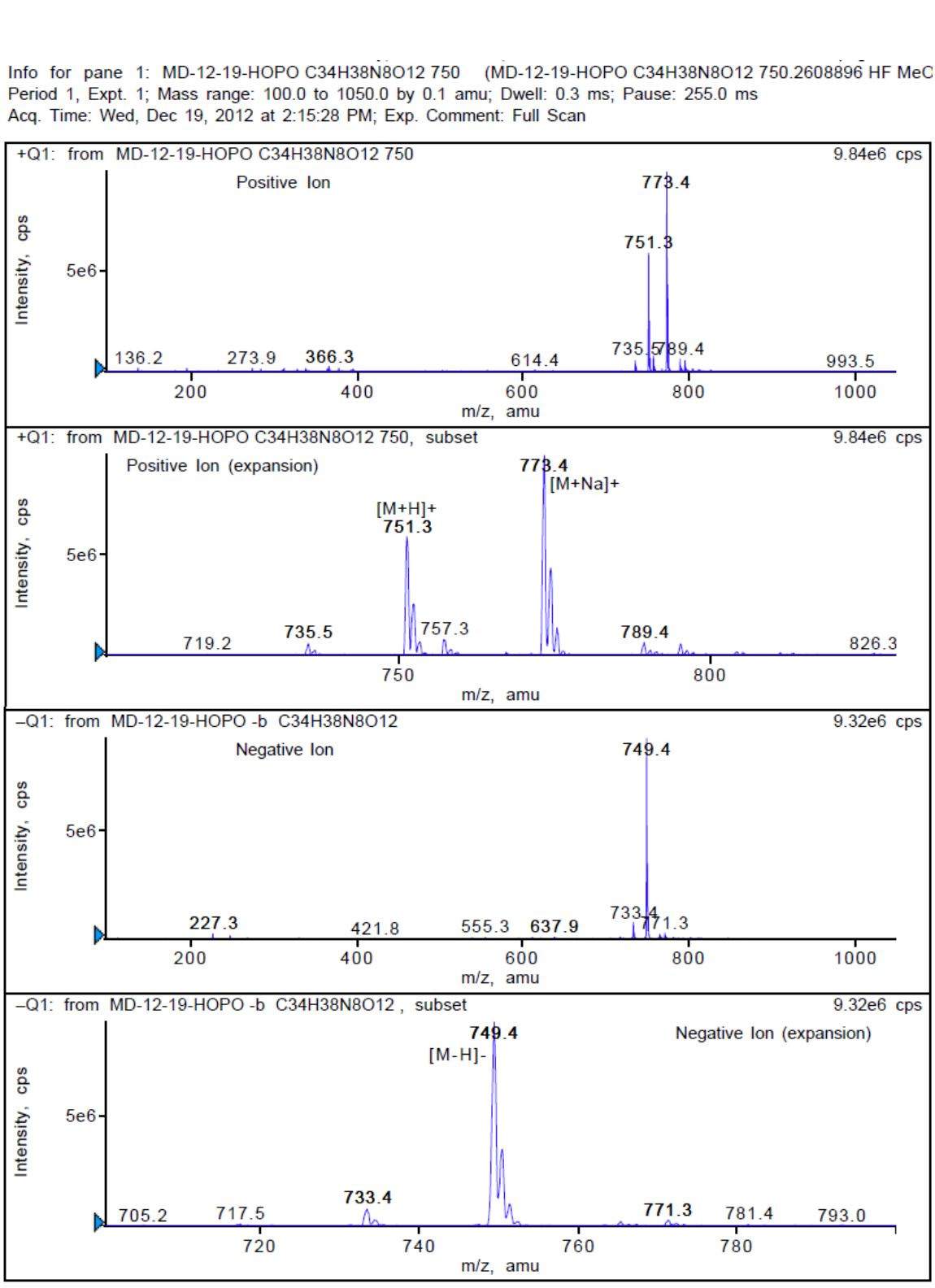


Figure S1. Mass spectrometry analysis of the HOPO ligand showing the expected mass signals.

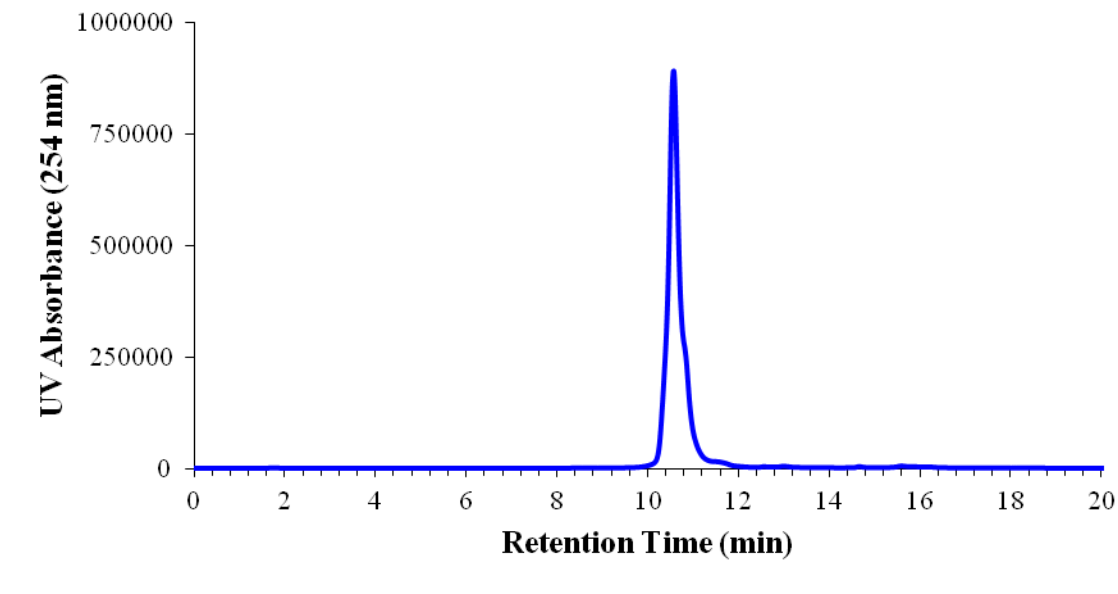


Figure S2. HPLC chromatogram of the HOPO ligand.

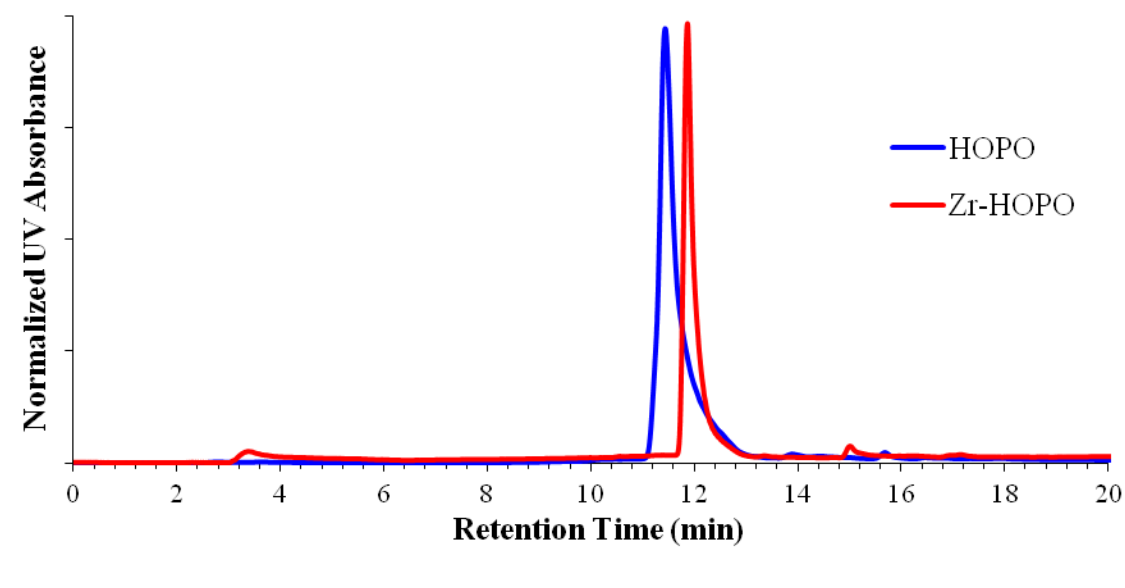


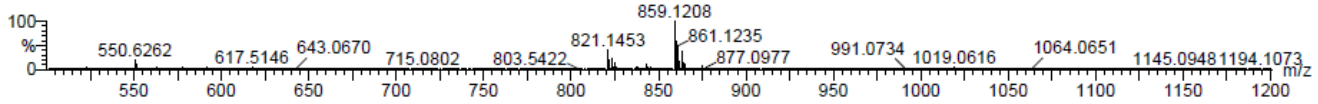
Figure S3. HPLC chromatogram of the HOPO ligand and the non-radioactive Zr-HOPO complex.

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 110.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
225 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 0-34 H: 0-34 N: 0-8 O: 0-12 Na: 1-1 Zr: 0-1

C34H34N8O12Zr
MD-11-5-Zr-HOPO-HRMS 6 (0.145) Cm (5:9)

1: TOF MS ES+
2.27e+003



Minimum:				-1.5		
Maximum:		5.0	5.0	110.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
859.1208	859.1241	-3.3	-3.8	22.5	5.7	C34 H34 N8 O12 Na Zr

Figure S4. High resolution mass spectrometry (HRMS) analysis of the Zr-HOPO complex showing the expected mass signal.

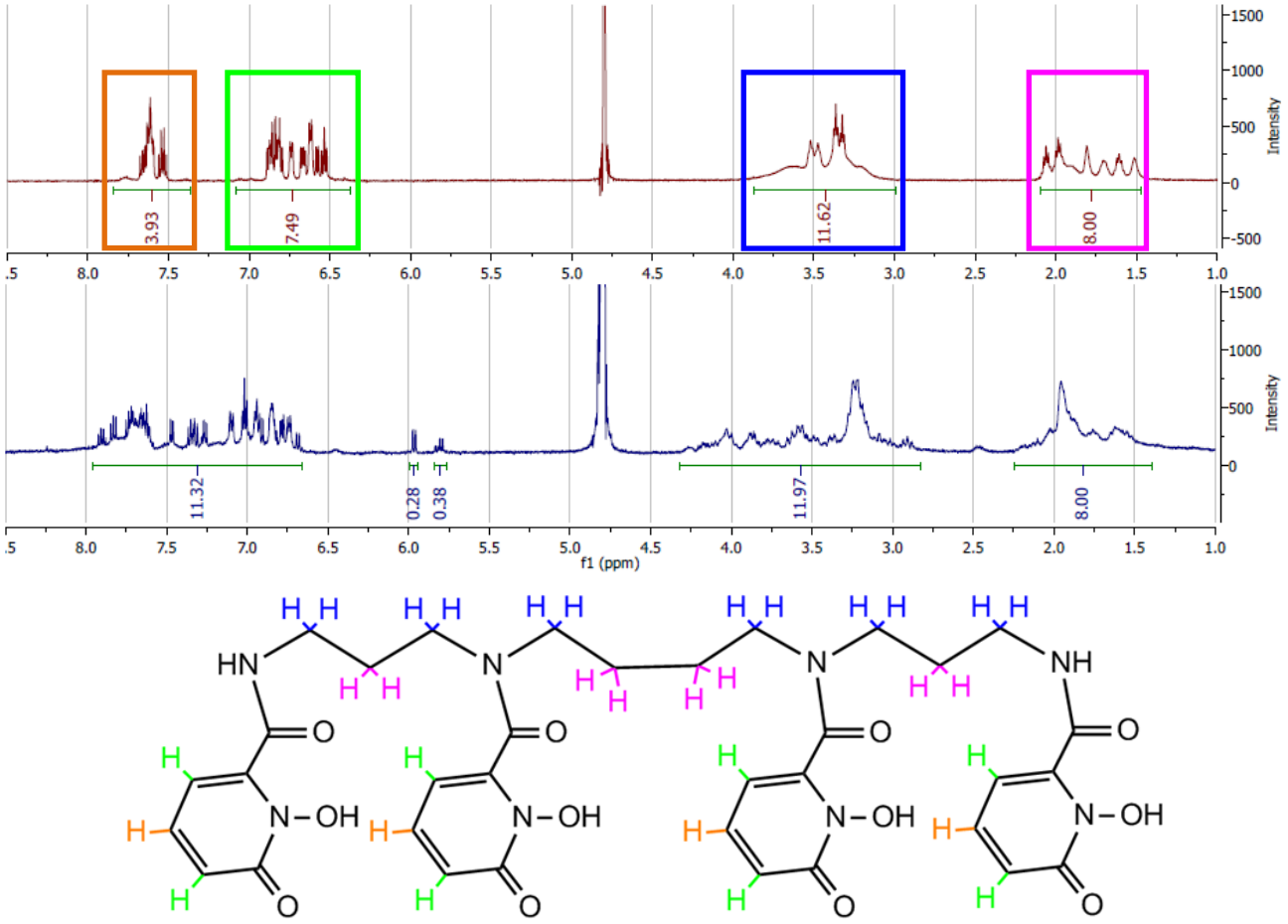


Figure S5. ^{1}H NMR comparison of the HOPO ligand (top) and the Zr-HOPO complex (bottom). Spectra were collected on a 500 MHz machine in D_2O.

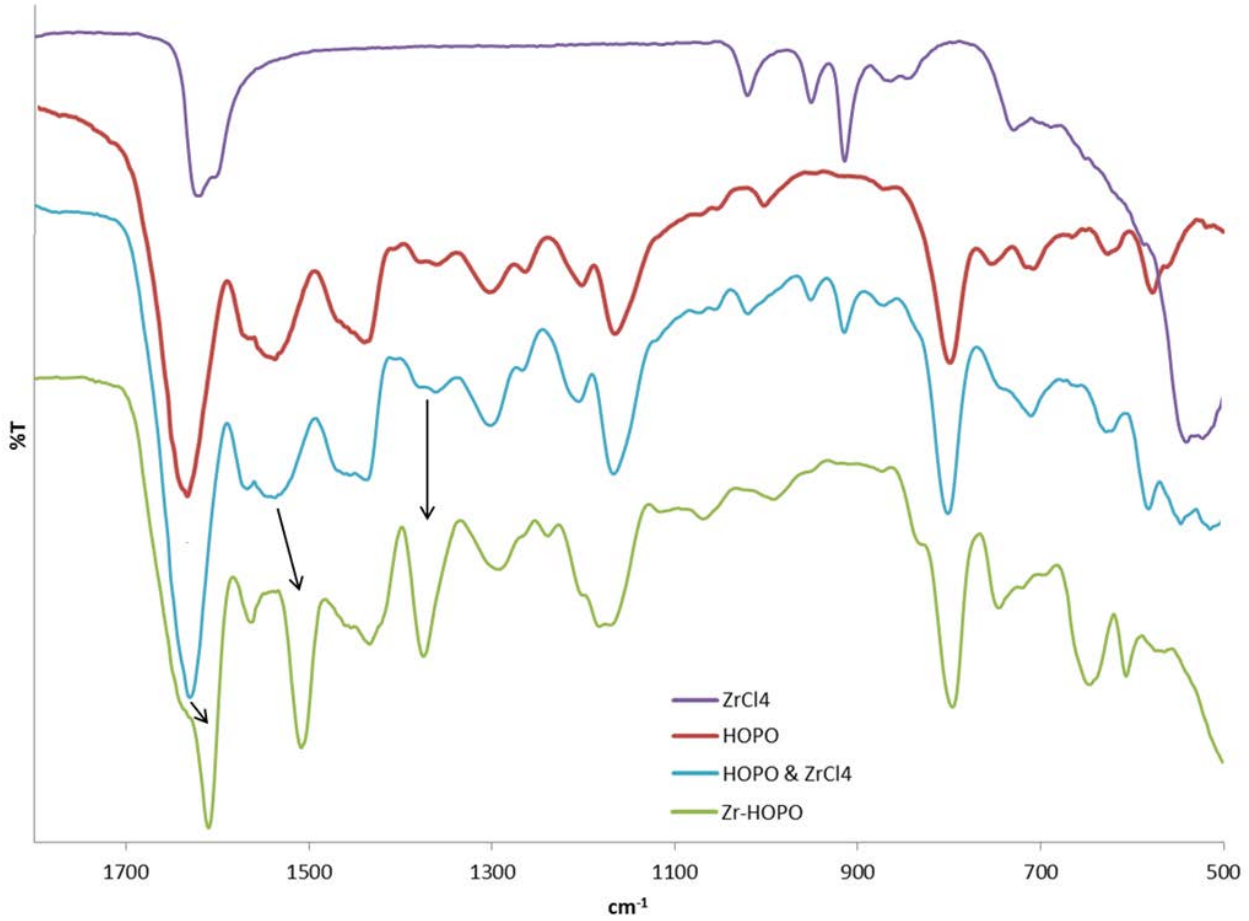


Figure S6. Experimental Zr-HOPO IR spectra. The purple line is powdered ZrCl4. The red line is solid HOPO. The blue line is a mixture of solid HOPO and $ZrCl_4$ powder while the green line is the lyophilized product of the complexation of HOPO and $ZrCl_4$. The three peaks pointed out in the figure correspond to changes in the spectra as a result of the complexation (from 1630 to 1610, 1564 to 1537, and 1375 to 1360 cm^{-1}). This red-shift is characteristic of a hydroxamate, or in this case a hydroxypyridinone, binding a metal. Furthermore, similar signals are seen in the DFT calculated IR spectra associated with a number of highly coupled asymmetric carbonyl stretches (see **Figure S7**).

