Supporting Information for: Charting the Coordinative Landscape of the ^{18}F-Sc/^{44}Sc/^{177}Lu triad with the Tri-aza-cyclononane (tacn) Scaffold

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Abbreviations

Ac	Acetate
AcN	Acetonitrile
API-ES	Atmospheric Pressure Ionization - Electrospray
Ar	Aromatic
Ar(Bz)	Aromatic Benzyl
Ar(Pa)	Aromatic Picolinic Acid
Asc	Ascorbate
Bz	Benzyl
CV	Column Volume
DCM	Dichloromethane
DFT	Density Functional Theory
DIPEA	N,N-diisopropylethylamine
DMAP	4-dimethylaminopyridine
DMEM	Dulbecco's Modified Eagle Medium
DMF	Dimethylformamide
DMSO	Dimethyl sulfoxide
ESI	Electrospray Ionization
EtOAc	Ethyl Acetate
FBS	Fetal Bovine Serum
HEPES	2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid
HPLC	High Performance Liquid Chromatography
HR	High Resolution
Hz	Hertz
ICP-OES	Inductively Coupled Plasma - Optical Emission Spectroscopy
IS	Internal Standard
LC	Liquid Chromatography
LR	Low Resolution
MeCN	Acetonitrile
MeOH	Methanol
MS	Mass Spectrometry
NMR	Nuclear Magnetic Resonance
PBS	Phosphate Buffered Saline
PVDF	Polyvinylidene Fluoride
QTAIM	Quantum Theory of Atoms in Molecules
RCY	Radiochemical Yield
RMSD	Root Mean Square Deviation
RT	Room Temperature
R_t	Retention time
SD	Standard Deviation

TACN	Triazacyclononane
TEA	Triethylamine
TFA	Trifluoroacetic acid
THF	Tetrahydrofuran
TLC	Thin Layer Chromatography
TOF	Time of Flight

1 Experimental procedures

1.1 General methods

All starting materials were purchased from commercial sources and used without further purification. ^{18}F and ^{44}Sc was received from the University of Wisconsin-Madison Cyclotron Lab (GE PETtrace cyclotron), and ^{177}Lu was received from the DOE isotope program, produced at the University of Missouri Research Reactor.

NMR spectra (^{1}H, $^{13}C\{^{1}H\}$, ^{19}F, ^{45}Sc, COSY, HSQC and HMBC) were collected at Stony Brook University on a 400, 500, or 700 MHz III Bruker instrument at 25 °C and processed using TopSpin 4.0.9. and at the University of Wisconsin-Madison Department of Chemistry Paul Bender Chemical Instrumentation Center (CIC) using a Bruker Avance III 500 with a DCH liquid He cryoprobe (Bender Fund), a Bruker Avance Neo 500 with a 5mm Prodigy-BBO liquid N_2 cryoprobe (NSF CHE-2017891), or a Bruker Avance III 600 with a TCI-F liquid He cryoprobe (NIH S10 OD012245). Data was processed using MestReNova 14.3.3-33362. Chemical shifts (δ) are reported in parts per million (ppm) relative to tetramethylsilane. ^{1}H, $^{13}C\{^{1}H\}$, COSY, HSQC and HMBC NMR spectra are referenced to residual solvent signals, ^{45}Sc NMR spectra are referenced in MestReNova using a ^{1}H NMR spectra as an absolute reference.

High resolution ESI mass spectrometry were carried out at the Stony Brook University Center for Advanced Study of Drug Action (CASDA) with a Bruker Impact II UHR QTOF MS system, and at the University of Wisconsin-Madison Department of Chemistry Paul Bender Chemical Instrumentation Center (CIC) using a Thermo Scientific Q Exactive Focus Orbitrap MS system, and at the University of Wisconsin-Madison School of Pharmacy Analytical Instrumentation Cluster using a Bruker MaXis Ultra-High Resolution Quadrupole Time-of-Flight MS system.

Ultraviolet-visible spectra were collected with the NanoDrop 1C instrument (AZY1706045). Spectra were recorded from 190 to 850 nm in a quartz cuvette with 1 cm path length. Copper titration and molar extinction measurements were made in sodium acetate buffer (10 mM, pH 5.5).

ICP-OES and MP-AES analyses were carried out using an Agilent 5110 inductively coupled plasma optical emission spectrometer and an Agilent 4210 microwave plasma atomic emission spectrometer, respectively. For both techniques, a 6-point standard curve (1-100 ppm) with respect to scandium, lutetium, or copper was used and fits were found to be $R^2 > 0.99$.

Analytical- and radio-HPLC methods were carried out using a Shimadzu HPLC-20AR equipped with a binary gradient pump, UV-vis detector, autoinjector, or an Agilent 1260 Infinity II system. Both instruments were set to detect UV absorption was recorded at 220 nm and 254 nm and were coupled to an in-line LabLogic Dual Scan-RAM detector and were controlled using the LabLogic Laura software package. RadioHPLC analyses utilised a LabLogic 1" NaI photomultiplier tube detector with 2" lead shielding and radioTLC analyses utilised a LabLogic plastic photomultiplier tube detector.

Semipreparative HPLC was carried out using a Shimadzu HPLC-20AR equipped with a binary gradient pump, UV-vis detector, and manual injector. UV absorption was recorded at 220 and 254 nm.

Flash chromatography was carried out using a Combi Flash Rf+ system with UV detection at 220 and 254 nm.

Liquid chromatography mass spectrometry (LCMS) was carried out on a Phenomenex Luna C18 column (5 µm, 150 mm × 3 mm, 100 Å, AXIA packed) at a flow rate of 0.8 mL/min using a single quadrupole Agilent 1200 Infinity II LC/MSD system equipped with a binary gradient pump,

UV- vis detector, automatic injector, and an atmospheric pressure electrospray ionization (AP-ESI) source. Ultraviolet absorption was recorded at 220 nm and 254 nm, and positive and negative mass spectra were collected from m/z = 100-1000.

Chromatography Solvent Systems:

Analytical HPLC - Method A: binary solvent system (A: water + 0.1% TFA; B: MeCN + 0.1% TFA); gradient (0–2 min: 5% B; 2–14 min: 5–95% B; 14–16 min: 95% B; 16–16.5 min: 95–5% B; 16.5–20 min 5% B); flow rate: 0.8 mL/min; column: Phenomenex Luna C18 column (5 μm, 150 mm × 3 mm, 100 Å, AXIA packed).

Analytical HPLC - Method B: binary solvent system (A: water + 0.1% TFA; B: MeCN + 0.1% TFA); gradient (0–2 min: 0% B; 2–14 min: 0–90% B; 14–16 min: 90% B; 16–16.5 min: 90–0% B; 16.5–20 min 0% B); flow rate: 1.0 mL/min; temperature: 50 °C; column: Restek Ultra AQ C18 column (5 μm, 250 mm × 3 mm).

Analytical HPLC - Method C: binary solvent system (A: 10 mM ammonium formate pH 9.0; B: MeCN); gradient (0–2 min: 0% B; 2–14 min: 0–90% B; 14–16 min: 90% B; 16–16.5 min: 90–0% B; 16.5–20 min 0% B); flow rate: 1.0 mL/min; temperature: 50 °C; column: Restek Ultra AQ C18 column (5 μm, 250 mm × 3 mm).

Analytical HPLC - Method D: binary solvent system (A: 10 mM ammonium formate pH 4.0; B: MeCN); gradient (0–2 min: 0% B; 2–14 min: 0–90% B; 14–16 min: 90% B; 16–16.5 min: 90–0% B; 16.5–20 min 0% B); flow rate: 1.0 mL/min; temperature: 50 °C; column: Restek Ultra AQ C18 column (5 μm, 250 mm × 3 mm).

Analytical HPLC – Method E: single solvent system (A: MeOH); no gradient; flow rate: 0.25 mL/ min; column: CHIRALPAK IE-3 (4.6x50mm, 3mi).

Semipreparative HPLC - Method F: binary solvent system (A: water + 0.1% TFA; B: MeCN + 0.1% TFA); gradient: (0–1 min: 5% B; 1–14 min: 5–50% B; 14–23 min: 50–95% B; 23–26 min: 95% B; 26–27 min: 95–5% B; 27–30 min: 5% B); flow rate: 15 mL/min; column: Phenomenex Luna C18 column (250 mm × 21.2 mm, 100 Å, AXIA packed).

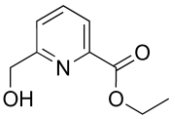
Flash chromatography - Method G: Binary solvent system (A: water + 0.1% TFA; B: MeCN + 0.1% TFA); flow rate: 60 mL/min; column: RediSep C18 column (100 g HP gold).

LCMS - Method H: binary solvent system (A: water + 0.1% FA; B: MeCN + 0.1% FA); gradient (0-3 min: 5% B; 3-10 min: 5-95% B; 10-13 min: 95% B; 13-13.5 min: 95-5% B; 13.5-16 min: 5% B); flow rate: 0.8 mL/min; column: Phenomenex Luna C18 column (5 μm, 150 mm × 3 mm, 100 Å, AXIA packed).

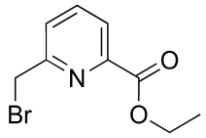
In vivo biodistribution in naïve BALB/C mice models. Animal experiments were conducted with the approval of the University of Wisconsin-Madison Institutional Animal Care and Use Committee (IACUC). All studies were conducted in accordance with the relevant guidelines and regulations. BALB/C mice were purchased from Jackson Laboratory.

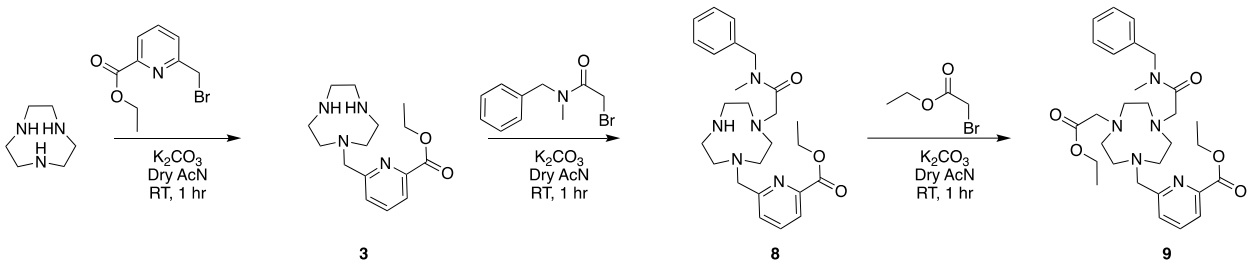
1.2 Ligand Synthesis

Ethyl 6-(hydroxymethyl)picolinate, ***1***. To a solution of diethyl-2,6-pyridinedicarboxylate (10.00 g, 44.80 mmol, 1 equiv.) in ethanol (200 mL) at 0 °C was added sodium borohydride (4.07 g, 107.51 mmol, 2.4 equiv.) in 4 portions over 1 h. After an additional 4 h at 0 °C, the reaction was quenched with acetone (150 mL) and the solvent was removed under reduced pressure. The residue was dissolved in water (100 mL) and extracted with dichloromethane (3 x 50 mL). The organic phase was dried over sodium sulfate and the solvent was removed under reduced pressure to give the desired product as a clear pale yellow oil that rapidly crystallized (6.28 g, 34.68 mmol, 77%). ^{1}H NMR (500 MHz, MeOD) δ 8.04 – 7.94 (m, 2H, Ar(Pa)), 7.79 – 7.73 (m, 1H, Ar(Pa)), 4.76 (s, 2H, CH_2OH)), 4.43 (q, *J* = 7.1 Hz, 2H, CH_2CH_3), 1.41 (t, *J* = 7.1 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 166.3 (COOEt), 163.4 (*C* CH_2OH), 148.2 (*C*COOEt), 139.5 (Ar(Pa)), 125.3 (Ar(Pa)), 124.5 (Ar(Pa)), 65.3 (CH_2OH), 62.9 (CH_2CH_3), 14.5 (CH_3). ESI-HRMS (+ve ion): [**1**+H]$^{+}$ *m/z* = 182.0812 (experimental); 182.0812 (calculated).



