Supporting Information for:

Th^{IV}-Desferrioxamine: Characterization of a Fluorescent Bacterial Probe

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Dalton Transactions

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General Considerations for NMR Spectroscopy Characterization:

All NMR data was collected on a Bruker (AVANCE™) 400 MHz instrument, operating at 400 MHz for ^{1}H and 101 MHZ for ^{13}C). ^{1}H NMR was referenced to the HDO peak as 4.79 ppm. ^{13}C NMR were referenced to the acetic acid-d_4 (-CHD_2, p) as 21.03 ppm.[1] Spectra were collected at 25 °C. *Note, samples containing ^{232}Th were doubly contained, with the radioactive material in a shatter-proof PTFE-tube liner fitted with a Teflon stopper (Sigma). This liner was placed inside of a standard 5 mm glass NMR tube for data acquisition.*

NMR solvents (D_2O, acetic acid-d_4, and ND_4OD or NaOD (38%) were purchased (Sigma-Aldrich) and used as received.

The following experiments (pulse sequences) provided, by Bruker, were utilized to conduct NMR experiments: ^{1}H (zg30), ^{13}C (zgpg30), COSY (cosygpppqf), HMBC (hmbcgplpndqf), HSQC (hsqcedetgp), DEPT-135 (deptsp153). The data was processed using MestReNova (V 14.1) NMR software.

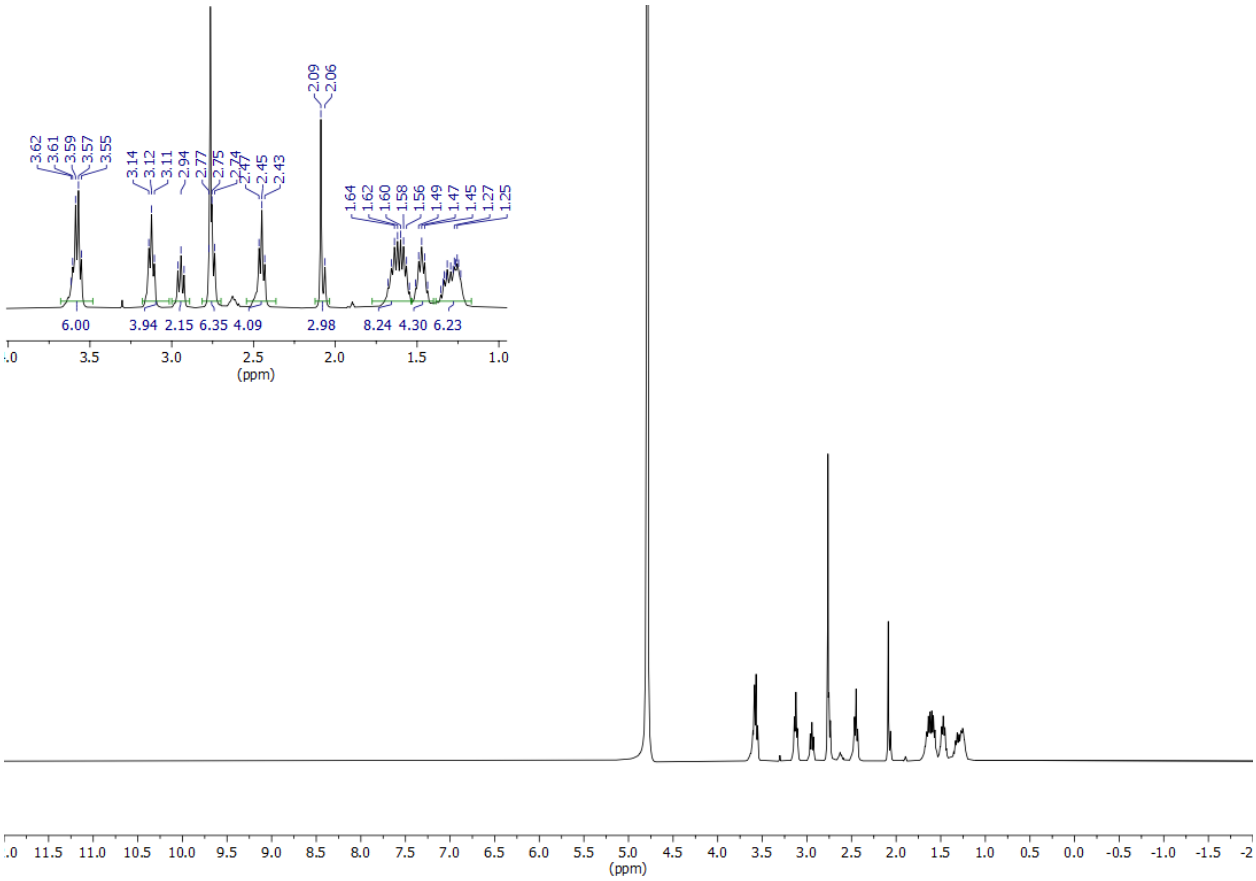

Figure S1. ^{1}H NMR of H_4DFO-mesylate. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

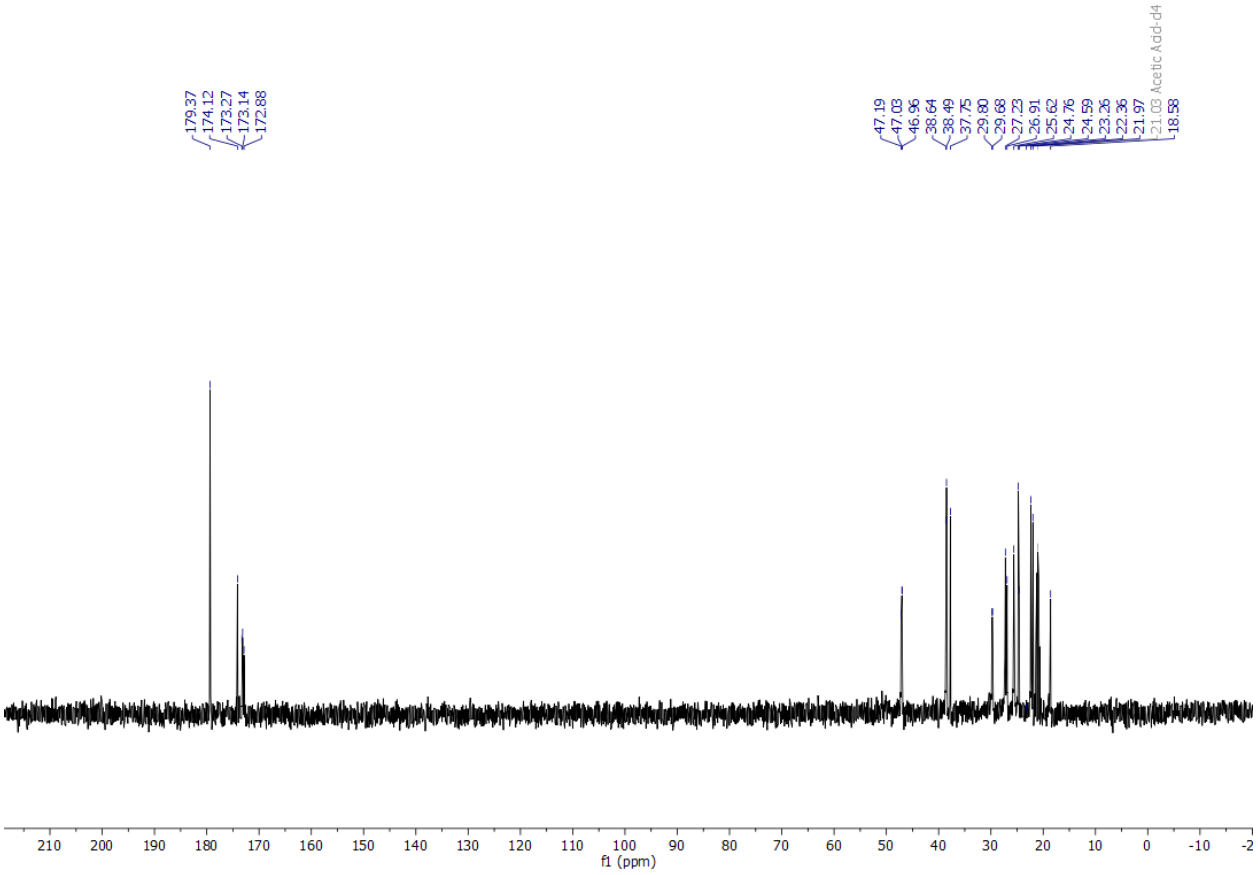

Figure S2. ^{13}C NMR of H_4DFO-mesylate. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

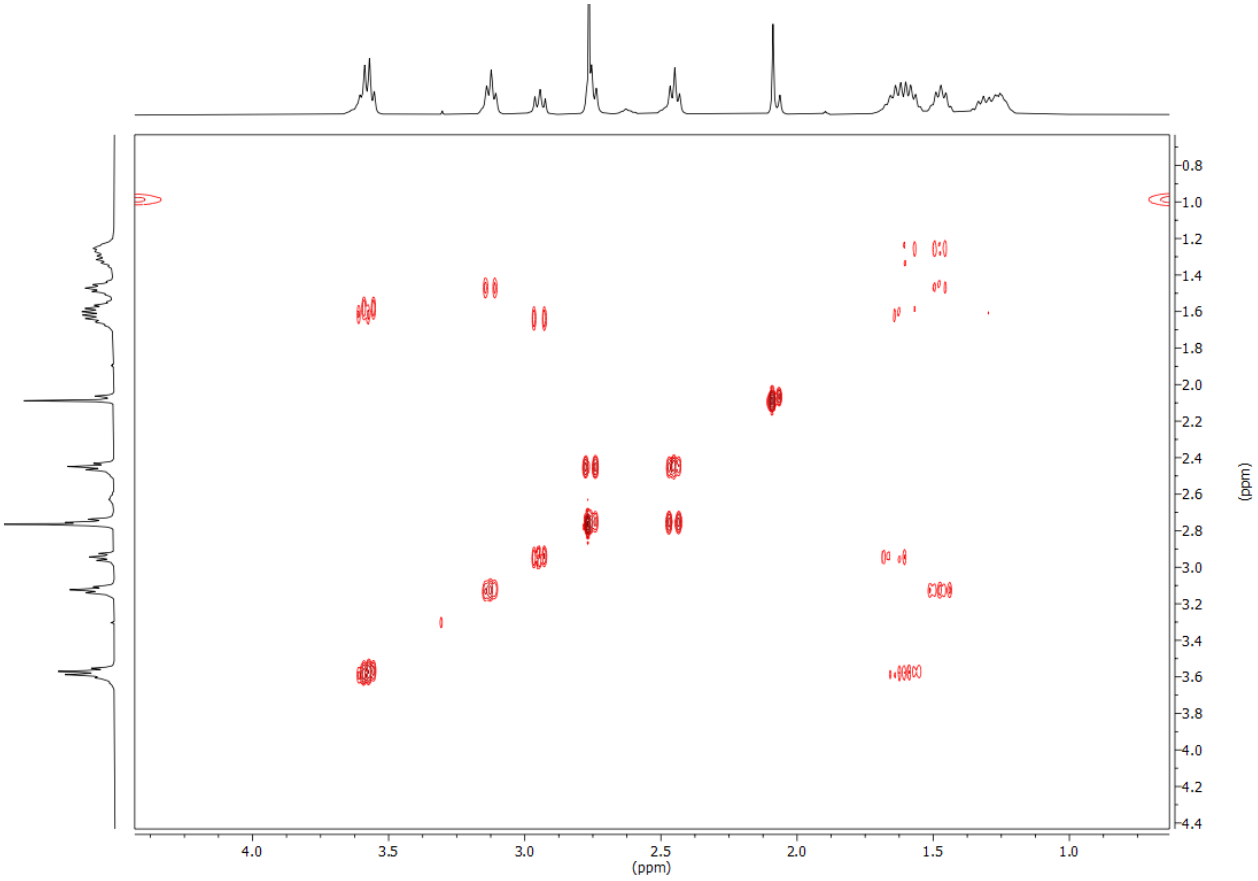

Figure S3. COSY NMR of H_4DFO-mesylate. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

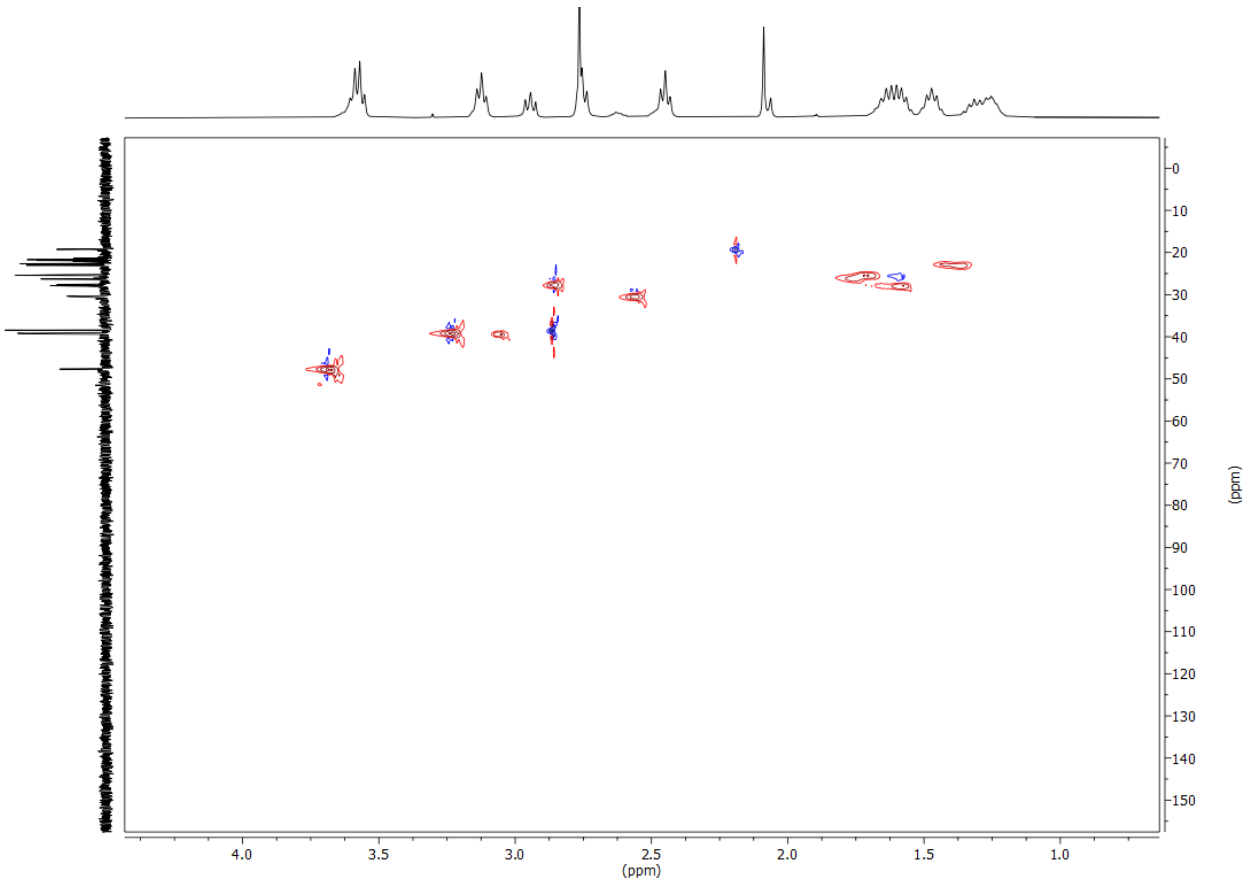

Figure S4. HSQC NMR of H_4DFO-mesylate. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

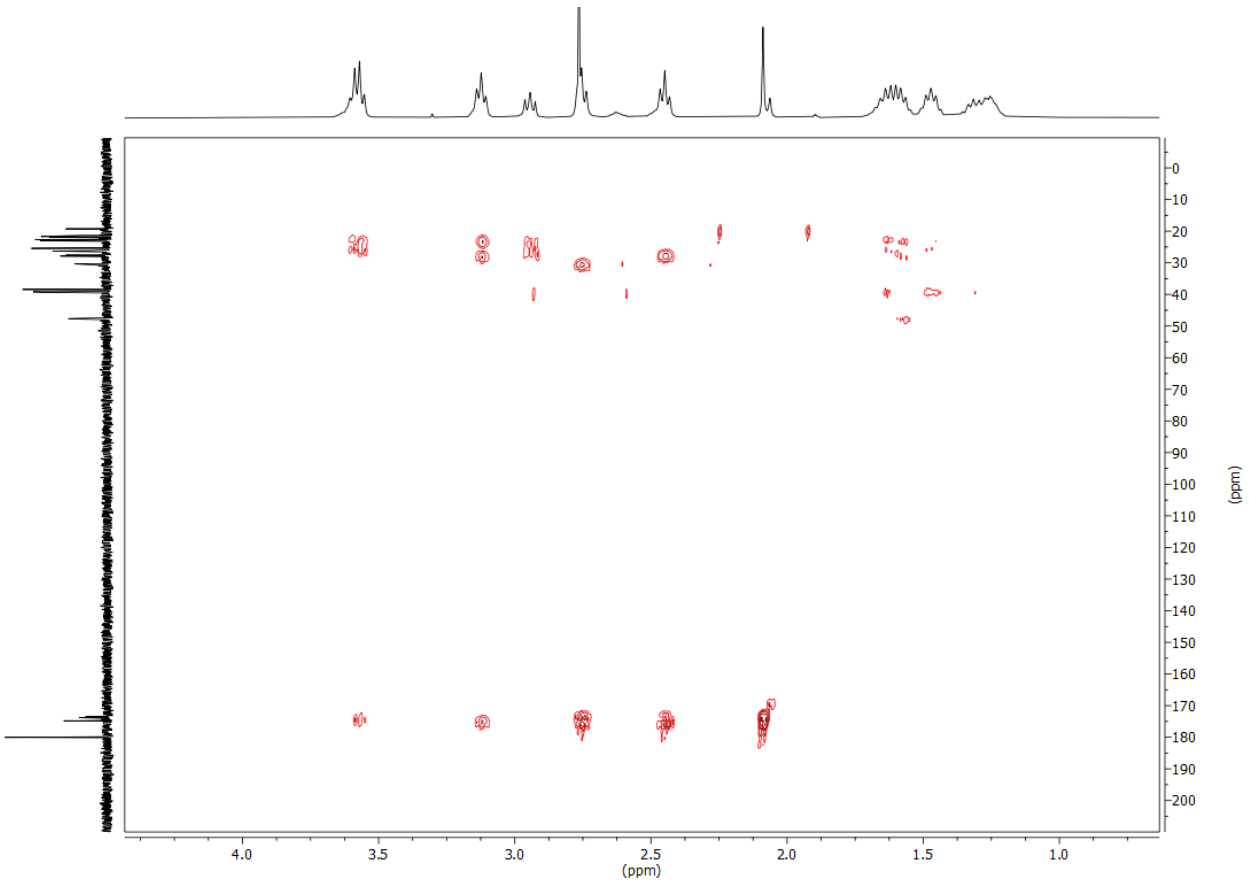

Figure S5. HMBC NMR of H_4DFO-mesylate. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