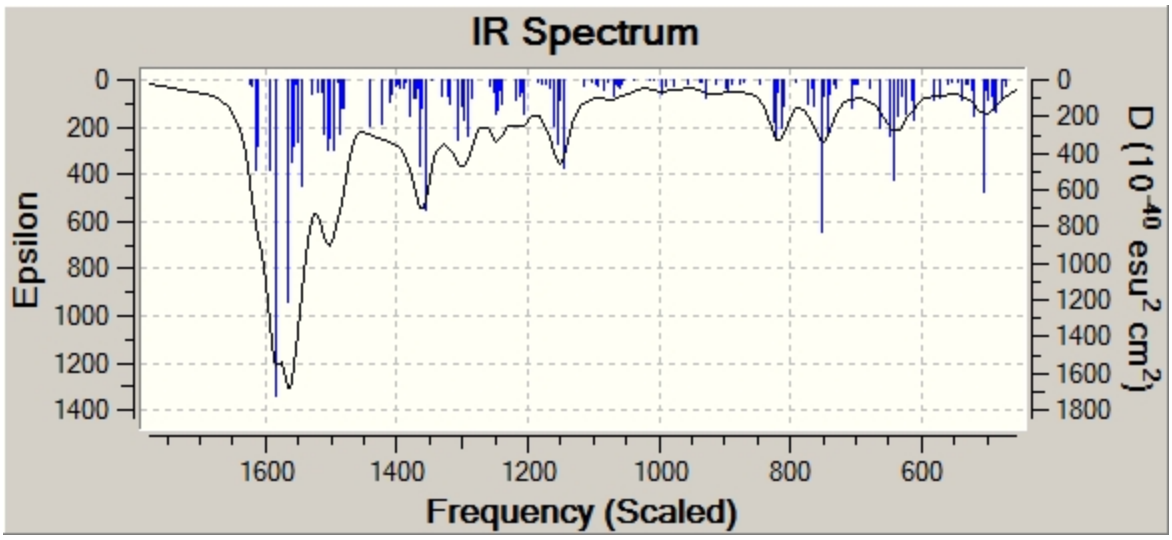


Figure S7. Computed Zr-HOPO IR spectrum. The spectrum is scaled by 0.992 and with a resolution of 15 cm^{-1}. The prominent peaks resembling those in the experimental (between 1600 and 1300 cm^{-1}) correspond to various highly coupled asymmetric carbonyl stretches.

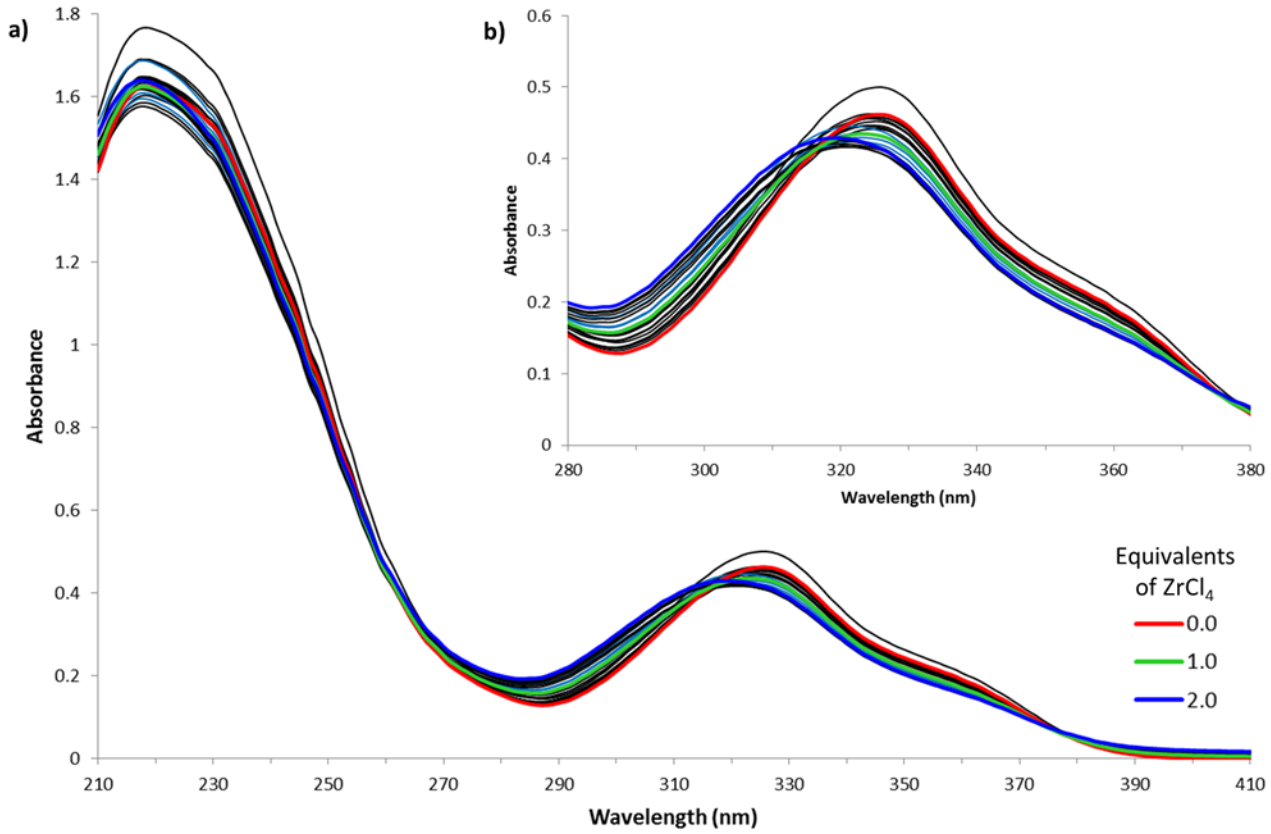


Figure S8. Zr-HOPO UV-Vis spectroscopy. Solutions of HOPO were prepared with 0.1 equivalent increments of $ZrCl_4$ from 0.0 to 2.0 equivalents in PBS at a pH of 7.4 and allowed to equilibrate at room temperature for 24 h. The figure above shows a) the full spectrum and b) a zoomed in section highlighting the peak which undergoes the greatest change. While the peak does shift slightly lower in absorbance and to slightly lower wavelengths, neither of these changes shows a consistent stopping point corresponding to a specific ratio of Zr:HOPO.

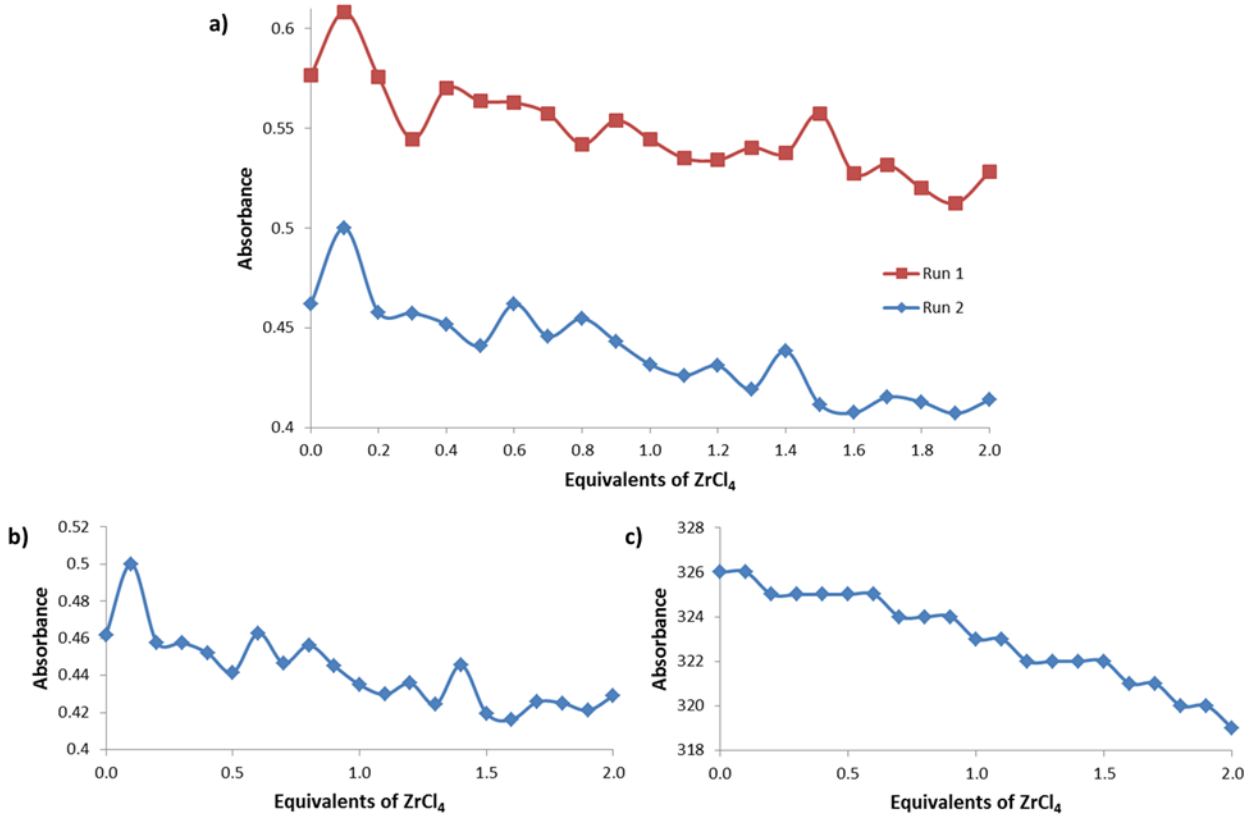


Figure S9. Zr-HOPO UV-Vis spectroscopy. The figure above shows a) a profile of the absorbance at 326 nm, b) a profile of the maximum peak absorbance, and c) a profile of the peak wavelength all according to the amount of $ZrCl_4$. None of these graphs demonstrate a distinct end point to the spectral changes. All of the shifts are small and continual over the entire range from 0.0 to 2.0 equivalents of $ZrCl_4$. There is no notable plateau at the 1:1 stoichiometry suggested by other experiments. These results are neither negative nor positive; they simply do not confer any information.

Complete reference for GAUSSIAN 09 (Ref. 48)

Gaussian 09, Revision A.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Gaussian 09, Revision C.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Basis set	MeOH to MeO^-	EtOH to EtO^-
cep-121g	381.5	377.5
cep-31g	387.6	384.7
LANL2DZ	389.9	385.5
QZVP	380.0	376.7
cc-pVTZ	385.6	381.6
aug-cc-pVTZ	377.6	374.7
cc-pVQZ	382.1	378.2
aug-cc-pVQZ	377.7	374.9
expt.	381.6 ± 0.7	378.6 ± 0.8

Table S1. Deprotonation enthalpies obtained with B3LYP using different basis sets.

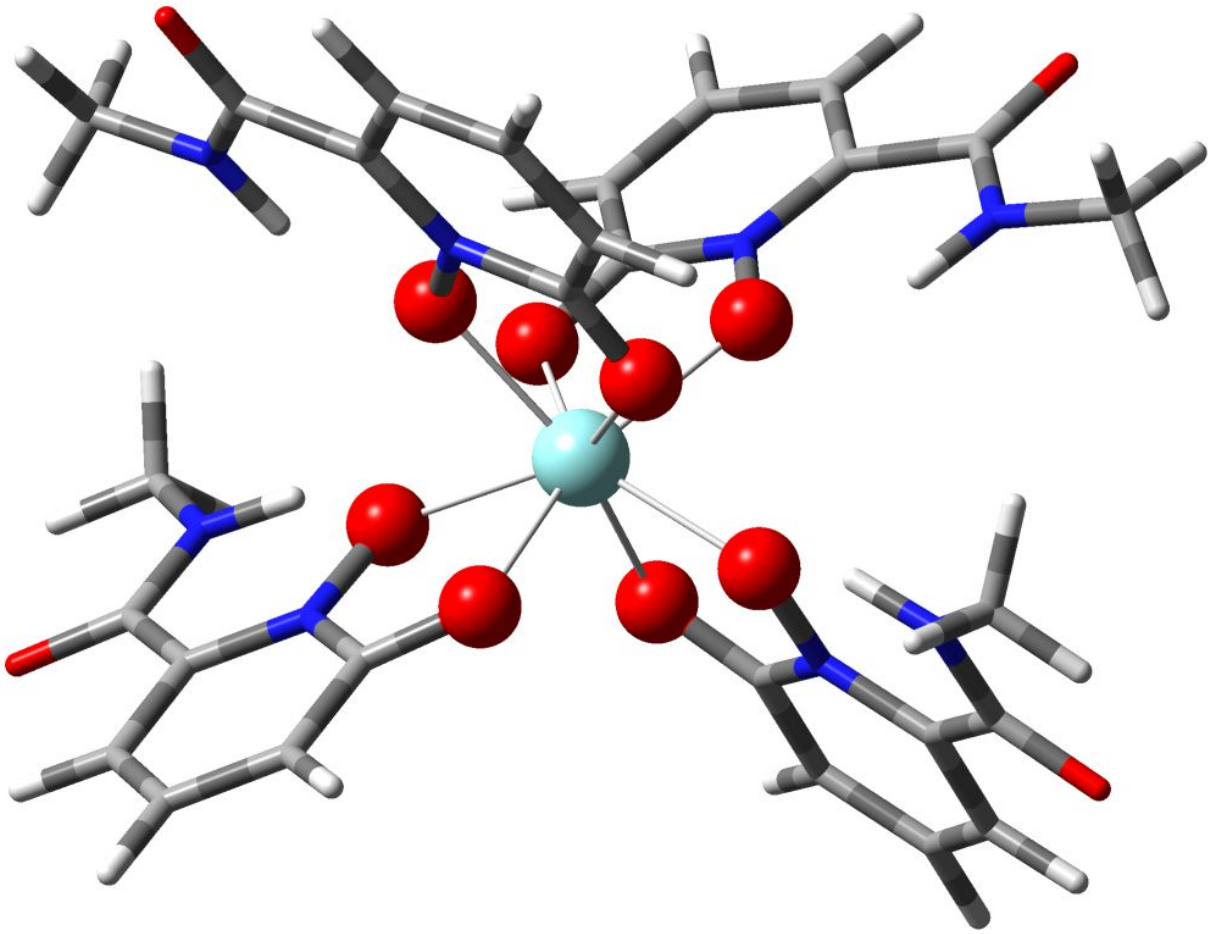


Figure S10. Optimized DFT structure of Zr bond by four free 1,2-HOPO groups. The geometry is a very close match to a previously reported crystal structure of Zr bound by four hydroxamate groups.[35]

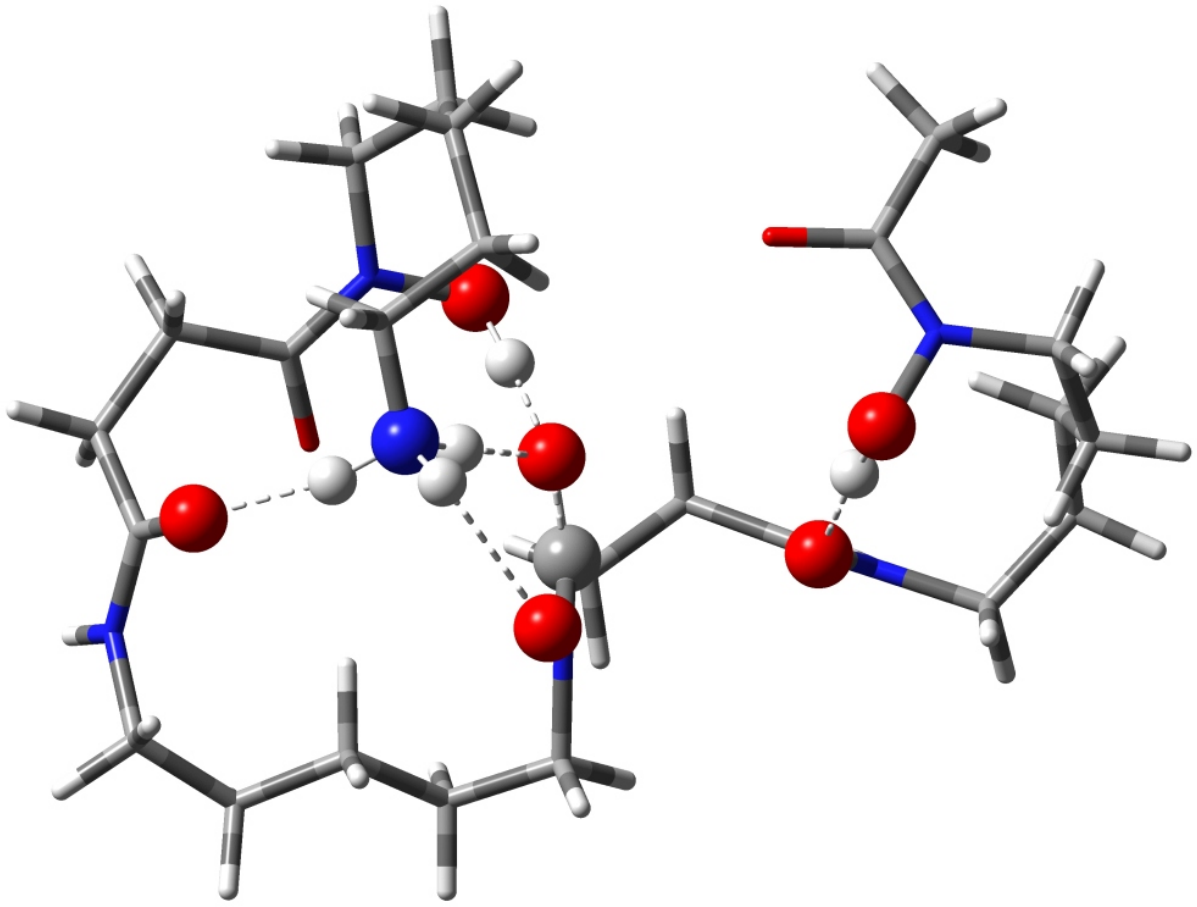


Figure S11. Optimized DFT structure of $DFOH_2$ (CPCM). The zwitterionic form was found to be more stable with the protonated amine tail forming hydrogen bonds with oxygens including a deprotonated hydroxylamine group.