Ethyl 6-(bromomethyl)picolinate, ***2***. To a solution of ethyl 6-(bromomethyl)picolinate (5.76 g, 31.79 mmol, 1 equiv.) in chloroform (300 mL) at 0 °C was slowly added phosphorus tribromide (12.91 g, 47.68 mmol, 1.5 equiv.). After 1 h at 0 °C, the reaction was quenched with saturated aqueous sodium bicarbonate (100 mL) and mixture was extracted with dichloromethane (3 x 50 mL). The organic phase was dried over sodium sulfate and the solvent was removed under reduced pressure to give the desired product as a dark red oil (5.63 g, 23.07 mmol, 73%). ^{1}H NMR (500 MHz, MeOD) δ 8.06 (dd, *J* = 7.8, 1.2 Hz, 1H, Ar(Pa)), 8.01 (t, *J* = 7.8 Hz, 1H, Ar(Pa)), 7.79 (dd, *J* = 7.7, 1.1 Hz, 1H, Ar(Pa)), 4.68 (s, 2H, CH_2OH)), 4.45 (q, *J* = 7.1 Hz, 2H, CH_2CH_3), 1.43 (t, *J* = 7.1 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 165.8 (COOEt), 159.2 (*C* CH_2Br), 148.7 (*C*COOEt), 140.3 (Ar(Pa)), 128.7 (Ar(Pa)), 125.4 (Ar(Pa)), 63.1 (CH_2CH_3), 32.9 (*C*H2Br), 14.5 (CH_3). ESI-HRMS (+ve ion): [**2**+H]$^{+}$ *m/z* = 243.9969 (experimental); 243.9968 (calculated) and 245.9948 (experimental); 245.9948 (calculated). HPLC: R_t = 9.60 min (Method A).

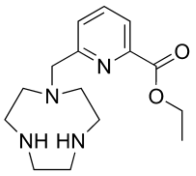




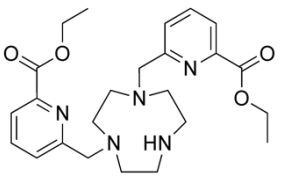
Scheme S1: General alkylation procedure.

1.2.1 General Alkylation Procedure

To a solution of the secondary amine and potassium carbonate in dry acetonitrile at 0 °C was added slowly the corresponding alkyl bromide as a solution in an equivalent volume of dry acetonitrile under N_2. After 1 h at 0 °C, the reaction mixture was filtered and the solvent was removed under reduced pressure. The resultant crude mixture was dissolved in acetonitrile/water (1:1) and the desired product(s) was isolated using either flash chromatography (Method C) or semi-preparative HPLC (Method B) in sufficient purity to use in following reactions. Example stoichiometry/reactants: 1,4,7-Triazacyclononane (1.00 g, 7.74 mmol, 3 equiv.); potassium carbonate (1.07 g, 7.74 mmol, 3 equiv.); ethyl 6-(bromomethyl)picolinate (0.63 g, 2.58 mmol, 1 equiv.); dry acetonitrile (40 mL). Products: **3** (457 mg, 1.55 mmol, 60%); **4**(131 mg, 0.288 mmol, 11%); **5** (15 mg, 0.024 mmol, 0.9%).

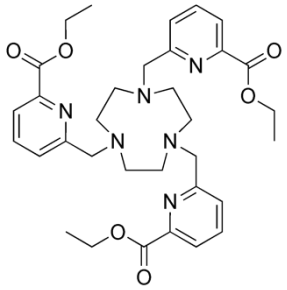


Ethyl 6-((1,4,7-triazonan-1-yl)methyl)picolinate, ***3****.* ^{1}H NMR (600 MHz, MeOD) δ = 8.12 (dd, *J* = 7.7, 1.1 Hz, 1H, Ar(Pa)), 8.05 (t, *J* = 7.8 Hz, 1H, Ar(Pa)), 7.61 (dd, *J* = 7.9, 1.0 Hz, 1H, Ar(Pa)), 4.50 (q, *J* = 7.1 Hz, 2H, CH_2 ethyl), 4.26 (s, 2H, CH_2 pic), 4.22 – 3.50 (m, 2H, tacn), 3.37 (t, *J* = 5.7 Hz, 4H, tacn), 3.28 – 2.89 (m, 6H, tacn), 1.44 (t, *J* = 7.2 Hz, 3H, CH_3 ethyl). ^{13}C{^{1}H} NMR (151 MHz, MeOD) δ 166.5 (*C*OOEt), 161.2 (*C*CH_2N), 147.8 (*C*COOEt), 140.6 (Ar(Pa)), 128.0 (Ar(Pa)), 125.3 (Ar(Pa)), 63.6 (CH_2 ethyl), 58.5 (CH_2 pic), 51.2 (tacn), 47.0 (tacn), 46.1 (tacn), 14.5 (CH_3 ethyl). ESI-HRMS (+ve ion): [**3**+H]$^+$ *m/z* = 293.1973 (experimental); 293.1972 (calculated). HPLC: R_t = 5.58 min (Method A).



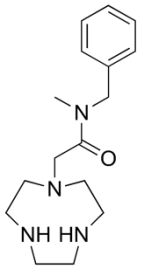
Diethyl 6,6'-((1,4,7-triazonane-1,4-diyl)bis(methylene))dipicolinate, ***4****.* ^{1}H NMR (500 MHz, MeOD) δ 7.98 – 7.91 (m, 4H, Ar(Pa)), 7.62 – 7.54 (m, 2H, Ar(Pa)), 4.58 (s, 4H, CH_2(Pa)), 4.33 (q, *J* = 7.1 Hz, 4H, CH_2 ethyl), 3.80 – 3.53 (m, 12H, tacn), 1.35 (t, *J* = 7.1 Hz, 6H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 165.9 (CO), 163.3 (*C*CH_2N), 147.8 (*C*COOEt), 140.1 (Ar(Pa)), 127.9 (Ar(Pa)), 125.5 (Ar(Pa)), 63.3 (CH_2 ethyl), 60.9 (CH_2(Pa)), 54.1 (tacn), 53.1 (tacn), 45.9 (tacn), 14.5 (CH_3). ESI-HRMS (+ve ion): [**4**+H]$^+$ *m/z* = 456.2606 (experimental); 456.2605 (calculated). HPLC: R_t = 6.92 min (Method A).

triethyl 6,6',6''-((1,4,7-triazonane-1,4,7-triyl)tris(methylene))tripicolinate, ***5***:^{1}H NMR (500 MHz, MeOD) δ 7.90 (t, *J* = 7.8 Hz, 3H, Ar(Pa)), 7.80 (d, *J* = 7.7 Hz, 3H, Ar(Pa)), 7.57 (d, *J* = 7.9 Hz, 3H, Ar(Pa)), 4.72 (s, 6H, CH_2(Pa)), 4.25 (q, *J* = 7.1 Hz, 6H, CH_2 CH_3), 4.19 – 3.66 (m, 12H, tacn), 1.30 (t, *J* = 7.1 Hz, 9H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 165.6 (COOEt), 156.1 (*C*CH_2N), 147.6 (*C*COOEt), 139.9 (Ar(Pa)), 127.8 (Ar(Pa)), 125.6 (Ar(Pa)), 63.2 (CH_2CH_3), 61.5 (CH_2 Pa), 54.3 (tacn), 14.5 (CH_3). ESI-HRMS (+ve ion): [**5**+H]$^{+}$ *m/z* = 619.3239 (experimental); 619.3239 (calculated). HPLC: R_t = 7.98 min (Method A).

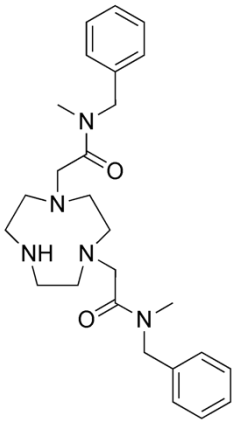


6/7/L^{030}:Sample reaction stoichiometry*:* 1,4,7-Triazacyclononane (1.00 g, 7.74 mmol, 3 equiv.); potassium carbonate (1.07 g, 7.74 mmol, 3 equiv.); *N*-benzyl-2-bromo-*N*-methylacetamide (0.62 g, 2.58 mmol, 1 equiv.); dry acetonitrile (40 mL). Products: **6** (808 mg); **7** (222 mg); **L^{030}** (47 mg).

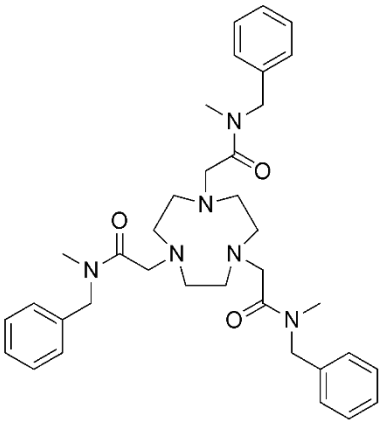
N-benzyl-N-methyl-2-(1,4,7-triazonan-1-yl)acetamide:^{1}H NMR (500 MHz, MeOD) δ 7.43 – 7.22 (m, 5H, (Ar(Bz)), 4.66 – 4.54 (m, 2H, CH_2(Bz)), 3.84 – 3.79 (m, 2H, CH_2 Ac), 3.69 (s, 4H, tacn), 3.37 – 3.28 (m, 4H, tacn), 3.13 – 3.02 (m, 4H, tacn), 2.98 – 2.93 (m, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 174.5 (CO), 174.4 (CO), 137.9 (C Bz), 137.1 (C Bz), 130.1 (Ar(Bz)), 129.8 (Ar(Bz)), 128.9 (Ar(Bz)), 128.7 (Ar(Bz)), 127.8 (Ar(Bz)), 56.3 (CH_2 Ac), 56.2 (CH_2 Ac), 53.1 (CH_2(Bz)), 52.5 (CH_2(Bz)), 51.4 (tacn), 51.2 (tacn), 46.4 (tacn), 46.2 (tacn), 45.3 (tacn), 45.1 (tacn), 34.7 (CH_3), 34.3 (CH_3). ESI-HRMS (+ve ion): [**6**+H]$^{+}$ *m/z* = 291.2180 (experimental); 291.2179 (calculated). HPLC: R_t = 6.15 min (Method A).



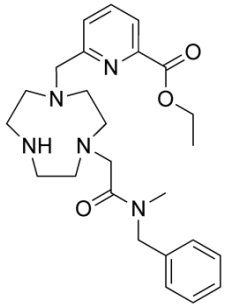
2,2'-(1,4,7-triazonane-1,4-diyl)bis(N-benzyl-N-methylacetamide). ^{1}H NMR (500 MHz, MeOD) δ 7.35 – 7.19 (m, 10H, Ar(Bz)), 4.67 – 4.55 (m, 4H, CH_2 Bz), 4.31 – 4.12 (m, 4H, CH_2 Ac), 3.58 – 3.24 (m, 12H, tacn), 2.98 – 2.92 (m, 6H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 172.0 (CO), 170.9 (CO), 170.0 (CO), 137.7 (C Bz), 137.6 (C Bz), 137.0 (C Bz), 136.9 (C Bz), 130.1 (Ar(Bz)), 129.8 (Ar(Bz)), 129.0 (Ar(Bz)), 128.7 (Ar(Bz)), 128.0 (Ar(Bz)), 127.9 (Ar(Bz)), 58.4 (CH_2 Ac), 58.1 (CH_2 Ac), 57.9 (CH_2 Ac), 53.7 (tacn), 53.3 (tacn), 53.2 (tacn), 52.8 (CH_2 Bz), 52.4 (tacn), 52.3 (tacn), 52.1 (CH_2 Bz), 51.7 (tacn), 44.6 (tacn), 44.4 (tacn), 34.6 (CH_3), 34.5 (CH_3), 34.2 (CH_3), 34.2 (CH_3). ESI-HRMS (+ve ion): [**7**+H]$^{+}$ *m/z* = 452.3021 (experimental); 452.3020 (calculated). HPLC: R_t = 7.80 min (Method A).



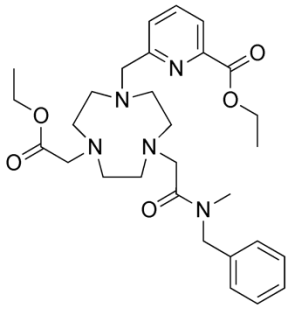
2,2',2''-(1,4,7-triazonane-1,4,7-triyl)tris(N-benzyl-N-methylacetamide), ***L^{030}****:* ^{1}H NMR (500 MHz, MeOD) δ 7.40 – 7.21 (m, 15H, Ar(Bz)), 4.62 – 4.55 (m, 6H, CH_2 Bz), 4.08 – 3.98 (m, 6H, CH_2 Ac), 3.30 – 3.10 (m, 12H, tacn), 2.93 (s, 8H, CH_3). $^{13}C\{^{1}H\}$ NMR (126 MHz, MeOD) δ 171.2 (CO), 171.0 (CO), 170.5 (CO), 170.3 (CO), 138.1 (C Bz), 137.6 (C Bz), 130.1 (Ar(Bz)), 129.7 (Ar(Bz)), 128.9 (Ar(Bz)), 128.8 (Ar(Bz)), 128.6 (Ar(Bz)), 127.7 (Ar(Bz)), 127.7 (Ar(Bz)), 57.0 (CH_2 Ac), 56.7 (CH_2 Ac), 52.0 (CH_2 Bz), 51.9 (CH_2 Bz), 51.8 (tacn), 51.6 (tacn), 51.3 (tacn), 34.4 (CH_3), 34.4 (CH_3), 34.3 (CH_3). ESI-HRMS (+ve ion): $[\mathbf{L^{030}}+H]^+$ *m/z* = 613.3865 (experimental); 613.3861 (calculated). HPLC: R_t = 9.48 min (Method A). UV-vis: ε = 571.7 $M^{-1}\cdot cm^{-1}$ at 258 nm.