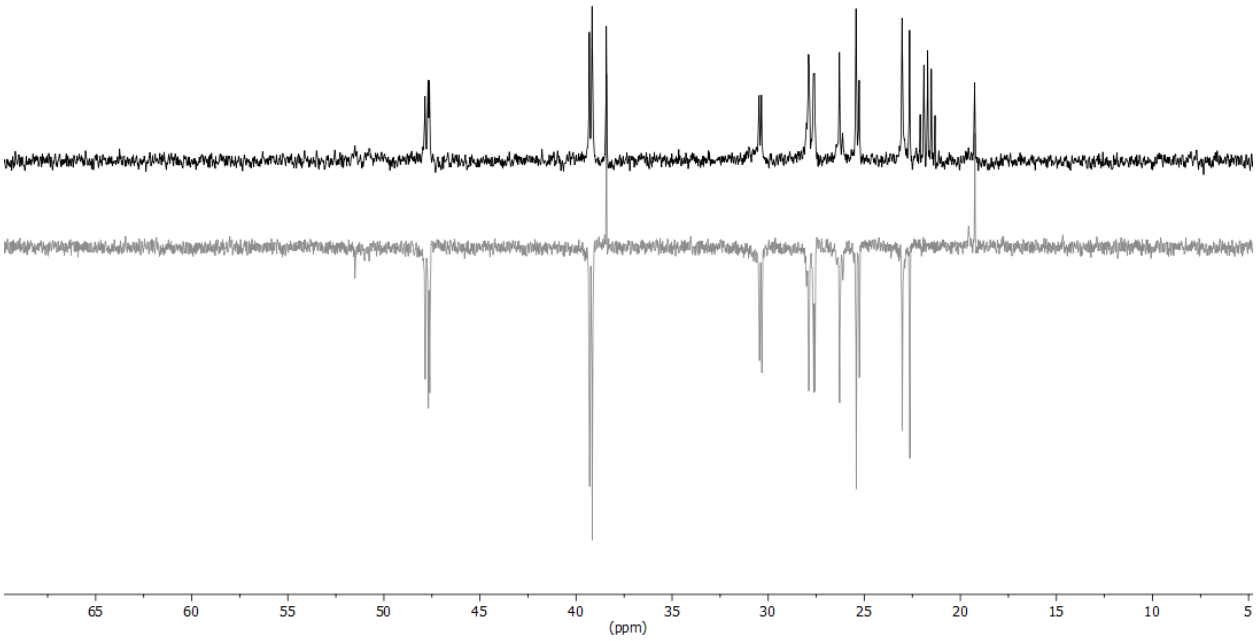

Figure S6. DEPT-135 NMR (*bottom*, grey) of H_4DFO-mesylate overlaid with ^{13}C NMR (*top*, black). The spectra were observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 (pentet at 21.03 ppm, top spectrum) on a 400 MHz spectrometer at 25 °C.

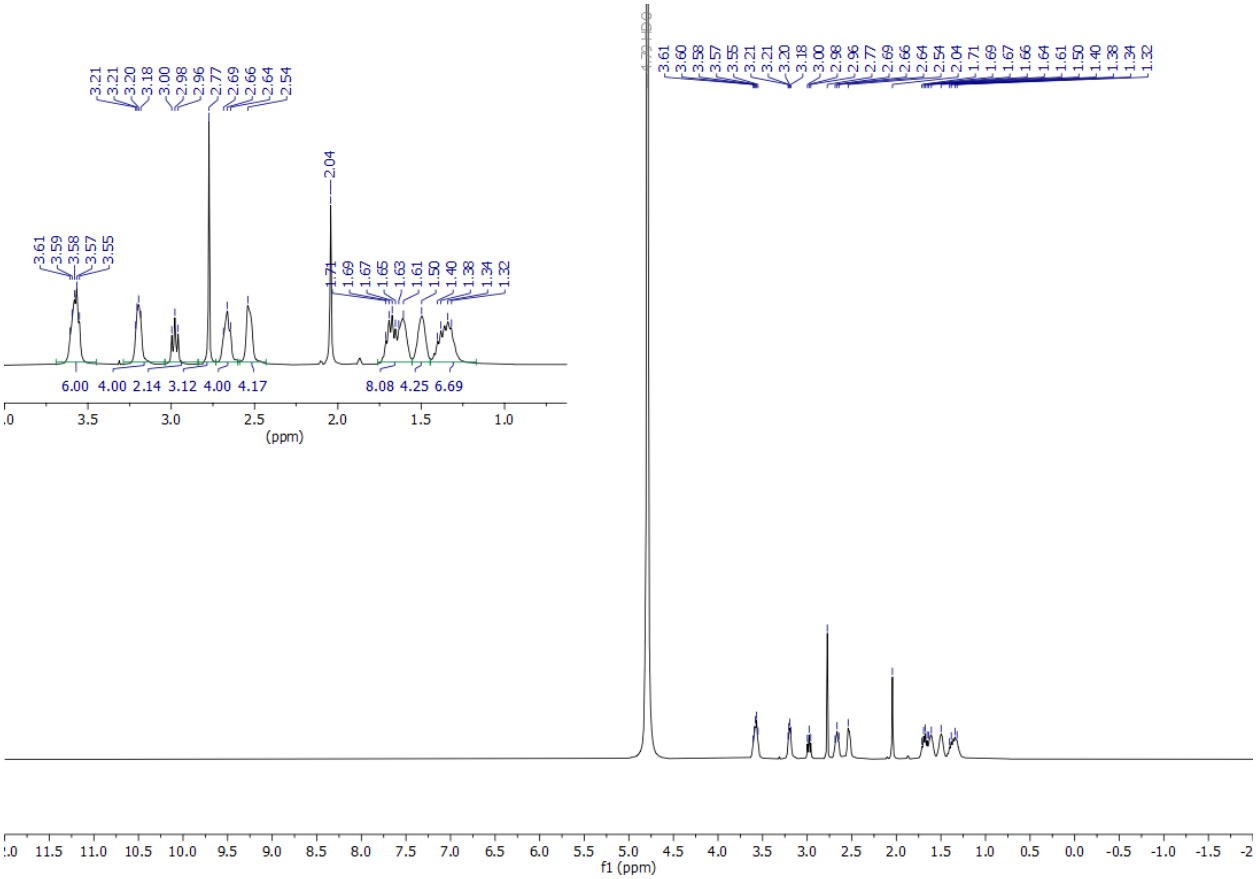

Figure S7. ^{1}H NMR of $[Th(HDFO)]^{2+}$. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

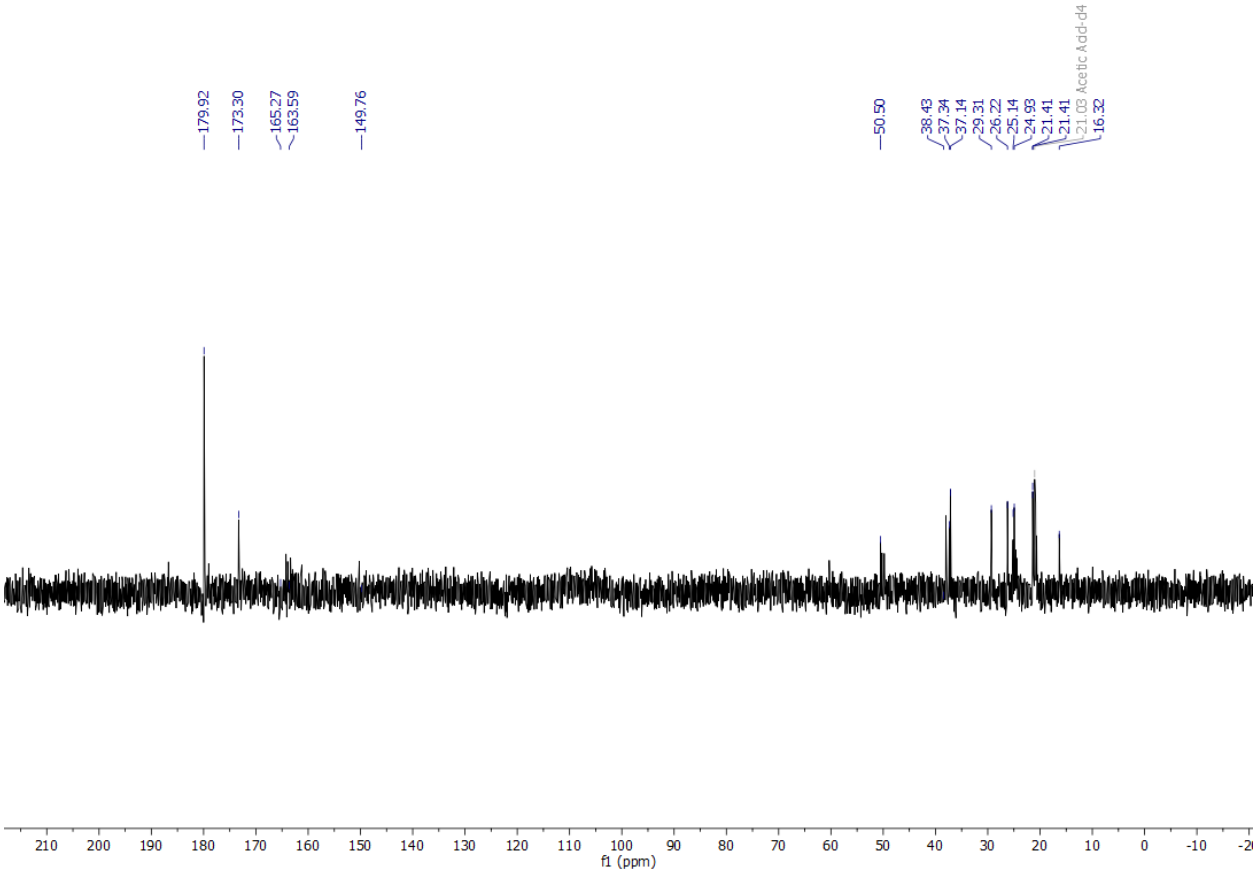

Figure S8. ^{13}C NMR of $[Th(HDFO)]^{2+}$. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

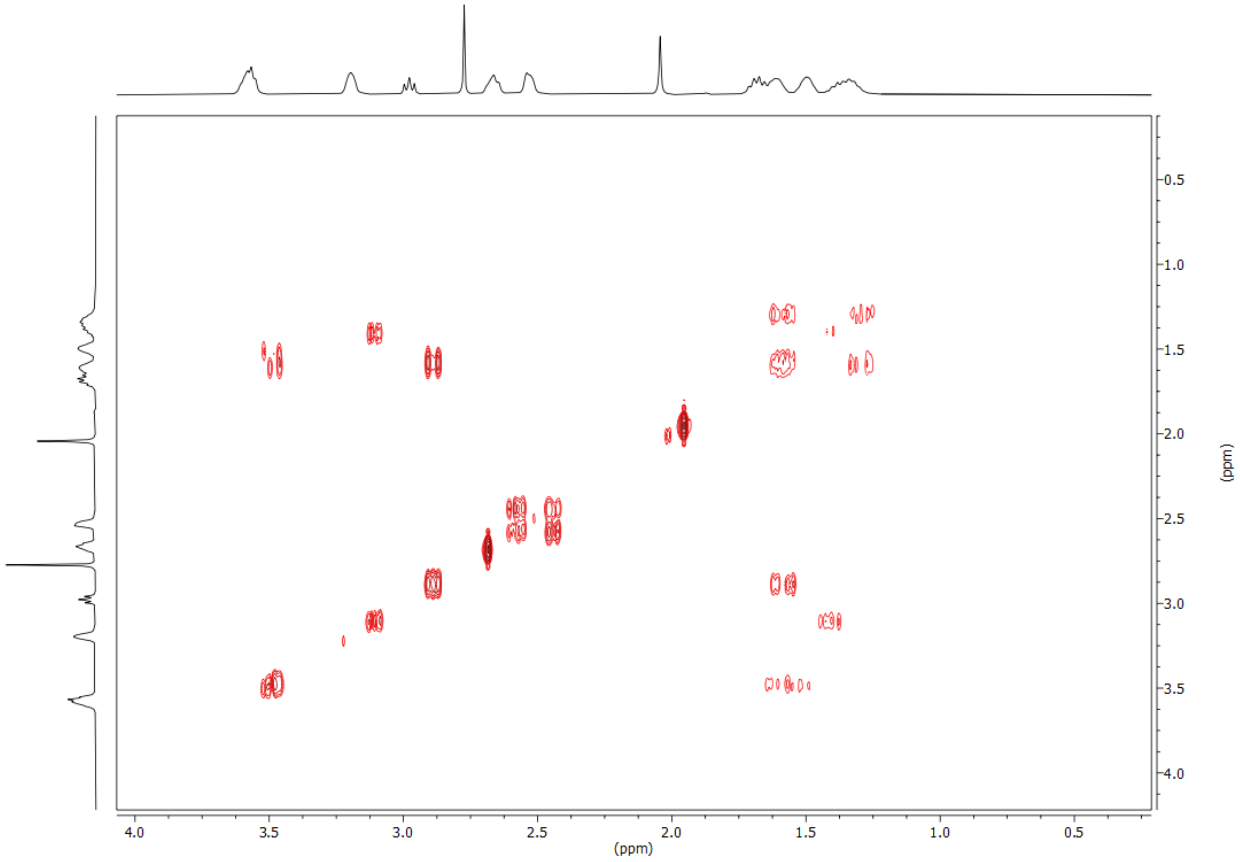

Figure S9. COSY NMR of $[Th(HDFO)]^{2+}$. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

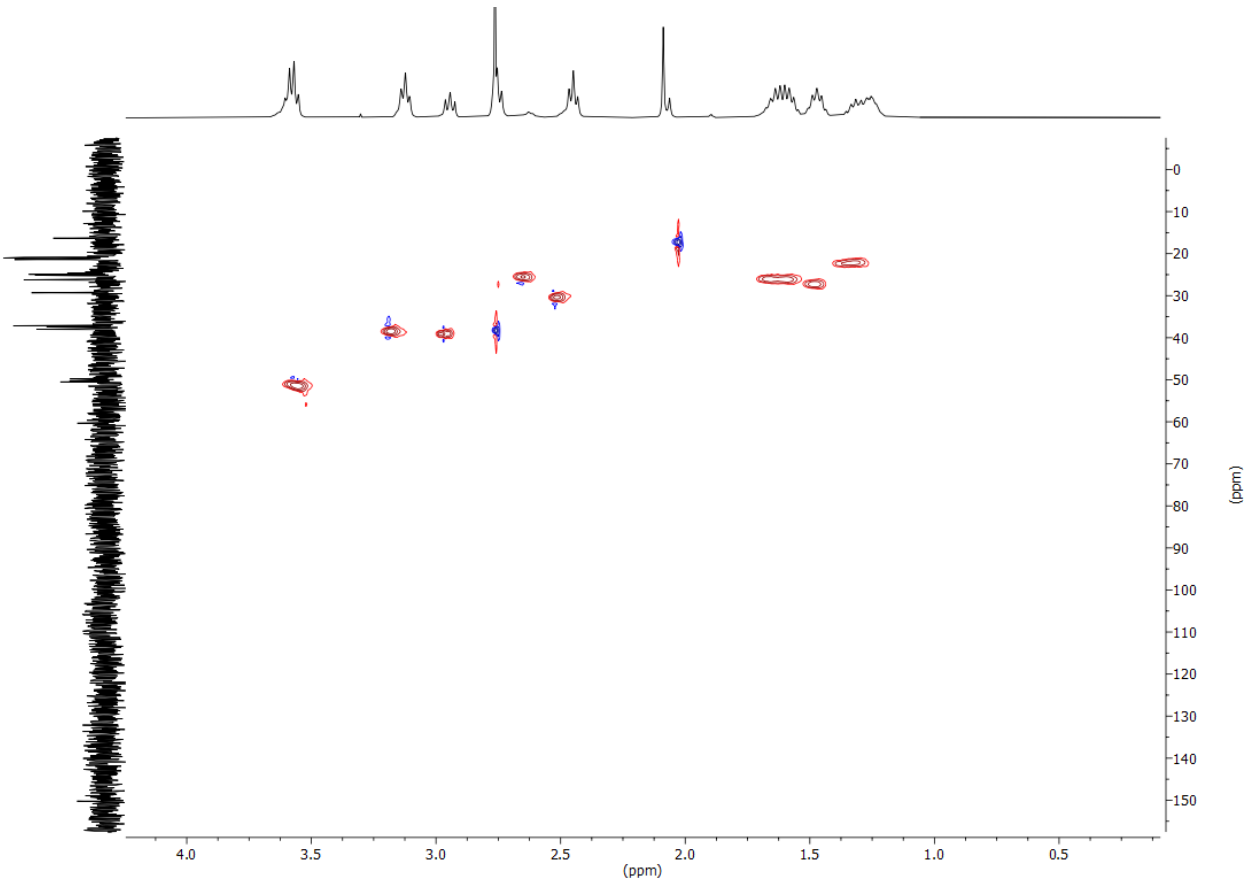

Figure S10. HSQC NMR of $[Th(HDFO)]^{2+}$. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