Cartesian coordinates of optimized structures (gas phase)

Zr[3,4,3-(LI-1,2-HOPO)], **I**

C	0	-1.23222400	1.60141000	-2.98443100	M
C	0	-0.77771400	1.91113600	-4.27624200	M
C	0	0.19081800	1.08409800	-4.90943400	M
C	0	0.67740500	-0.06858800	-4.27771900	M
C	0	0.20918400	-0.40120300	-2.97100800	H
N	0	-0.70732800	0.47741000	-2.37676900	H
H	0	0.54247800	1.34155300	-5.90519700	M
H	0	-1.21969800	2.76002600	-4.78322500	M
H	0	1.39696600	-0.73290900	-4.74243600	M
O	0	-1.12462800	0.07982700	-1.10260700	H
O	0	0.53746700	-1.43737000	-2.23719100	H
C	0	-2.43003700	2.37135800	-2.42180900	M
O	0	-3.37992500	2.58309800	-3.24876000	M
N	0	-2.47721800	2.86782100	-1.13646400	M
C	0	-1.40004800	2.81003500	-0.11008700	M
H	0	-1.89769600	2.59825600	0.84485300	M
H	0	-0.75881800	1.95292000	-0.29558700	M
C	0	4.28088800	-1.35477400	-1.13329500	M
C	0	5.13414200	-2.33810900	-1.65603700	M
C	0	4.70397400	-3.69036000	-1.73127600	M
C	0	3.42047800	-4.05712100	-1.30613300	M
C	0	2.53963400	-3.06097900	-0.78813400	H
N	0	3.02770900	-1.75196500	-0.69651800	H
H	0	5.37572000	-4.44446900	-2.13371100	M
H	0	6.10912000	-2.01115200	-1.99617000	M
H	0	3.04744300	-5.07328500	-1.36387400	M
O	0	2.12534800	-0.85524800	-0.09288000	H
O	0	1.30694700	-3.24771500	-0.37396200	H
C	0	4.76962900	0.09246400	-1.10173300	M
O	0	5.92902800	0.34459800	-1.57047600	M
N	0	3.94257400	1.05656100	-0.59343100	M
H	0	3.06081000	0.74650000	-0.18471800	M
C	0	4.40629700	2.46063100	-0.50249600	M
H	0	5.10286300	2.55840200	0.34021700	M
H	0	4.97238600	2.66732100	-1.41809300	M
C	0	1.87019800	0.77539800	3.16906400	M
C	0	2.30090200	0.41829100	4.45568600	M
C	0	1.88456600	-0.81223100	5.03263200	M
C	0	1.13124200	-1.72335500	4.28270700	M
C	0	0.74005700	-1.38588700	2.95217800	H
N	0	1.00881500	-0.08137800	2.50394700	H
H	0	2.20223200	-1.06962100	6.03971700	M
H	0	3.01282900	1.06344900	4.95688300	M
H	0	0.86267600	-2.70786900	4.64867200	M
O	0	0.39396700	0.26281200	1.28425800	H
O	0	0.17330900	-2.18178100	2.07790300	H
C	0	2.60942900	1.88918500	2.43149800	M
O	0	3.87999900	1.79601000	2.43254000	M
N	0	1.94895100	2.93266500	1.81730200	M
C	0	2.81960900	3.90616900	1.08314900	M
H	0	2.27236600	4.84904100	1.01882000	M
H	0	3.72249800	4.07902700	1.68375100	M

C	0	-4.47294000	-1.81500700	0.82513400	M
C	0	-5.37183400	-2.87717100	0.63626500	M
C	0	-4.91088600	-4.12311200	0.13713400	M
C	0	-3.56225600	-4.29189900	-0.21158300	M
C	0	-2.65186000	-3.21385100	-0.02513800	H
N	0	-3.13163900	-2.03700600	0.55578200	H
H	0	-5.61283000	-4.94131700	0.00000400	M
H	0	-6.41451900	-2.68243500	0.85618700	M
H	0	-3.17199700	-5.21010200	-0.63542000	M
O	0	-2.14650600	-1.09057300	0.84800500	H
O	0	-1.37373100	-3.19969200	-0.35714400	H
C	0	-5.02956000	-0.44035500	1.17421300	M
O	0	-6.25674300	-0.35026900	1.50393700	M
N	0	-4.20324300	0.64416200	1.00550700	M
H	0	-3.21870100	0.44982100	0.81134500	M
C	0	-4.73459100	2.02065700	1.10307100	M
H	0	-4.08548000	2.60806700	1.76952600	M
H	0	-5.71224000	1.93518600	1.58594100	M
C	0	3.23975500	3.48132700	-0.35931200	M
H	0	2.36213400	3.12262000	-0.91540800	M
H	0	3.56401200	4.40894700	-0.85605900	M
C	0	0.54840000	3.26490900	2.26327500	M
H	0	-0.03541400	2.34322400	2.18440200	M
H	0	0.58615600	3.55392900	3.32581500	M
C	0	-0.17926100	4.40307300	1.50229000	M
H	0	0.38635900	5.34260400	1.57040600	M
H	0	-1.10400700	4.57786000	2.07632400	M
C	0	-0.57932100	4.12753600	0.02532400	M
H	0	0.30569700	4.08239300	-0.62267700	M
H	0	-1.17784100	4.97971900	-0.32745900	M
C	0	-3.71785900	3.61911900	-0.75985300	M
H	0	-4.04482100	4.18477700	-1.63841100	M
H	0	-3.43556600	4.33306700	0.02539400	M
C	0	-4.90642900	2.74291600	-0.27304600	M
H	0	-5.16190400	2.00740900	-1.04476900	M
H	0	-5.76930100	3.42226600	-0.18892700	M
Zr	0	-0.03898100	-1.53592300	-0.02999300	H

Zr[3,3,3-(LI-1,2-HOPO)], **II**

C	0	-0.80378600	1.81417600	-2.88042100	M
C	0	-0.22144600	2.14064800	-4.11534000	M
C	0	0.66673500	1.22707700	-4.74739700	M
C	0	0.95253000	-0.01759800	-4.16897100	M
C	0	0.35905400	-0.36258500	-2.91735800	H
N	0	-0.49140300	0.58558100	-2.33105000	H
H	0	1.11889200	1.49493300	-5.69888100	M
H	0	-0.50156500	3.07832800	-4.57945700	M
H	0	1.61462700	-0.74051600	-4.63180000	M
O	0	-1.06311900	0.16218100	-1.12756000	H
O	0	0.51925800	-1.46578700	-2.22576400	H
C	0	-1.90911200	2.71095000	-2.31850200	M
O	0	-2.76043000	3.13205500	-3.17133800	M
N	0	-1.96933000	3.09215900	-0.99019500	M
C	0	-0.98434000	2.68901100	0.05881900	M
C	0	4.21006100	-1.36716000	-0.99402900	M
C	0	5.07821200	-2.35472600	-1.48272700	M
C	0	4.64871300	-3.70742800	-1.55959800	M
C	0	3.35304500	-4.07099100	-1.16994200	M
C	0	2.45615900	-3.07079000	-0.68794700	H
N	0	2.94412500	-1.76121700	-0.59344800	H
H	0	5.33168800	-4.46516000	-1.93542000	M
H	0	6.06317700	-2.03189100	-1.79702900	M
H	0	2.98221300	-5.08777000	-1.23088000	M
O	0	2.02711700	-0.85602800	-0.02553200	H
O	0	1.21105100	-3.25266400	-0.30958600	H
C	0	4.69596200	0.08131600	-0.95667600	M
O	0	5.86168100	0.33375700	-1.40875900	M
N	0	3.86242700	1.04602400	-0.45693000	M
H	0	2.97512600	0.73548400	-0.06075200	M
C	0	4.32595500	2.44965000	-0.35953500	M
H	0	4.99075200	2.55216900	0.50872700	M
H	0	4.92799400	2.64640700	-1.25373000	M
C	0	1.59852300	0.80088900	3.26491600	M
C	0	1.95022000	0.46090200	4.57972400	M
C	0	1.51145900	-0.77143900	5.13710200	M
C	0	0.81693000	-1.69856600	4.34931900	M
C	0	0.50427500	-1.37593600	2.99426300	H
N	0	0.79250900	-0.07281800	2.55668500	H
H	0	1.76764100	-1.01793800	6.16423600	M
H	0	2.62117500	1.11736700	5.12125000	M
H	0	0.53674600	-2.68232100	4.70861700	M
O	0	0.25960000	0.26224900	1.30278500	H
O	0	-0.00693800	-2.17616900	2.08927200	H
C	0	2.37898200	1.89836000	2.54413700	M
O	0	3.64675100	1.80325500	2.62012800	M
N	0	1.76976700	2.91986800	1.84115700	M
C	0	2.69194300	3.88862400	1.16405700	M
H	0	2.15745200	4.84333900	1.10257700	M
H	0	3.56987500	4.03165800	1.80668800	M
C	0	-4.59923200	-1.56767300	0.52412900	M
C	0	-5.55262200	-2.55566500	0.23236100	M
C	0	-5.14039600	-3.81988500	-0.26552900	M
C	0	-3.78332000	-4.08135100	-0.50980100	M

C	0	-2.81547800	-3.07766800	-0.22191100	H
N	0	-3.26102000	-1.88305000	0.35046300	H
H	0	-5.88531800	-4.58073900	-0.48288800	M
H	0	-6.59366100	-2.29263900	0.37620000	M
H	0	-3.42846900	-5.01657600	-0.92746800	M
O	0	-2.23753600	-1.01552000	0.74064000	H
O	0	-1.51607800	-3.14241500	-0.45025000	H
C	0	-5.07443900	-0.16477900	0.88749400	M
O	0	-6.31166000	0.01304800	1.13139500	M
N	0	-4.14892900	0.84777800	0.83092600	M
H	0	-3.17529100	0.57007900	0.69256400	M
C	0	-4.54324700	2.26379400	0.97882200	M
H	0	-3.91142200	2.72915200	1.75111500	M
H	0	-5.57118000	2.25669400	1.35264600	M
C	0	3.16336600	3.48156900	-0.26491300	M
H	0	2.30673700	3.14016400	-0.86314500	M
H	0	3.52167100	4.40946700	-0.73673800	M
C	0	0.37873600	3.37277300	2.14307000	M
H	0	-0.14182500	2.55019000	2.64308600	M
H	0	0.45101900	4.20552400	2.86322600	M
C	0	-0.46426800	3.85829000	0.93164100	M
C	0	-3.17664800	3.89713100	-0.61175700	M
H	0	-3.36825600	4.58935300	-1.43761600	M
H	0	-2.92525900	4.48834100	0.27421200	M
C	0	-4.48064900	3.08992900	-0.34706900	M
H	0	-4.69489400	2.43654700	-1.20086500	M
H	0	-5.29147900	3.83437600	-0.31381200	M
Zr	0	-0.13388400	-1.52716300	-0.03042700	H
H	0	0.09691000	4.57530000	0.31675200	M
H	0	-1.30089700	4.41885200	1.36962000	M
H	0	-0.13917900	2.20489000	-0.42609700	M
H	0	-1.42550900	1.92436300	0.70284300	M

$[ZrDFO(H_2O)_2]^{2+}$ with non hydrogen bonded amine group, **III**

Zr	0.51294000	-0.56367600	1.31312000
N	-8.36488900	-4.47147000	-2.52212900
C	-7.40649400	-3.24073600	-2.58617200
C	-6.41532600	-3.23871700	-1.40213900
C	-5.47950400	-1.99378200	-1.47141700
C	-4.46685500	-1.94006200	-0.29190300
C	-3.59193900	-0.66363500	-0.39101600
N	-2.55856400	-0.57508900	0.67107200
C	-2.48120400	0.27028000	1.71587000
C	-3.69248100	1.00100600	2.28535300
C	-3.57444600	2.54780600	2.24813900
C	-3.78174000	3.09453000	0.82001400
O	-4.31054200	2.37463100	-0.08849800
N	-3.36066700	4.38154100	0.59771100
C	-3.36756400	5.02339400	-0.74385900
C	-1.94301100	5.07915300	-1.36485600
C	-1.30279900	3.67618700	-1.52974500
C	0.16049900	3.72034500	-2.03768600
C	0.84878300	2.33199900	-2.03720200
N	1.02154800	1.74791200	-0.67417100
C	2.05775600	1.84597300	0.16414300
C	3.18312900	2.85532700	0.00683700
C	4.58411500	2.18673100	-0.01275100
C	4.75797600	1.29918800	-1.26064300
O	3.77603800	1.06811200	-2.03699400
N	6.00511700	0.75846200	-1.47091200
C	6.29117200	-0.17789200	-2.58920500
C	6.61179000	-1.61945200	-2.10359900
C	5.54197700	-2.26450900	-1.17794700
C	4.15711900	-2.50302600	-1.84128200
C	3.18164500	-3.32691900	-0.95632600
N	2.61354300	-2.55440800	0.18632400
C	3.01311000	-2.43684800	1.46303900
C	4.18486200	-3.19323300	2.05627100
O	-1.39225800	-1.35897700	0.42185600
O	-1.31295000	0.37412700	2.31508100
O	0.04313100	0.78606300	-0.28472600
O	2.04412800	1.02725200	1.20749200
O	1.49365600	-1.75338300	-0.17507100
O	2.31089500	-1.62241300	2.22473100
H	-9.02445800	-4.46740400	-3.31171500
H	-7.82803800	-5.34804900	-2.55365600
H	-8.90701900	-4.46010500	-1.64826700
H	-8.05540500	-2.35900500	-2.58480500
H	-6.89843300	-3.30989300	-3.55343200
H	-6.96830100	-3.22541800	-0.45006300
H	-5.80604400	-4.15560700	-1.41879300
H	-6.09000000	-1.07809500	-1.46797600
H	-4.92769100	-2.00446600	-2.42372400
H	-3.81879800	-2.82745700	-0.30813500
H	-5.01016100	-1.94541400	0.66537900
H	-4.18597400	0.25487600	-0.36070900
H	-3.02450100	-0.66383400	-1.32875700
H	-4.60712300	0.69353800	1.77400700

H	-3.76352700	0.68131900	3.33409700
H	-2.59967400	2.86252300	2.64217800
H	-4.34483200	2.97580000	2.90515300
H	-2.94987200	4.89710000	1.36875000
H	-4.04231500	4.43408600	-1.37187100
H	-3.78452200	6.03360300	-0.64620800
H	-2.01624300	5.58548000	-2.33945300
H	-1.29607200	5.71168000	-0.73422700
H	-1.91263100	3.07341800	-2.21994600
H	-1.32418500	3.14951300	-0.56687700
H	0.19428000	4.10393400	-3.06892600
H	0.74871800	4.42333200	-1.42665200
H	1.83832300	2.35365700	-2.50272900
H	0.24338200	1.59507800	-2.57361500
H	3.03820900	3.45121800	-0.89731000
H	3.13362600	3.53344600	0.87014200
H	4.71264900	1.57421500	0.88978800
H	5.35692900	2.96696500	0.00796500
H	6.76058400	1.00693900	-0.84114300
H	5.40925800	-0.16214600	-3.23486000
H	7.13797800	0.21085400	-3.16968800
H	6.75832300	-2.24496800	-2.99755800
H	7.57596200	-1.61524300	-1.57143800
H	5.42157400	-1.63452500	-0.28312800
H	5.94419300	-3.23011400	-0.83090100
H	3.67457800	-1.55456600	-2.10678500
H	4.29393200	-3.07072000	-2.77490200
H	3.67046200	-4.22535600	-0.55988700
H	2.30889000	-3.63890800	-1.53813600
H	4.96526900	-2.47999900	2.34670700
H	3.85207000	-3.70051700	2.96874400
H	4.61732500	-3.92627700	1.37348100
O	-0.26060200	-2.64698400	2.20488600
H	-1.03059300	-2.81089700	1.61288900
H	0.08949800	-3.41120900	2.69538200
O	0.86709300	-0.06962200	3.51260300
H	1.72608600	-0.31741400	3.90156600
H	0.24194700	0.40434100	4.08759100