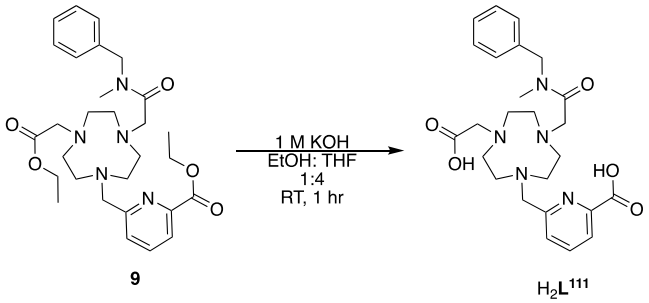


ethyl 6-((4-(2-(benzyl(methyl)amino)-2-oxoethyl)-1,4,7-triazonan-1-yl)methyl)picolinate, ***8****.* **3** (100 mg, 0.19 mmol, 1 equiv.); potassium carbonate (107 mg, 0.77 mmol, 4 equiv.); *N*-benzyl-2-bromo-*N*-methylacetamide (38 mg, 0.15 mmol, 0.8 equiv.); dry acetonitrile (3 mL). Product: **8** (23 mg, 0.04 mmol, 27%). OR **6** (0.50 g, 0.95 mmol, 1 equiv.); potassium carbonate (0.54 g, 3.75 mmol, 4 equiv.); ethyl 6-(bromomethyl)picolinate (0.19 g, 0.75 mmol, 0.8 equiv.); dry acetonitrile (10 mL). Product: **8** (0.11 g, 0.2 mmol, 21%).HPLC: R_t = 8.02 min (Method A). Product was used without further characterization for subsequent alkylation step.



ethyl 6-((4-(2-(benzyl(methyl)amino)-2-oxoethyl)-7-(2-ethoxy-2-oxoethyl)-1,4,7-triazonan-1-yl)methyl)picolinate, ***9****:* **8** (111 mg, 0.20 mmol, 1 equiv.); potassium carbonate (81 mg, 0.59 mmol, 3 equiv.); ethyl 2-bromoacetate (36 mg, 0.22 mmol, 1.1 equiv.); dry acetonitrile (2 mL). Product: **9** (50mg, 0.16 mmol, 57%). HPLC: R_t = 8.52 min (Method A). Product was used without further characterization for subsequent deprotection step.



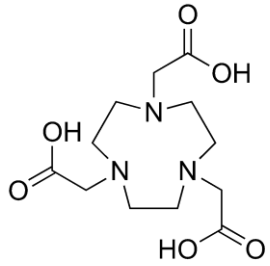


Scheme S2: General deprotection procedure.

General Deprotection Procedure

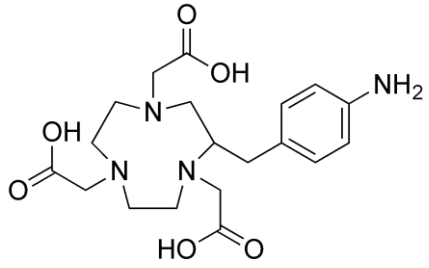
To a solution of ester in ethanol/tetrahydrofuran (1 mL, 1:4) was added potassium hydroxide (1 M, 13 equiv.). After 1 h at room temperature, the reaction mixture was filtered and the solvent was removed under reduced pressure. The resultant crude mixture was dissolved in acetonitrile/water (1:1) and purified using semi-preparative HPLC (Method E). The products were isolated and concentrated under reduced pressure then lyophilized.

2,2',2''-(1,4,7-triazonane-1,4,7-triyl)triacetic acid, $H_3\mathbf{L}^{300}$:



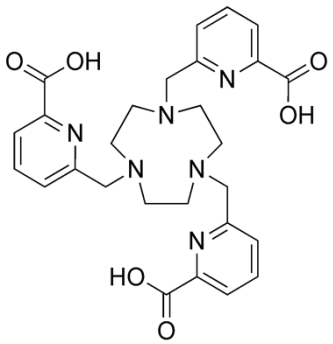
HPLC: R_t = 2.02 min (Method A). UV-vis: ε = 397.7 $M^{-1}\cdot cm^{-1}$ at 231 nm.

2,2',2''-(2-(4-aminobenzyl)-1,4,7-triazonane-1,4,7-triyl)triacetic acid, $H_3\mathbf{L}^{300\text{-}BzNH2}$:



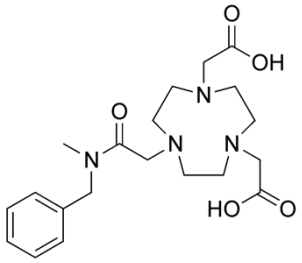
HPLC: R_t = 4.57 min (Method A). UV-vis: ε = 5254 $M^{-1}\cdot cm^{-1}$ at 220 nm.

6,6',6''-((1,4,7-triazonane-1,4,7-triyl)tris(methylene))tripicolinic acid, $H_3\mathbf{L}^{003}$:



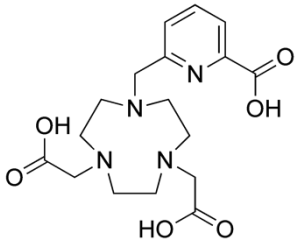
^{1}H NMR (500 MHz, MeOD) δ 7.96 (dd, *J* = 7.7, 1.2 Hz, 3H, Ar(Pa)), 7.92 (t, *J* = 7.7 Hz, 3H, Ar(Pa)), 7.59 (dd, *J* = 7.6, 1.3 Hz, 3H, Ar(Pa)), 4.42 (s, 6H, CH_2(Pa)), 3.48 (s, 12H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 167.4 (CO), 157.0 (*C*CH_2N), 148.9 (*C*COOH), 139.8 (Ar(Pa)), 128.1 (Ar(Pa)), 125.6 (Ar(Pa)), 61.4 (CH_2 Pa), 53.5 (tacn). ESI-HRMS (+ve ion): $[H_3\mathbf{L}^{003}+H]^+$ *m/z* = 535.2295 (experimental); 535.2300 (calculated). HPLC: R_t = 5.53 min (Method A). UV-vis: ε = 12674 $M^{-1}\cdot cm^{-1}$ at 268 nm.

2,2'-(7-(2-(benzyl(methyl)amino)-2-oxoethyl)-1,4,7-triazonane-1,4-diyl)diacetic acid, $H_2\mathbf{L}^{210}$:



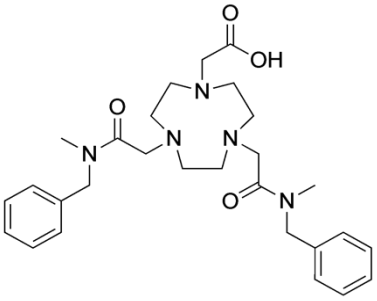
^{1}H NMR (500 MHz, MeOD) δ 7.41 – 7.26 (m, 5H, Ar(Bz)), 4.63 – 4.54 (m, 2H, CH_2(Bz)), 4.20 – 4.14 (m, 2H, CH_2 (Am)), 3.73 (s, 4H, CH_2(Ac)), 3.27 – 3.00 (m, 12H, tacn), 2.96 – 2.93 (m, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 173.6 (CO Ac), 173.5 (CO Ac), 169.3 (CO Am), 169.1 (CO Am), 138.0 (C(Bz)), 137.3 (C(Bz)), 130.1 (Ar(Bz)), 129.8 (Ar(Bz)), 129.1 (Ar(Bz)), 128.9 (Ar(Bz)), 128.6 (Ar(Bz)), 127.8 (Ar(Bz)), 56.6 (CH_2 (Am)), 56.5 (CH_2 (Am)), 56.0 (CH_2(Ac)), 53.3 (CH_2(Bz)), 52.5 (CH_2(Bz)), 52.4 (tacn), 52.1 (CH_2(Bz)), 51.1 (tacn), 49.6 (tacn), 34.4 (CH_3), 34.2 (CH_3). ESI-HRMS (+ve ion): $[H_2\mathbf{L}^{210}+H]^+$ *m/z* = 407.2285 (experimental); 407.2289 (calculated). HPLC: R_t = 6.85 min (Method A). UV-vis: ε = 299.7 $M^{-1}\cdot cm^{-1}$ at 257 nm.

2,2'-(7-((6-carboxypyridin-2-yl)methyl)-1,4,7-triazonane-1,4-diyl)diacetic acid, $H_3\mathbf{L}^{201}$:



^{1}H NMR (600 MHz, MeOD) δ 8.12 (dd, *J* = 7.6, 1.0 Hz, 1H, Ar(Pa)), 8.01 (t, *J* = 7.7 Hz, 1H, Ar(Pa)), 7.88 (dd, *J* = 7.8, 1.1 Hz, 1H, Ar(Pa)), 4.31 (s, 2H, CH_2(Pa)), 3.62 (s, 4H, CH_2(Ac)), 3.08 (d, *J* = 23.7 Hz, 12H, tacn). ^{13}C{^{1}H} NMR (151 MHz, MeOD) δ 173.5 (CO(Ac)), 167.9 (CO(Pa)), 157.5 (*C*CH_2N), 149.5 (*C*COOH(Pa)), 140.1 (Ar(Pa)), 128.9 (Ar(Pa)), 125.6 (Ar(Pa)), 61.1 (CH_2(Pa)), 56.8(Pa(Ac)), 51.3 (tacn), 51.1 (tacn), 51.0 (tacn). ESI-HRMS (+ve ion): $[H_3\mathbf{L}^{201}+H]^+$ *m/z* = 381.1766 (experimental); 381.1769 (calculated). HPLC: R_t = 3.23 min (Method A). UV-vis: ε = 5526 $M^{-1}\cdot cm^{-1}$ at 271 nm.

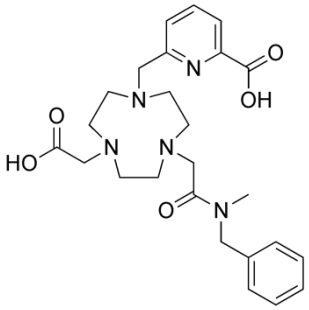
2-(4,7-bis(2-(benzyl(methyl)amino)-2-oxoethyl)-1,4,7-triazonan-1-yl)acetic acid, $H\mathbf{L}^{120}$:



^{1}H NMR (600 MHz, MeOD) δ 7.39 – 7.23 (m, 10H, Ar(Bz)), 4.67 – 4.53 (m, 4H, CH_2(Bz)), 4.13 – 4.02 (m, 4H, CH_2 (Am)), 3.73 – 3.64 (m, 2H, CH_2(Ac)), 3.16 (s, 12H, tacn), 2.95 – 2.91 (m, 6H, CH_3). ^{13}C{^{1}H} NMR (151 MHz, MeOD) δ 174.1 (CO(Ac)), 174.0 (CO(Ac)), 170.5 (CO (Am)), 170.3 (CO (Am)), 170.1 (CO (Am)), 169.9 (CO (Am)), 138.1 (C(Bz)), 137.5 (C(Bz)), 130.1 (Ar(Bz)), 130.1 (Ar(Bz)), 129.7 (Ar(Bz)), 129.0 (Ar(Bz)), 128.9 (Ar(Bz)), 128.8 (Ar(Bz)), 128.6 (Ar(Bz)), 127.8 (Ar(Bz)), 56.6 (CH_2 (Am)), 56.4 (CH_2 (Am)), 56.3 (CH_2(Ac)), 56.2 (CH_2(Ac)), 53.3 (CH_2(Bz)),

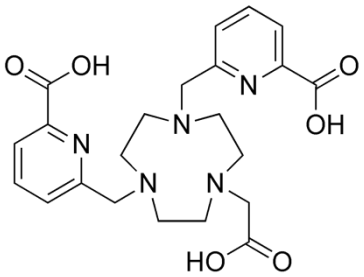
52.5 (tacn), 52.3 (tacn), 52.0 (CH_2(Bz)), 51.4 (tacn), 51.1 (tacn), 50.2 (tacn), 50.0 (tacn), 34.4, (CH_3) 34.3 (CH_3), 34.2 (CH_3). ESI-HRMS (+ve ion): [H**L**^{120}+H]$^+$ *m/z* = 510.3071 (experimental); 510.3075 (calculated). HPLC: R_t = 8.57 min (Method A). UV-vis: ε = 489.9 $M^{-1}\cdot cm^{-1}$ at 258 nm.