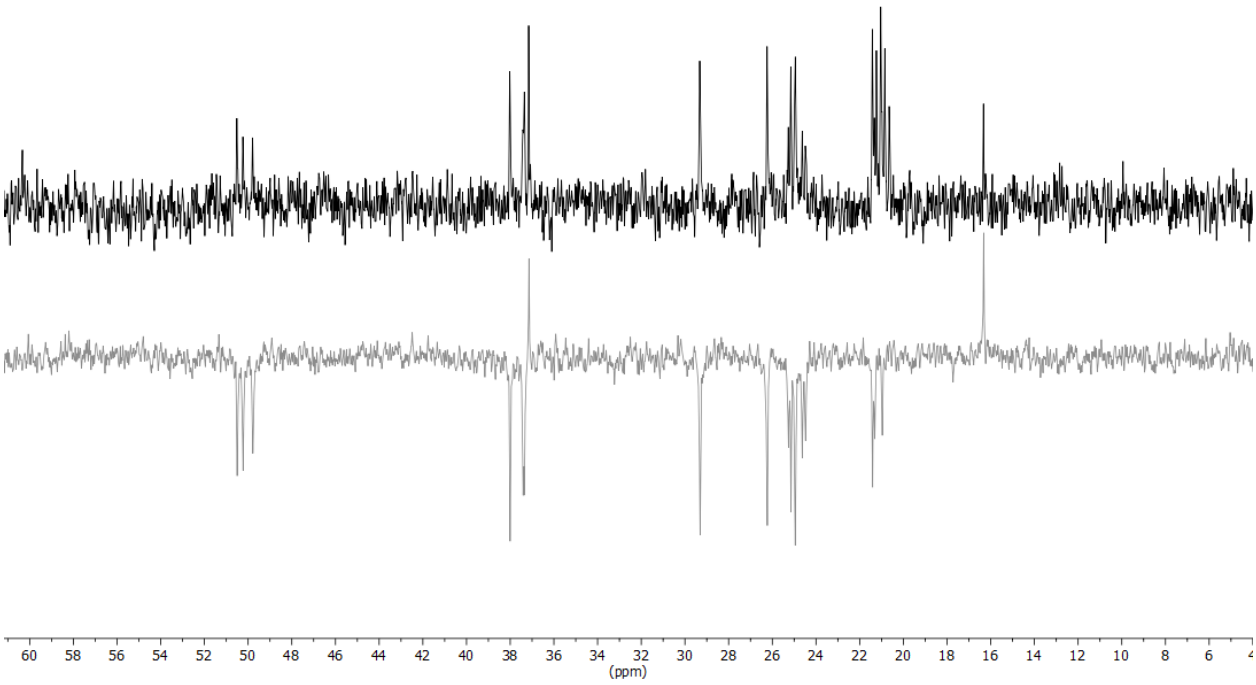

Figure S11. DEPT-135 NMR of $[Th(HDFO)]^{2+}$ (*bottom*, grey) overlaid with ^{13}C NMR (*top*, black). The spectra were observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

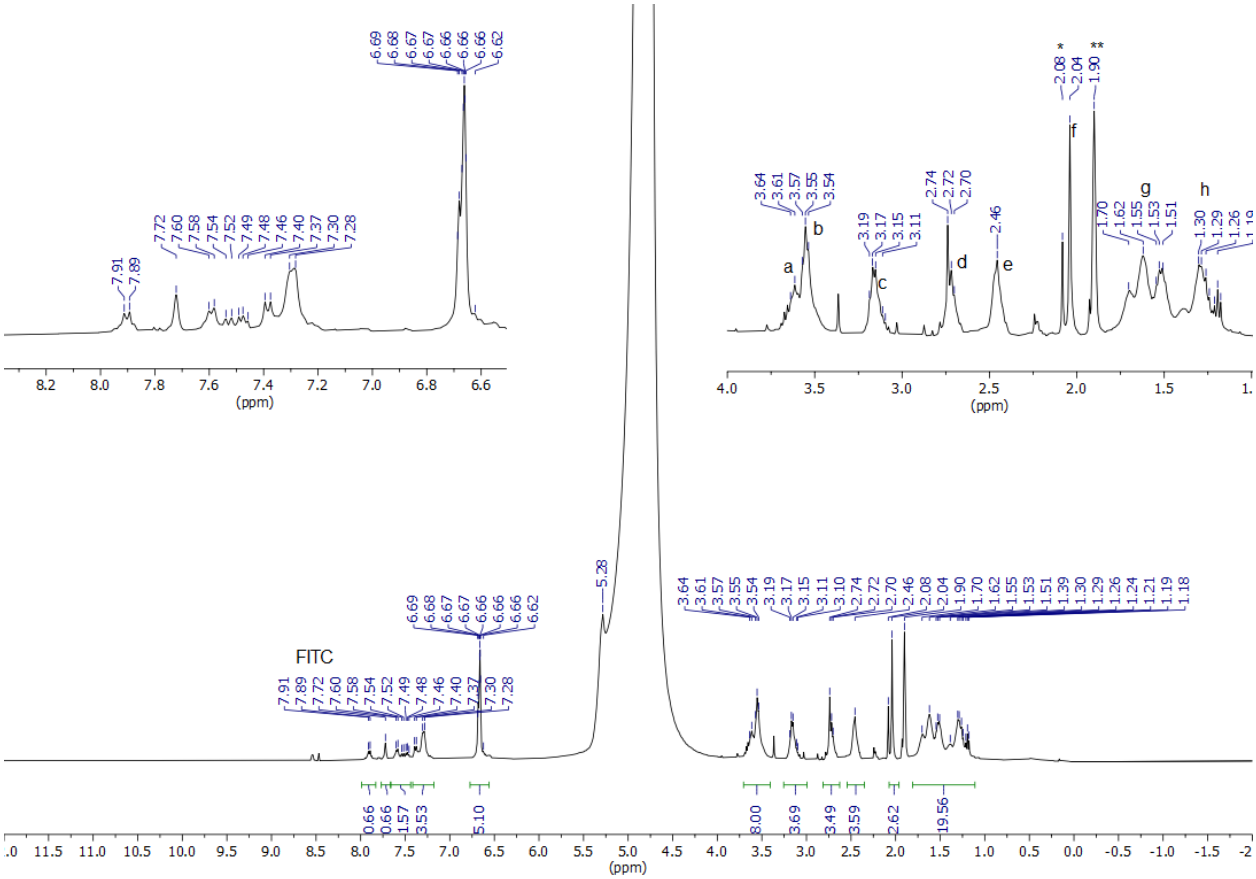

Figure S12. ^{1}H NMR of DFO_FITC. (* = acetate, ** = dmso) The spectrum was observed in D_2O buffered (pD = 8) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

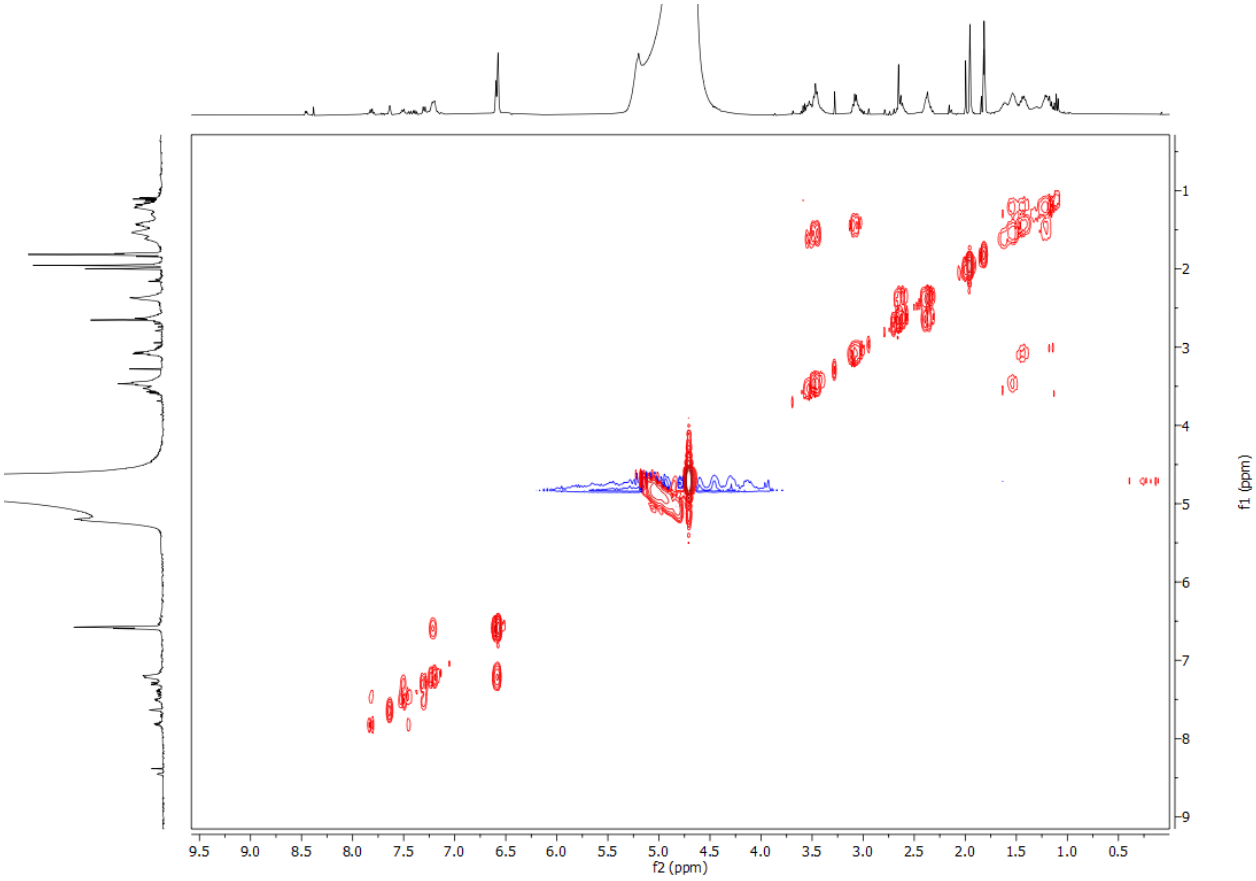

Figure S13. COSY NMR of DFO_FITC. The spectrum was observed in D_2O buffered (pD = 8) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

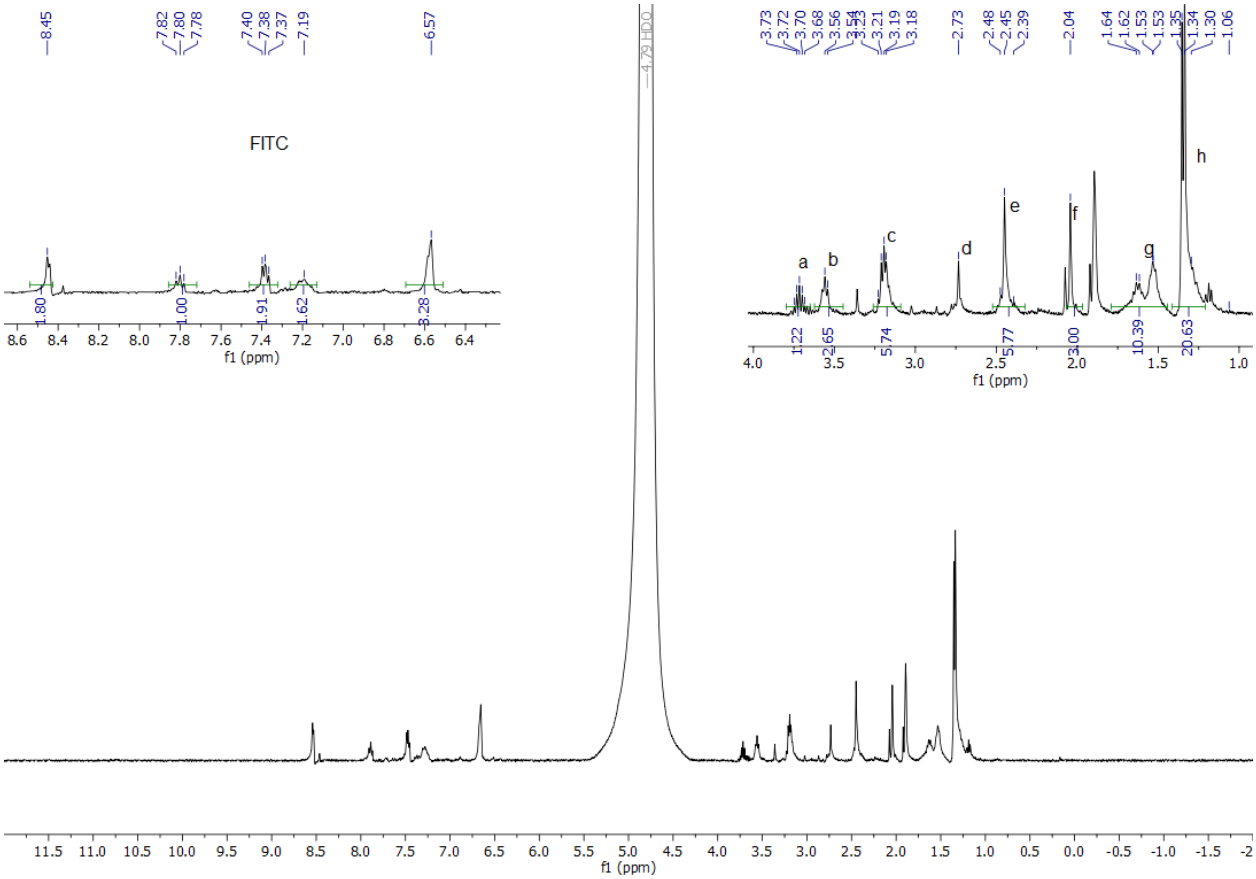

Figure S14. ^{1}H NMR of [Th(DFO_FITC)]. The spectrum was observed in D_2O buffered (pD = 8) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C. (sharp peaks at 1.89 and 1.35 ppm respectively assigned as dmso and acetate impurities, respectively)

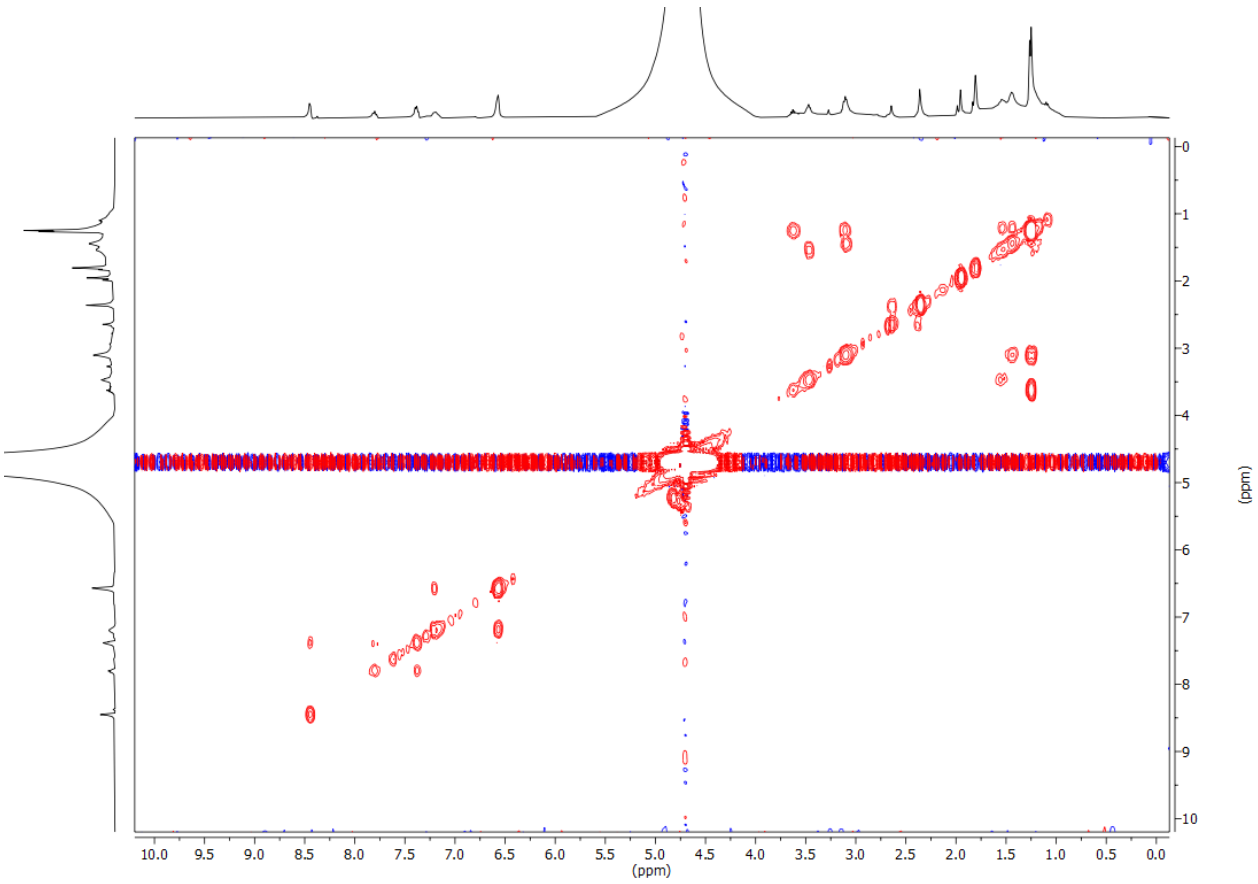

Figure S15. COSY NMR of [Th(DFO_FITC)]. The spectrum was observed in D_2O buffered (pH = 8) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25s °C.