$[ZrDFO(H_2O)_2]^{2+}$ with hydrogen bonded amine group, **IIIa**

Zr	0.07347200	-0.92732700	-1.26674700
N	-0.89282600	0.00719600	2.23131500
C	-0.89247200	-0.24855200	3.73860200
C	-0.54621200	-1.70477500	4.15699500
C	0.95958300	-2.12057200	4.30389100
C	1.62984200	-2.84551300	3.08656300
C	2.56330600	-1.94448400	2.22154000
N	2.17431300	-1.94804000	0.77890200
C	2.92510600	-1.83318100	-0.32477800
C	4.40013100	-2.20275300	-0.39282600
C	5.30075900	-1.05884900	-0.92759800
C	5.28552900	0.14530400	0.03571800
O	4.70224700	0.06139600	1.16358900
N	5.90128500	1.28991000	-0.40841900
C	5.92834400	2.55341800	0.37791100
C	4.73927300	3.49923900	0.04573600
C	3.36471100	2.83268400	0.31563700
C	2.15711700	3.79298200	0.18318500
C	0.82028400	3.13250700	0.61103400
N	0.32439600	2.07036500	-0.31356900
C	-0.67750200	2.10890700	-1.20112400
C	-1.49507900	3.35645100	-1.48581700
C	-3.00853400	3.09803400	-1.24473100
C	-3.35827700	2.59722600	0.17340500
O	-2.48862800	2.04124100	0.93195300
N	-4.67253100	2.72462600	0.52619100
C	-5.29222400	2.08956800	1.71981900
C	-6.27861800	0.95417400	1.31760900
C	-5.66849400	-0.16756400	0.42955100
C	-4.61898600	-1.05478000	1.15090000
C	-3.99950200	-2.15523700	0.25053400
N	-2.93056100	-1.66455300	-0.67095800
C	-2.85991900	-1.74872600	-2.01385100
C	-4.05510300	-2.09124900	-2.88367100
O	0.77532900	-1.76363400	0.57589800
O	2.28036600	-1.47937100	-1.43223800
O	0.81032300	0.74735200	-0.06639100
O	-0.97021600	0.97501300	-1.81152500
O	-1.68349300	-1.38671400	-0.02879600
O	-1.67819000	-1.54763900	-2.55659500
H	0.04913100	0.07560600	1.81563300
H	-1.34344100	-0.75693700	1.68959000
H	-1.41580900	0.86549600	1.97362100
H	-1.90550300	-0.00468500	4.07743800
H	-0.20531400	0.47441600	4.19302300
H	-1.01359000	-1.82573200	5.14451000
H	-1.06863900	-2.41147100	3.49348800
H	1.00539600	-2.80539700	5.16008000
H	1.55790400	-1.24467600	4.60215000
H	0.85505000	-3.27615600	2.44324400
H	2.22379600	-3.68478700	3.46871300
H	3.60936600	-2.24919600	2.28484300
H	2.53553900	-0.89369600	2.53787000
H	4.75695200	-2.52703900	0.58590400

H	4.47661800	-3.05826000	-1.07981100
H	4.96968600	-0.74548200	-1.92661500
H	6.32609600	-1.43908100	-1.03150600
H	6.37157300	1.27396900	-1.30695300
H	5.90460600	2.27797300	1.43761100
H	6.88304000	3.05362300	0.17735000
H	4.85084700	4.40107100	0.66774000
H	4.80669100	3.82934300	-1.00317700
H	3.37358400	2.40610100	1.32865900
H	3.22326500	1.98329300	-0.36442700
H	2.30164900	4.66584900	0.83856500
H	2.06861500	4.18227800	-0.84256000
H	0.02712600	3.87862200	0.71504400
H	0.94407000	2.64554300	1.58548400
H	-1.14657900	4.20367300	-0.89089900
H	-1.36275900	3.62343700	-2.54246300
H	-3.35061200	2.33008000	-1.95197100
H	-3.56463600	4.01693200	-1.47018500
H	-5.29197100	3.21803800	-0.10953900
H	-4.47488500	1.71988700	2.34393300
H	-5.82481600	2.85853400	2.29242700
H	-6.68856100	0.52233500	2.24283200
H	-7.13345600	1.39875400	0.78607600
H	-5.21992000	0.28326900	-0.46959100
H	-6.49255400	-0.80766900	0.07938500
H	-3.81091300	-0.43680100	1.56193300
H	-5.09816300	-1.56386100	2.00017300
H	-4.77168100	-2.64049800	-0.35660600
H	-3.51930500	-2.92926800	0.86212000
H	-3.90664900	-1.63057900	-3.86347700
H	-4.12339700	-3.17800500	-3.02975200
H	-4.99970000	-1.74010000	-2.46077600
O	0.34993100	-3.00396900	-2.37585900
H	-0.34544200	-3.21689800	-3.02867700
O	1.01877500	-0.31861000	-3.27477500
H	1.95412300	-0.59866200	-3.34092100
H	1.17997000	-3.50120100	-2.49773900
H	0.68624600	0.20849900	-4.02364900

$ZrDFO(OH)_2$, **IV**

Zr	0.38923500	0.30749800	1.25615500
N	-1.28893100	0.80555000	-1.94847600
C	-0.95999200	1.99042200	-2.84091000
C	-1.19578600	3.35709900	-2.12724800
C	-0.12330900	4.44556500	-2.45209700
C	1.09586700	4.52315500	-1.47764000
C	2.15447900	3.37934500	-1.57499200
N	2.03229500	2.37997000	-0.48834700
C	3.02139900	1.69574700	0.12344300
C	4.49245500	2.08630600	-0.08361100
C	5.44922600	1.19945000	0.75331000
C	5.68536300	-0.15986600	0.07247300
O	5.99186600	-0.22606100	-1.16272500
N	5.57805400	-1.27941200	0.87466800
C	5.74750600	-2.65847400	0.36204100
C	4.40280200	-3.39640200	0.10796200
C	3.45656500	-2.63784400	-0.86184900
C	2.26787600	-3.51292000	-1.33971900
C	1.16916400	-2.70501400	-2.09020200
N	0.34259300	-1.87248000	-1.18689600
C	-0.70510600	-2.24647300	-0.42092900
C	-1.44404000	-3.55634900	-0.70940200
C	-2.95377400	-3.40330300	-0.41496300
C	-3.65790500	-2.33689500	-1.28026900
O	-3.04133900	-1.56236100	-2.08237300
N	-5.02029800	-2.25342200	-1.08524800
C	-5.87544200	-1.17638300	-1.63648800
C	-6.63886700	-0.41818700	-0.51369300
C	-5.74339000	0.18649900	0.60344200
C	-4.84382300	1.36928700	0.15579800
C	-3.95631700	1.93274900	1.30245100
N	-2.75537300	1.11571300	1.59251200
C	-2.46489900	0.42013300	2.71791100
C	-3.50944000	0.22349000	3.81494800
O	0.70271600	1.98902500	-0.17321500
O	2.69011600	0.71529500	0.91470600
O	0.79582800	-0.52659100	-0.97521400
O	-1.13627000	-1.44489800	0.50439900
O	-1.66877800	1.33290400	0.69038600
O	-1.27042900	-0.06161700	2.87364300
H	-0.37684400	0.29869700	-1.66675600
H	-1.66760000	1.09850700	-1.01020400
H	-1.93178800	0.10960400	-2.34654400
H	-1.56029500	1.91556200	-3.75638300
H	0.09034600	1.88001200	-3.12626600
H	-2.19069900	3.73551100	-2.40870400
H	-1.19700100	3.18835300	-1.04642500
H	-0.61548200	5.43013000	-2.42256200
H	0.24127700	4.32696700	-3.48771700
H	0.73276500	4.56929800	-0.44395300
H	1.61501200	5.47229100	-1.68452600
H	3.16436300	3.80154800	-1.51908000
H	2.07258500	2.86071200	-2.54373100
H	4.77220000	1.98778700	-1.14071400

H	4.62732100	3.14108300	0.19849500
H	5.06054900	1.07734600	1.76942900
H	6.42424100	1.70606400	0.81397100
H	5.22962000	-1.15552700	1.81778700
H	6.31091600	-2.57481500	-0.57335300
H	6.36046200	-3.22966000	1.07938500
H	4.65061600	-4.39536600	-0.29384400
H	3.88086000	-3.56718900	1.06582100
H	4.02842200	-2.28979200	-1.73523400
H	3.06772200	-1.74287000	-0.36589300
H	2.63516400	-4.30526600	-2.01411800
H	1.80464300	-4.01747000	-0.47752700
H	0.51272700	-3.38483100	-2.65032500
H	1.62179600	-2.00737400	-2.80351800
H	-1.29059400	-3.86549000	-1.74825800
H	-1.04304400	-4.34984000	-0.06193800
H	-3.07904000	-3.10567200	0.63417400
H	-3.45839400	-4.37113500	-0.55113100
H	-5.45483000	-2.92319300	-0.45675900
H	-5.21627200	-0.51239600	-2.20231000
H	-6.59956200	-1.60549700	-2.34694400
H	-7.23925900	0.37596400	-0.98855900
H	-7.36478500	-1.10900100	-0.05066200
H	-5.11144400	-0.60669700	1.02890200
H	-6.40378000	0.53290900	1.41702300
H	-4.19092200	1.07000500	-0.67400900
H	-5.47831200	2.19047200	-0.21465100
H	-4.54905000	2.03561500	2.22072400
H	-3.57907400	2.92704000	1.03135300
H	-3.11871400	-0.53097800	4.50153900
H	-3.67204700	1.15352200	4.37911600
H	-4.47525400	-0.11251300	3.42349600
O	0.88658700	1.51136900	2.82176700
H	0.42339500	1.49627800	3.68413500
O	1.32747100	-1.40627200	1.85676700
H	2.30351700	-1.36323200	1.90980200

$Zr(1,2\text{-}HOPO)_4$

C	0	2.24941700	2.76647900	-2.47700200	M
C	0	1.93531200	3.38461000	-3.69591300	M
C	0	0.70521100	3.10123300	-4.34706500	M
C	0	-0.20909300	2.20183500	-3.78364100	M
C	0	0.10008500	1.56785000	-2.54304300	H
N	0	1.32269100	1.88257200	-1.94069200	H
H	0	0.47417800	3.58678500	-5.29149800	M
H	0	2.66970700	4.07093900	-4.09947400	M
H	0	-1.15660700	1.95811900	-4.25032300	M
O	0	1.53776700	1.22363600	-0.71964500	H
O	0	-0.65240300	0.70931900	-1.89204600	H
C	0	3.58799100	3.09567200	-1.81784800	M
O	0	4.35293000	3.92955900	-2.40260700	M
N	0	3.89616200	2.47007500	-0.63933700	M
H	0	3.20014600	1.82903800	-0.25550000	M
C	0	5.16794800	2.72338600	0.06082600	M
H	0	5.00070300	3.30461800	0.97814400	M
H	0	5.64539800	1.77231600	0.32546200	M
H	0	5.82567800	3.29187700	-0.60018600	M
Zr	0	0.00024700	-0.25688200	-0.00029000	H
C	0	-3.76927600	-2.68057000	-0.33573300	M
C	0	-4.35757100	-3.61145600	0.53382200	M
C	0	-3.73352600	-3.93222100	1.76854700	M
C	0	-2.52289000	-3.32718500	2.13493700	M
C	0	-1.91903800	-2.38053400	1.25669100	H
N	0	-2.57530300	-2.09369000	0.05662900	H
H	0	-4.19991200	-4.65446700	2.43333900	M
H	0	-5.29031100	-4.05883700	0.21253900	M
H	0	-2.01273400	-3.54663400	3.06591600	M
O	0	-1.91753000	-1.15042300	-0.74256200	H
O	0	-0.78734200	-1.73139900	1.44902000	H
C	0	-4.46670400	-2.37001900	-1.65879000	M
O	0	-5.56922900	-2.95951200	-1.90591600	M
N	0	-3.86610100	-1.47884300	-2.50786500	M
H	0	-2.97609300	-1.07317900	-2.20774500	M
C	0	-4.45096700	-1.14598200	-3.81802700	M
H	0	-4.59600000	-0.06154900	-3.90645500	M
H	0	-3.79288200	-1.48200600	-4.63060600	M
H	0	-5.41621500	-1.64861300	-3.90976600	M
C	0	-2.24951800	2.76404200	2.47881300	M
C	0	-1.93520100	3.38189300	3.69780900	M
C	0	-0.70477700	3.09871100	4.34844100	M
C	0	0.20964600	2.19981600	3.78439900	M
C	0	-0.09973200	1.56615600	2.54368200	H
N	0	-1.32264600	1.88068500	1.94186400	H
H	0	-0.47357800	3.58402600	5.29295600	M
H	0	-2.66969700	4.06782900	4.10185900	M
H	0	1.15740700	1.95627700	4.25067300	M
O	0	-1.53794600	1.22209100	0.72067000	H
O	0	0.65282000	0.70809600	1.89213200	H
C	0	-3.58846200	3.09287400	1.82024300	M
O	0	-4.35352200	3.92638800	2.40536400	M
N	0	-3.89702500	2.46719500	0.64189800	M
H	0	-3.20078900	1.82682500	0.25735400	M

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C                  0   -5.16933800    2.72023400   -0.05740100 M
H                  0   -5.00499400    3.31324400   -0.96773500 M
H                  0   -5.63946000    1.76888300   -0.33360400 M
H                  0   -5.83208000    3.27677200    0.60880100 M
C                  0    3.76933900   -2.68139600    0.33399100 M
C                  0    4.35767200   -3.61167300   -0.53618700 M
C                  0    3.73399500   -3.93113300   -1.77143700 M
C                  0    2.52369300   -3.32538100   -2.13774000 M
C                  0    1.91981100   -2.37932800   -1.25886900 H
N                  0    2.57573300   -2.09373200   -0.05832500 H
H                  0    4.20040300   -4.65293500   -2.43669600 M
H                  0    5.29013000   -4.05966500   -0.21493700 M
H                  0    2.01380300   -3.54384200   -3.06909800 M
O                  0    1.91803700   -1.15085200    0.74138700 H
O                  0    0.78836900   -1.72969500   -1.45103300 H
C                  0    4.46630900   -2.37234700    1.65764300 M
O                  0    5.56858200   -2.96239400    1.90459700 M
N                  0    3.86540800   -1.48211800    2.50749400 M
H                  0    2.97592600   -1.07548700    2.20711300 M
C                  0    4.44972900   -1.15071100    3.81826800 M
H                  0    4.60839000   -0.06782000    3.90308000 M
H                  0    3.78417900   -1.47500600    4.62944100 M
H                  0    5.40834500   -1.66484400    3.91550800 M
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3,4,3-(LI-1,2-HOPO)H_4

C	-2.20811500	2.82795000	2.11987900
C	-1.22503700	3.31664700	2.98040600
C	-0.58246300	4.56188200	2.68518300
C	-0.93253500	5.31722900	1.56809700
C	-1.96329400	4.86100600	0.66874100
N	-2.53951000	3.60492500	1.03134500
H	0.20110000	4.92436100	3.34529300
H	-0.97313000	2.74338400	3.86461000
H	-0.43625400	6.25060200	1.33167900
O	-3.56324600	3.15601200	0.13498700
O	-2.43205600	5.40416500	-0.40169100
C	-2.95586100	1.53242200	2.42931100
O	-3.65749600	1.48638600	3.48869100
N	-2.77181300	0.44123700	1.60654700
C	-1.92854100	0.44143100	0.37596800
H	-2.30765200	-0.36069000	-0.26923600
H	-2.08473700	1.37569200	-0.17106900
C	8.37401600	-3.08409600	0.79645900
C	8.45381600	-3.62065400	2.08251200
C	9.72641000	-3.79793000	2.71216900
C	10.91171500	-3.44478200	2.07132700
C	10.88193500	-2.88545000	0.74144000
N	9.57253800	-2.74428700	0.18812900
H	9.76362000	-4.21789500	3.71419300
H	7.52123200	-3.88871600	2.56325700
H	11.88541200	-3.57042400	2.53125700
O	9.60573900	-2.18350100	-1.13144000
O	11.84844300	-2.49763100	-0.01510800
C	6.99909900	-2.91148600	0.15658200
O	5.97266500	-3.25918200	0.82497100
N	6.91774300	-2.40051200	-1.11278300
H	7.77104000	-2.12452900	-1.58820500
C	5.60386500	-2.22704200	-1.77147900
H	5.77285300	-2.24128100	-2.85559000
H	4.97869100	-3.08837500	-1.50632700
C	2.20837300	2.82808700	-2.11979000
C	1.22536300	3.31696000	-2.98029200
C	0.58301200	4.56230400	-2.68503500
C	0.93322100	5.31757200	-1.56793900
C	1.96387900	4.86113800	-0.66857000
N	2.53989100	3.60497900	-1.03123000
H	-0.20048500	4.92493600	-3.34514100
H	0.97333800	2.74376800	-3.86450700
H	0.43712200	6.25104400	-1.33152700
O	3.56354400	3.15584400	-0.13489100
O	2.43273100	5.40418800	0.40187200
C	2.95600900	1.53250000	-2.42927000
O	3.65785500	1.48651300	-3.48850400
N	2.77169500	0.44124300	-1.60665200
C	3.47597500	-0.82113900	-1.97760500
H	2.85276900	-1.66066600	-1.64183100
H	3.54726600	-0.85536300	-3.06985100
C	-8.37429900	-3.08372400	-0.79654800
C	-8.45407700	-3.62007300	-2.08269000