*6-((4-(2-(benzyl(methyl)amino)-2-oxoethyl)-7-(carboxymethyl)-1,4,7-triazonan-1-yl)methyl)picolinic acid, H_2**L**^{111}*:



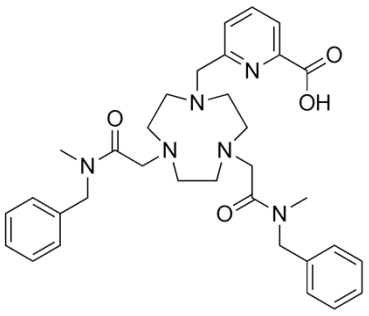
^{1}H NMR (500 MHz, MeOD) δ 8.10 (t, *J* = 7.2 Hz, 1H, Ar(Pa)), 8.00 – 7.91 (m, 1H, Ar(Pa)), 7.85 – 7.78 (m, 1H, Ar(Pa)), 7.40 – 7.17 (m, 5H, Ar(Bz)), 4.63 – 4.49 (m, 2H, CH_2(Bz)), 4.40 – 4.35 (m, 2H, CH_2(Pa)), 4.18 – 3.95 (m, 2H, CH_2 (Am)), 3.75 – 3.61 (m, 2H, CH_2(Ac)), 3.39 – 3.04 (m, 12H, tacn), 2.94 – 2.90 (m, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 173.4 (CO Ac), 173.3 (CO Ac), 170.2 (CO Am), 169.6 (CO Am), 167.6 (CO Pa), 167.4 (CO Pa), 157.4 (*C*CH_2N), 157.1 (*C*CH_2N), 149.0 (*C*COOH Pa), 148.9 (*C*COOH Pa), 140.1 (Ar(Pa)), 140.0 (Ar(Pa)), 138.0 (C Bz), 137.4 (C Bz), 130.1 (Ar(Bz)), 129.8 (Ar(Bz)), 129.0 (Ar(Bz)), 128.9 (Ar(Bz)), 128.8 (Ar(Pa)), 128.6 (Ar(Pa)), 127.7 (Ar(Bz)), 125.7 (Ar(Pa)), 60.8 (CH_2(Pa)), 57.4 (CH_2 (Am)), 56.7 (CH_2 (Am)), 56.5 (CH_2(Ac)), 56.3 (CH_2(Ac)), 53.3 (CH_2(Bz)), 53.0 (CH_2(Bz)), 52.5 (tacn), 52.4 (tacn), 52.3 (tacn), 52.1 (tacn), 51.8 (tacn), 51.4 (tacn), 51.2 (tacn), 50.9 (tacn), 50.8 (tacn), 34.5 (CH_3), 34.3 (CH_3). ESI-HRMS (+ve ion): [H_2**L**^{111}+H]$^+$ *m/z* = 484.2554 (experimental); 484.2554 (calculated). HPLC: R_t = 6.87 min (Method A). UV-vis: ε = 8360 $M^{-1}\cdot cm^{-1}$ at 271 nm.

*6,6'-((7-(carboxymethyl)-1,4,7-triazonane-1,4-diyl)bis(methylene))dipicolinic acid, H_3**L**^{102}*:



^{1}H NMR (500 MHz, MeOD) δ 8.05 (dd, *J* = 7.8, 1.1 Hz, 2H, Ar(Pa)), 7.96 (t, *J* = 7.7 Hz, 2H, Ar(Pa)), 7.70 (dd, *J* = 7.8, 1.1 Hz, 2H, Ar(Pa)), 4.40 (s, 4H, CH_2(Pa)), 3.62 (s, 2H, CH_2(Ac)), 3.38 – 3.09 (m, 12H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 173.6 (CO(Ac)), 167.5 (CO(Pa)), 156.7 (C(Pa)), 149.1 (*C*CH_2N), 139.9 (Ar(Pa)), 128.5 (Ar(Pa)), 125.7 (Ar(Pa)), 61.0 (CH_2(Pa)), 56.8 (CH_2(Ac)), 53.1 (tacn), 52.1 (tacn), 51.4 (tacn). ESI-HRMS (+ve ion): [H_3**L**^{102}+H]$^+$ *m/z* = 458.2032 (experimental); 458.2034 (calculated). HPLC: R_t = 5.05 min (Method A). UV-vis: ε = 8056 $M^{-1}\cdot cm^{-1}$ at 269 nm.

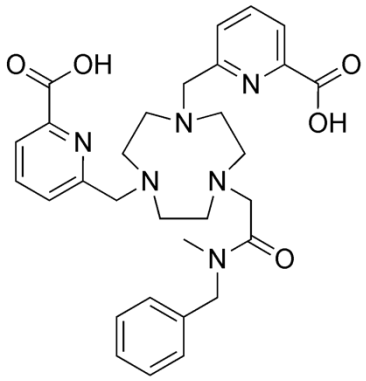
*6-((4,7-bis(2-(benzyl(methyl)amino)-2-oxoethyl)-1,4,7-triazonan-1-yl)methyl)picolinic acid, H**L**^{021}*:



^{1}H NMR (500 MHz, MeOD) δ 8.15 – 7.05 (m, 1H, Ar(Pa)), 8.02 – 7.90 (m, 1H, Ar(Pa)), 7.81 – 7.71 (m, 1H, Ar(Pa)), 7.39 – 7.14 (m, 10H, Ar(Bz)), 4.63 – 4.49 (m, 4H, CH_2(Bz)), 4.49 – 4.41 (m, 2H, CH_2(Pa)), 4.35 – 4.23 (m, 4H, CH_2 (Am)), 3.84 – 3.25 (m, 12H, tacn), 2.96 – 2.88 (m, 6H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 169.9 (CO (Am)), 169.0 (CO (Am)), 168.8 (CO (Am)), 167.7 (CO(Pa)), 167.5 (CO(Pa)), 157.3 (C(Pa)), 148.6 (*C*CH_2N), 148.4 (*C*CH_2N), 140.3 (Ar(Pa)), 137.8 (C(Bz)), 137.7 (C(Bz)), 137.1 (C(Bz)), 130.4 (Ar(Bz)), 130.1 (Ar(Bz)), 130.0 (Ar(Bz)), 129.7 (Ar(Bz)), 129.1 (Ar(Bz)), 129.0 (Ar(Bz)), 128.8 (Ar(Bz)), 128.7 (Ar(Bz)), 128.6 (Ar(Bz)), 128.5 (Ar(Bz)), 128.3 (Ar(Pa)), 127.8 (Ar(Bz)), 125.8

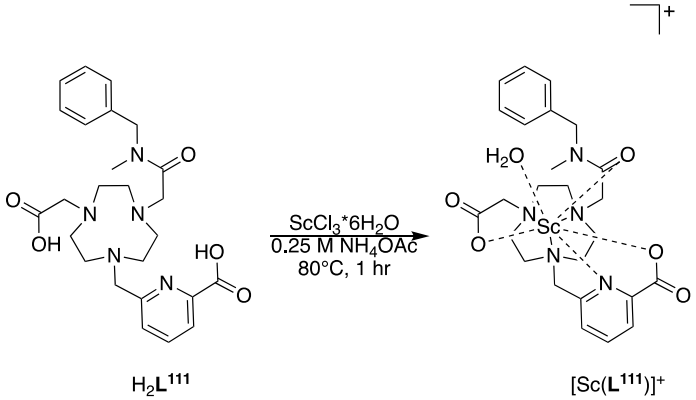
(Ar(Pa)), 61.3 (CH_2(Pa)), 60.9 (CH_2(Pa)), 60.6 (CH_2(Pa)), 58.8 (CH_2 (Am)), 58.4 (CH_2 (Am)), 58.0 (CH_2 (Am)), 53.6 (CH_2(Bz)), 53.3 (CH_2(Bz)), 53.0 (tacn), 52.7 (tacn), 52.2 (tacn), 52.0 (CH_2(Bz)), 51.9 (CH_2(Bz)), 51.7 (CH_2(Bz)), 34.4 (CH_3), 34.3 (CH_3) 33.4 (CH_3). ESI-HRMS (+ve ion): $[H\mathbf{L}^{021}+H]^+$ *m/z* = 587.3339 (experimental); 587.3340 (calculated). HPLC: R_t = 8.27 min (Method A). UV-vis: ε = 4174 $M^{-1}\cdot cm^{-1}$ at 268 nm.

6,6'-((7-(2-(benzyl(methyl)amino)-2-oxoethyl)-1,4,7-triazonane-1,4-diyl)bis(methylene))dipicolinic acid, $H_2\mathbf{L}^{012}$:



^{1}H NMR (500 MHz, MeOD) δ 8.03 – 7.97 (m, 2H, Ar(Pa)), 7.95 – 7.87 (m, 2H, Ar(Pa)), 7.72 – 7.63 (m, 2H, Ar(Pa)), 7.39 – 7.09 (m, 5H, Ar(Bz)), 4.51 – 4.42 (m, 2H, CH_2(Bz)), 4.50 – 4.38 (m, 4H, CH_2(Pa)), 4.19 – 3.94 (m, 2H, CH_2 (Am)), 3.71 – 3.20 (m, 12H, tacn), 2.94 – 2.82 (m, 3H, CH_3). $^{13}C\{^1H\}$ NMR (126 MHz, MeOD) δ 170.1 (CO (Am)), 169.4 (CO (Am)), 167.4 (CO(Pa)), 157.0 (C(Pa)), 156.8 (C(Pa)), 148.8 (*C*CH_2N), 148.6 (*C*CH_2N), 139.9 (Ar(Pa)), 137.8 (C(Bz)), 137.3 (C(Bz)), 130.1 (Ar(Bz)), 129.7 (Ar(Bz)), 128.9 (Ar(Bz)), 128.6 (Ar(Bz)), 128.5 (Ar(Bz)), 128.2 (Ar(Pa)), 127.6 (Ar(Bz)), 125.7 (Ar(Pa)), 61.2 (CH_2(Pa)), 58.4 (CH_2 (Am)), 57.5 (CH_2 (Am)), 53.3 (CH_2(Bz)), 53.2 (CH_2(Bz)), 52.8 (tacn), 52.7 (tacn), 52.4 (tacn), 52.2 (CH_2(Bz)), 34.4 (CH_3), 34.3 (CH_3). ESI-HRMS (+ve ion): $[H_2\mathbf{L}^{012}+H]^+$ *m/z* = 561.2817 (experimental); 561.2820 (calculated). HPLC: R_t = 6.90 min (Method A). UV-vis: ε = 13511 $M^{-1}\cdot cm^{-1}$ at 268 nm.

1.3 Synthesis and characterization of coordination complexes

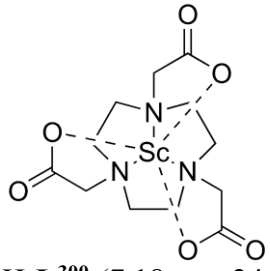


Scheme S3: General scandium complexation procedure.

1.3.1 General Scandium Complexation Procedure

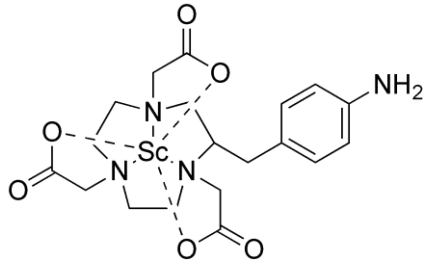
To a solution of ligand in ammonium acetate (0.25 M, pH 4.5, 5-10 mL) was added scandium(III) chloride hexahydrate and the reaction mixture was heated to 80 °C for 1 hour, then checked via LCMS to ensure complete complexation. The scandium complexes were isolated and analyzed as crude product.