General Considerations for DOSY NMR with Molecular Weight Calibrations:

The DOSY NMR data was collected with a 2D stimulated echo experiment using the stegp1s pulse sequence provided by Bruker. Prior to the experiment, relaxation delay, 90 degree pulse width, gradient range, diffusion delay, and mixing time were optimized, such that the compound signals were ~10 % of their initial intensities. The Molecular weight calibration standards were included as internal standards with the "unknown"complex under study. The samples were contained in PTFE NMR tube liners fitted with Teflon stoppers (inner diameter 3 mm, Sigma-Aldrich), placed inside of standard 5 mm glass NMR tubes (Wilmad, 400 MHz).

DOSY NMR processing was accomplished using the Bayesian DOSY Transform method in MestReNova.

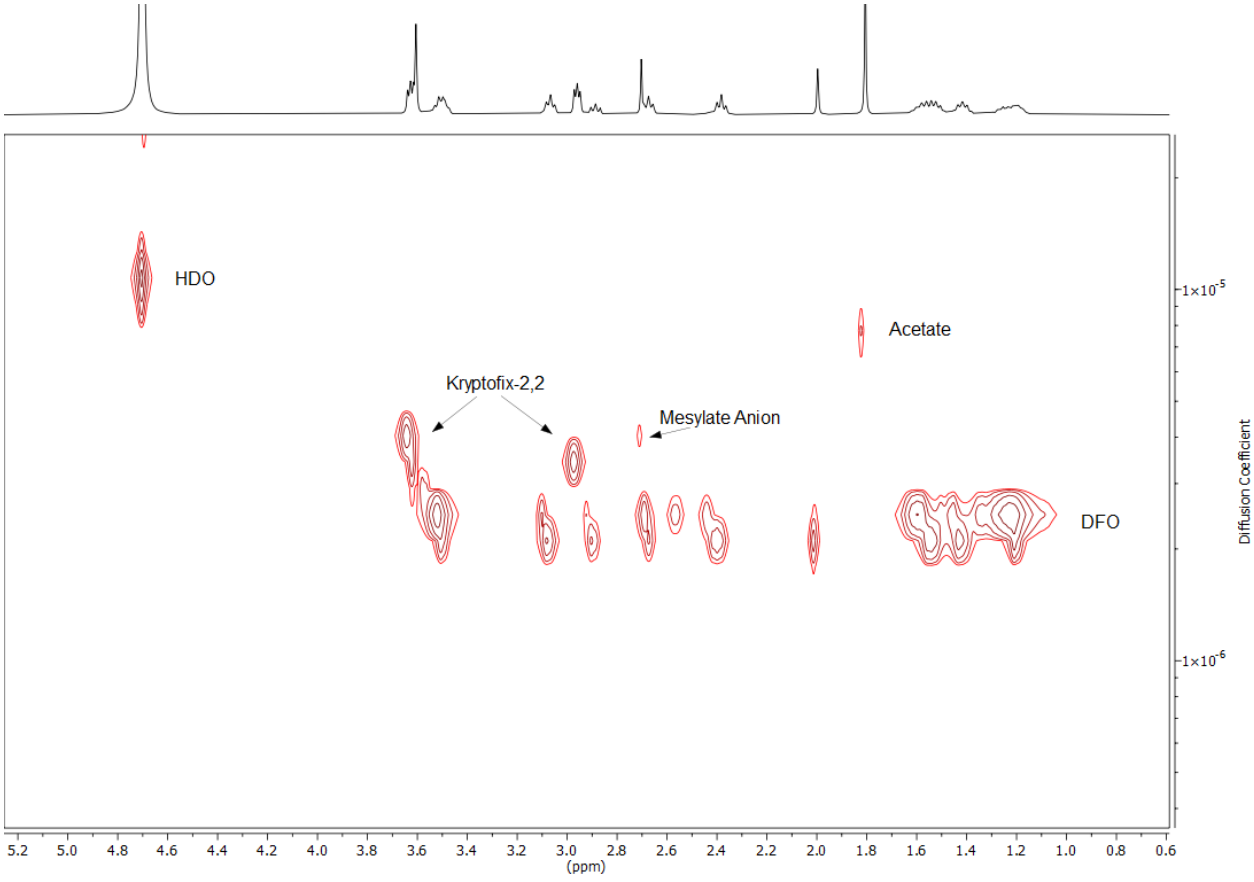

Figure S16. DOSY NMR of DFO-mesylate with molecular weight calibration standards. The spectrum was observed in D_2O buffered with NaOAc and pH adjusted with acetic acid-d_4 to pD = 5.5 Note, diffusion coefficient is in units of cm^2s^{-1}.

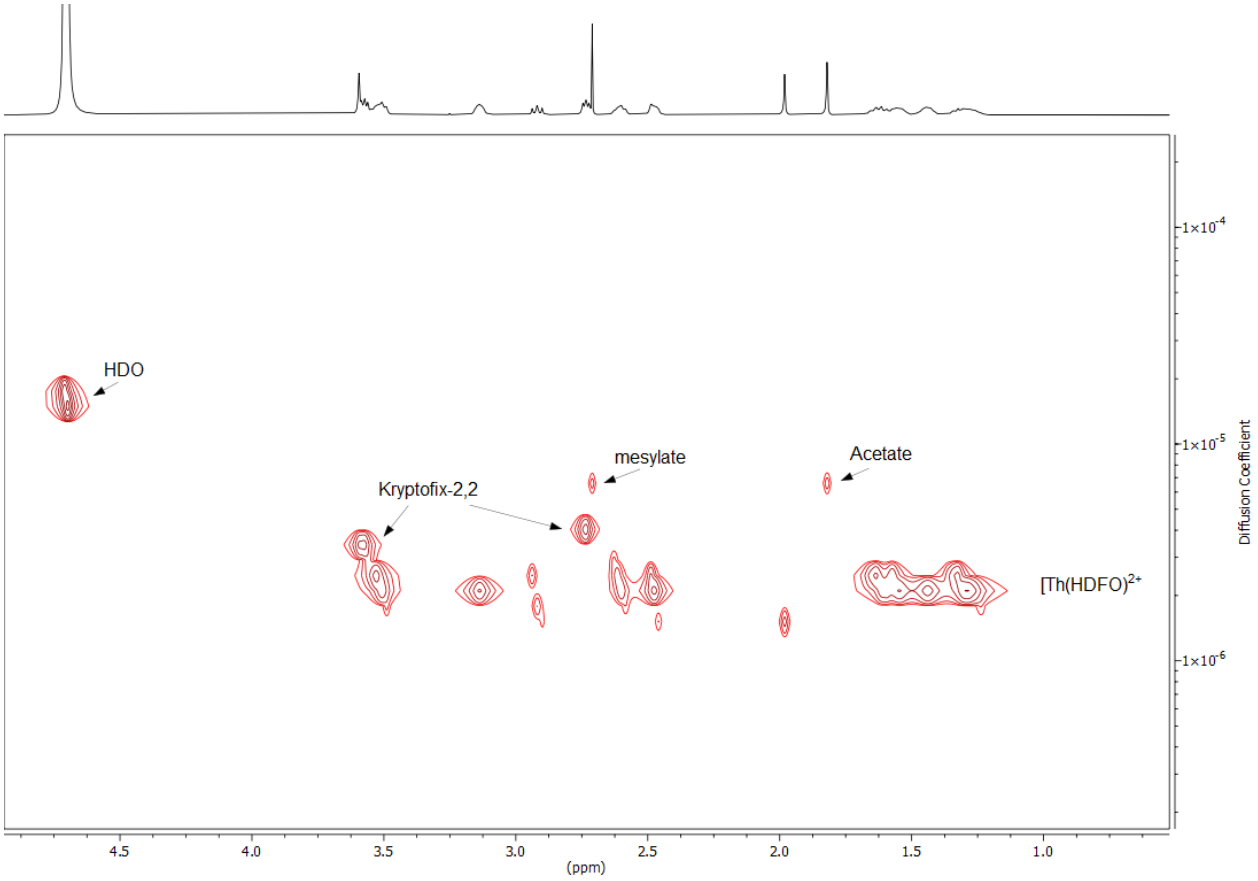

Figure S17. DOSY NMR of $[Th(HDFO)]^{2+}$ with molecular weight calibration standards.The spectrum was observed in D_2O buffered with NaOAc and pH adjusted with acetic acid-d_4 to pD = 5.5 Note, diffusion coefficient is in units of cm^2s^{-1}.

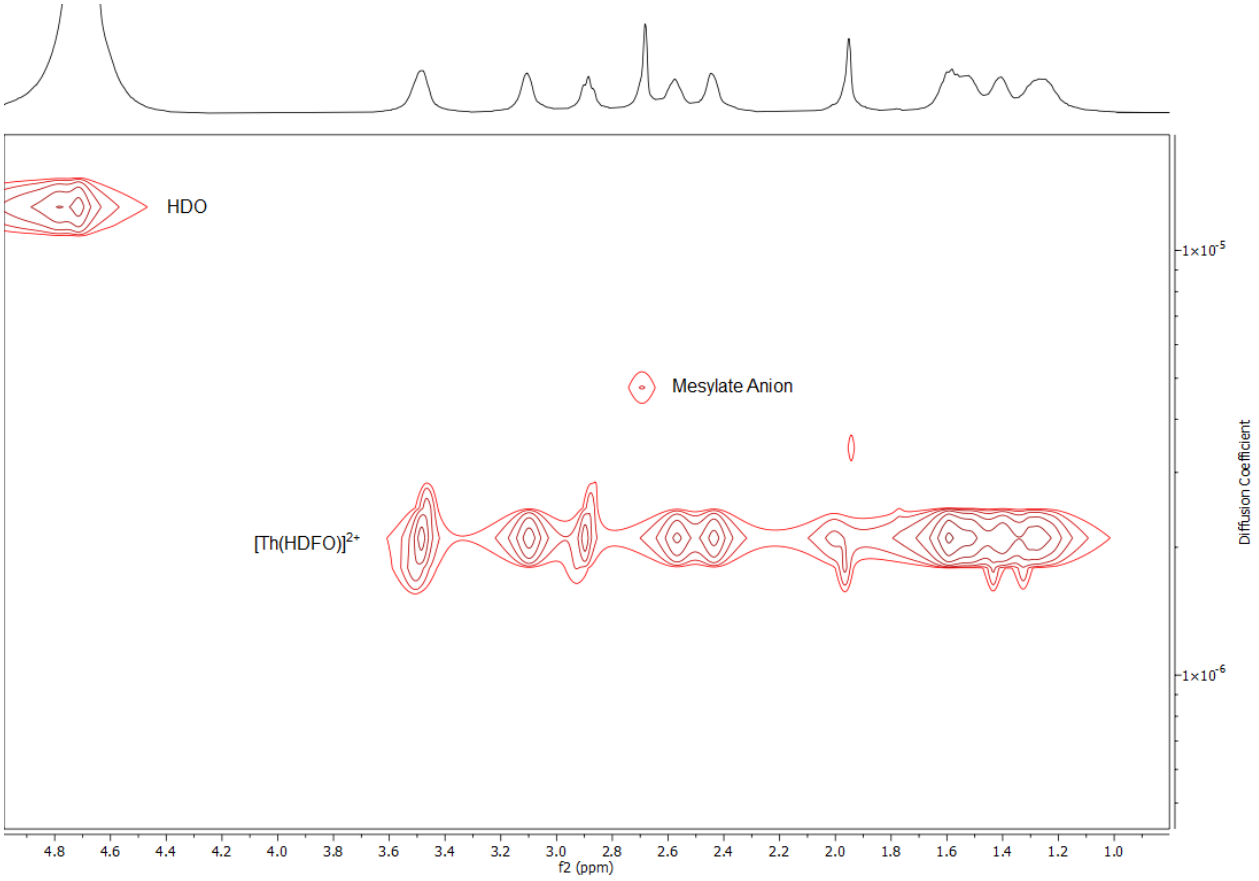

Figure S18. DOSY NMR of $[Th(HDFO)]^{2+}$. The spectrum was observed in D_2O buffered (pD = 5) with ND_4OD and acetic acid-d_4 on a 400 MHz spectrometer at 25 °C.

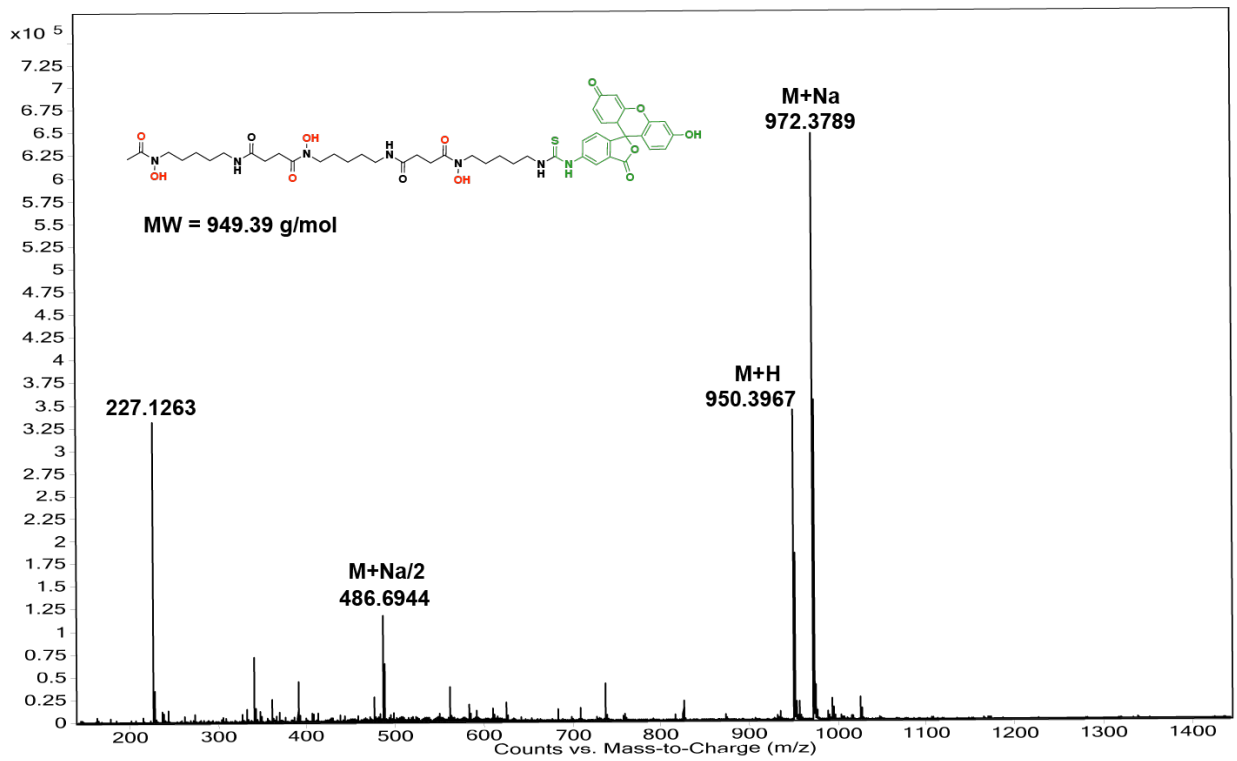

Figure S19. High resolution mass spectrum of DFO_FITC. The ion flies as M+H and M+Na, the M+Na/2 peak is also observed. The peak at m/*z* = 227.1263 likely arises from a degradation product of nylon 66 from the 15 mL conical tube in which the sample is stored.