C	-9.72666400	-3.79732400	-2.71236800
C	-10.91198600	-3.44436200	-2.07145700
C	-10.88223200	-2.88525500	-0.74147600
N	-9.57283900	-2.74408800	-0.18815300
H	-9.76385300	-4.21712400	-3.71446200
H	-7.52148100	-3.88800000	-2.56348700
H	-11.88567900	-3.56999200	-2.53140000
O	-9.60606900	-2.18353300	1.13151200
O	-11.84876400	-2.49765000	0.01515300
C	-6.99938500	-2.91113000	-0.15665900
O	-5.97294100	-3.25871100	-0.82509700
N	-6.91802300	-2.40028800	1.11275400
H	-7.77131700	-2.12443900	1.58825400
C	-5.60413600	-2.22687100	1.77145000
H	-4.97899800	-3.08824400	1.50633200
H	-5.77313400	-2.24106800	2.85555900
C	4.89192500	-0.91264400	-1.34894600
H	5.48467600	-0.04675200	-1.66896200
H	4.81862000	-0.88653800	-0.25428300
C	1.92840800	0.44144700	-0.37608100
H	2.30750600	-0.36067300	0.26913400
H	2.08459800	1.37570900	0.17095400
C	0.41527000	0.22615200	-0.65722100
H	0.26750100	-0.71760300	-1.20292900
H	0.06196800	1.03182200	-1.31675000
C	-0.41539900	0.22614600	0.65709900
H	-0.06210100	1.03181600	1.31663000
H	-0.26761600	-0.71760900	1.20280500
C	-3.47613800	-0.82112500	1.97748800
H	-3.54736500	-0.85540000	3.06973600
H	-2.85299900	-1.66067000	1.64163300
C	-4.89212400	-0.91251800	1.34889600
H	-4.81886600	-0.88640100	0.25423300
H	-5.48480000	-0.04659000	1.66895600
H	-10.60632800	-2.06118500	1.24773000
H	-3.60440700	3.93956500	-0.49926300
H	3.60483100	3.93933900	0.49941200
H	10.60598900	-2.06107200	-1.24763700

3,3,3-(LI-1,2-HOPO)H_4

C	-0.51872700	5.01900300	0.50295100
C	0.20588700	5.91439900	1.28802900
C	1.39704500	6.51138600	0.75973000
C	1.84357600	6.23587100	-0.53120800
C	1.11000400	5.32981900	-1.38405600
N	-0.05292700	4.77034400	-0.77095400
H	1.96004300	7.20175700	1.38323400
H	-0.16088800	6.15846100	2.27780300
H	2.73983700	6.68420500	-0.94488500
O	-0.77635200	3.86873400	-1.61713000
O	1.33874000	4.95883000	-2.59338100
C	-1.85412300	4.43682900	0.95928800
O	-2.80343100	5.24977300	1.18882900
N	-1.96184000	3.07133400	1.14323300
C	-0.84127800	2.11046800	0.93267900
H	-1.07941200	1.46817600	0.07635000
H	0.05195200	2.68100800	0.66551200
C	7.26148800	-0.75510800	-1.00392000
C	8.20989200	0.01608600	-0.32988600
C	9.58384300	-0.38250100	-0.31394700
C	10.01449500	-1.53857200	-0.96099200
C	9.07251500	-2.36965900	-1.67073400
N	7.72463900	-1.89793100	-1.63722800
H	10.30452500	0.23432600	0.21705900
H	7.85443100	0.91036000	0.16669000
H	11.05054200	-1.85798100	-0.96027800
O	6.83588800	-2.76328400	-2.35694500
O	9.26133600	-3.46293600	-2.32385900
C	5.80531800	-0.29739300	-0.99915100
O	5.51038200	0.77385400	-0.37741900
N	4.87203600	-1.04613900	-1.66753200
H	5.16609000	-1.89888700	-2.13270900
C	3.45240400	-0.62629400	-1.69651100
H	3.42329600	0.45812400	-1.86136800
H	2.98078800	-1.11936200	-2.55572000
C	-0.79677000	-2.22321600	2.34523100
C	-2.18041300	-2.30999800	2.49057000
C	-2.72179900	-2.73641700	3.74826700
C	-1.90666600	-3.08323200	4.82460900
C	-0.46924200	-3.02001100	4.70455400
N	-0.01571600	-2.57516400	3.42690100
H	-3.80246000	-2.79516900	3.85426600
H	-2.83054900	-2.05968100	1.66031700
H	-2.30707900	-3.41425100	5.77646500
O	1.41152400	-2.51450400	3.30781100
O	0.44965500	-3.30407600	5.55985200
C	-0.13294200	-1.88553600	1.01222500
O	-0.25915000	-2.70731600	0.05163900
N	0.53721200	-0.68410900	0.88595500
C	1.24918600	-0.43154300	-0.40310900
H	0.67402600	-0.91292600	-1.20065600
H	1.25194500	0.65112700	-0.58071900
C	-5.85367100	-1.97899200	-1.51177100
C	-5.26993400	-3.24078000	-1.63189000

C	-5.71677200	-4.14696900	-2.64631700
C	-6.73467500	-3.80369700	-3.53231400
C	-7.36911100	-2.50957200	-3.44885300
N	-6.86192100	-1.66863900	-2.41261000
H	-5.24490600	-5.12311300	-2.72251800
H	-4.47513000	-3.49108300	-0.94037000
H	-7.08659100	-4.47568900	-4.30689900
O	-7.52758700	-0.39850600	-2.37746500
O	-8.31384400	-2.00323100	-4.16091500
C	-5.35236200	-1.03239200	-0.42885600
O	-4.47753800	-1.45800800	0.39137900
N	-5.84202300	0.24487300	-0.37893300
H	-6.55091300	0.52599000	-1.04932900
C	-5.34110200	1.19876300	0.63809800
H	-5.27027600	0.66625600	1.59488100
H	-6.08650900	1.99595200	0.74238300
C	2.70268400	-0.97559600	-0.38193900
H	3.25180300	-0.53556900	0.45973800
H	2.68101900	-2.06294200	-0.23841500
C	0.69400500	0.31109400	1.98905600
H	0.91282300	-0.21179500	2.92439100
H	1.58585900	0.90471300	1.75283000
C	-0.53356400	1.24694800	2.18448700
H	-0.32412600	1.90762200	3.03903400
H	-1.40248200	0.63483500	2.45440100
C	-3.31196200	2.52436900	1.46699400
H	-3.93056700	3.37291300	1.77140500
H	-3.22287000	1.84328900	2.32279300
C	-3.94988300	1.78188500	0.26277700
H	-3.30775000	0.95009000	-0.05018800
H	-4.04368000	2.46955800	-0.58767100
H	1.68348800	-2.87274600	4.21111300
H	-0.23719800	3.94727000	-2.46619400
H	-8.17878800	-0.51851800	-3.14635100
H	7.49244700	-3.46959300	-2.67192500

DFOH$_2$

N	-0.75175200	2.00718300	-1.81725700
C	0.02321200	3.22952100	-2.25505600
C	0.41235100	4.11088700	-1.03877900
C	1.58064800	3.49536200	-0.20417600
C	1.50597100	3.83320900	1.30841100
C	2.56836300	3.09307000	2.16836200
N	2.47273700	1.61862500	2.02121400
C	3.47046100	0.70831100	1.75973400
C	4.91149200	1.26779800	1.65211700
C	6.00974500	0.16294200	1.63288800
C	6.28800100	-0.45776900	0.24757700
O	7.37457300	-0.21895200	-0.37484700
N	5.31316200	-1.28240700	-0.25740100
C	5.47288900	-1.97037800	-1.56027300
C	4.31775300	-2.97558100	-1.78926200
C	2.95073800	-2.29310000	-2.08197400
C	1.74983300	-3.24289900	-1.83162900
C	0.35918200	-2.59330400	-2.08411100
N	0.24166600	-1.20210200	-1.54689300
C	0.13921100	-0.87588800	-0.25113700
C	0.09692500	-1.93765000	0.85176300
C	-1.05522700	-1.67495900	1.87010600
C	-2.43501200	-2.01913500	1.30379800
O	-2.80622200	-1.65805000	0.13631500
N	-3.27149800	-2.76024900	2.10708700
C	-4.60929500	-3.24727900	1.67774200
C	-5.78956500	-2.30466500	2.04926800
C	-5.81694700	-0.94275100	1.29829600
C	-6.04327000	-1.07754400	-0.23070600
C	-6.00647300	0.27282100	-0.98940400
N	-4.67311900	0.93609500	-0.91512700
C	-4.44689000	2.29976900	-0.80641000
C	-5.59057800	3.16408800	-0.25837700
O	1.16401500	1.11640900	2.34130600
O	3.22560300	-0.53966400	1.61776000
O	0.37162900	-0.22709600	-2.56180300
O	0.09807900	0.38795500	0.15196400
O	-3.64840700	0.19821200	-1.62100300
O	-3.33544000	2.83624600	-1.11200600
H	-0.42711100	1.63761300	-0.89102500
H	-1.76842500	2.19016400	-1.74567000
H	-0.50678800	1.13142100	-2.38355300
H	-0.59912600	3.78561800	-2.96554400
H	0.91807700	2.87831000	-2.78234300
H	0.68682900	5.11379200	-1.39746400
H	-0.48103400	4.24005600	-0.40879200
H	2.54306900	3.83525600	-0.62006500
H	1.56822100	2.40368700	-0.31380400
H	0.51141600	3.56800000	1.68948400
H	1.63670300	4.91461200	1.47318600
H	2.42599400	3.34888600	3.22907400
H	3.57582800	3.40268800	1.87356200
H	4.99937800	1.89960900	0.75612500
H	5.09691100	1.92095000	2.51571800

H	5.74028300	-0.62535200	2.34680600
H	6.95792600	0.60886800	1.94900900
H	4.45271800	-1.37325300	0.28480700
H	5.50692300	-1.22762300	-2.37214600
H	6.44493200	-2.48145300	-1.56404300
H	4.58962500	-3.63826200	-2.62477900
H	4.23315400	-3.61860500	-0.89746500
H	2.92887300	-1.92072700	-3.11592500
H	2.83255200	-1.40709200	-1.44519500
H	1.82378800	-4.13144100	-2.48009600
H	1.80858000	-3.61175300	-0.79565600
H	-0.44507400	-3.22211300	-1.67858800
H	0.18287900	-2.46086100	-3.15351600
H	0.01886500	-2.95181500	0.45063400
H	1.04898000	-1.85540500	1.39558000
H	-1.04565300	-0.61170400	2.13917700
H	-0.86642900	-2.24713400	2.78805700
H	-2.93722100	-3.02521200	3.02611800
H	-4.56365600	-3.40410900	0.59541600
H	-4.76363300	-4.22602100	2.15104400
H	-6.72372300	-2.85407900	1.84563800
H	-5.76632200	-2.12057600	3.13459900
H	-4.87837000	-0.40237700	1.48047900
H	-6.62231100	-0.32751000	1.73271900
H	-5.28646400	-1.73695800	-0.66886300
H	-7.02589500	-1.53645900	-0.42565100
H	-6.75016600	0.96142600	-0.57579900
H	-6.23970300	0.10899900	-2.05193100
H	-6.39002400	3.27974200	-1.00233400
H	-6.02712000	2.74734100	0.65617000
H	-5.17239800	4.14891700	-0.04196900
H	0.73540600	0.79107500	1.44886300
H	-3.23137000	-0.42887800	-0.95549300

Cartesian coordinates of optimized structures (CPCM, water)

Zr[3,4,3-(LI-1,2-HOPO)], **I**, CPCM

C	-1.11977300	1.68752700	-2.92473200
C	-0.54350100	2.10061100	-4.13392300
C	0.46292500	1.30306000	-4.74769100
C	0.86883700	0.08875700	-4.17484000
C	0.28220700	-0.33139200	-2.94805000
N	-0.67476900	0.50305800	-2.37379700
H	0.91371800	1.63648500	-5.67753700
H	-0.88782100	3.01873500	-4.59398600
H	1.62152900	-0.54287500	-4.63198700
O	-1.22269400	0.01694800	-1.17526300
O	0.54884600	-1.43101900	-2.25910400
C	-2.34416500	2.41534800	-2.36902000
O	-3.31691400	2.57314100	-3.20204000
N	-2.39029400	2.91150700	-1.10131800
C	-1.28229900	2.84992900	-0.09819400
H	-1.74809000	2.57264100	0.85281700
H	-0.60697700	2.03927400	-0.35863500
C	4.30599000	-1.40039000	-1.07411800
C	5.16545100	-2.39192400	-1.56773400
C	4.72732000	-3.74112500	-1.65895700
C	3.42961300	-4.09517300	-1.26765500
C	2.55093000	-3.09092400	-0.77146400
N	3.03354300	-1.78808300	-0.67827000
H	5.40253500	-4.49931800	-2.04321000
H	6.15775400	-2.09483000	-1.88093300
H	3.06062100	-5.11196500	-1.33612000
O	2.12410300	-0.88143300	-0.10246200
O	1.29816700	-3.27462300	-0.37806700
C	4.78889500	0.04454200	-1.02468600
O	6.00862200	0.28791800	-1.36479400
N	3.92637700	1.02436300	-0.65698000
H	2.99517800	0.73737400	-0.35193800
C	4.34596400	2.44993100	-0.62420300
H	5.13137200	2.57820100	0.13210700
H	4.79635000	2.68252200	-1.59764100
C	1.73472900	0.75944800	3.20579600
C	2.07466000	0.45123000	4.52894000
C	1.62424400	-0.76617000	5.11299300
C	0.93392500	-1.70920000	4.34014000
C	0.62140700	-1.40716600	2.98370700
N	0.91808000	-0.12355900	2.51923700
H	1.86774600	-0.98801400	6.14761500
H	2.72780600	1.12330000	5.07297400
H	0.65019900	-2.68070200	4.72843600
O	0.34671200	0.20951200	1.27194500
O	0.08514500	-2.22257800	2.09271100
C	2.53428600	1.80759700	2.43333600
O	3.79456700	1.56130000	2.35706000
N	1.95923300	2.90745500	1.87306400
C	2.86671500	3.83364800	1.11713900
H	2.38824200	4.81323000	1.11469200
H	3.80651900	3.92412700	1.67466000

C	-4.51496700	-1.80233700	0.60774500
C	-5.41342900	-2.84881100	0.35331500
C	-4.93765100	-4.12335300	-0.05300100
C	-3.56526500	-4.33809800	-0.23879800
C	-2.65442000	-3.27582100	0.01034600
N	-3.15744700	-2.06461900	0.47697800
H	-5.64349500	-4.92579000	-0.24261300
H	-6.47112700	-2.64308700	0.45297600
H	-3.16665000	-5.28614500	-0.58064200
O	-2.17443000	-1.12413000	0.82671700
O	-1.33834500	-3.32071200	-0.17386600
C	-5.06652300	-0.41701700	0.91751100
O	-6.33958900	-0.29432700	1.06514200
N	-4.20596600	0.63502900	0.96388400
H	-3.21088700	0.42367800	0.86983100
C	-4.67769100	2.03303100	1.11617700
H	-3.98131600	2.55312600	1.78354400
H	-5.65026400	1.99242700	1.61317200
C	3.16902300	3.42968100	-0.36085600
H	2.25589100	3.05530400	-0.84140000
H	3.42612400	4.36605500	-0.87439300
C	0.58833800	3.34229500	2.34341900
H	-0.04413800	2.45026700	2.35432000
H	0.68976300	3.69012900	3.38082000
C	-0.11177400	4.47044900	1.54368400
H	0.47456200	5.39700000	1.59469100
H	-1.03329300	4.66954800	2.11225900
C	-0.51025300	4.19187300	0.06567600
H	0.36849500	4.19188700	-0.58962100
H	-1.14261600	5.02740200	-0.26311100
C	-3.62057300	3.66720000	-0.68855200
H	-3.93379100	4.28620000	-1.53564200
H	-3.32221500	4.33483600	0.12597500
C	-4.83051800	2.80264400	-0.23589500
H	-5.11308300	2.09931700	-1.02864100
H	-5.66817900	3.50636100	-0.12318100
Zr	-0.06953100	-1.52930400	-0.06471100