*[Sc(**L**^{300})]*



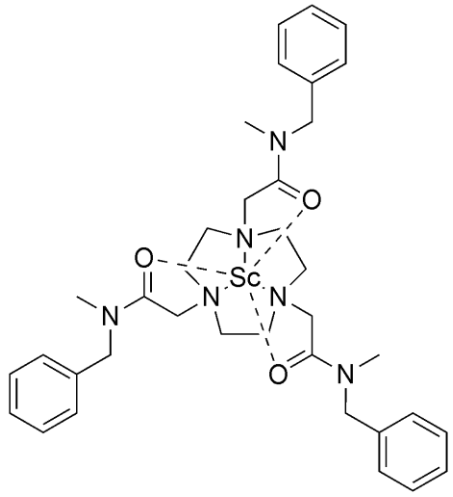
H_3**L**^{300} (7.18 mg, 24.1 μmol, 1 equiv.); scandium(III) chloride hexahydrate (6.25 mg, 24.1 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 3.77 (d, *J* = 15.9 Hz, 2H, Ac(CH_2)), 3.70 (s, 2H, Ac(CH_2)), 3.35 (d, *J* = 15.7 Hz, 2H, Ac(CH_2)), 3.25 – 2.95 (m, 12H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 66.6(Ac(CH_2)), 65.6(Ac(CH_2)), 56.1 (tacn), 54.5 (tacn). ^{45}Sc NMR (122 MHz, MeOD) δ 102.9. ^{45}Sc NMR (122 MHz, D_2O) δ 101.5. ESI-HRMS (+ve ion): [Sc(**L**^{300})+H]$^{+}$ *m/z* = 346.0830 (experimental); 346.0827 (calculated). HPLC: R_t = 2.93 min (Method B).

*[Sc(**L**$^{300\text{-}BzNH2}$)]*



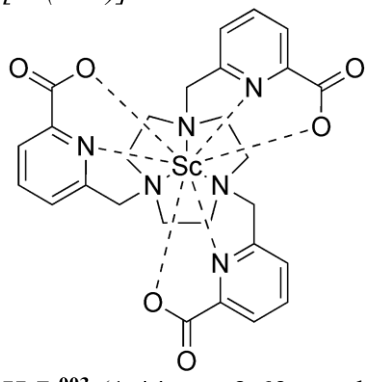
H_3**L**$^{300\text{-}BzNH2}$ (51.7 mg, 100 μmol, 1 equiv.); scandium(III) chloride hexahydrate (25.9 mg, 100 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 7.63 – 7.21 (m, 7H, Ar(Bz) + NH_3^+), 4.59 – 2.58 (m, 19H, CH_2 Bz) + CH_2(Ac) + tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 190.1, 182.6, 181.6, 179.8, 139.4 (CNH2), 131.9 (Ar(Bz)), 130.7 (CH_2(Bz)), 124.4 (Ar(Bz)), 68.0 (CH_2), 66.6 (CH_2), 65.3 (CH_2), 63.8 (CH_2), 58.6 (CH_2), 57.2 (CH_2), 57.0 (CH_2), 55.7 (CH_2), 51.7 (CH_2), 51.6 (CH_2), 51.4 (CH_2), 51.2 (CH_2), 51.0 (CH_2), 32.5 (CH_2(Bz)). ^{45}Sc NMR (122 MHz, MeOD) δ 95.0. ^{45}Sc NMR (122 MHz, D_2O) δ 91.7. ESI-HRMS (+ve ion): [Sc(**L**$^{300\text{-}BzNH2}$)+H]$^+$ *m/z* = 451.1407 (experimental); 451.1406 (calculated). HPLC: R_t = 1.51 min (Method B).

*[Sc(**L**^{030})]$^{3+}$*



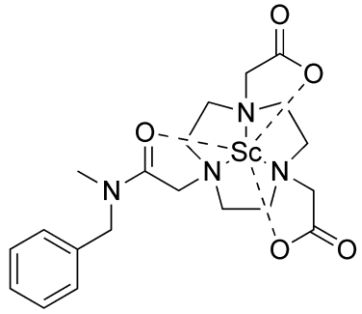
L^{030} (11.6 mg, 19.0 μmol, 1 equiv.); scandium(III) chloride hexahydrate (4.93 mg, 19.0 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 7.52 – 7.02 (m, 15H, Ar(Bz)), 5.01 – 4.09 (m, 12H, CH_2(Bz) & CH_2 (Am)), 3.87 – 3.64 (m, 4H, CH_2(Ac)), 3.50 – 3.11 (m, 12H, tacn), 3.12 – 2.88 (m, 9H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 178.2 (CO), 176.3 (CO), 130.4 (CH(Bz)), 130.1 (CH(Bz)), 129.8 (CH(Bz)), 129.6 (CH(Bz)), 128.5 (CH(Bz)), 128.3 (CH(Bz)), 56.7 (tacn), 55.2 (tacn), 53.4 (CH_2(Bz)), 35.7 (CH_3). ^{45}Sc NMR (122 MHz, MeOD) δ 98.9. ^{45}Sc NMR (122 MHz, D_2O) δ 100.9. ESI-HRMS (+ve ion): [Sc(**L**^{030})+HCOO]$^{2+}$ *m/z* = 351.1662 (experimental); 351.1657 (calculated). HPLC: R_t = 12.13 min (Method B).

*[Sc(**L**^{003})]*



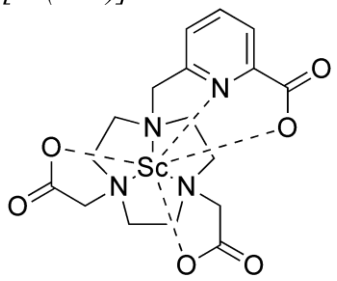
H_3**L**^{003} (1.44 mg, 2.69 μmol, 1 equiv.); scandium(III) chloride hexahydrate (0.70 mg, 2.69 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.13 (t, *J* = 7.7 Hz, 3H, Ar(Pa)), 8.01 (d, *J* = 7.6 Hz, 3H, Ar(Pa)), 7.67 (d, *J* = 7.7 Hz, 3H, Ar(Pa)), 4.04 (dd, *J* = 37.2, 14.2 Hz, 6H, CH_2(Pa)), 3.67 – 3.52 (m, 3H, tacn), 2.80 (dd, *J* = 16.1, 5.9 Hz, 3H, tacn), 2.54 (dd, *J* = 12.5, 5.2 Hz, 3H, tacn), 2.15 (td, *J* = 13.2, 5.9 Hz, 4H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 169.4 (COOSc), 156.1 (CCH_2N), 150.7 (*C*COOSc), 141.9 (CH(Pa)), 126.4 (CH(Pa)), 124.3 (CH(Pa)), 66.6 (CH_2(Pa)), 59.0 (tacn), 57.6 (tacn). ^{45}Sc NMR (122 MHz, MeOD) δ 39.9. ^{45}Sc NMR (122 MHz, D_2O) δ 45.6. ESI-HRMS (+ve ion): [Sc(**L**^{003})+H]$^+$ *m/z* = 577.1623 (experimental); 577.1624 (calculated). HPLC: R_t = 7.35 min (Method B). Crystals suitable for single crystal X-ray diffraction were grown from slow evaporation of the aqueous reaction solution (CCDC: 2369298).

*[Sc(**L**^{210})]$^+$*



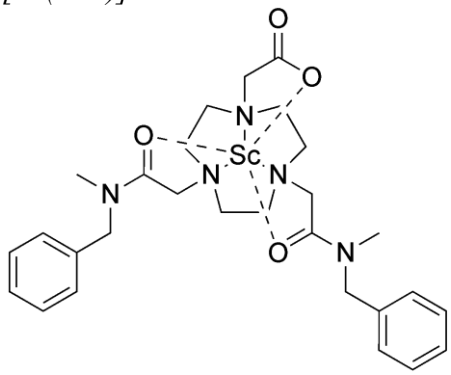
H_2**L**^{210} (7.73 mg, 19.0 μmol, 1 equiv.); scandium(III) chloride hexahydrate (4.93 mg, 19.0 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 7.49 – 7.23 (m, 5H, Ar(Bz)), 4.94 – 4.41 (m, 2H, CH_2(Bz)), 4.13 – 4.06 (m, 2H, CH_2 (Am)), 3.87 – 3.64 (m, 4H, CH_2(Ac)), 3.41 – 2.91 (m, 12H, tacn), 3.06 (d, *J* = 16.3 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 179.1 (CO(Ac)), 176.1 (CO(Am)), 136.5 (C(Bz)), 130.3 (CH(Bz)), 130.0 (CH(Bz)), 129.7 (CH(Bz)), 129.3 (CH(Bz)), 128.3 (CH(Bz)), 66.7 (CH_2(Ac)), 62.9 (CH_2 (Am)), 56.1 (tacn), 55.1 (tacn), 54.5 (CH_2(Bz)), 53.2 (CH_2(Bz)), 35.6 (CH_3). ^{45}Sc NMR (122 MHz, MeOD) δ 100.5. ^{45}Sc NMR (122 MHz, D_2O) δ 101.0. ESI-HRMS (+ve ion): [Sc(**L**^{210})]$^+$ *m/z* = 449.1610 (experimental); 449.1613 (calculated). HPLC: R_t = 8.63 min (Method B).

*[Sc(**L**^{201})]*



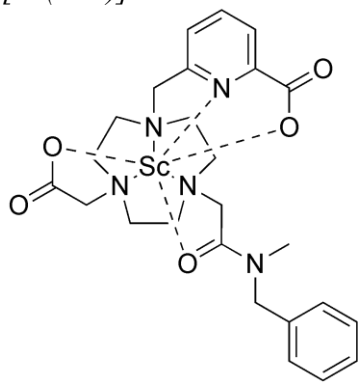
H_3**L**^{201} (9.9 mg, 26 μmol, 1 equiv.); scandium(III) chloride hexahydrate (6.8 mg, 26 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.12 (t, *J* = 7.7 Hz, 1H, Ar(Pa)), 8.03 (dd, *J* = 7.6, 1.2 Hz, 1H, Ar(Pa)), 7.61 (dd, *J* = 7.7, 1.2 Hz, 1H, Ar(Pa)), 4.38 (s, 2H, CH_2 Pa), 4.01 (d, *J* = 15.3 Hz, 2H, CH_2 Ac a), 3.28* (d, 2H, CH_2 Ac a), 3.27 – 2.96 (m, 12H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 180.2 (CO(Ac)), 172.1 (CO(Pa)), 157.7 (CH_2*C*(Pa)), 153.0 (*C*CO(Pa)), 142.4 (Ar(Pa)), 125.2 (Ar(Pa)), 124.2 (Ar(Pa)), 67.2 (CH_2(Ac)), 65.4 (CH_2(Pa)), 56.7 (tacn), 55.4 (tacn), 54.9 (tacn). *Overlapping residual solvent peak confirmed by ^{1}H-^{1}H COSY NMR. ^{45}Sc NMR (122 MHz, MeOD) δ 67.8. ^{45}Sc NMR (122 MHz, D_2O) δ 84.8, 69.8. ESI-HRMS (+ve ion): [Sc(**L**^{201})+H]$^+$ *m/z* = 423.1097 (experimental); 423.1093 (calculated). HPLC: R_t = 5.85 min (Method B).

*[Sc(**L**^{120})]$^{2+}$*



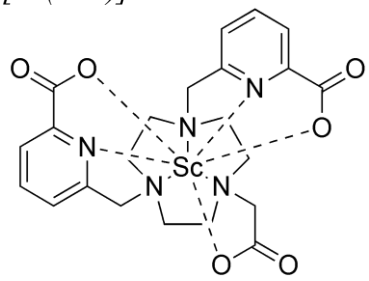
H**L**^{120} (2.58 mg, 5.06 μmol, 1 equiv.); scandium(III) chloride hexahydrate (1.31 mg, 5.06 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 7.56 – 7.08 (m, 10H, Ar(Bz)), 5.21 – 3.58 (m, 10H, CH_2(Bz) & CH_2 (Am) & CH_2(Ac)), 3.47 – 3.11 (m, 12H, tacn), 3.10 – 3.04 (m, 6H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 178.7 (CO(Ac)), 178.3 (CO(Ac)), 176.4 (CO(Am)), 176.0 (CO(Am)), 136.3 (C(Bz)), 130.9 (Ar(Bz)), 130.7 (Ar(Bz)), 130.5 (Ar(Bz)), 130.3 (Ar(Bz)), 130.0 (Ar(Bz)), 129.7 (Ar(Bz)), 129.6 (Ar(Bz)), 129.4 (Ar(Bz)), 128.5 (Ar(Bz)), 128.2 (Ar(Bz)), 127.8 (Ar(Bz)), 65.7 (CH_2(Ac)), 63.7 (CH_2 (Am)), 62.8 (CH_2 (Am)), 56.6 (tacn), 56.4 (tacn), 55.3 (tacn), 54.4 (CH_2(Bz)), 54.1 (CH_2(Bz)), 53.6 (CH_2(Bz)), 53.2 (CH_2(Bz)), 35.3 (CH_3 (Am)), 33.1 (CH_3 (Am)), 32.7 (CH_3 (Am)). ^{45}Sc NMR (122 MHz, MeOD) δ 97.8, 70.7. ^{45}Sc NMR (122 MHz, D_2O) δ 101.1. ESI-HRMS (+ve ion): [Sc(**L**^{120})+OAc]$^+$ *m/z* = 612.2621 (experimental); 612.2610 (calculated). HPLC: R_t = 11.58 min (Method B).