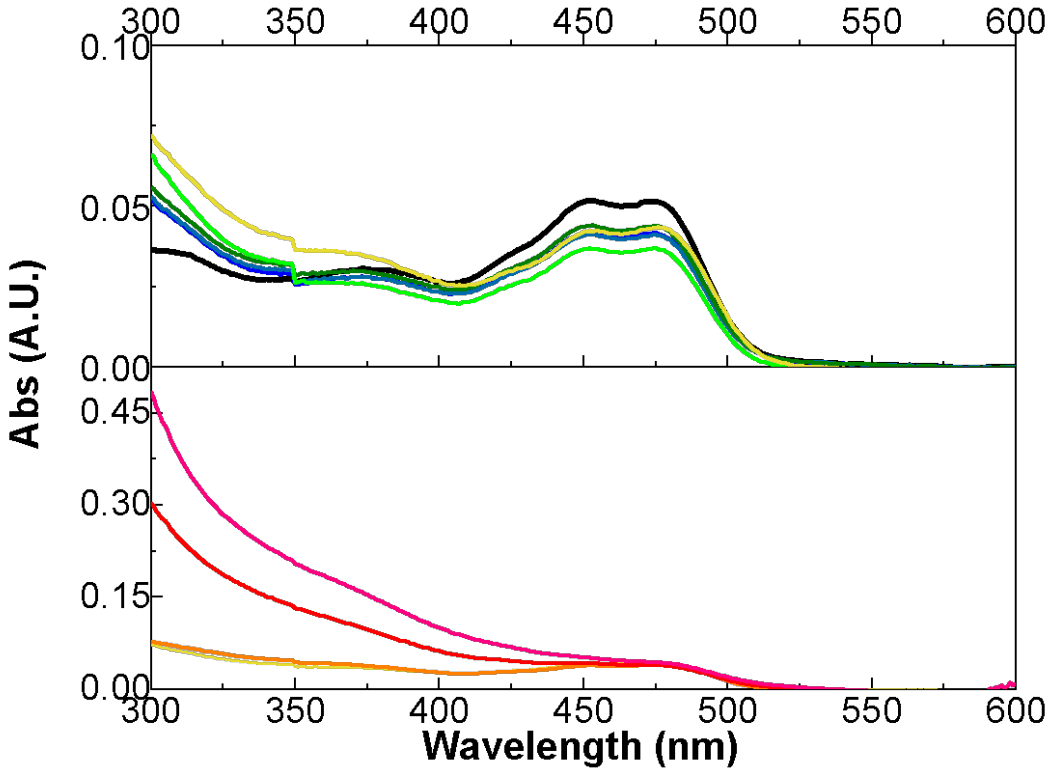

Figure S20. Absorption spectra of Fluorescein Fe^{III} UV-Visible titration. The initial Fluorescein concentration is 0.005 mM with 0 mM Fe^{III} (black), 0.0025mM Fe^{III} (blue), 0.005 mM Fe^{III} (teal), 0.075 mM Fe^{III} (dark green), 0.01 mM FeIII (green), 0.05 mM FeIII (yellow), 0.1 mM Fe^{III} (orange), 0.5 mM Fe^{III} (red) and 1 mM Fe^{III} (pink).

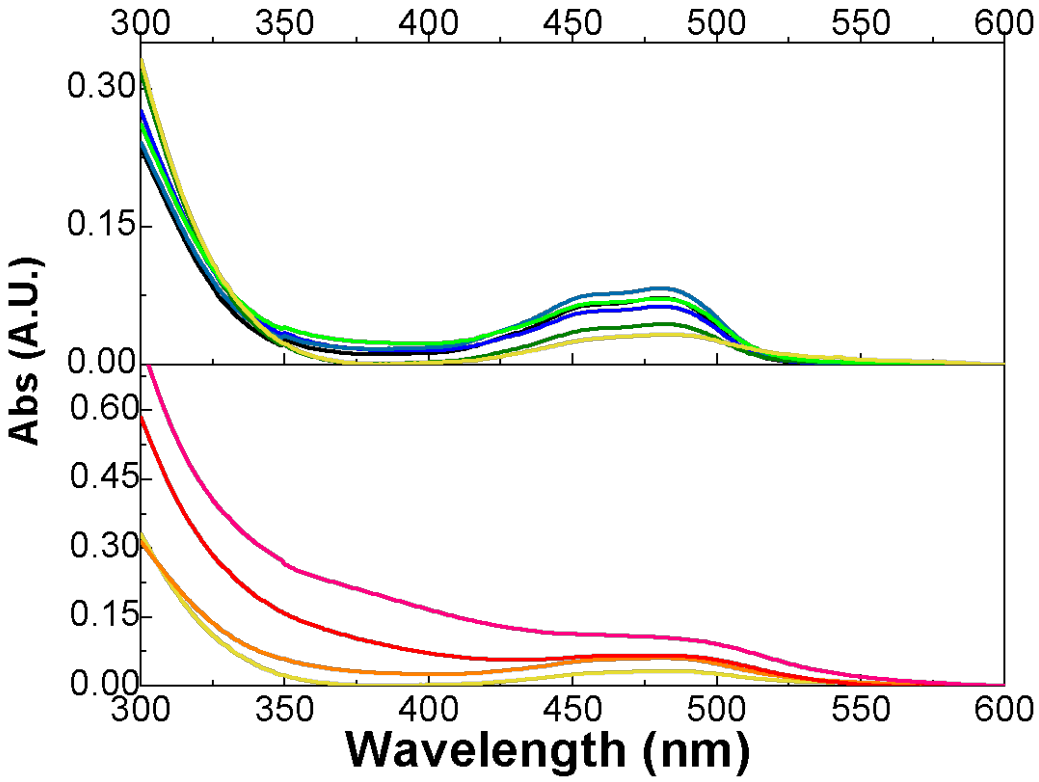

Figure S21. Absorption spectra of DFO_FITC Fe^{III} UV-Visible titration. The initial DFO_FITC concentration is 0.01 mM with 0 mM Fe^{III} (black), 0.0025mM Fe^{III} (blue), 0.005 mM Fe^{III} (teal), 0.075 mM Fe^{III} (dark green), 0.01 mM Fe^{III} (green), 0.05 mM Fe^{III} (yellow), 0.1 mM Fe^{III} (orange), 0.5 mM Fe^{III} (red) and 1 mM Fe^{III} (pink).

DFO_FITC Fluorescence Fe^{III} Titration Excitation/Emission

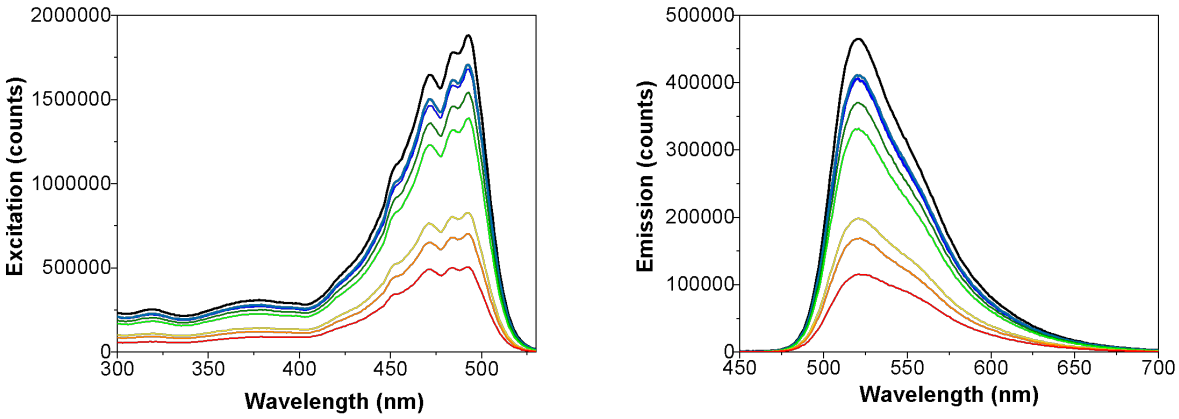

Figure S22. Excitation (left) and Emission (right) of DFO_FITC with varying quantities of Fe^{III} in acetate buffer solution. For each experiment 0.01 mM DFO_FITC was mixed with 0 mM Fe^{III} (black), 0.0025mM Fe^{III} (blue), 0.005 mM Fe^{III} (teal), 0.075 mM Fe^{III} (dark green), 0.01 mM Fe^{III} (green), 0.05 mM Fe^{III} (yellow), 0.1 mM Fe^{III} (orange) and 0.5 mM Fe^{III} (red).

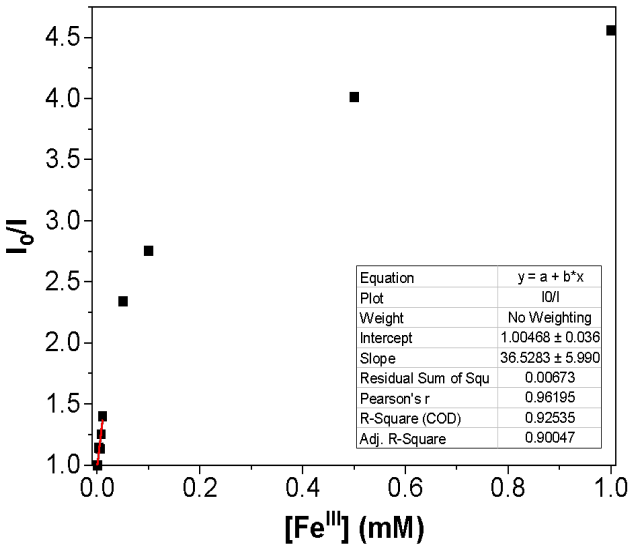

Figure S23. Stern-Volmer plot of DFO_FITC with of Fe^{III} in acetate buffer solution.

DFO_FITC Fluorescence Th^{IV} Titration Excitation/Emission

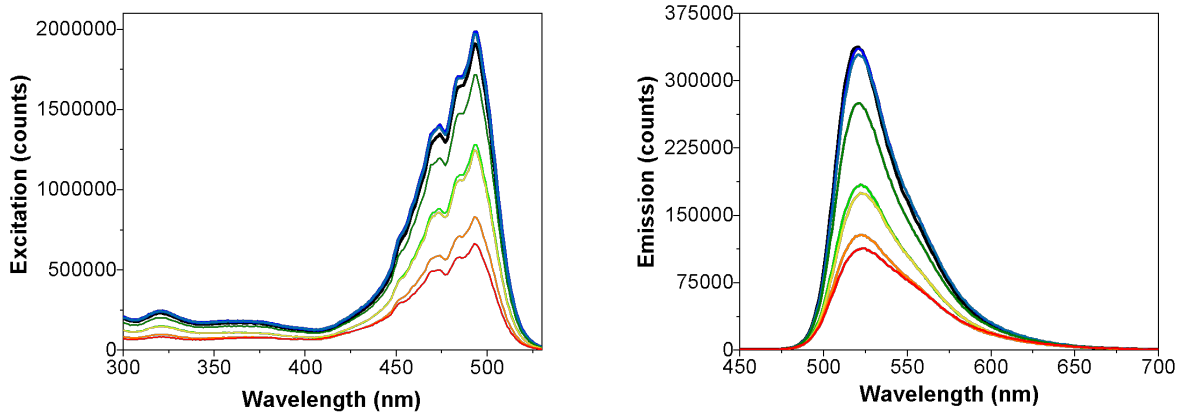

Figure S24. Excitation (left) and Emission (right) of DFO_FITC with varying quantities of Th^{IV} in acetate buffer solution. For each experiment 0.01 mM DFO_FITC was mixed with 0 mM Th^{IV} (black), 0.005mM Th^{IV} (blue), 0.0075 mM Th^{IV} (teal), 0.01 mM Th^{IV} (dark green), 0.05 mM Th^{IV} (green), 0.1 mM Th^{IV} (yellow), 0.5 mM Th^{IV} (orange) and 1 mM Th^{IV} (red).

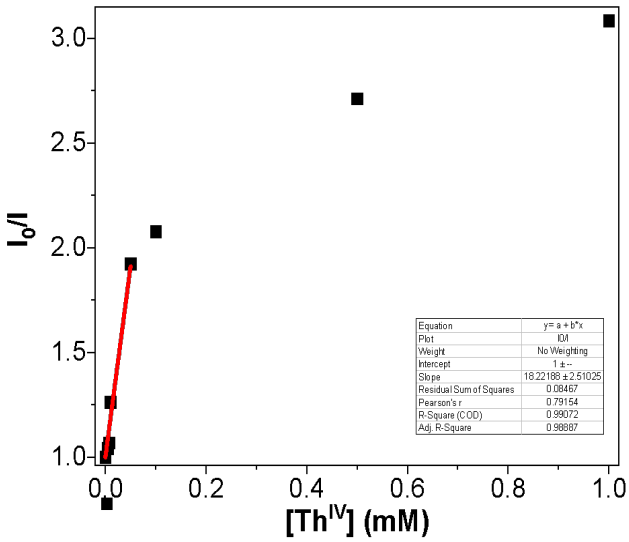

Figure S25. Stern-Volmer plot of DFO_FITC with of Th^{IV} in acetate buffer solution.

Fluorescein Fluorescence Fe^{III} Titration Excitation/Emission

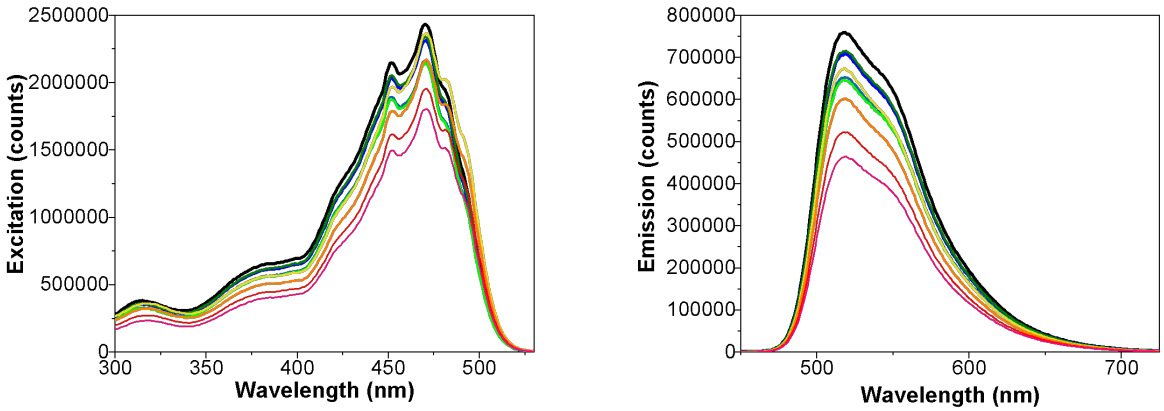

Figure S26. Excitation (left) and Emission (right) of Fluorescein with varying quantities of Fe^{III} in acetate buffer solution. For each experiment 0.005 mM Fluorescein was mixed with 0 mM Fe^{III} (black), 0.0025mM Fe^{III} (blue), 0.005 mM Fe^{III} (teal), 0.075 mM Fe^{III} (dark green), 0.01 mM Fe^{III} (green), 0.05 mM Fe^{III} (yellow), 0.1 mM Fe^{III} (orange), 0.5 mM Fe^{III} (red) and 1 mM Fe^{III} (pink).

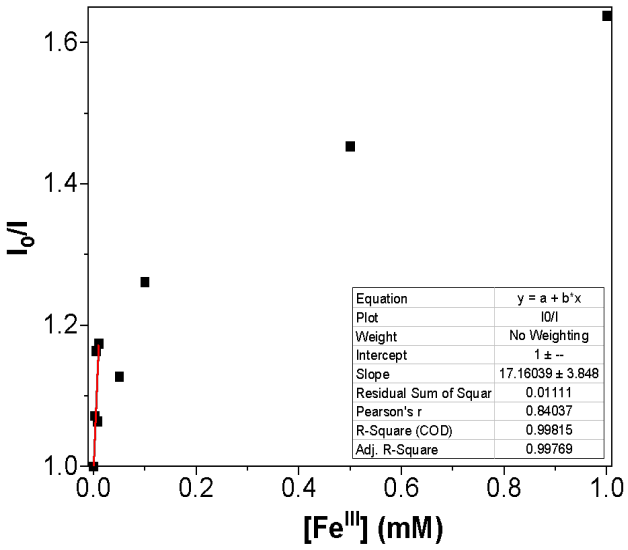

Figure S27. Stern-Volmer plot of Fluorescein with of Fe^{III} in acetate buffer solution.

Fluorescein Fluorescence Th^{IV} Titration Excitation/Emission

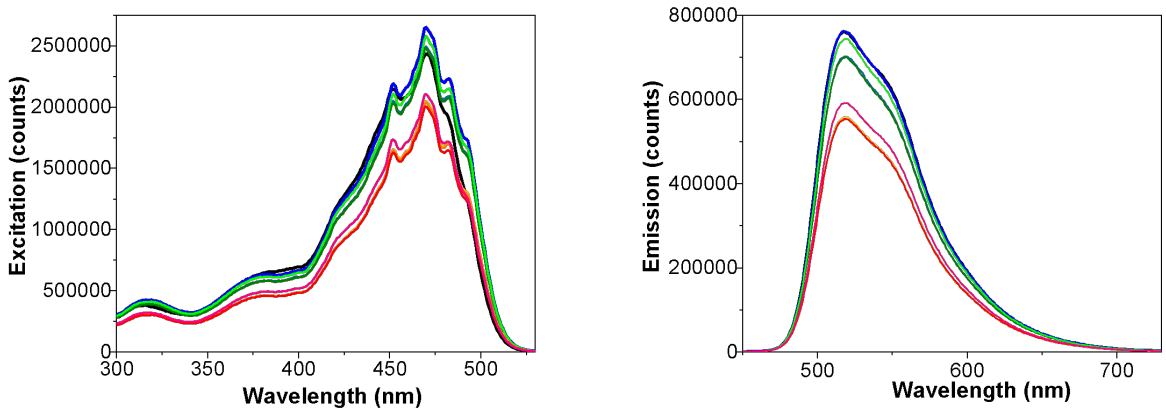

Figure S28. Excitation (left) and Emission (right) of Fluorescein with varying quantities of Th^{IV} in acetate buffer solution. For each experiment 0.005 mM Fluorescein was mixed with 0 mM Th^{IV} (black), 0.005mM Th^{IV} (blue), 0.0075 mM Th^{IV} (teal), 0.01 mM Th^{IV} (dark green), 0.05 mM Th^{IV} (green), 0.1 mM Th^{IV} (yellow), 0.5 mM Th^{IV} (orange) and 1 mM Th^{IV} (red).