Zr[3,3,3-(LI-1,2-HOPO)], **II**, CPCM

C	-0.79686800	1.79162900	-2.83027500
C	-0.14014800	2.18645500	-4.00420400
C	0.81158800	1.31922000	-4.61011400
C	1.08829200	0.05785900	-4.06200900
C	0.42378100	-0.34267300	-2.86906300
N	-0.48664500	0.55189100	-2.30797600
H	1.32387000	1.63778000	-5.51287100
H	-0.38067200	3.14702700	-4.44281800
H	1.80169700	-0.62339800	-4.51095200
O	-1.12634900	0.07714400	-1.15151100
O	0.58147300	-1.47335100	-2.19602500
C	-1.96646800	2.61594000	-2.28951200
O	-2.87077300	2.91851300	-3.15830200
N	-2.03433700	3.04358400	-0.99361400
C	-1.00829000	2.72146500	0.05132200
C	4.28015500	-1.37388700	-0.87970800
C	5.17773800	-2.36255700	-1.30567800
C	4.76975500	-3.72346400	-1.36128100
C	3.46375000	-4.09251100	-1.01165600
C	2.54473900	-3.09146100	-0.58682200
N	3.00554100	-1.77898200	-0.51169000
H	5.47532700	-4.48028200	-1.68963500
H	6.17337600	-2.05598300	-1.59865400
H	3.11993600	-5.11912700	-1.06101800
O	2.07059500	-0.87204200	0.01890300
O	1.27586700	-3.28226700	-0.24591800
C	4.71619000	0.08800900	-0.88733200
O	5.93534300	0.35325100	-1.21134700
N	3.81265300	1.05865100	-0.59872300
H	2.88251600	0.75986600	-0.30233700
C	4.17766700	2.49773900	-0.67576100
H	4.97620300	2.70774100	0.04862300
H	4.59841100	2.67809100	-1.67364900
C	1.48890800	0.92885200	3.25044700
C	1.76584000	0.68536900	4.60180600
C	1.33263200	-0.52900100	5.20496300
C	0.72037200	-1.52938000	4.43526600
C	0.46788100	-1.29057900	3.05479100
N	0.75018600	-0.01576100	2.55994100
H	1.52859300	-0.70327700	6.25860400
H	2.35882000	1.40349900	5.15586400
H	0.45417500	-2.49509200	4.84945800
O	0.24909700	0.25250900	1.27457600
O	0.00110400	-2.15127700	2.16272000
C	2.29895900	1.95703700	2.45762500
O	3.56677600	1.73508900	2.45880800
N	1.74134800	2.99888600	1.78044800
C	2.66859700	3.89671000	1.01291200
H	2.19422000	4.88166800	0.99116500
H	3.60255200	3.98872600	1.57785500
C	-4.57876800	-1.62021900	0.40339900
C	-5.51419700	-2.59906200	0.03924000
C	-5.08281700	-3.86403900	-0.44191800
C	-3.71612900	-4.13149100	-0.59670300

C	-2.76759900	-3.13605800	-0.23606200
N	-3.23049500	-1.94107100	0.30719700
H	-5.81718600	-4.61548400	-0.71402600
H	-6.56442400	-2.34786200	0.11133100
H	-3.34853700	-5.07000300	-0.99504300
O	-2.21962700	-1.08189400	0.77740900
O	-1.44981200	-3.22837200	-0.38038800
C	-5.06974000	-0.22652400	0.77127600
O	-6.33779300	-0.04038700	0.88876100
N	-4.15100500	0.76856300	0.88404900
H	-3.16914400	0.49400500	0.81612700
C	-4.52868700	2.19193700	1.05031800
H	-3.83461800	2.64262500	1.76882400
H	-5.52993800	2.21209400	1.48811700
C	2.97668000	3.45758200	-0.45206900
H	2.07214700	3.05075800	-0.92237800
H	3.21919400	4.38100200	-0.99529100
C	0.36513500	3.52018400	2.07413200
H	-0.17216200	2.76082500	2.65083300
H	0.49080600	4.39952500	2.72133700
C	-0.47551700	3.94241300	0.83882800
C	-3.25600200	3.82666900	-0.60421800
H	-3.48111100	4.50655400	-1.43169800
H	-2.99670000	4.43317300	0.26515700
C	-4.53441300	2.99871200	-0.28931000
H	-4.77164400	2.32582700	-1.12249200
H	-5.35172500	3.73221100	-0.23251900
Zr	-0.09754700	-1.52700200	-0.01249400
H	0.09390400	4.60905900	0.17968700
H	-1.30190000	4.53469800	1.24892000
H	-0.17716300	2.21574100	-0.43438600
H	-1.44297200	2.00717800	0.75293800

$[ZrDFO(H_2O)_2]^{2+}$ with non hydrogen bonded amine group, **III**, CPCM

Zr	0.29537800	-0.31543800	1.16681300
N	-8.15471000	-5.01405300	-1.65216500
C	-7.38446300	-3.76034900	-2.08030900
C	-6.32197900	-3.37389400	-1.03226200
C	-5.55838200	-2.09129800	-1.45883600
C	-4.48329500	-1.68000800	-0.41826700
C	-3.74740700	-0.38893000	-0.85561600
N	-2.63834700	-0.02408000	0.06624700
C	-2.60973300	0.85526000	1.07405700
C	-3.82720200	1.64161300	1.53519700
C	-3.56264100	3.16056300	1.69805700
C	-3.34975400	3.87892700	0.35503700
O	-3.89548400	3.44932900	-0.72906300
N	-2.57099500	4.99991100	0.39181700
C	-2.19489200	5.80238700	-0.79983700
C	-0.68719500	5.66224200	-1.14489200
C	-0.25908900	4.20137500	-1.43869100
C	1.24844600	4.07316600	-1.77308200
C	1.72777200	2.61235300	-1.97520500
N	1.65363100	1.78057300	-0.73604100
C	2.53827200	1.66199900	0.25869500
C	3.85751800	2.41520800	0.29847500
C	5.09412200	1.47186400	0.24960400
C	5.18681300	0.69607300	-1.07490600
O	4.78711300	1.21290900	-2.18431700
N	5.70441900	-0.56277500	-1.01173500
C	5.80577300	-1.46962600	-2.18529300
C	5.91042200	-2.94927600	-1.73489000
C	4.74208600	-3.45664600	-0.84237900
C	3.35880400	-3.49344900	-1.54356900
C	2.21144700	-3.96268400	-0.60877100
N	1.81843500	-2.92784100	0.38986900
C	2.15011500	-2.77761400	1.68053900
C	3.00813400	-3.75429400	2.45317500
O	-1.44636900	-0.78813500	-0.12727100
O	-1.45959700	0.97267100	1.72124300
O	0.47362300	0.99178200	-0.58195100
O	2.20836200	0.83461900	1.23962200
O	0.98482200	-1.89759700	-0.14750300
O	1.67012100	-1.70958700	2.29452100
H	-8.88112500	-5.24501300	-2.33645900
H	-7.52977400	-5.82230300	-1.57151400
H	-8.61031000	-4.87376400	-0.74509400
H	-8.13062900	-2.97152600	-2.20919500
H	-6.93446500	-3.99063000	-3.04969700
H	-6.80839800	-3.20643900	-0.06016700
H	-5.61040300	-4.20295500	-0.90598500
H	-6.27541300	-1.26648400	-1.59199400
H	-5.07820000	-2.25894800	-2.43509600
H	-3.75239600	-2.49170800	-0.29902500
H	-4.95505500	-1.51349400	0.56071400
H	-4.43835200	0.45573500	-0.91665500
H	-3.28564100	-0.52062300	-1.83976600
H	-4.66996200	1.47630500	0.86334900

H	-4.10558800	1.23561600	2.51728900
H	-2.70843200	3.33616700	2.36024100
H	-4.44304800	3.60531200	2.18204500
H	-2.15708700	5.26621900	1.27935300
H	-2.81399400	5.45912300	-1.63367800
H	-2.43842400	6.85409800	-0.60240900
H	-0.48282000	6.30028000	-2.01857000
H	-0.08684700	6.06106500	-0.31177600
H	-0.85319400	3.80460600	-2.27727600
H	-0.48867900	3.57750400	-0.56453100
H	1.47123000	4.61323400	-2.70602900
H	1.84843600	4.54674300	-0.98186900
H	2.76187500	2.57832600	-2.32836200
H	1.10091400	2.09420800	-2.70726200
H	3.91014700	3.13909300	-0.51549600
H	3.88535300	2.97199400	1.24300100
H	5.08456800	0.77811300	1.09689700
H	5.99431000	2.09363500	0.34744300
H	6.03881600	-0.90403000	-0.11724700
H	4.92343900	-1.30317600	-2.81300900
H	6.68690600	-1.20488400	-2.78710100
H	5.98226400	-3.56637800	-2.64244500
H	6.85506000	-3.08535000	-1.18613800
H	4.68023000	-2.83360900	0.06141700
H	4.98969900	-4.47270200	-0.49920600
H	3.09779600	-2.50981200	-1.95587500
H	3.39366200	-4.19500100	-2.39027700
H	2.49133100	-4.87149900	-0.06863600
H	1.30533900	-4.17426600	-1.18470900
H	3.90341100	-3.23298900	2.81064700
H	2.44508100	-4.09484900	3.32929000
H	3.31412500	-4.61802800	1.86318500
O	-1.04210300	-1.89677400	2.25505600
H	-1.79404300	-2.30502300	1.78753600
H	-0.75630000	-2.42380800	3.02378600
O	0.40828600	0.33028200	3.33421000
H	1.08472600	0.04595400	3.97408600
H	-0.29463000	0.87558800	3.73122600

$[ZrDFO(H_2O)_2]^{2+}$ with hydrogen bonded amine group, **IIIa**, CPCM

Zr	0.09593700	-0.90110900	-1.06389700
N	-1.23474300	0.18668800	2.32465400
C	-1.05209400	0.02372800	3.82895800
C	-0.39117200	-1.33147000	4.16965400
C	1.07274400	-1.48431600	3.64369200
C	1.40367100	-2.93651300	3.18761500
C	2.51062700	-3.02668400	2.11129800
N	2.14088800	-2.27480500	0.86456500
C	2.94319600	-1.85243800	-0.12427500
C	4.43563100	-2.15918900	-0.13330800
C	5.29107600	-1.16062500	-0.94775300
C	5.54115500	0.16232700	-0.20353300
O	5.64298200	0.19610400	1.07932400
N	5.68305300	1.27741700	-0.97993000
C	5.91353300	2.64446000	-0.44456700
C	4.62748600	3.51744700	-0.45993900
C	3.45376800	2.87046300	0.31717300
C	2.19046600	3.76378700	0.39723800
C	0.97960300	3.03699400	1.03821700
N	0.36472900	2.01353500	0.14449800
C	-0.65286500	2.13705200	-0.71725600
C	-1.36834900	3.45542500	-0.96233000
C	-2.90634700	3.29020500	-1.01857600
C	-3.51517700	2.69444700	0.26354000
O	-2.78294200	2.32005400	1.25498100
N	-4.86971400	2.56645500	0.26643100
C	-5.65543500	1.84928400	1.30311300
C	-6.51113400	0.71491100	0.67344100
C	-5.70246900	-0.35562400	-0.11034000
C	-4.80863500	-1.25661900	0.78257500
C	-4.03089200	-2.34208200	-0.00664400
N	-2.88184700	-1.81054300	-0.79347000
C	-2.73986600	-1.68891800	-2.12193500
C	-3.86073200	-1.99669600	-3.09336800
O	0.74471800	-2.12284800	0.60540400
O	2.35645600	-1.24031100	-1.13743800
O	0.87187000	0.67988700	0.27861400
O	-1.01425400	1.04848400	-1.37111100
O	-1.70240800	-1.54342500	-0.03037900
O	-1.55489100	-1.30782900	-2.56231500
H	-0.33200500	0.29000900	1.83250200
H	-1.68779800	-0.63109300	1.89286200
H	-1.81141600	1.01440400	2.08203000
H	-2.04658700	0.09598300	4.27835500
H	-0.44947800	0.87242700	4.16750500
H	-0.42222800	-1.44906600	5.26115400
H	-1.02229100	-2.13153900	3.75427200
H	1.78188400	-1.16350800	4.42017700
H	1.23044900	-0.81293300	2.79134100
H	0.49877200	-3.41436800	2.79581200
H	1.74119800	-3.54392100	4.03925500
H	2.68990800	-4.07582800	1.84313400
H	3.44686700	-2.59722200	2.48271400
H	4.81387300	-2.22299800	0.88977200

H	4.54565800	-3.16007000	-0.57562100
H	4.84456600	-0.97162500	-1.92848400
H	6.27141900	-1.62531000	-1.12215200
H	5.56151700	1.18299700	-1.98273000
H	6.28573500	2.53662300	0.57879700
H	6.69811200	3.11777900	-1.04737800
H	4.88318700	4.49493100	-0.02214900
H	4.32346400	3.70310200	-1.50217100
H	3.78095700	2.62876000	1.34062100
H	3.19097200	1.91936500	-0.16240500
H	2.40174100	4.65383000	1.00884100
H	1.90621700	4.12330500	-0.60281500
H	0.19960700	3.75056300	1.31714200
H	1.28116400	2.49978900	1.94297200
H	-1.09004700	4.19024700	-0.20493000
H	-1.03074700	3.84663100	-1.93151800
H	-3.18877800	2.64531200	-1.85937600
H	-3.35865100	4.27167100	-1.20759700
H	-5.37598100	2.90149700	-0.54754600
H	-4.94641900	1.45876600	2.03749600
H	-6.31287200	2.56327000	1.81642100
H	-7.08084200	0.23694600	1.48503400
H	-7.24987000	1.16960600	-0.00435100
H	-5.08436100	0.14297500	-0.87115600
H	-6.41315900	-0.99620300	-0.65478100
H	-4.09590400	-0.65426800	1.36008600
H	-5.43956500	-1.78641200	1.51201100
H	-4.69289100	-2.86822200	-0.70149700
H	-3.60191800	-3.08064600	0.67910400
H	-3.56684900	-1.64017000	-4.08233000
H	-4.03192400	-3.07936100	-3.14399000
H	-4.79631500	-1.51562100	-2.79713100
O	0.48348200	-2.87358900	-2.23591000
H	-0.11465900	-3.13169500	-2.96146600
O	0.94682300	-0.10890200	-3.00379200
H	1.87673400	-0.27168400	-3.24683400
H	1.32648900	-3.36155600	-2.26200800
H	0.46760200	0.41052000	-3.67354700

$ZrDFO(OH)_2$, **IV**, CPCM

Zr	-0.19003800	-0.46726400	1.46791600
N	1.15924900	-0.65663700	-2.01812900
C	1.28625000	-1.49762200	-3.28188000
C	1.17770100	-3.03804200	-3.06642700
C	-0.18405400	-3.74692800	-3.37789200
C	-1.19014800	-3.94678500	-2.20241500
C	-2.08922800	-2.71084300	-1.89069400
N	-1.95581400	-2.23114500	-0.48876300
C	-2.89358500	-1.79178400	0.37439300
C	-4.35426400	-2.23342500	0.26642700
C	-5.36571300	-1.26177800	0.92457400
C	-5.68593200	-0.04272100	0.04524500
O	-5.87599400	-0.17492600	-1.22205400
N	-5.79307300	1.16223000	0.68003300
C	-6.08387400	2.44538800	-0.01057100
C	-4.81850300	3.32867800	-0.19833000
C	-3.66928500	2.59064700	-0.93007600
C	-2.45196800	3.49484600	-1.25240400
C	-1.22151900	2.69175700	-1.75628300
N	-0.52168800	1.95361700	-0.66988600
C	0.54068900	2.33081200	0.05586600
C	1.24393200	3.66499400	-0.16098100
C	2.78433800	3.53207600	-0.11120500
C	3.36396800	2.55110900	-1.14696100
O	2.61648900	1.85783900	-1.93417000
N	4.72241900	2.44783900	-1.15022500
C	5.50210700	1.43143200	-1.90053200
C	6.43668900	0.63389300	-0.94844400
C	5.70950700	-0.10291400	0.21103800
C	4.83429200	-1.29971000	-0.24616100
C	4.10626400	-2.01688300	0.92131400
N	2.93699400	-1.26450200	1.45387500
C	2.77970300	-0.69394400	2.66238500
C	3.92024700	-0.62282300	3.66382400
O	-0.60865400	-1.95796100	-0.11767200
O	-2.47987000	-1.06355800	1.38694200
O	-0.99782600	0.63161700	-0.40299600
O	0.97096800	1.49858600	0.98154500
O	1.76495700	-1.32670100	0.63803900
O	1.59485500	-0.21635500	2.96869700
H	0.18606400	-0.51653900	-1.70303600
H	1.62911900	-1.08557400	-1.19547300
H	1.59356000	0.27316400	-2.14646600
H	2.27334100	-1.25921400	-3.68907200
H	0.53280600	-1.13518600	-3.98848400
H	1.92285800	-3.47813900	-3.74367800
H	1.50969700	-3.29440400	-2.04999200
H	0.06390600	-4.74947200	-3.75682300
H	-0.68589500	-3.22600400	-4.20941400
H	-0.64034400	-4.23174300	-1.29716900
H	-1.84421100	-4.79263900	-2.45456900
H	-3.14242100	-2.93598500	-2.07124100
H	-1.81445100	-1.86573200	-2.53655100
H	-4.63499900	-2.40512300	-0.77531500

H	-4.42294800	-3.20422400	0.77801000
H	-5.01589400	-0.94915500	1.91268300
H	-6.30827100	-1.80800800	1.06803600
H	-5.59856300	1.19876200	1.67477100
H	-6.52107200	2.19926100	-0.98301800
H	-6.83641100	2.98504500	0.57743700
H	-5.12079300	4.22405300	-0.76400300
H	-4.46462200	3.67658200	0.78496200
H	-4.04880400	2.16104300	-1.87051900
H	-3.33358800	1.74880100	-0.31261400
H	-2.72431800	4.22036300	-2.03400300
H	-2.15742600	4.07638100	-0.36590400
H	-0.50149100	3.35619100	-2.24121900
H	-1.52452900	1.93612000	-2.48930700
H	0.93393200	4.11993300	-1.10375300
H	0.93589200	4.34846900	0.64219900
H	3.10307100	3.19680200	0.88324800
H	3.23107200	4.52215600	-0.26864800
H	5.23927000	3.04294400	-0.51021500
H	4.78677800	0.77645700	-2.40424900
H	6.10310700	1.92925800	-2.67325900
H	7.00067100	-0.08755500	-1.55931400
H	7.17533300	1.32991400	-0.52138700
H	5.09115800	0.61734100	0.76674900
H	6.46858700	-0.47317800	0.91736300
H	4.09152800	-0.98130600	-0.98896500
H	5.47242600	-2.04930600	-0.73830200
H	4.79695600	-2.20371700	1.74961400
H	3.71197800	-2.98309700	0.58508700
H	3.63707300	0.07138100	4.45788100
H	4.09938300	-1.61023100	4.10867300
H	4.85075700	-0.28190600	3.20196000
O	-0.33366200	-2.11374700	2.80329500
H	0.29281000	-2.14752400	3.55369100
O	-1.11186900	0.83771800	2.82302700
H	-2.00801400	0.63861200	3.15853200