*[Sc(**L**^{111})]$^{+}$*



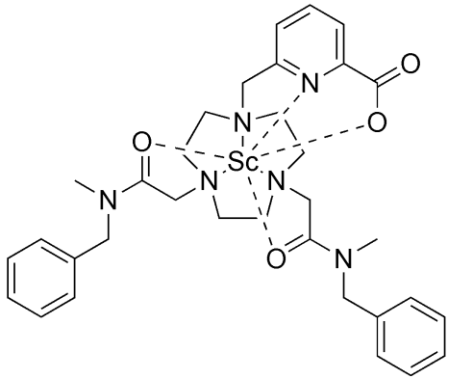
H_2**L**^{111} (5.00 mg, 10.3 μmol, 1 equiv.); scandium(III) chloride hexahydrate (2.68 mg, 10.3 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.18 – 8.08 (m, 1H, Ar(Pa)), 8.07 – 7.98 (m, 1H, Ar(Pa)), 7.68 – 7.62 (m, 1H, Ar(Pa)), 7.41 – 6.98 (m, 5H, Ar(Bz)), 4.66 – 3.98 (m, 8H, CH_2(Pa) & CH_2(Bz) & CH_2 (Am) & CH_2(Ac)), 3.58 – 3.32 (m, 12H, tacn), 3.03 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 179.86, 179.68, 176.66, 176.38, 176.24, 171.49, 157.81, 153.27, 142.71, 142.66, 136.57, 135.93, 130.24, 129.82, 129.29, 128.42, 128.08, 125.31, 124.03, 123.90, 121.73, 119.40, 117.07, 114.75, 74.24, 66.53, 66.38, 65.24, 64.85, 64.64, 57.06, 56.68, 56.45, 56.29, 56.23, 56.06, 54.59, 54.37, 54.28, 54.06, 53.77, 53.55, 53.27, 35.59, 34.90. ^{45}Sc NMR (122 MHz, MeOD) δ 68.5. ^{45}Sc NMR (122 MHz, D_2O) δ 87.0, 71.0. ESI-HRMS (+ve ion): [Sc(**L**^{111})]$^{+}$ *m/z* = 526.1889 (experimental); 526.1879 (calculated). HPLC: R_t = 7.95 min (Method B).

*[Sc(**L**^{102})]*



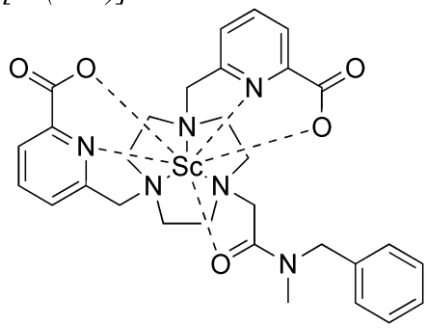
H_3**L**^{102} (5.76 mg, 12.6 μmol, 1 equiv.); scandium(III) chloride hexahydrate (3.27 mg, 12.6 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.33 – 7.48 (m, 6H, Ar(Pa)), 4.74 (d, J = 15.7 Hz, 1H, CH_2(Pa)), 4.33 (dd, J = 14.9, 10.3 Hz, 2H, CH_2(Pa)), 4.11 (d, J = 14.0 Hz, 1H, CH_2(Pa)), 4.03 (d, J = 15.9 Hz, 1H, CH_2(Ac)), 3.64 – 2.74 (m, 12H, tacn), 3.48 (d, J = 15.8 Hz, 1H, CH_2(Ac)). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 176.5 (CO(Ac)), 172.6 (CO(Pa)), 171.4 (CO(Pa)), 158.0 (CH_2*C*(Pa)), 155.8 (*C*CO(Pa)), 154.3 (*C*CO(Pa)), 151.7 (Ar(Pa)), 144.2 (Ar(Pa)), 138.7 (Ar(Pa)), 128.2 (Ar(Pa)), 126.9 (Ar(Pa)), 124.5 (Ar(Pa)), 123.9 (Ar(Pa)), 66.6 (CH_2(Ac)), 65.2 (CH_2(Pa)), 63.3 (CH_2(Pa)), 55.7 (tacn), 55.5 (tacn), 54.8 (tacn), 54.6 (tacn), 52.2 (tacn). ^{45}Sc NMR (122 MHz, MeOD) δ 129.6. ^{45}Sc NMR (122 MHz, D_2O) δ 131.8. ESI-HRMS (+ve ion): [Sc(**L**^{102})+H]$^+$ *m/z* = 500.1355 (experimental); 500.1358 (calculated). HPLC: R_t = 6.95 min (Method B).

*[Sc(**L**^{021})]*$^{2+}$

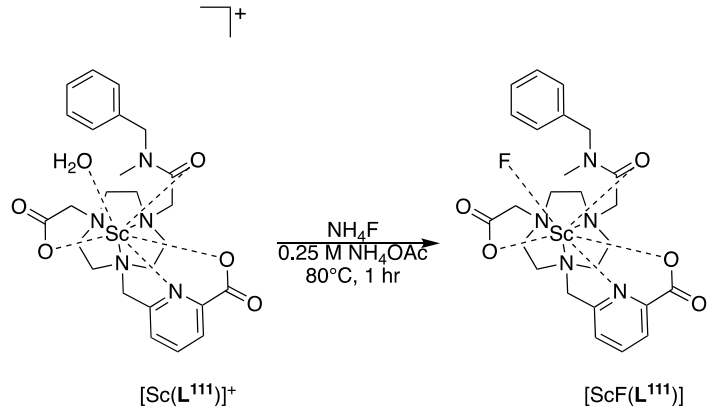


H**L**^{021} (50.0 mg, 85.2 μmol, 1 equiv.); scandium(III) chloride hexahydrate (22.1 mg, 85.2 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.24 – 8.11 (m, 1H, Ar(Pa)), 8.10 – 7.98 (m, 1H, Ar(Pa)), 7.75 – 7.62 (m, 1H, Ar(Pa)), 7.44 – 7.11 (m, 10H, Ar(Bz)), 4.78 – 4.02 (m, 10H, CH_2(Pa + Am + Bz)), 3.08 – 2.97 (m, 6H, CH_3), 3.55 – 2.65 (m, 12H, tacn), 1.98 (s, 6H, OAc- counter anion). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 179.3, 176.7, 176.6, 176.5, 176.4, 176.3, 176.2, 171.3, 170.9, 157.9, 153.4, 153.2, 143.3, 143.1, 136.9, 136.3, 136.1, 135.7, 135.5, 130.4, 130.2, 129.9, 129.8, 129.7, 129.4, 129.1, 129.1, 128.8, 128.5, 128.4, 128.0, 127.8, 125.4, 124.3, 124.2, 124.1, 65.5, 65.3, 64.6, 64.3, 64.2, 64.1, 63.9, 63.8, 57.2, 57.1, 56.8, 56.7, 56.6, 56.0, 55.8, 55.5, 55.4, 55.2, 55.1, 55.0, 54.7, 54.4, 53.8, 53.6, 52.8, 52.1, 35.5, 35.4, 35.2, 25.3, 25.2, 21.3. ^{45}Sc NMR (122 MHz, MeOD) δ 76.2, 69.1. ^{45}Sc NMR (122 MHz, D_2O) δ 87.5, 71.8. ESI-HRMS (+ve ion): [Sc(**L**^{021})]$^{2+}$ *m/z* = 315.1363 (experimental); 315.1369 (calculated). HPLC: R_t = 9.30 min (Method B).

*[Sc(**L**^{012})]$^{+}$*



H_2**L**^{012} (10.6 mg, 19.0 μmol, 1 equiv.); scandium(III) chloride hexahydrate (4.93 mg, 19.0 μmol, 1 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.20 – 7.53 (m, 6H, Ar(Pa)), 7.40 – 7.09 (m, 5H, Ar(Bz)), 4.66 – 3.59 (m, 10H, CH_2(Pa) + CH_2Bz) + CH_2 (Am)), 3.60 – 2.62 (m, 12H, Ar(Pa)), 3.00 – 2.90 (m, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 172.3 (CO (Am)), 171.4 (CO (Am)), 163.2 (CO (Am)), 162.9 (CO (Am)), 156.6 (CH_2*C*(Pa)), 152.5 (*C*CO(Pa)), 143.1 (Ar(Pa)), 142.6 (Ar(Pa)), 139.2 (C(Bz)), 130.1 (Ar(Bz)), 129.8 (Ar(Bz)), 129.7 (Ar(Bz)), 129.1 (Ar(Bz)), 128.9 (Ar(Bz)), 128.7 (Ar(Bz)), 128.5 (Ar(Bz)), 128.4 (Ar(Bz)), 127.6 (Ar(Bz)), 127.1 (Ar(Bz)), 126.2 (Ar(Pa)), 126.1 (Ar(Pa)), 124.7 (Ar(Pa)), 124.3 (Ar(Pa)), 123.7 (Ar(Pa)), 67.0 (CH_2(Pa)), 66.6 (CH_2(Pa)), 66.0 (CH_2(Pa)), 65.0 (CH_2 (Am)), 62.0 (CH_2(Pa)), 58.7 (tacn), 57.3 (CH_2(Bz)), 56.8 (tacn), 54.9 (tacn), 52.3 (tacn), 51.9 (tacn), 35.1 (CH_3(Am)), 34.7 (CH_3(Am)). ^{45}Sc NMR (122 MHz, MeOD) δ 127.4, 73.3, 60.5, 43.4. ^{45}Sc NMR (122 MHz, D_2O) δ 141.1, 81.0. ESI-HRMS (+ve ion): [Sc(**L**^{012})]$^{+}$ *m/z* = 603.2144 (experimental); 603.2144 (calculated). HPLC: R_t = 8.8 min (Method B).

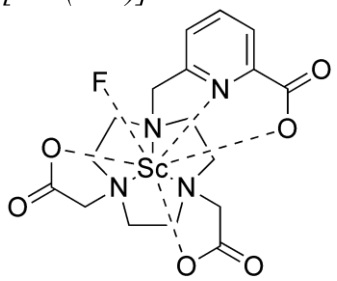


Scheme S4: General fluorination procedure.

1.3.2 General Fluorination Procedure

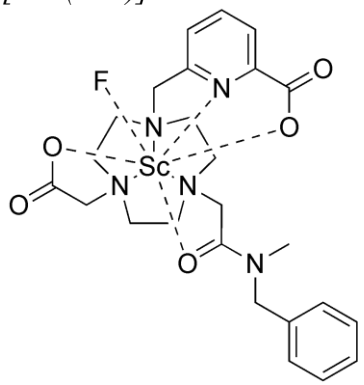
To a solution of complex in ammonium acetate (0.25 M, pH 4.5, 4 mL) was added cesium fluoride or ammonium fluoride and the reaction mixture was heated to 100 °C for 1 hour, then checked via LCMS to ensure complete fluorination. The scandium-fluoride ternary complexes were lyophilised and redissolved in acetonitrile to remove excess ammonium acetate and were used without further purification.