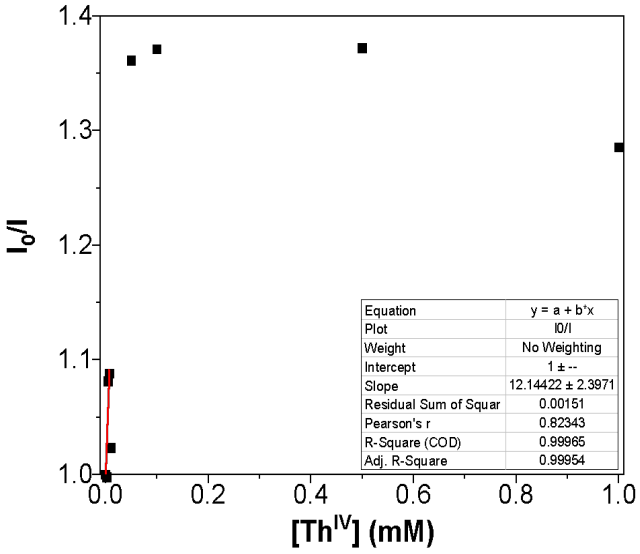

Figure S29. Stern-Volmer plot of Fluorescein with of Th^{IV} in acetate buffer solution.

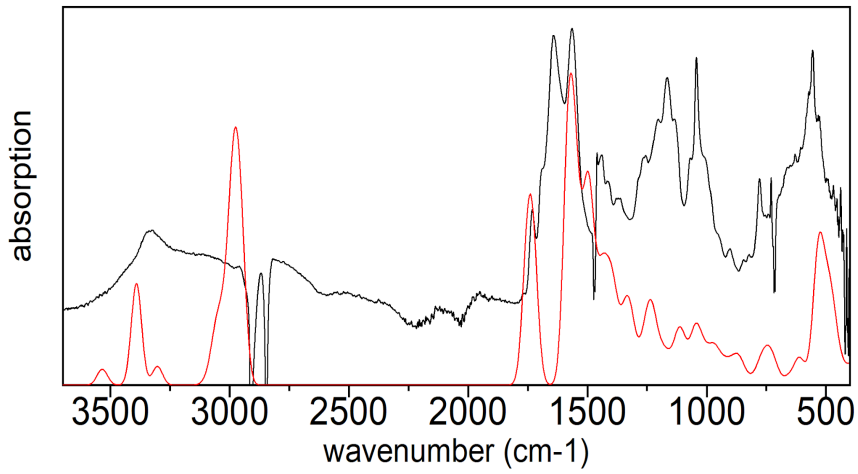

Figure S30. Experimental and Calculated IR spectrum of $[Fe(HDFO)]^+$ using an IR card. Residual solvent (methanol) vibrations are also observed with similar intensity to the $[Fe(HDFO)]^+$.

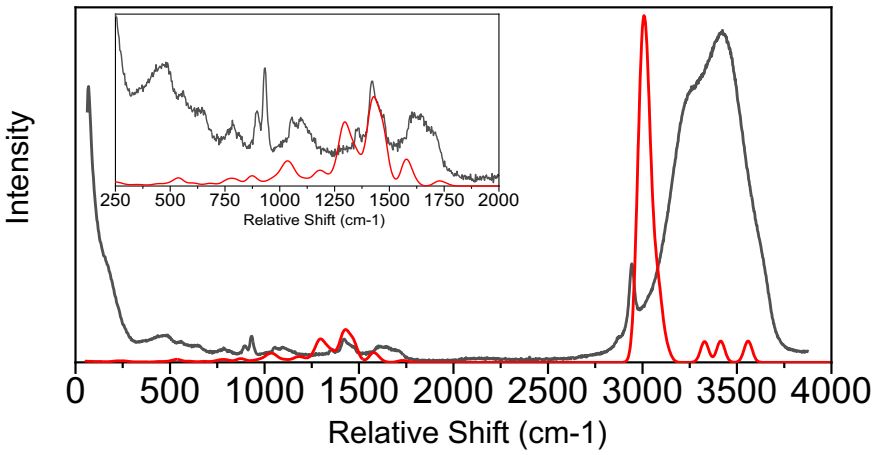

Figure S31. 514.5 nm Raman of $[Th(HDFO)]^{2+}$ in 0.1M NH_4CH_3COO (Black) with calculated Raman of $[Th(HDFO)]^{2+}$ (Red).

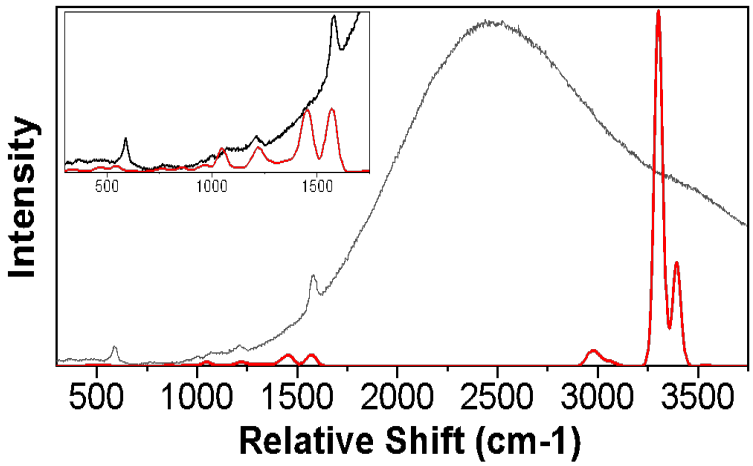

Figure S32. 514.5 nm Raman of $[Fe(HDFO)]^+$ in 0.1M NH_4CH_3COO (Black) with calculated Raman of $[Fe(HDFO)]^+$ (Red).

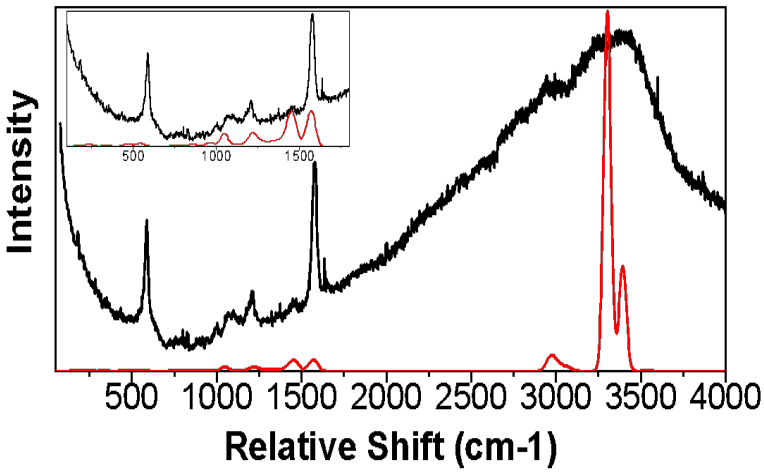

Figure S33. 632.8 nm Raman of $[Fe(HDFO)]^+$ in 0.1M NH_4CH_3COO (Black) with calculated Raman of $[Fe(HDFO)]^+$ (Red).

Fluorescence Microscopy of *S. aureus*

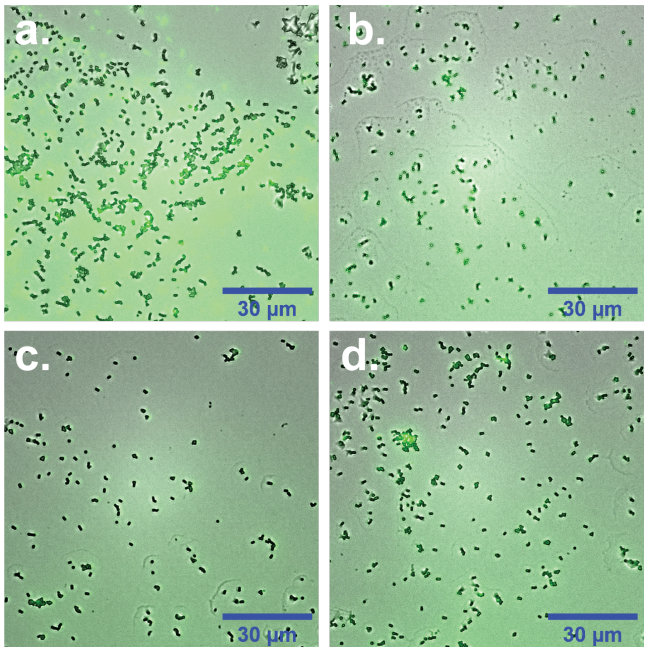

Figure S34. Overlay of fluorescent and transmission microscopy images of *S. aureus* labeled with FITC, DFO_FITC, [Fe(DFO_FITC)], and [Th(DFO_FITC)]. Slides were mounted in 1x DPBS diluted in water then fixed. Images were acquired at 40x magnification and fluorescent EX: 470 nm/EM 525 nm.

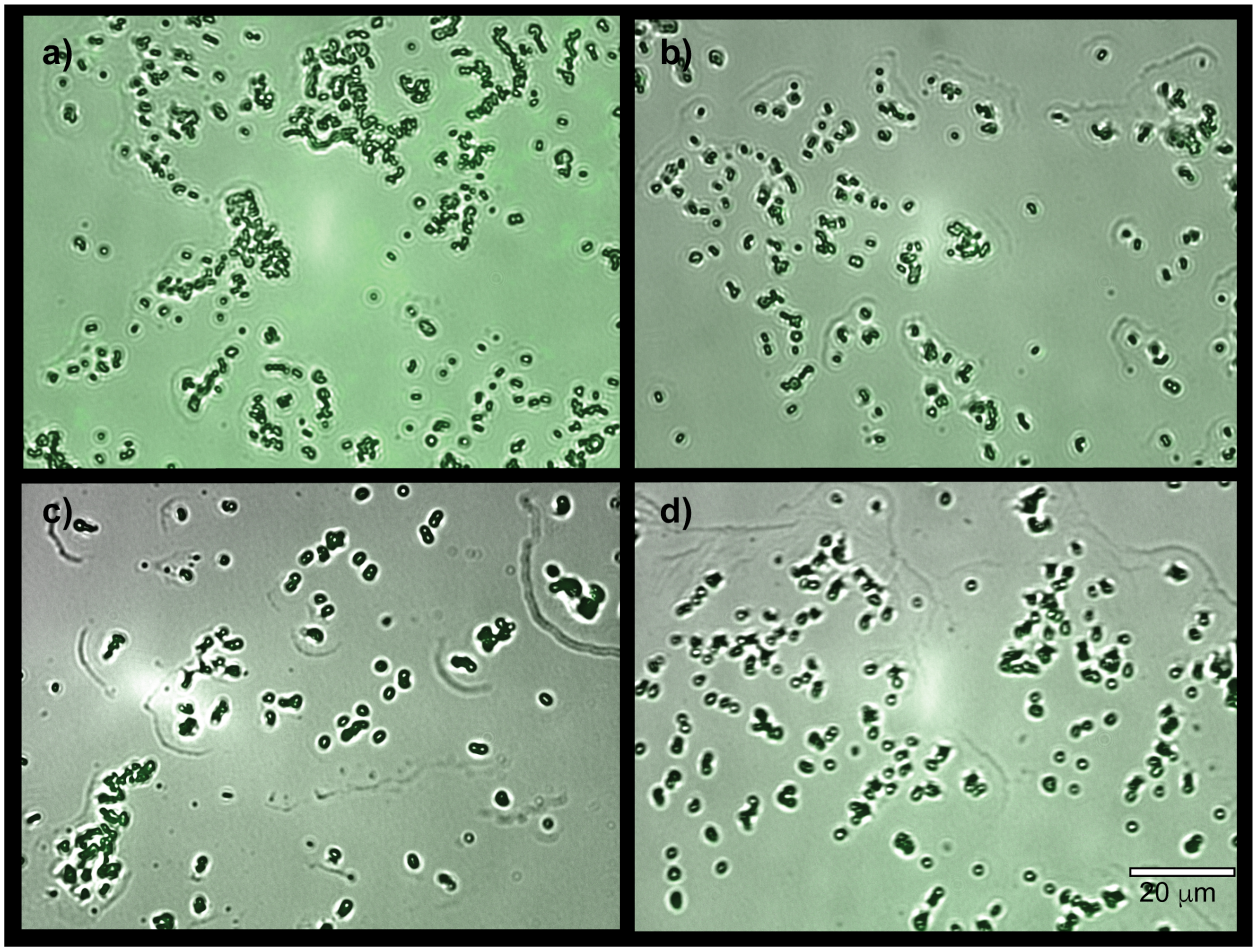

Figure S35. Overlay of fluorescent and transmission microscopy images of *S. aureus* labeled with a) FITC, b) H_3DFO_FITC, c) [Fe(HDFO_FITC)], and d) [Th(DFO_FITC)]. Slides were mounted in 1x DPBS diluted in water then fixed. Images were acquired at 60x magnification and fluorescent EX: 470 nm/EM 525 nm.

Vibrational Calculation of $[Fe(HDFO)]^{+}$

DFT Calculations were performed using ORCA 4.2.1 suit running in Microsoft MPI v10. The geometry optimization and frequency calculation were performed using the following input.

```
! UKS BP Opt Freq PBE def2-SVP def2/J FinalGrid6 SlowConv RIJCOSX
%scf
MaxIter 1500
end
%maxcore 2000
%pal
nprocs 4
end
%basis Newgto 26 "def2-TZVPP" end
        Newauxgto 26 "def2/J" end
end

* xyz 1 6
 Fe    -0.170352     1.324749    -0.422260
 O     -0.921840     2.898671    -1.404441
 O      1.211483     2.892180     0.019075
 O     -1.697208     0.061547    -0.776595
 O      1.113899     0.671908    -1.919461
 O     -1.407461     1.603320     1.269238
 O      1.061558     0.105222     0.578609
 C      2.175509     0.155427    -1.433806
 C      3.394933    -0.016300    -2.294106
 O     -4.492023     3.832127     2.389066
 N     -2.592932     0.003617     0.230281
 C     -3.517983    -1.109826     0.111294
 C     -2.750540    -2.440263     0.057350
 C     -3.602734    -3.621717    -0.409253
 C     -2.765207    -4.901991    -0.558251
 C     -3.583857    -6.067042    -1.092331
 N     -0.177670     4.018354    -1.346876
 C     -0.778029     5.195320    -1.981112
 C     -1.563200     6.081911    -1.000280
 C     -2.703372     5.395819    -0.234156
 C     -3.908769     5.023334    -1.104991
 C     -5.130563     4.529731    -0.314386
 N     -5.013180     3.192729     0.249213
 C      3.295842    -0.701409     0.658934
 C      4.267385     0.351151     1.204407
 C      3.627246     1.392744     2.129148
 C      4.625521     2.406654     2.704549
 C      5.345832     3.286614     1.668451
```

N	2.184350	-0.157639	-0.122475
C	4.131540	3.846135	-0.434291
N	4.465855	4.123152	0.864412
O	4.568583	2.866049	-1.044473
C	-2.412307	0.833376	1.286274
C	-4.741572	2.949748	1.571429
C	-4.802670	1.470857	1.981928
C	-3.430663	0.909022	2.408877
C	3.239320	4.893134	-1.114620
C	1.860451	5.163611	-0.468561
C	0.928252	3.978335	-0.577543
N	-2.722633	-7.310818	-1.255688
H	3.063602	-0.171476	-3.337452
H	4.049770	-0.852822	-1.984762
H	3.983499	0.926396	-2.250219
H	2.810773	-1.262977	1.483130
H	3.843628	-1.433690	0.031197
H	4.747529	0.862351	0.343501
H	5.075020	-0.195463	1.743077
H	3.117589	0.878382	2.972513
H	2.827662	1.931456	1.578995
H	4.095912	3.065627	3.428176
H	5.411638	1.883364	3.294679
H	6.078225	3.941379	2.187885
H	5.918034	2.666105	0.950605
H	4.042657	4.937469	1.311781
H	3.111537	4.554911	-2.160193
H	3.802091	5.851147	-1.145187
H	1.421903	6.068805	-0.926618
H	1.970716	5.388702	0.614072
H	0.016555	5.783002	-2.483399
H	-1.426280	4.786458	-2.780205
H	-0.847422	6.515621	-0.268397
H	-1.960032	6.946289	-1.578793
H	-3.044394	6.081987	0.570103
H	-2.318839	4.493972	0.287399
H	-3.622373	4.251588	-1.852897
H	-4.232228	5.916824	-1.685539
H	-6.027828	4.547273	-0.969639
H	-5.327471	5.209549	0.539736
H	-5.139002	2.396271	-0.375685
H	-5.483611	1.430758	2.857209
H	-5.264156	0.850968	1.184372
H	-2.990840	1.584147	3.168030
H	-3.562633	-0.082734	2.893072

H	-4.095086	-0.975062	-0.832007
H	-4.234921	-1.087618	0.955316
H	-1.904443	-2.279635	-0.643476
H	-2.306514	-2.650193	1.054535
H	-4.069753	-3.375799	-1.389285
H	-4.442023	-3.808688	0.297379
H	-1.914033	-4.695202	-1.245438
H	-2.324076	-5.171948	0.427664
H	-4.412471	-6.351615	-0.413862
H	-4.012187	-5.856007	-2.092227
H	-2.303136	-7.598981	-0.351117
H	-1.931784	-7.134264	-1.904625
H	-3.253706	-8.121967	-1.624561

Further numerical frequency calculation of the optimized $[Fe(HDFO)]^{+}$ structure to generate the IR and Raman spectra was performed using the following input:

```
! UKS BP NumFreq PBE def2-SVP def2/J FinalGrid6 SlowConv RIJCOSX
%maxcore 2000
%pal
nprocs 12
end
%basis Newgto 26 "def2-TZVPP" end
      Newauxgto 26 "def2/J" end
end
%elprop Polar 1 end

* xyz 1 6
Fe     -0.1702060000     1.3248370000    -0.4226810000
O      -0.9216770000     2.8987220000    -1.4047630000
O       1.2116880000     2.8922550000     0.0188200000
O      -1.6970680000     0.0615620000    -0.7771440000
O       1.1138960000     0.6711960000    -1.9194950000
O      -1.4078360000     1.6033750000     1.2684320000
O       1.0611950000     0.1054800000     0.5791500000
C       2.1754050000     0.1551080000    -1.4332460000
C       3.3949700000    -0.0172610000    -2.2932460000
O      -4.4919740000     3.8317150000     2.3896810000
N      -2.5930760000     0.0035920000     0.2294590000
C      -3.5180090000    -1.1099280000     0.1102910000
C      -2.7504890000    -2.4402990000     0.0566540000
C      -3.6026330000    -3.6220230000    -0.4093950000
C      -2.7648640000    -4.9021190000    -0.5584990000
C      -3.5834370000    -6.0675020000    -1.0919740000
```