3,4,3-(LI-1,2-HOPO)H_4, CPCM

C	-1.63787300	-3.85791800	-0.60821300
C	-0.36246600	-4.17890200	-1.06558700
C	0.40445300	-5.16251800	-0.36156800
C	-0.10086600	-5.80530400	0.76908400
C	-1.41805600	-5.49385700	1.26250300
N	-2.10981000	-4.51800900	0.50727600
H	1.40029500	-5.40942700	-0.71834300
H	0.02856700	-3.68341800	-1.94577200
H	0.47201000	-6.55004100	1.31038600
O	-3.41694100	-4.18068800	0.98284200
O	-2.04376600	-5.98078500	2.29209200
C	-2.59426400	-2.92198100	-1.34023300
O	-3.35936000	-3.42833300	-2.24119000
N	-2.57673900	-1.60024500	-1.01968500
C	-1.68970000	-1.01009000	0.03197300
H	-2.28791800	-0.27583800	0.58416700
H	-1.40104600	-1.79334900	0.73868500
C	8.98027700	-1.19216800	-0.32575500
C	9.32743300	-2.06891200	-1.35543300
C	10.65212200	-2.06939300	-1.89165100
C	11.62653400	-1.20053500	-1.40432500
C	11.31150900	-0.28045600	-0.34394300
N	9.97901700	-0.34168100	0.13229600
H	10.89792600	-2.76058200	-2.69220100
H	8.56552200	-2.74040100	-1.72789200
H	12.63681000	-1.18519100	-1.79728400
O	9.71345000	0.59386200	1.18299700
O	12.08209700	0.59553000	0.23037900
C	7.55677200	-1.22122100	0.22244400
O	6.72881700	-2.05631000	-0.29719400
N	7.21316600	-0.38230800	1.23533000
H	7.91074900	0.26302500	1.59307200
C	5.84932500	-0.34965100	1.81481400
H	5.43364000	-1.36218300	1.78299400
H	5.95226700	-0.05033300	2.86370200
C	1.63804700	3.85807300	0.60895900
C	0.36275300	4.17906000	1.06665600
C	-0.40426600	5.16281400	0.36294000
C	0.10084900	5.80574400	-0.76772300
C	1.41791800	5.49430100	-1.26146300
N	2.10977300	4.51829200	-0.50653700
H	-1.40002000	5.40972000	0.71996300
H	-0.02811100	3.68347400	1.94685800
H	-0.47210100	6.55059200	-1.30879300
O	3.41678100	4.18097200	-0.98244100
O	2.04343700	5.98134400	-2.29111500
C	2.59452200	2.92200000	1.34070000
O	3.35974700	3.42820700	2.24162800
N	2.57691100	1.60030700	1.01998600
C	3.51289500	0.67569300	1.73186000
H	3.59854900	1.00570000	2.77205500
H	3.05973200	-0.32059300	1.72411100
C	-8.98046200	1.19204200	0.32487500
C	-9.32785900	2.06911000	1.35419500

C	-10.65262500	2.06963100	1.89022500
C	-11.62686900	1.20049200	1.40306600
C	-11.31159000	0.28005100	0.34307000
N	-9.97903000	0.34125500	-0.13299300
H	-10.89862300	2.76107900	2.69049100
H	-8.56608100	2.74082600	1.72651600
H	-12.63720500	1.18518600	1.79587400
O	-9.71314200	-0.59467000	-1.18326700
O	-12.08201900	-0.59620100	-0.23105100
C	-7.55689000	1.22109300	-0.22315400
O	-6.72905600	2.05632400	0.29644700
N	-7.21309800	0.38203400	-1.23585400
H	-7.91058200	-0.26342600	-1.59355700
C	-5.84918700	0.34938400	-1.81517000
H	-5.43357900	1.36195100	-1.78346600
H	-5.95198200	0.04988800	-2.86402200
C	4.91343400	0.63772000	1.06485500
H	4.81693800	0.32733200	0.01643100
H	5.35724100	1.64104800	1.07929300
C	1.68973000	1.01031200	-0.03163900
H	1.40104800	1.79366000	-0.73824200
H	2.28786200	0.27609200	-0.58396800
C	0.42466400	0.33364100	0.55761600
H	-0.17451000	1.08947700	1.08428500
H	0.72067400	-0.42275400	1.29820900
C	-0.42461000	-0.33343300	-0.55724600
H	0.17457000	-1.08928500	-1.08388500
H	-0.72059300	0.42295000	-1.29786200
C	-3.51268600	-0.67575500	-1.73176900
H	-3.59819100	-1.00588000	-2.77193800
H	-3.05958400	0.32055900	-1.72407100
C	-4.91331300	-0.63780200	-1.06494700
H	-4.81698200	-0.32726400	-0.01655300
H	-5.35703500	-1.64117000	-1.07930500
H	-3.50561700	-4.76919900	1.78868500
H	-10.60355100	-1.05408300	-1.27769000
H	3.50530900	4.76961600	-1.78820500
H	10.60397200	1.05308500	1.27741800

3,3,3-(LI-1,2-HOPO)H_4, CPCM

C	-0.96116800	-3.59363300	-1.48149300
C	0.19362600	-3.80111100	-2.23137200
C	1.16164800	-4.75251600	-1.77336500
C	0.96877000	-5.47578000	-0.59589200
C	-0.21745500	-5.28177000	0.19831300
N	-1.12149300	-4.32811100	-0.32482200
H	2.06307700	-4.91139900	-2.35825900
H	0.34113600	-3.24588300	-3.14945900
H	1.69504600	-6.19830900	-0.24054200
O	-2.30129400	-4.10445800	0.45372600
O	-0.56015300	-5.85559000	1.31268600
C	-2.12518300	-2.71426700	-1.92638600
O	-3.06190900	-3.26259800	-2.61518000
N	-2.11072900	-1.39629200	-1.58810200
C	-1.02768400	-0.75441800	-0.78040000
H	-1.51149400	-0.05976700	-0.08376700
H	-0.52397700	-1.51820300	-0.18118400
C	8.06955500	-0.85444400	1.51869600
C	8.13559200	-1.61203600	2.68971400
C	9.25064000	-1.48503600	3.57438900
C	10.29478200	-0.60586800	3.29452400
C	10.26805800	0.19279600	2.09778700
N	9.13068900	0.00810700	1.27330300
H	9.27851600	-2.08511500	4.47891800
H	7.31982700	-2.29013600	2.90142900
H	11.14909400	-0.49355300	3.95250000
O	9.15189500	0.81752400	0.09310800
O	11.14486000	1.05480500	1.67523900
C	6.85984900	-1.01481500	0.60341000
O	5.97108600	-1.88512900	0.92849600
N	6.75638200	-0.24367100	-0.51144500
H	7.48823000	0.43207700	-0.70909900
C	5.59731600	-0.32613000	-1.43215700
H	5.95718400	-0.04131900	-2.42704200
H	5.25661300	-1.36595200	-1.47242400
C	0.96157000	3.59393100	-1.48196200
C	-0.19334300	3.80136900	-2.23167500
C	-1.16123900	4.75287800	-1.77362600
C	-0.96811200	5.47631400	-0.59629300
C	0.21829900	5.28244600	0.19765300
N	1.12216400	4.32861400	-0.32546900
H	-2.06279600	4.91167400	-2.35834400
H	-0.34104700	3.24599100	-3.14964100
H	-1.69432200	6.19887900	-0.24088400
O	2.30216300	4.10516400	0.45282800
O	0.56118600	5.85629800	1.31195900
C	2.12545300	2.71444100	-1.92694800
O	3.06211200	3.26262200	-2.61595200
N	2.11098500	1.39654400	-1.58837300
C	3.25995900	0.53511700	-2.00839400
H	2.88830800	-0.49093600	-2.09361000
H	3.59312300	0.86292500	-2.99802200
C	-8.07017200	0.85394000	1.51797700
C	-8.13654900	1.61146400	2.68901600

C	-9.25182300	1.48435900	3.57339600
C	-10.29585700	0.60516800	3.29319800
C	-10.26879800	-0.19341700	2.09640800
N	-9.13120200	-0.00865500	1.27225800
H	-9.27995800	2.08438000	4.47795500
H	-7.32088000	2.28960200	2.90097900
H	-11.15033300	0.49276300	3.95094500
O	-9.15203600	-0.81798100	0.09199400
O	-11.14542000	-1.05549200	1.67364000
C	-6.86027300	1.01448700	0.60298600
O	-5.97162300	1.88479800	0.92838300
N	-6.75649200	0.24344500	-0.51191200
H	-7.48820200	-0.43240600	-0.70973200
C	-5.59723700	0.32610500	-1.43236600
H	-5.25666300	1.36597300	-1.47248100
H	-5.95685100	0.04132700	-2.42735200
C	4.43295100	0.60430800	-0.99434600
H	4.80021100	1.63578800	-0.92451000
H	4.07923300	0.30518300	0.00079600
C	1.02790400	0.75491400	-0.78052700
H	1.51161900	0.06030700	-0.08378500
H	0.52430800	1.51887000	-0.18143700
C	0.00003900	0.00026800	-1.66463700
H	0.51704400	-0.71891900	-2.31139600
H	-0.51706000	0.71950700	-2.31126400
C	-3.25974900	-0.53501400	-2.00829600
H	-3.59278500	-0.86293700	-2.99793100
H	-2.88817900	0.49106300	-2.09356300
C	-4.43284600	-0.60421500	-0.99437100
H	-4.07924800	-0.30498900	0.00078300
H	-4.80004500	-1.63571500	-0.92450500
H	-10.01636300	-1.32102800	0.20226300
H	-2.17056100	-4.73735900	1.21894200
H	2.17175900	4.73849400	1.21775400
H	10.01622300	1.32051800	0.20372300

DFOH$_2$, CPCM

N	-2.21171500	1.03373600	1.95342200
C	-2.32889200	2.54685100	1.85768100
C	-0.95665800	3.24086700	1.66407600
C	-1.07442800	4.55132200	0.82508200
C	-0.89500300	4.39421900	-0.71563500
C	-2.00182200	3.67462900	-1.53369800
N	-1.97851300	2.18104800	-1.44946300
C	-3.05025200	1.32872600	-1.63267800
C	-4.46600700	1.89064400	-1.41253700
C	-5.52624200	0.76923400	-1.31415900
C	-5.29597200	-0.21255200	-0.15128000
O	-4.76358500	0.16833200	0.96028800
N	-5.73330100	-1.48766100	-0.35233700
C	-5.72239500	-2.59117100	0.64703500
C	-4.56871000	-3.61015400	0.41810400
C	-3.20274000	-3.10285700	0.95056300
C	-1.99366400	-3.95202800	0.47648200
C	-0.63746300	-3.52346300	1.10963600
N	-0.45251900	-2.03591200	1.13880100
C	-0.15539600	-1.26454600	0.08238300
C	0.24806000	-1.86656000	-1.26472400
C	1.60581200	-1.31338300	-1.80482900
C	2.81716200	-1.80799600	-1.01227900
O	2.89392400	-1.61978200	0.26699100
N	3.79741100	-2.44911000	-1.69852700
C	5.06199700	-2.95686400	-1.10160200
C	6.28366800	-2.04636600	-1.41475100
C	6.19538500	-0.61196700	-0.82295200
C	6.31736900	-0.56146300	0.72386500
C	5.95704100	0.81994400	1.32916100
N	4.52330800	1.17067700	1.12755900
C	3.98162000	2.28895200	0.53696600
C	4.94963600	3.26339700	-0.13953600
O	-0.68007900	1.63111300	-1.78272500
O	-2.87492800	0.08980100	-1.92028200
O	-0.78274900	-1.44345400	2.38425800
O	-0.22235800	0.06229100	0.18564000
O	3.62279800	0.32022500	1.87080300
O	2.71571800	2.50843000	0.53422700
H	-1.48075700	0.65255600	1.30306600
H	-1.93632900	0.71658500	2.88497900
H	-3.12044300	0.60128300	1.70638000
H	-2.83524200	2.89812000	2.76185000
H	-2.98341600	2.74593100	1.01121600
H	-0.52491000	3.46849400	2.64805200
H	-0.25890200	2.55545600	1.16623200
H	-0.29201500	5.24765900	1.16042100
H	-2.03604000	5.04601800	1.03838800
H	0.06856500	3.91074100	-0.92173800
H	-0.83310700	5.40597300	-1.14435200
H	-1.88051600	3.94305400	-2.59395400
H	-2.99388400	4.00905000	-1.21676500
H	-4.49540400	2.51381600	-0.51344200
H	-4.72503100	2.54452500	-2.25657500

H	-5.58560900	0.21525900	-2.25651700
H	-6.50630400	1.24168400	-1.15496500
H	-6.12125400	-1.71209700	-1.26273100
H	-5.65003400	-2.14498800	1.64425800
H	-6.69109700	-3.09932600	0.56940800
H	-4.83701300	-4.55134000	0.92169300
H	-4.50333000	-3.83381800	-0.65818800
H	-3.23634500	-3.08051100	2.05029600
H	-3.05189200	-2.06657700	0.62215100
H	-2.15046900	-5.01325200	0.72527800
H	-1.92379700	-3.89086700	-0.61990900
H	0.19995500	-4.00160500	0.58915400
H	-0.59311100	-3.81727300	2.16143400
H	0.28339600	-2.95752500	-1.23028600
H	-0.52612000	-1.58854500	-1.99148000
H	1.60167000	-0.21793100	-1.75118700
H	1.70432800	-1.59370900	-2.85872700
H	3.67469500	-2.57384000	-2.69806800
H	4.90264900	-3.05249300	-0.02457200
H	5.23854100	-3.95901300	-1.50963000
H	7.18118100	-2.55562000	-1.03036400
H	6.39939400	-1.98245200	-2.50717800
H	5.24669400	-0.15037200	-1.13393100
H	6.99595400	0.00155500	-1.26391000
H	5.67780200	-1.32258000	1.18885500
H	7.35031000	-0.79236700	1.02415500
H	6.56250800	1.60979500	0.87799800
H	6.14665100	0.82141200	2.41080400
H	5.62529500	3.72184800	0.59221000
H	5.55821200	2.76579000	-0.90212500
H	4.35499000	4.04759800	-0.61266500
H	-0.44614300	0.97108300	-1.01107800
H	3.31045700	-0.40675900	1.23404200

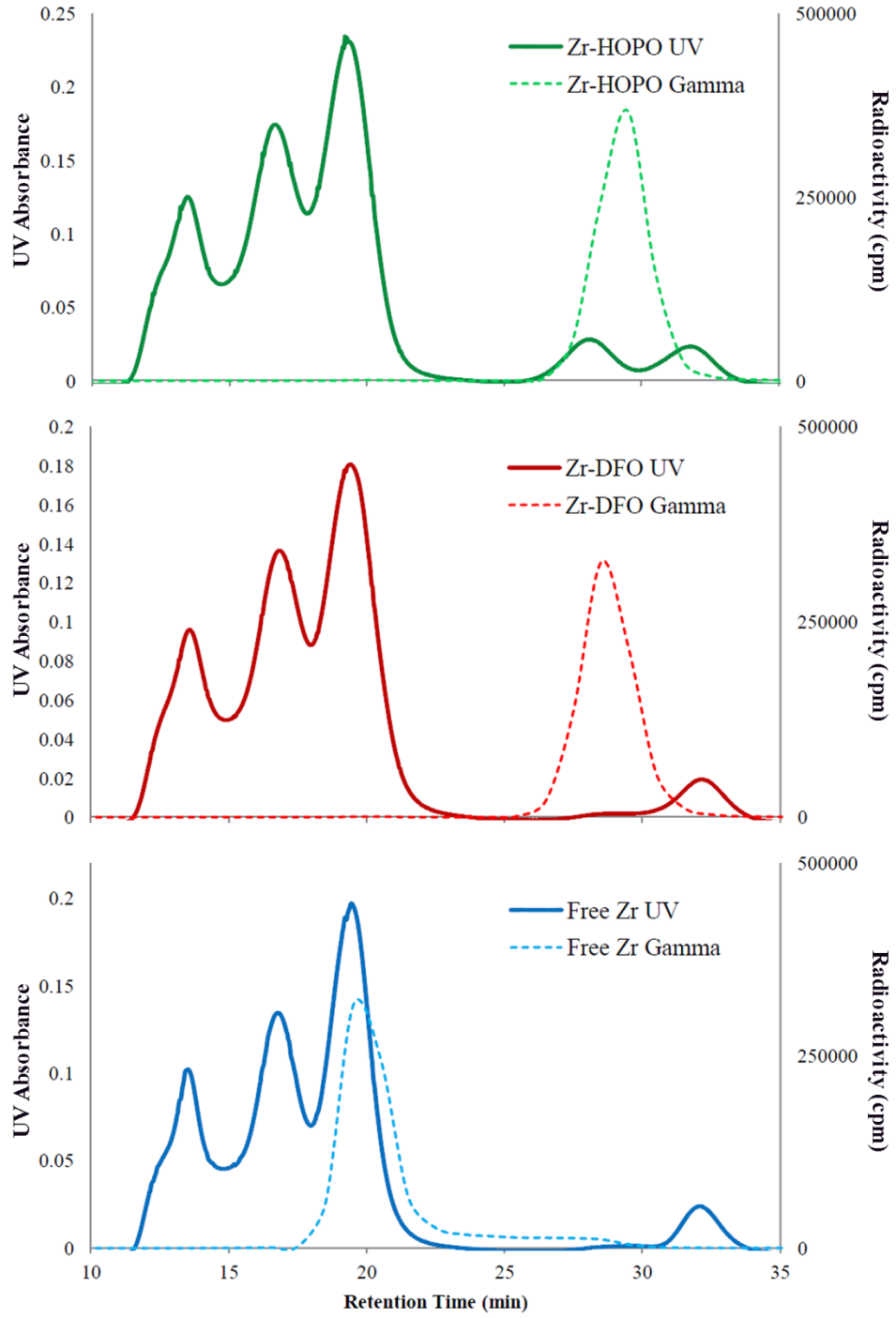

Figure S12. SEC chromatograms of ^{89}Zr-HOPO, ^{89}Zr-DFO, and free ^{89}Zr in serum after 7 days. Solid lines are the UV absorbance due to the serum components and to the HOPO ligand itself. Dotted lines are the radiotrace associated with the ^{89}Zr.