*[ScF(**L**^{201})]$^{-}$*



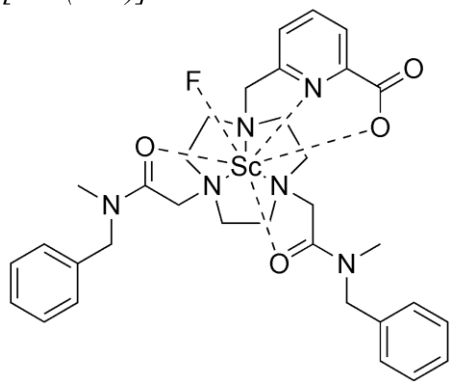
[Sc(**L**^{201})] (17.6 mg, 41.7 μmol, 1 equiv.); ammonium fluoride (7.73 mg, 209 μmol, 5 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.14 – 8.07 (m, 1H, Ar(Pa)), 8.05 – 7.99 (m, 1H, Ar(Pa)), 7.63 – 7.55 (m, 1H, Ar(Pa)), 4.38 (s, 1H, CH_2(Pa)), 4.35 (s, 1H, CH_2(Pa)), 4.01 (d, J = 15.3 Hz, 1H, CH_2(Ac)), 3.89 (d, J = 15.1 Hz, 1H, CH_2(Ac)), 3.26 (d, J = 16.2 Hz, 2H, CH_2(Ac)), 3.29 – 2.91 (m, 12H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 13C NMR (126 MHz, MeOD) δ 180.2(CO(Ac)), 179.9 (CO(Ac)), 179.3 (CO(Ac)), 172.0 (CO(Pa)), 171.8 (CO(Pa)), 157.6 (CH_2*C*(Pa)), 153.2 (*C*CO(Pa)), 153.1 (*C*CO(Pa)), 142.3 (Ar(Pa)), 142.0 (Ar(Pa)), 125.2 (Ar(Pa)), 125.1 (Ar(Pa)), 124.1 (Ar(Pa)), 67.2 (CH_2(Ac)), 66.3 (CH_2(Ac)), 65.3 (CH_2(Pa)), 56.7 (tacn), 55.8 (tacn), 55.4 (tacn), 54.9 (tacn), 54.6 (tacn), 45.0 (tacn). ^{45}Sc NMR (122 MHz, MeOD) δ 67.0. ^{45}Sc NMR (122 MHz, D_2O) δ 85.6. ^{19}F NMR (564 MHz, MeOD) δ -9.23. ESI-HRMS (+ve ion): [ScF(**L**^{201})+2H]$^{+}$ *m/z* = 443.1160 (experimental); 443.1155 (calculated). HPLC: R_t = 1.33 min (Method A).

*[ScF(**L**^{111})]*



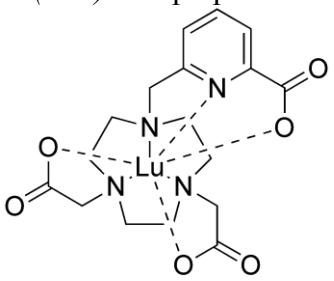
[Sc(**L**^{111})]$^{+}$ (5.27 mg, 10.0 μmol, 1 equiv.); ammonium fluoride (1.85 mg, 50.0 μmol, 5 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.13 (t, J = 7.7 Hz, 0.8H, Ar(Pa)), 8.03 (t, J = 7.2 Hz, 0.8H, Ar(Pa)), 7.64 (d, J = 7.8 Hz, 0.8H, Ar(Pa)), 7.39 (t, J = 7.5 Hz, 0.2H, Ar(Pa)), 7.33 (t, J = 7.5 Hz, 0.2H, Ar(Pa)), 7.24 (d, J = 7.0 Hz, 0.2H, Ar(Pa)), 7.36 – 7.18 (m, 3.5H, Ar(Bz)), 6.99 – 6.92 (m, 1.5H, Ar(Bz)), 4.74 – 3.89 (m, 8H, CH_2(Ac) + CH_2(Pa) + CH_2 (Am) + CH_2(Bz)), 3.59 – 2.66 (m, 12H, tacn), 3.07 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 179.7, 176.1, 175.8, 171.5, 157.8, 153.2, 142.6, 136.6, 136.0, 130.2, 129.8, 129.3, 129.0, 128.1, 125.5, 124.1, 123.9, 65.7, 65.4, 65.1, 63.8, 56.5, 56.3, 56.2, 55.7, 55.3, 54.7, 54.3, 53.9, 53.7, 53.3, 36.0, 35.1. ^{45}Sc NMR (122 MHz, MeOD) δ 67.8. ^{45}Sc NMR (122 MHz, D_2O) δ 68.3. ^{19}F NMR (564 MHz, MeOD) δ -5.65. ESI-HRMS (+ve ion): [ScF(**L**^{111})+H]$^{+}$ *m/z* = 546.1951 (experimental); 546.1941 (calculated). HPLC: R_t = 8.27 min (Method B).

*[ScF(**L**^{021})]*$^{+}$

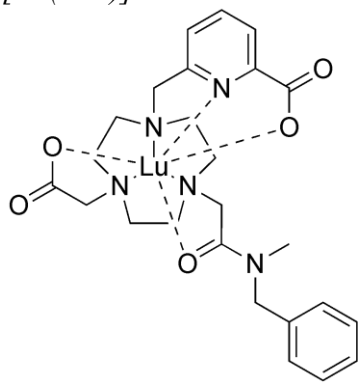


[Sc(**L**^{021})]$^{2+}$ (24.3 mg, 38.6 μmol, 1 equiv.); caesium fluoride (2.93 mg, 193 μmol, 5 equiv.). ^{1}H NMR (500 MHz, MeOD) δ 8.24 – 8.14 (m, 1H, Ar(Pa)), 8.11 – 8.02 (m, 1H, Ar(Pa)), 7.73 – 7.63 (m, 1H, Ar(Pa)), 7.42 – 7.11 (m, 10H, Ar(Bz)), 4.76 – 4.01 (m, 10H, Ar(Pa)), 3.11 – 3.00 (m, 6H, CH_3), 3.60 – 2.78 (m, 12H, tacn). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 176.31, 176.24, 176.12, 171.63, 163.06, 162.79, 158.03, 157.82, 153.48, 143.36, 136.43, 136.22, 136.11, 135.52, 130.85, 130.33, 130.27, 130.20, 129.95, 129.87, 129.80, 129.65, 129.58, 129.53, 129.19, 129.06, 128.42, 128.16, 125.56, 125.33, 124.32, 124.23, 119.42, 117.09, 65.49, 65.37, 65.13, 64.26, 63.71, 57.12, 56.74, 56.06, 55.85, 55.47, 55.21, 54.37, 53.85, 53.75, 35.68, 35.42, 35.27, 33.07. ^{45}Sc NMR (122 MHz, MeOD) δ 75.4. ^{45}Sc NMR (122 MHz, D_2O) δ 86.2, 76.0. ^{19}F NMR (564 MHz, MeOD) δ 2.52, 1.58. ESI-HRMS (+ve ion): [ScF(**L**^{021})]$^{+}$ *m/z* = 649.2733 (experimental); 649.2727 (calculated). HPLC: R_t = 8.93 min (Method D).

*Lu(**L**^{201})* was prepared according to a literature procedure.[1]



*[Lu(**L**^{111})]$^{+}$*



To a solution of H_2**L**^{111} (1.93 mg, 4.00 µmol, 1 equiv.) in water (2 mL) was added lutetium(III) chloride hexahydrate (2.34 mg, 6.00 µmol, 1.5 equiv.) and the reaction mixture was heated to 80 °C for 1 hour, then checked via LCMS to ensure complete complexation. The lutetium complex was isolated and analyzed as crude product. ^{1}H NMR (500 MHz, MeOD) δ 8.13 (t, J = 7.7 Hz, 0.8H, Ar(Pa)), 8.03 (t, J = 7.2 Hz, 0.8H, Ar(Pa)), 7.64 (d, J = 7.8 Hz, 0.8H, Ar(Pa)), 7.39 (t, J = 7.5 Hz, 0.2H, Ar(Pa)), 7.33 (t, J = 7.5 Hz, 0.2H, Ar(Pa)), 7.24 (d, J = 7.0 Hz, 0.2H, Ar(Pa)), 7.36 – 7.18 (m, 3.5H, Ar(Bz)), 6.99 – 6.92 (m, 1.5H, Ar(Bz)), 4.74 – 3.89 (m, 8H, CH_2(Ac) + CH_2(Pa) + CH_2 (Am) + CH_2(Bz)), 3.59 – 2.66 (m, 12H, tacn), 3.07 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, MeOD) δ 181.18, 180.05, 175.07, 172.08, 157.26, 150.59, 142.56, 135.52, 129.14, 128.73, 127.65, 127.04, 126.80, 125.57, 123.60, 115.15, 64.06, 63.39, 62.75, 55.36, 55.16, 54.37, 53.85, 53.18, 51.82, 51.06, 36.55, 22.93. ESI-HRMS (+ve ion): [Lu(**L**^{111})]$^{+}$ *m/z* = 656.1721 (experimental); 656.1728 (calculated). HPLC: R_t = 6.46, 6.76 min (Method A).

1.4 Ultraviolet-Visible Spectroscopy Data

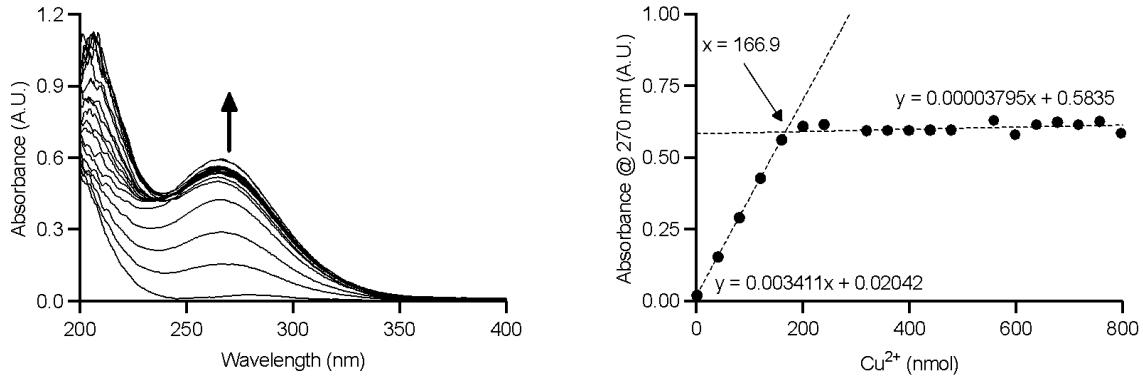


Figure S1. Spectrophotometric titration of $H_3\mathbf{L}^{300}$ (H_3nota) with Cu^{2+}. UV-vis absorbance spectra of $H_3\mathbf{L}^{300}$ (H_3nota) upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

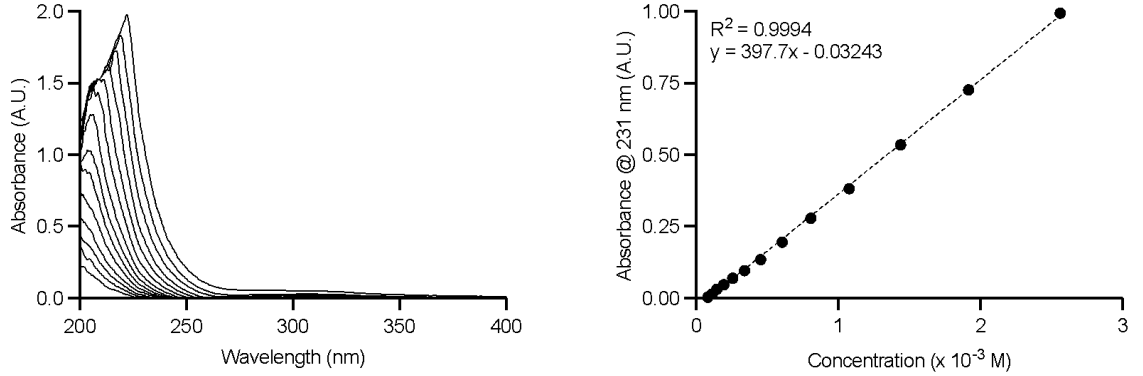


Figure S2. UV-vis analysis of $H_3\mathbf{L}^{300}$ (H_3nota) to determine molar extinction coefficient. UV-vis absorbance spectra of $H_3\mathbf{L}^{300}$ (H_3nota) at decreasing concentration (left) and analysis of spectra at 231 nm used to determine the molar extinction coefficient (right).