N	-0.1777630000	4.0186070000	-1.3466530000
C	-0.7782540000	5.1954860000	-1.9809770000
C	-1.5630320000	6.0822870000	-1.0000530000
C	-2.7031350000	5.3963130000	-0.2337000000
C	-3.9089720000	5.0244290000	-1.1041940000
C	-5.1305700000	4.5307790000	-0.3133270000
N	-5.0133710000	3.1934510000	0.2495490000
C	3.2954040000	-0.7015560000	0.6597390000
C	4.2671870000	0.3510660000	1.2049420000
C	3.6271610000	1.3930490000	2.1292500000
C	4.6254840000	2.4070190000	2.7044110000
C	5.3456340000	3.2868180000	1.6681220000
N	2.1839460000	-0.1577970000	-0.1218340000
C	4.1313180000	3.8459040000	-0.4346950000
N	4.4657470000	4.1233180000	0.8639550000
O	4.5682680000	2.8655840000	-1.0445440000
C	-2.4125530000	0.8332910000	1.2855280000
C	-4.7417470000	2.9497780000	1.5716370000
C	-4.8028230000	1.4706830000	1.9814200000
C	-3.4308280000	0.9087100000	2.4082030000
C	3.2391960000	4.8928210000	-1.1152730000
C	1.8605360000	5.1636980000	-0.4689260000
C	0.9282430000	3.9784830000	-0.5775640000
N	-2.7219100000	-7.3110210000	-1.2556480000
H	3.0636120000	-0.1737430000	-3.3363890000
H	4.0500110000	-0.8531690000	-1.9826870000
H	3.9837160000	0.9253460000	-2.2503540000
H	2.8102340000	-1.2630800000	1.4839030000
H	3.8433000000	-1.4338400000	0.0321160000
H	4.7471900000	0.8616900000	0.3436250000
H	5.0747040000	-0.1955820000	1.7437290000
H	3.1173110000	0.8791800000	2.9727990000
H	2.8277230000	1.9315860000	1.5787100000
H	4.0961970000	3.0658820000	3.4283520000
H	5.4117430000	1.8835210000	3.2941930000
H	6.0783220000	3.9415510000	2.1871930000
H	5.9176570000	2.6660670000	0.9503340000
H	4.0426380000	4.9378230000	1.3110590000
H	3.1110830000	4.5543820000	-2.1607380000
H	3.8022920000	5.8506360000	-1.1461840000
H	1.4217430000	6.0689400000	-0.9266580000
H	1.9714540000	5.3888100000	0.6136430000
H	0.0160020000	5.7829710000	-2.4840320000
H	-1.4269650000	4.7862280000	-2.7794910000
H	-0.8471240000	6.5160010000	-0.2683020000

H	-1.9599070000	6.9466770000	-1.5785220000
H	-3.0436810000	6.0823850000	0.5708430000
H	-2.3186910000	4.4942350000	0.2875280000
H	-3.6230460000	4.2529400000	-1.8525450000
H	-4.2324290000	5.9182490000	-1.6842290000
H	-6.0281220000	4.5489710000	-0.9681670000
H	-5.3268770000	5.2101790000	0.5412680000
H	-5.1394340000	2.3973290000	-0.3757280000
H	-5.4837570000	1.4302370000	2.8566930000
H	-5.2642710000	0.8511060000	1.1835970000
H	-2.9909830000	1.5836100000	3.1675390000
H	-3.5627840000	-0.0831810000	2.8921230000
H	-4.0948640000	-0.9752460000	-0.8331730000
H	-4.2352250000	-1.0876480000	0.9540890000
H	-1.9045040000	-2.2798490000	-0.6443440000
H	-2.3062730000	-2.6498400000	1.0538380000
H	-4.0700960000	-3.3763720000	-1.3892880000
H	-4.4415910000	-3.8090690000	0.2976060000
H	-1.9140430000	-4.6952460000	-1.2460990000
H	-2.3232240000	-5.1717720000	0.4272760000
H	-4.4115820000	-6.3522630000	-0.4130110000
H	-4.0123810000	-5.8567130000	-2.0916630000
H	-2.3017960000	-7.5989320000	-0.3512820000
H	-1.9314940000	-7.1343040000	-1.9050660000
H	-3.2529410000	-8.1223900000	-1.6240920000

*

Table S1. Table of vibrational transition assignments for $[Fe(HDFO)]^+$

Vibrational Mode	frequency	IR	Raman
6	10.48	14.05691	9.846319
7	15.98	11.75783	5.130086
8	18.5	5.782264	0.420178
9	21.19	1.634214	10.16115
10	29.19	2.780977	2.805112
11	44.91	1.276219	4.201866
12	47.67	4.889689	1.265611
13	49.26	2.112635	2.892019
14	51.51	8.115471	4.201331
15	57.63	2.773541	2.890089
16	58.86	1.64736	2.547438
17	77.29	0.163164	3.010576
18	80.59	2.553492	3.303326
19	83.67	5.971534	0.900218
20	90.91	7.823866	2.371552
21	92.09	0.302025	3.063561

22	102.63	1.655086	1.334976
23	106.8	1.855474	1.419307
24	113.11	6.111039	1.518082
25	120.12	0.166289	9.439907
26	126.35	0.668786	0.912379
27	127.84	3.541434	1.75746
28	135.36	1.29875	1.423349
29	146.43	1.71895	20.29104
30	153.72	4.845419	0.505887
31	165.28	3.502369	2.31001
32	169.57	0.280429	4.711582
33	176.46	0.761519	6.286235
34	179.37	0.72842	3.468499
35	194.14	1.987444	5.830411
36	195.09	0.727089	17.2683
37	201.14	0.726701	1.479784
38	214.3	0.579736	5.985961
39	216.65	6.447235	4.854499

40	221.95	3.810953	8.389341
41	225.95	0.02286	8.351417
42	233.91	0.975185	2.586542
43	234.67	0.353816	16.94313
44	243.78	4.179264	59.53019
45	253.8	18.35196	10.27403
46	261.9	3.023172	1.112524
47	273.59	2.325714	2.121582
48	284.21	6.412833	2.455099
49	299.09	17.07255	11.23213
50	303.7	5.092711	2.266155
51	313.31	2.562094	5.18137
52	322.49	15.85879	6.905282
53	330.52	13.46122	11.725
54	343.8	15.79228	10.6304
55	344.79	0.350544	5.22306
56	346.65	25.15781	12.98661
57	357.07	17.22286	14.75557

58	367.58	0.97505	0.868325
59	374.2	18.16117	1.893398
60	407.51	20.08648	7.749259
61	421.83	0.874624	5.118529
62	435.45	6.605646	5.983657
63	448.58	15.83684	5.329954
64	455.71	9.555388	59.68893
65	468.99	40.54595	3.931913
66	475.66	5.985531	5.268312
67	480.93	25.42215	40.49211
68	488.78	15.28062	3.144574
69	491.79	29.80938	16.97515
70	494.93	38.90871	7.718641
71	518.49	30.64581	3.682893
72	525.43	113.3285	8.543051
73	535.25	17.42162	1.747357
74	542.27	74.20562	3.066202
75	545.33	0.20993	137.1935

76	577.21	1.677767	1.087974
77	580	3.970848	3.797991
78	597.29	3.423622	11.81775
79	607.67	16.0103	7.991526
80	616.19	10.86081	2.587575
81	618.7	12.39731	11.67994
82	652.51	6.289176	2.30352
83	660.25	6.324419	2.397916
84	679.87	0.709711	2.828464
85	703.72	3.422265	8.873054
86	714.26	13.86715	2.188295
87	718.26	6.957011	6.72328
88	729.81	3.904022	2.709192
89	741.66	23.61286	3.665777
90	748.42	5.693141	4.676739
91	748.75	12.38803	36.04566
92	772.01	11.87706	3.462068
93	777.42	17.63242	52.70827

94	804.18	2.688253	1.130522
95	814.04	3.366048	2.119042
96	822.8	0.663158	7.170014
97	826.88	1.583195	1.799486
98	835.96	4.998426	28.33336
99	855.54	3.403606	3.302118
100	863.98	29.44958	90.36848
101	873.71	1.915884	0.868548
102	882.28	0.430993	2.50482
103	885.26	9.007883	5.34942
104	900.03	19.22593	1.000316
105	911.13	2.992473	2.281911
106	928.33	17.14933	3.717443
107	936.86	4.265656	10.83328
108	938.71	3.353166	57.50631
109	954.2	8.776632	12.03933
110	960.29	10.62349	8.416514
111	967.16	10.02082	2.643042

112	967.83	3.148354	58.63186
113	974.64	12.54041	30.95124
114	980.08	10.55684	35.0739
115	997.02	15.28682	10.72332
116	1004.75	4.779783	7.914879
117	1014.94	17.60163	3.6074
118	1017.23	6.539541	2.75681
119	1032.35	13.19265	4.741368
120	1036.74	5.70139	10.7509
121	1044.77	15.12725	353.849
122	1046.84	24.97342	10.56474
123	1050.84	8.625812	33.4287
124	1053.77	9.019336	155.0569
125	1056.76	10.52704	18.80353
126	1074.37	0.894713	4.148512
127	1078.37	0.988673	1.301759
128	1083.94	17.59968	33.88086
129	1091.08	6.350719	7.802968

130	1104.68	14.39055	9.576735
131	1113.22	11.60629	12.87909
132	1113.91	23.96495	12.8235
133	1119.66	23.74845	40.53063
134	1137.5	5.614402	23.33948
135	1142.38	13.63273	7.251954
136	1158.37	3.034116	2.202933
137	1164.13	1.324906	4.373055
138	1167.96	16.95167	40.00216
139	1171.56	6.80274	4.953762
140	1186.79	8.244982	96.37587
141	1192.09	15.71212	4.220293
142	1192.71	4.122243	17.13353
143	1205.97	0.629649	49.67715
144	1207.22	1.81449	33.13004
145	1207.48	5.887666	2.667335
146	1220.27	26.22923	295.1665
147	1224.99	23.46529	137.8001

148	1235.54	32.64736	30.20548
149	1241.33	13.92603	20.37014
150	1246.73	15.62583	7.904027
151	1251.33	25.36105	47.40467
152	1258.24	2.968066	43.73175
153	1260.27	0.668867	11.79142
154	1267.18	15.83294	29.86088
155	1273.48	1.01239	44.24883
156	1278.15	7.99881	24.55137
157	1280.44	1.895273	9.633843
158	1281.91	4.737104	24.04812
159	1290.97	0.892968	13.64085
160	1292.8	4.368949	2.406758
161	1294.62	1.466938	26.1264
162	1296.53	3.817843	10.86841
163	1302.76	1.613323	4.808789
164	1310.17	4.907326	44.61906
165	1310.56	13.20766	6.779921

166	1321.62	33.25611	22.8812
167	1326.29	9.919848	22.37576
168	1329.48	29.95768	19.89616
169	1330.56	12.9178	26.36485
170	1334.91	3.868382	11.45473
171	1335.69	4.322535	6.676256
172	1345.56	0.678931	5.210598
173	1350.18	3.5111	4.430462
174	1352.89	39.27007	101.1006
175	1354.69	13.02339	15.72183
176	1361.94	0.009016	5.006541
177	1369.17	1.167588	42.71453
178	1377.88	1.734	16.32208
179	1380.63	12.82623	24.99323
180	1382.26	8.330684	29.92276
181	1389.37	9.682759	21.77011
182	1392.6	10.96396	34.89128
183	1393.24	30.76011	20.89249

184	1395.61	8.625847	8.21263
185	1396.38	2.834534	13.90882
186	1396.61	7.655302	6.997113
187	1399.7	14.59146	5.869696
188	1400.51	8.330655	8.835364
189	1402.54	8.158267	11.19254
190	1405.98	13.47101	14.07712
191	1408.36	12.27379	6.206237
192	1410.19	1.126762	14.85747
193	1410.64	5.737461	9.398403
194	1412.7	0.236311	21.50473
195	1414.85	5.329105	20.79686
196	1423.36	6.968773	4.48226
197	1424.82	1.885296	23.30549
198	1434.1	51.30577	99.27672
199	1436.71	81.3324	741.618
200	1463.29	23.46278	582.4846
201	1466.34	28.54443	261.1777

202	1475.81	58.21004	288.293
203	1495.84	129.933	12.86491
204	1504.48	145.9869	3.199007
205	1543.79	181.3841	406.9439
206	1559.93	112.785	455.2495
207	1569.18	44.30522	55.13838
208	1578.61	23.42659	364.1119
209	1582.69	289.8384	705.7958
210	1727.4	185.8792	17.77456
211	1753.62	181.0483	3.689018
212	2946.36	41.95466	89.99575
213	2948.34	11.09722	158.6879
214	2950.24	13.91173	36.0957
215	2951.67	53.87577	248.0846
216	2952.12	12.99536	93.15826
217	2955.81	23.49291	95.42318
218	2959.98	28.30523	191.0613
219	2967.9	19.27262	202.6081

220	2975.09	57.7692	213.2552
221	2975.34	21.22462	38.87684
222	2975.83	4.556101	76.59159
223	2976.84	17.50465	61.10449
224	2979.65	51.68361	321.6185
225	2981.13	25.36847	166.7056
226	2981.52	11.7996	73.2162
227	2984.4	10.02589	78.17766
228	2987.32	43.21967	114.5605
229	2989.68	11.61709	78.29532
230	2992.09	1.766809	120.5219
231	2998.18	29.68789	126.9765
232	3001.53	13.75066	133.3966
233	3003.81	25.14905	161.5837
234	3008.78	23.45826	77.48989
235	3011.04	16.03984	7.49276
236	3017.67	2.64262	185.2406
237	3017.91	4.626758	89.7332

238	3033.06	8.941766	62.69632
239	3035.82	23.09881	18.00867
240	3037.93	13.53346	152.4376
241	3039.67	4.513226	15.6219
242	3042.61	7.702367	53.97102
243	3048.38	9.958884	53.63738
244	3053.5	12.06454	52.22393
245	3056.42	4.845093	40.2674
246	3063.64	5.983978	50.78559
247	3064.2	17.08456	109.1025
248	3067.1	1.761467	34.47288
249	3068.31	6.448277	73.41322
250	3072.26	10.72939	97.85255
251	3084.71	0.478119	48.15951
252	3099.82	4.966066	93.20582
253	3303.5	29.85041	50523.07
254	3388.42	86.8624	870.2007
255	3394.7	76.47397	13857.54

256	3529.81	14.40902	46.40616
257	3540.96	11.67086	110.0222

Vibrational calculation of $[Th(HDFO)]^{2+}$

DFT Calculations were performed using ORCA 4.2.1 suit running in Microsoft MPI v10. The geometry optimization and frequency calculation were performed using the following input.

```
! TightOpt Freq PBE ZORA ZORA-def2-SVP Sarc/J TightSCF FinalGrid6 RIJCOSX
%maxcore 2000
%pal
nprocs 12
end
%basis Newgto 90 "SARC-ZORA-TZVPP" end
      Newauxgto 90 "Sarc/J" end
end
%freq
Hess2ElFlags 1,2,2,1
end

* xyz 2 1
 Th     0.167415     1.203264     0.067563
 O     -0.526727     3.089636    -1.021534
 O      1.245893     3.231027     0.726086
 O     -1.423520    -0.423602    -0.449927
 O      1.813357     0.164916    -1.297627
 O     -1.786963     1.187776     1.451588
 O      1.853805     0.170811     1.223475
 C      2.875794    -0.337312    -0.751965
 C      3.984140    -0.856685    -1.614134
 O     -4.460031     3.405992     1.832766
 N     -2.624742    -0.459310     0.198938
 C     -3.553049    -1.478024    -0.286179
 C     -3.000696    -2.901387    -0.127199
 C     -3.948307    -3.960531    -0.710386
 C     -3.420729    -5.395589    -0.519689
 C     -4.360534    -6.417658    -1.148963
 N     -0.028542     4.332938    -0.747348
 C     -0.645029     5.463122    -1.463125
 C     -1.653515     6.266914    -0.626412
 C     -2.875720     5.495686    -0.105252
 C     -3.947874     5.222366    -1.170791
 C     -5.263963     4.650288    -0.614338
 N     -5.249217     3.219597    -0.309905
 C      4.069647    -0.720929     1.439073
 C      5.204718     0.319846     1.430994
 C      4.725026     1.776567     1.468904
 C      5.882193     2.802153     1.497155
```