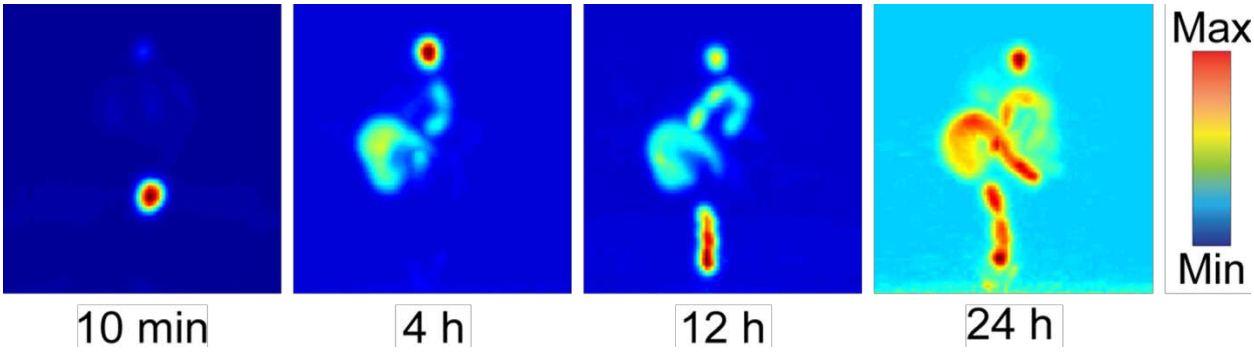

Figure S13. Maximum intensity projection PET images

	10 min		1 h		4 h		12 h		24 h	
	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO
Blood	3.24 ± 0.66	5.11 ± 0.90	0.17 ± 0.10	0.10 ± 0.04	0.05 ± 0.04	0.03 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	0.02 ± 0.00	0.02 ± 0.02
Heart	1.57 ± 0.22	2.17 ± 0.62	0.12 ± 0.06	0.06 ± 0.02	0.06 ± 0.01	0.03 ± 0.01	0.06 ± 0.01	0.02 ± 0.00	0.07 ± 0.01	0.02 ± 0.01
Lung	1.07 ± 0.17	2.16 ± 1.08	0.17 ± 0.09	0.14 ± 0.04	0.08 ± 0.01	0.04 ± 0.02	0.06 ± 0.01	0.02 ± 0.01	0.09 ± 0.05	0.04 ± 0.01
Gall Bladder	6.61 ± 2.87	1.57 ± 0.25	6.94 ± 3.38	0.47 ± 0.14	1.00 ± 0.41	0.26 ± 0.15	2.45 ± 1.02	0.16 ± 0.14	1.15 ± 0.59	0.23 ± 0.21
Liver	3.29 ± 0.75	0.88 ± 0.49	0.22 ± 0.09	0.24 ± 0.07	0.13 ± 0.01	0.12 ± 0.03	0.09 ± 0.02	0.06 ± 0.02	0.06 ± 0.03	0.11 ± 0.02
Spleen	0.31 ± 0.04	0.37 ± 0.22	0.09 ± 0.03	0.06 ± 0.02	0.06 ± 0.01	0.03 ± 0.01	0.05 ± 0.01	0.02 ± 0.01	0.06 ± 0.01	0.02 ± 0.01
Stomach	1.22 ± 0.39	0.62 ± 0.28	0.30 ± 0.15	1.10 ± 0.51	0.50 ± 0.74	0.06 ± 0.02	0.01 ± 0.00	0.01 ± 0.00	0.02 ± 0.00	0.01 ± 0.01
Large Intestine	0.26 ± 0.15	0.43 ± 0.13	0.09 ± 0.06	0.02 ± 0.01	7.17 ± 2.15	0.62 ± 0.55	0.10 ± 0.03	0.07 ± 0.05	0.03 ± 0.02	0.02 ± 0.01
Small Intestine	5.99 ± 1.18	0.94 ± 0.16	1.11 ± 0.35	0.35 ± 0.17	0.12 ± 0.13	0.04 ± 0.02	0.02 ± 0.01	0.01 ± 0.01	0.02 ± 0.00	0.02 ± 0.01
Kidney	9.46 ± 2.71	14.44 ± 5.88	1.05 ± 0.51	1.39 ± 0.55	0.40 ± 0.14	1.10 ± 0.44	0.53 ± 0.23	0.36 ± 0.13	0.51 ± 0.29	1.12 ± 0.33
Bladder	2.04 ± 1.06	2.50 ± 0.48	0.73 ± 0.36	2.47 ± 1.30	0.58 ± 0.27	1.22 ± 0.77	0.54 ± 0.26	0.69 ± 0.31	0.28 ± 0.14	0.56 ± 0.41
Muscle	0.36 ± 0.06	0.73 ± 0.56	0.10 ± 0.03	0.02 ± 0.01	0.09 ± 0.06	0.01 ± 0.01	0.06 ± 0.01	0.01 ± 0.00	0.06 ± 0.01	0.01 ± 0.00
Bone	1.04 ± 0.44	0.43 ± 0.10	0.29 ± 0.09	0.07 ± 0.04	0.23 ± 0.12	0.04 ± 0.02	0.25 ± 0.07	0.03 ± 0.01	0.17 ± 0.03	0.06 ± 0.01
Tail	4.25 ± 1.46	5.13 ± 2.92	0.81 ± 0.34	0.26 ± 0.05	0.29 ± 0.18	0.14 ± 0.08	0.11 ± 0.04	0.13 ± 0.05	0.05 ± 0.01	0.08 ± 0.02

Table S2. Full biodistribution data including all tissues collected. All values expressed as %ID/g.

	10 min		1 h		4 h		12 h		24 h	
	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO	Zr-HOPO	Zr-DFO
Blood	1.28 ± 0.39	2.71 ± 0.94	0.08 ± 0.03	0.04 ± 0.01	0.03 ± 0.01	0.01 ± 0.01	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.01
Heart	0.27 ± 0.02	0.33 ± 0.10	0.02 ± 0.01	0.01 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
Lung	0.13 ± 0.04	0.30 ± 0.21	0.03 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.01 ± 0.00
Gall Bladder	0.34 ± 0.29	0.13 ± 0.09	0.10 ± 0.16	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
Liver	1.20 ± 0.09	0.31 ± 0.10	0.10 ± 0.01	0.12 ± 0.02	0.04 ± 0.01	0.05 ± 0.02	0.04 ± 0.01	0.02 ± 0.01	0.02 ± 0.01	0.05 ± 0.02
Spleen	0.04 ± 0.01	0.07 ± 0.02	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
Stomach	0.67 ± 0.68	0.22 ± 0.10	0.16 ± 0.08	0.66 ± 0.26	0.45 ± 0.50	0.02 ± 0.01	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00
Large Intestine	0.23 ± 0.11	0.41 ± 0.13	1.05 ± 1.93	0.02 ± 0.00	6.53 ± 1.86	1.37 ± 1.58	0.11 ± 0.02	0.07 ± 0.04	0.04 ± 0.01	0.02 ± 0.01
Small Intestine	2.18 ± 1.25	0.43 ± 0.13	0.77 ± 0.33	0.19 ± 0.13	0.35 ± 0.62	0.02 ± 0.01	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00
Kidney	2.78 ± 1.57	6.11 ± 2.87	0.40 ± 0.20	0.57 ± 0.18	0.16 ± 0.07	0.44 ± 0.17	0.21 ± 0.10	0.14 ± 0.05	0.21 ± 0.12	0.46 ± 0.16
Bladder	0.08 ± 0.09	0.07 ± 0.04	0.01 ± 0.01	0.05 ± 0.03	0.01 ± 0.00	0.02 ± 0.01	0.01 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	0.01 ± 0.01
Muscle	0.04 ± 0.01	0.10 ± 0.10	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
Bone	0.05 ± 0.04	0.02 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
Tail	2.55 ± 0.95	1.74 ± 0.72	0.27 ± 0.05	0.12 ± 0.03	0.14 ± 0.07	0.07 ± 0.03	0.05 ± 0.01	0.07 ± 0.03	0.03 ± 0.01	0.04 ± 0.01

Table S3. Biodistribution data without normalization. All values expressed as %ID.

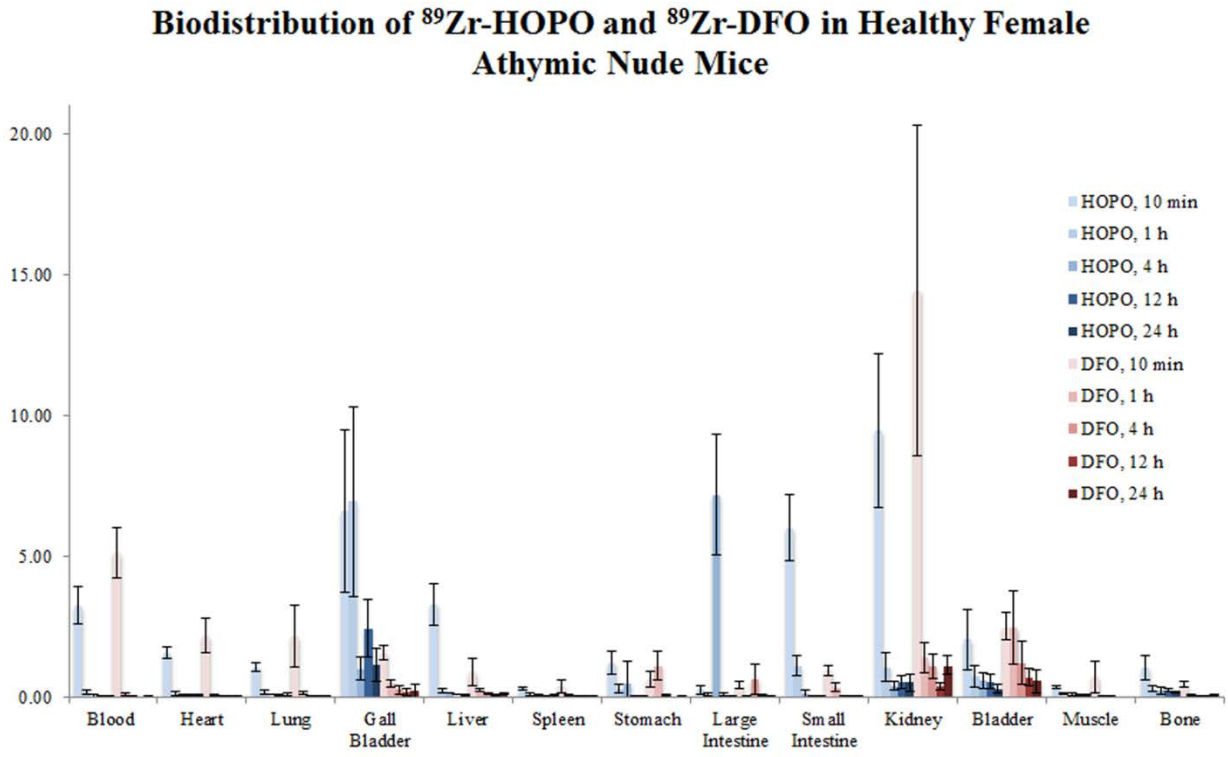

Figure S14. Graphical biodistribution data.

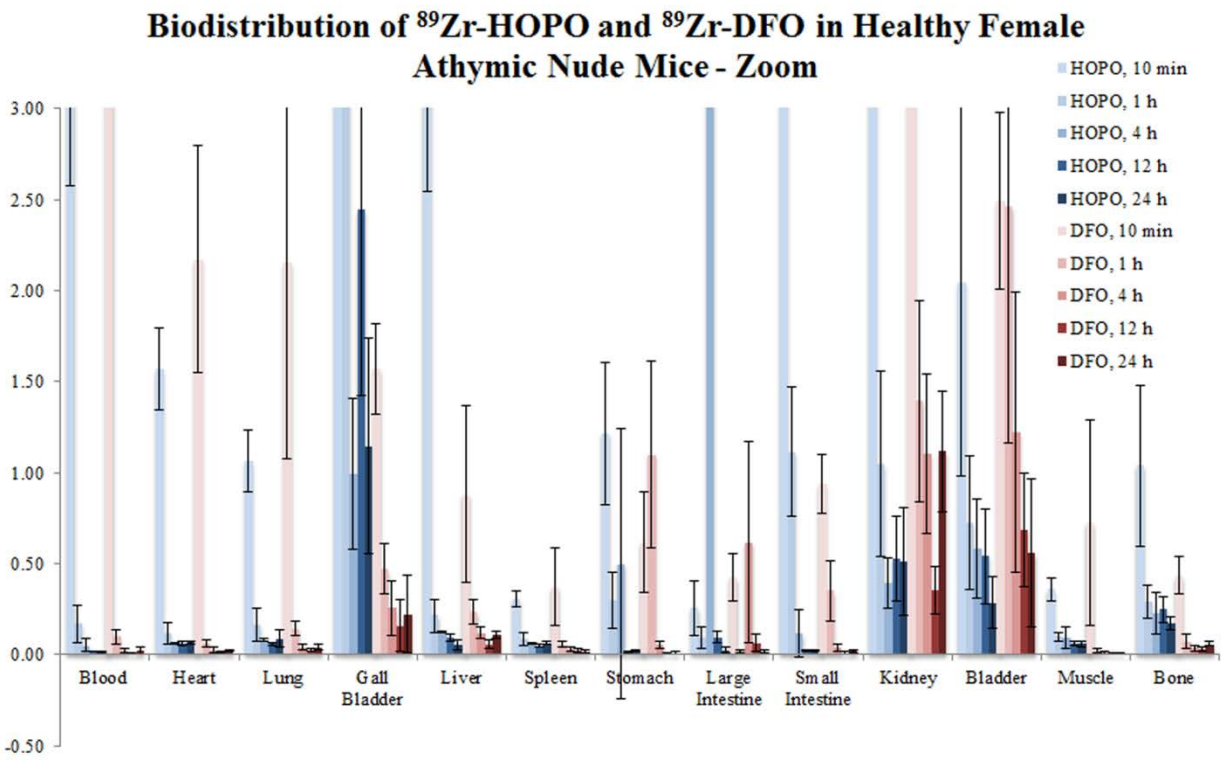

Figure S15. Zoomed in biodistribution data.

	10 min	1 h	4 h	12 h	24 h
Blood	**0.01529**	0.25713	0.27915	n/a	0.35592
Heart	0.11823	0.16419	**0.00164**	**0.00013**	**0.00011**
Lung	0.09260	0.63237	**0.00928**	**0.00042**	0.14603
Gall Bladder	**0.01283**	**0.01075**	**0.01512**	**0.00447**	**0.02669**
Liver	**0.00169**	0.70805	0.63334	0.08529	**0.02658**
Spleen	0.57396	0.19204	**0.00677**	**0.00144**	**0.00015**
Stomach	0.14010	**0.02319**	0.18904	0.13398	0.20703
Large Intestine	0.12945	**0.04036**	**0.00384**	0.37090	0.34642
Small Intestine	**0.03807**	**0.00781**	0.30326	0.11353	1.00000
Kidney	0.11012	0.39845	**0.02181**	0.24716	**0.03458**
Bladder	0.46929	**0.04248**	0.17054	0.49863	0.24675
Muscle	0.24602	**0.00310**	**0.03876**	**0.00003**	**0.00036**
Bone	**0.03801**	**0.00481**	**0.01486**	**0.00090**	**0.00088**
Tail	0.60666	**0.02000**	0.15382	0.47791	0.03349

Table S4. Calculated P values for the comparison of ^{89}Zr-HOPO and ^{89}Zr-DFO biodistribution data. Multiple unpaired t tests were carried out using GraphPad Prism. Significant values are shown in bold ($P < 0.05$).