C	5.763704	3.891031	0.428012
N	2.931526	-0.347272	0.578797
C	3.927210	5.162276	-0.622766
N	4.516691	4.643324	0.502293
O	4.365201	4.963347	-1.753526
C	-2.782439	0.424308	1.201020
C	-4.918229	2.723628	0.918911
C	-5.202599	1.224878	1.116499
C	-4.094883	0.544016	1.951376
C	2.712255	6.077401	-0.413114
C	1.614635	5.643265	0.584664
C	0.920032	4.359453	0.196993
N	-3.858295	-7.842625	-0.972456
H	3.540640	-1.469611	-2.417782
H	4.736708	-1.453547	-1.077096
H	4.492440	-0.007840	-2.107635
H	3.638276	-0.818555	2.447618
H	4.431398	-1.720001	1.136978
H	5.850634	0.167168	0.544182
H	5.843607	0.108571	2.310414
H	4.040489	1.922655	2.326421
H	4.104583	1.977731	0.574912
H	5.980278	3.254475	2.503530
H	6.849097	2.294195	1.318721
H	6.638545	4.570747	0.480490
H	5.783019	3.444123	-0.583310
H	4.135547	4.854296	1.421926
H	2.292407	6.197836	-1.426053
H	3.081865	7.076789	-0.113140
H	0.870496	6.454043	0.675049
H	2.012526	5.489366	1.602560
H	0.165613	6.115463	-1.832362
H	-1.121988	5.011967	-2.348175
H	-1.128540	6.733553	0.227550
H	-1.982327	7.114050	-1.260682
H	-3.339462	6.091339	0.702375
H	-2.563990	4.554677	0.384833
H	-3.565293	4.547613	-1.962672
H	-4.198151	6.177102	-1.675949
H	-6.076789	4.820650	-1.342622
H	-5.538580	5.186501	0.313701
H	-5.645149	2.587254	-1.001076
H	-6.152691	1.155173	1.680674
H	-5.371214	0.708580	0.153167
H	-3.900522	1.174397	2.834729

```
 H     -4.426725    -0.448599     2.305045
 H     -3.747323    -1.256553    -1.354180
 H     -4.502310    -1.356376     0.259957
 H     -2.022990    -2.935824    -0.644003
 H     -2.810663    -3.093737     0.946236
 H     -4.101536    -3.762715    -1.789926
 H     -4.950745    -3.885067    -0.238286
 H     -2.407260    -5.479623    -0.968882
 H     -3.308210    -5.597543     0.566231
 H     -5.367867    -6.391181    -0.691672
 H     -4.473982    -6.267059    -2.238666
 H     -3.750820    -8.083113     0.028794
 H     -2.932324    -7.970881    -1.418670
 H     -4.500466    -8.537185    -1.390305
*
```

Further numerical frequency calculation of the optimized[Th(HDFO)]$^{2+}$ structure to generate the IR and Raman spectra was performed using the following input:

```
! NumFreq PBE ZORA ZORA-def2-SVP Sarc/J TightSCF FinalGrid6 RIJCOSX
%maxcore 2000
%pal
nprocs 12
end
%basis Newgto 90 "SARC-ZORA-TZVPP" end
      Newauxgto 90 "Sarc/J" end
end
%elprop Polar 1 end

* xyz 2 1
Th      0.0592980000     1.1820000000     0.0336100000
O      -0.6977050000     3.0573180000    -1.0270550000
O       1.0814380000     3.2148910000     0.7401900000
O      -1.5054280000    -0.5004540000    -0.4212970000
O       1.6533990000     0.5723740000    -1.5877900000
O      -1.8293420000     1.0759180000     1.5191030000
O       1.8615090000     0.0517170000     0.8565170000
C       2.8279800000     0.1884760000    -1.2079320000
C       3.9593030000     0.1428950000    -2.1820070000
O      -4.3378990000     3.3865140000     1.8397440000
N      -2.6981640000    -0.5278070000     0.2301680000
C      -3.6290540000    -1.5483580000    -0.2355550000
C      -3.0798280000    -2.9700190000    -0.0306940000
C      -4.0131880000    -4.0393430000    -0.6177510000
```

C	-3.4749470000	-5.4698850000	-0.4242130000
C	-4.4219820000	-6.5086740000	-1.0195120000
N	-0.0908900000	4.2643780000	-0.8591570000
C	-0.6545590000	5.3875360000	-1.6242530000
C	-1.6180920000	6.2636710000	-0.8064260000
C	-2.8410810000	5.5556190000	-0.2012640000
C	-3.9492200000	5.2187820000	-1.2105580000
C	-5.2410190000	4.6742820000	-0.5688120000
N	-5.2460270000	3.2446190000	-0.2595910000
C	4.1925390000	-0.5457880000	0.7865890000
C	5.1740030000	0.5906210000	1.0971680000
C	4.6409900000	1.6800070000	2.0364750000
C	5.6612920000	2.8063320000	2.2784430000
C	5.9670610000	3.6884610000	1.0541880000
N	2.9754520000	-0.1126730000	0.0860690000
C	3.9436990000	4.3647710000	-0.2512720000
N	4.9015590000	4.6179300000	0.6861300000
O	3.8261090000	3.2817880000	-0.8370680000
C	-2.8414840000	0.3368640000	1.2512900000
C	-4.8719980000	2.7289010000	0.9503840000
C	-5.2208220000	1.2414590000	1.1543620000
C	-4.1487920000	0.5074410000	1.9868530000
C	2.9969610000	5.5407710000	-0.5296250000
C	1.6991220000	5.5247160000	0.3224130000
C	0.8584360000	4.2991020000	0.0830150000
N	-3.9003700000	-7.9255370000	-0.8222000000
H	3.5721090000	-0.1862080000	-3.1594170000
H	4.7882640000	-0.5102360000	-1.8709790000
H	4.3405770000	1.1753030000	-2.2949100000
H	3.8290120000	-1.0313280000	1.7078920000
H	4.6822850000	-1.3254630000	0.1756140000
H	5.4967920000	1.0424970000	0.1413740000
H	6.0764980000	0.1237220000	1.5386310000
H	4.3727380000	1.2248510000	3.0092610000
H	3.7078250000	2.1073280000	1.6252420000
H	5.3097200000	3.4553720000	3.1032130000
H	6.6179240000	2.3690700000	2.6262510000
H	6.8745600000	4.2875280000	1.2498670000
H	6.1801590000	3.0690240000	0.1647520000
H	4.9264530000	5.5450590000	1.1056030000
H	2.7471810000	5.4933990000	-1.6040860000
H	3.5057770000	6.5072340000	-0.3550960000
H	1.1265310000	6.4443480000	0.1170470000
H	1.9497290000	5.5288740000	1.3979360000
H	0.1802670000	5.9899950000	-2.0255200000

H	-1.1526840000	4.9193190000	-2.4889740000
H	-1.0480040000	6.7497520000	0.0084070000
H	-1.9459150000	7.0883350000	-1.4701190000
H	-3.2706540000	6.2245970000	0.5683480000
H	-2.5346880000	4.6488210000	0.3527190000
H	-3.5937020000	4.4960000000	-1.9716180000
H	-4.2186400000	6.1417680000	-1.7617930000
H	-6.0939480000	4.8595150000	-1.2459200000
H	-5.4460080000	5.2195690000	0.3715050000
H	-5.6885360000	2.6228860000	-0.9322090000
H	-6.1716360000	1.2163470000	1.7205850000
H	-5.4149840000	0.7342340000	0.1899230000
H	-3.9230590000	1.1303140000	2.8694120000
H	-4.5338340000	-0.4643510000	2.3453210000
H	-3.8162740000	-1.3629030000	-1.3114450000
H	-4.5836320000	-1.4145800000	0.2996540000
H	-2.0839470000	-3.0237330000	-0.5073800000
H	-2.9286710000	-3.1458860000	1.0521200000
H	-4.1601700000	-3.8472110000	-1.6992310000
H	-5.0146310000	-3.9615750000	-0.1490620000
H	-2.4771060000	-5.5515530000	-0.9003350000
H	-3.3343850000	-5.6646720000	0.6582280000
H	-5.4193340000	-6.4796210000	-0.5479680000
H	-4.5525290000	-6.3770510000	-2.1077220000
H	-3.7844040000	-8.1494160000	0.1816740000
H	-2.9753150000	-8.0527520000	-1.2686290000
H	-4.5380770000	-8.6339320000	-1.2254230000

*

Table S2. Table of vibrational transition assignments for $[Th(HDFO)]^{2+}$

Vibrational Mode	Frequency	IR	Raman
6	9.44	9.239171	0.252616
7	11.63	5.01141	0.252218
8	17.7	9.899253	0.637325
9	21.91	1.188684	0.46873
10	23.25	2.499045	0.472342
11	34.57	1.259987	0.358307
12	35.51	2.723927	0.308329
13	39.98	2.170154	1.02426
14	44.51	0.52485	0.119247
15	48.33	7.698119	1.026205
16	57.91	0.177313	1.272715
17	59.76	4.370488	0.358552
18	64.96	2.164917	1.705605
19	72.96	7.451189	0.536671
20	79.05	9.69873	0.160979
21	88.13	1.312905	1.355004

22	96.96	4.052338	0.23079
23	104.92	2.249669	1.23442
24	110.78	2.948937	0.810813
25	117.17	1.165184	0.494172
26	122.47	3.054631	0.231375
27	125.04	4.192814	0.675408
28	129.38	12.641433	0.422332
29	137.62	1.810334	0.984383
30	143.35	2.941441	0.488682
31	147.96	0.257545	0.17034
32	161.14	0.808768	0.109064
33	161.63	4.03596	1.046247
34	167.75	0.246766	0.50252
35	173.42	6.623955	0.47902
36	181.71	6.113123	0.272431
37	190.58	0.169168	0.104205
38	203.06	3.208518	2.258962
39	211.64	1.818579	0.61586

40	213.47	6.733193	2.337749
41	222.18	1.160952	0.913713
42	226.89	0.125206	0.096197
43	236.75	18.828276	0.68261
44	238.21	4.963211	1.833701
45	245.59	3.471618	1.993172
46	251.6	3.296647	0.436452
47	255.5	9.172937	1.267109
48	264.48	66.24419	1.760496
49	270.69	22.72726	1.423948
50	283.16	47.16732	0.614297
51	293.22	12.756778	0.799757
52	296.16	6.479119	0.855353
53	314.48	8.075519	0.258699
54	329.48	3.154777	0.094026
55	336.21	6.231126	0.586013
56	337.47	4.06975	1.153778
57	347.11	5.701629	0.755928

58	370.93	4.599846	1.503695
59	380.1	6.158507	0.523034
60	401.43	7.845364	0.30309
61	422.67	14.728936	1.695699
62	438.54	7.959167	1.301737
63	450.1	10.042327	1.740164
64	456.22	7.266392	0.681266
65	467.53	13.607511	0.528898
66	474.72	37.975438	1.003227
67	485.28	92.03279	0.257837
68	487.28	52.663554	0.249824
69	492.19	30.965028	1.063074
70	504.6	116.810801	1.529033
71	507.84	55.244148	2.100846
72	513.62	11.576029	0.874357
73	515.52	52.594428	0.780791
74	533.31	49.312092	1.015905
75	540.99	10.914825	15.63689

76	581	2.608419	1.012392
77	585.79	4.453792	1.535464
78	597.67	8.479546	1.377556
79	608.21	13.276737	1.500826
80	608.99	8.380147	0.891627
81	622.04	16.817868	2.253512
82	663.84	0.242815	1.769259
83	679.14	15.400763	2.232217
84	688.95	7.482222	2.216307
85	699.66	15.711157	0.244662
86	713.65	29.911005	1.145446
87	725.47	6.359975	0.228695
88	726	7.774216	0.033897
89	741.36	39.244546	0.790311
90	746.99	4.400772	0.347298
91	750.52	48.541415	4.279526
92	762.35	22.466515	5.272995
93	779.13	49.075266	5.819207

94	797.83	3.96068	8.008361
95	804.33	4.057208	0.472346
96	816.17	2.232811	2.634654
97	821.11	1.453967	0.890118
98	830.53	7.285802	0.803185
99	858.86	3.783411	1.866495
100	870.39	20.956436	17.50587
101	886.11	0.722476	0.517748
102	888.19	1.281638	3.063335
103	891.78	15.529915	1.381727
104	904.53	15.463588	2.360266
105	910.7	38.703427	0.428899
106	928.44	11.587865	2.931111
107	939.07	0.241996	1.555768
108	944.98	1.308687	2.241453
109	949.4	16.895929	1.100451
110	968.28	17.557364	5.591246
111	975.03	43.955375	1.544327

112	978.87	0.261264	0.300973
113	979.62	1.739438	2.078977
114	981.91	2.314283	6.997826
115	1006.78	17.520688	1.079082
116	1009.53	4.167415	2.257008
117	1015.14	8.364899	14.17113
118	1018.14	10.523121	6.360064
119	1026.35	19.45249	13.07999
120	1029.62	31.370448	1.233084
121	1044.87	51.119037	11.58054
122	1048.84	21.329488	2.670867
123	1051.27	9.951402	5.937305
124	1052.11	1.498813	9.819931
125	1053.57	32.907545	6.464252
126	1072.85	11.896087	1.392091
127	1076.53	0.827327	1.752936
128	1083.92	10.87412	3.761737
129	1089.38	1.380388	5.026701

130	1105.57	7.560758	3.295953
131	1111.26	18.507124	2.101879
132	1121.92	37.976464	2.325339
133	1124.02	11.460112	4.58831
134	1141.43	14.587923	2.382631
135	1152.39	5.653318	1.555588
136	1160.58	1.794463	3.752339
137	1164.88	17.452202	7.943737
138	1173.68	11.691177	2.532786
139	1180.83	18.269587	7.93128
140	1186.15	5.61795	3.629482
141	1187.42	0.616389	7.860918
142	1201.24	9.795065	2.473481
143	1211	6.090321	3.199542
144	1211.41	23.415126	5.576723
145	1217.87	22.191997	3.087774
146	1224.35	35.862032	1.337099
147	1227.35	78.561437	1.088531

148	1246.03	25.324916	6.623109
149	1250.08	16.407491	1.853305
150	1259.9	23.014559	11.11427
151	1263.24	4.940199	6.593428
152	1270.86	0.220089	6.511771
153	1273.34	1.732761	6.835364
154	1283.47	13.245446	18.77105
155	1288.27	1.571657	2.765657
156	1289.41	4.882235	7.086182
157	1292.75	4.246081	14.86875
158	1294.32	0.293049	16.91948
159	1296	6.391109	37.70498
160	1299.7	0.593072	8.41009
161	1300.91	10.749561	6.176284
162	1304.07	0.676817	8.977423
163	1314.44	3.260815	1.856525
164	1320.41	7.168066	11.90097
165	1329.01	25.042886	13.52913

166	1329.18	11.96914	4.347977
167	1331.91	12.094449	18.27511
168	1337.59	27.004636	9.086011
169	1340.12	1.576787	4.780283
170	1341.85	5.384644	2.270705
171	1347.59	14.23987	5.755918
172	1355.59	6.242746	5.359653
173	1356.17	3.135738	2.103453
174	1363.77	0.467246	3.263972
175	1364.48	22.676106	22.00918
176	1367.5	0.596858	4.281029
177	1369.73	8.434792	1.653161
178	1401.17	34.022546	12.78664
179	1402.54	3.1443	11.8255
180	1404.25	6.960032	13.47636
181	1409.5	20.845012	10.64406
182	1411.3	40.522896	13.1614
183	1414.92	15.152654	10.72389

184	1418.14	4.735989	14.78258
185	1418.53	11.181467	4.373152
186	1423.74	33.77792	27.65397
187	1425.6	14.759366	17.2845
188	1425.94	15.52435	3.574259
189	1426.59	11.59374	10.59273
190	1430.66	6.389886	6.723357
191	1431.66	16.563584	0.778693
192	1432.67	14.010491	14.09909
193	1434.81	2.972187	14.10025
194	1439.96	0.265343	37.0184
195	1440.24	13.291178	0.747974
196	1440.87	3.580948	0.917834
197	1452.13	2.291776	9.334137
198	1459.66	28.193081	1.849664
199	1463.79	133.573941	3.345422
200	1466.36	123.326533	26.2466
201	1469.87	273.274688	6.82546

202	1473.21	27.930672	73.00908
203	1499.89	158.774744	5.374534
204	1513.06	175.051611	6.65151
205	1566.06	459.824936	11.25933
206	1575.29	294.262273	16.07411
207	1577.01	204.717015	30.34873
208	1604.18	53.091384	7.854418
209	1609.36	38.171357	9.075203
210	1722.89	245.664826	10.05014
211	1755.52	161.578741	4.901084
212	2970.79	4.861492	184.4506
213	2974.33	14.326452	110.3634
214	2979.35	14.603983	11.0197
215	2986.09	18.270675	149.7004
216	2986.83	14.073242	42.7408
217	2990.13	13.283647	115.9183
218	2990.92	12.898202	294.7502
219	2991.58	3.065892	145.1257

220	2997.27	18.580044	24.85905
221	3001.48	24.543301	15.65695
222	3001.72	10.526347	197.3642
223	3002.67	10.192682	15.30944
224	3004.32	5.303813	181.2903
225	3008.66	10.228343	166.5486
226	3012.24	16.289109	162.0274
227	3015.21	0.437523	111.9794
228	3017.19	14.598385	140.6849
229	3019.2	15.438924	174.0315
230	3021.48	8.513355	103.7225
231	3022.36	15.541325	110.4726
232	3027.54	3.588745	163.0469
233	3032.35	12.707924	71.33835
234	3033.5	11.709032	3.559521
235	3035.49	10.77148	177.5264
236	3037.12	0.955556	74.57472
237	3043.34	5.859465	46.17313

238	3045.76	7.271387	151.11
239	3053.75	25.473616	7.868773
240	3057.01	5.673244	45.42244
241	3057.78	20.475329	6.165471
242	3060.79	5.653346	88.22558
243	3067.43	7.17419	60.39851
244	3072.33	4.113154	75.44353
245	3082.71	1.713623	26.42393
246	3084.01	2.797723	46.08358
247	3084.4	7.204553	46.13174
248	3088.08	2.814096	51.57878
249	3090.43	2.46306	43.58387
250	3095.37	4.797339	71.25259
251	3101.76	0.088207	37.5952
252	3130.62	2.139483	67.97403
253	3328.76	62.305311	131.7859
254	3412.71	97.697304	30.49683
255	3414.57	118.40475	104.7345

256	3557.15	39.729985	77.62734
257	3561.43	22.346357	58.33811

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