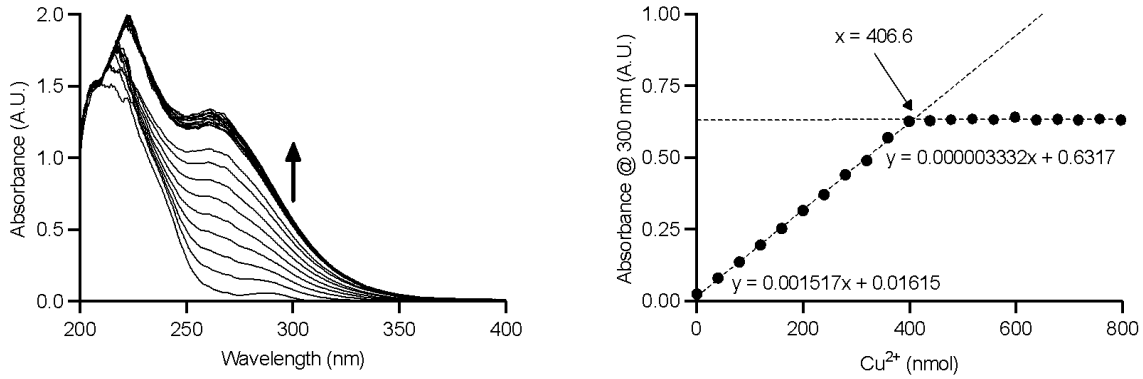


Figure S3. Spectrophotometric titration of $H_3\mathbf{L}^{\mathbf{300\text{-}NBzNH2}}$ with Cu^{2+}. UV-vis absorbance spectra of $H_3\mathbf{L}^{\mathbf{300\text{-}BzNH2}}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

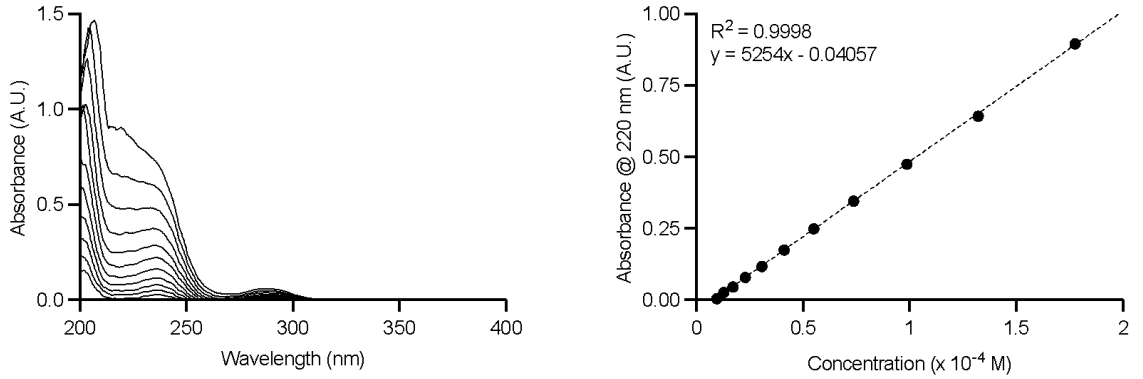


Figure S4. UV-vis analysis of $H_3\mathbf{L}^{\mathbf{300\text{-}BzNH2}}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H_3\mathbf{L}^{\mathbf{300\text{-}BzNH2}}$ at decreasing concentration (left) and analysis of spectra at 231 nm used to determine the molar extinction coefficient (right).

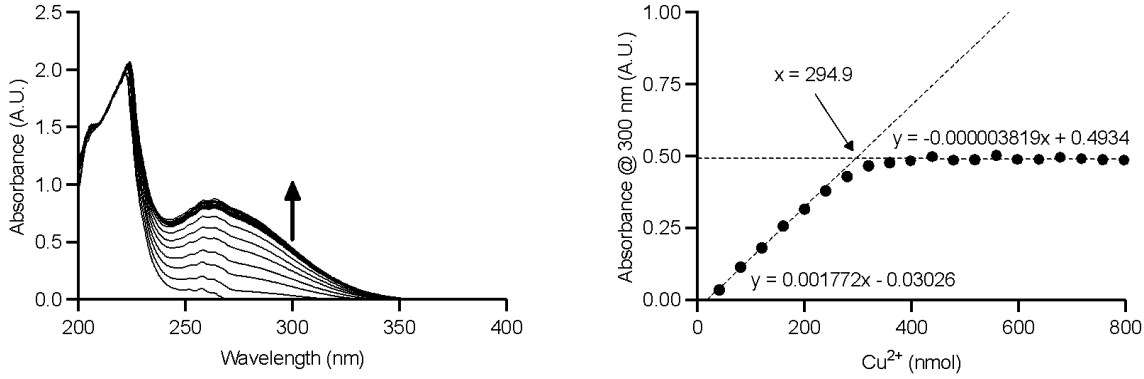


Figure S5. Spectrophotometric titration of $\mathbf{L}^{\mathbf{030}}$ with Cu^{2+}. UV-vis absorbance spectra of $\mathbf{L}^{\mathbf{030}}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

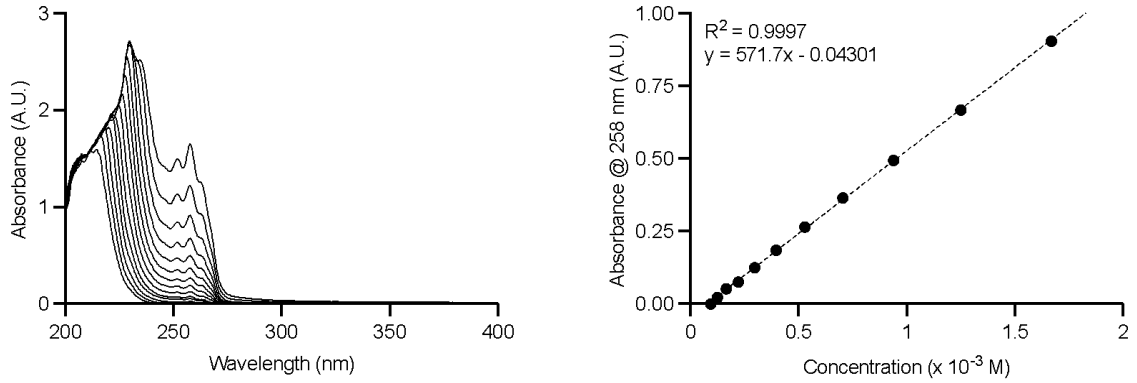


Figure S6. UV-vis analysis of $\mathbf{L^{030}}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $\mathbf{L^{030}}$ at decreasing concentration (left) and analysis of spectra at 258 nm used to determine the molar extinction coefficient (right).

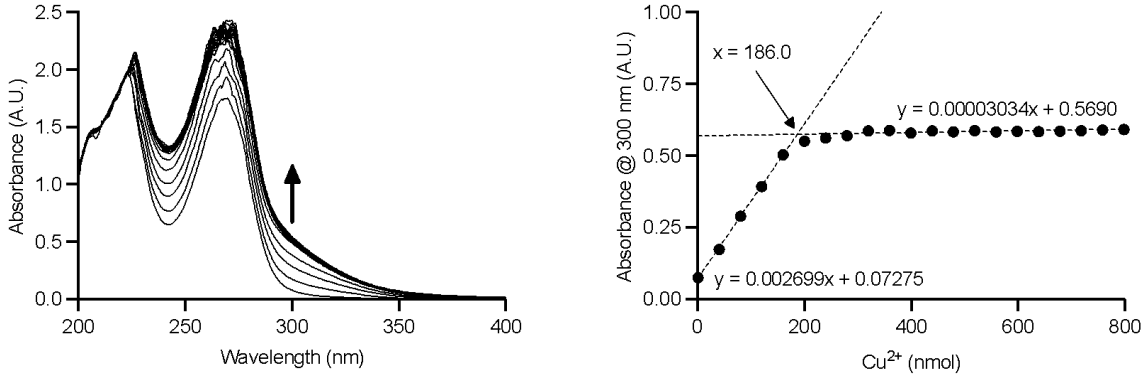


Figure S7. Spectrophotometric titration of $H_3\mathbf{L^{003}}$ with Cu^{2+}. UV-vis absorbance spectra of $H_3\mathbf{L^{003}}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

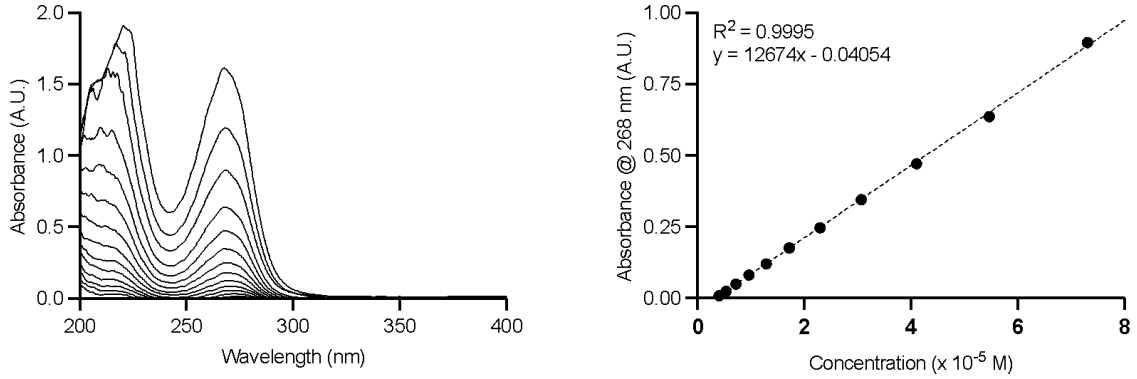


Figure S8. UV-vis analysis of $H_3\mathbf{L^{003}}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H_3\mathbf{L^{003}}$ at decreasing concentration (left) and analysis of spectra at 268 nm used to determine the molar extinction coefficient (right).

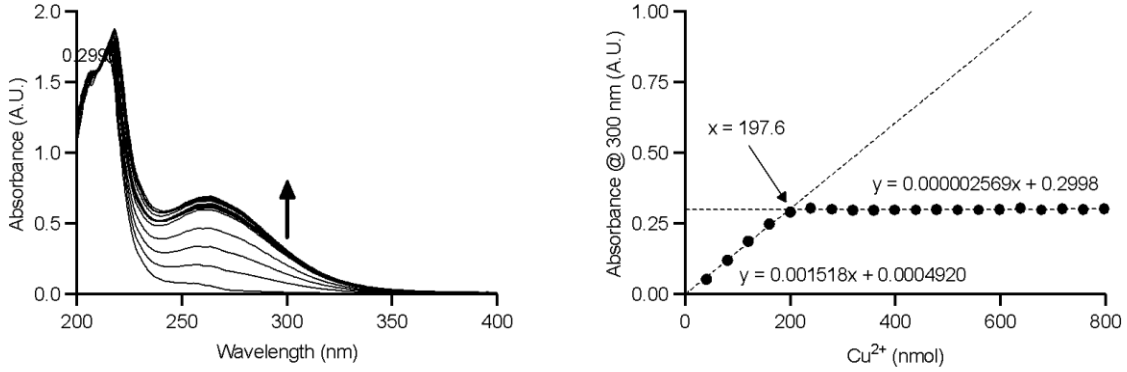


Figure S9. Spectrophotometric titration of $H_2\mathbf{L}^{\mathbf{210}}$ with Cu^{2+}. UV-vis absorbance spectra of $H_2\mathbf{L}^{\mathbf{210}}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

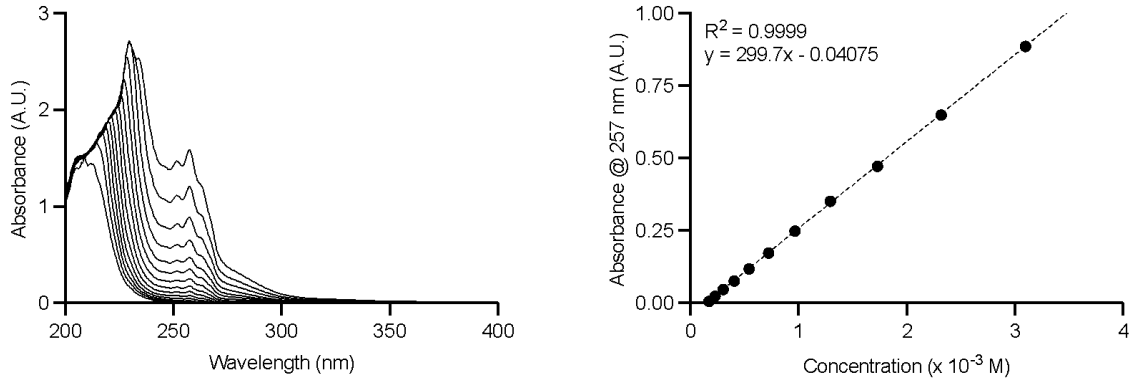


Figure S10. UV-vis analysis of $H_2\mathbf{L}^{\mathbf{210}}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H_2\mathbf{L}^{\mathbf{210}}$ at decreasing concentration (left) and analysis of spectra at 257 nm used to determine the molar extinction coefficient (right).

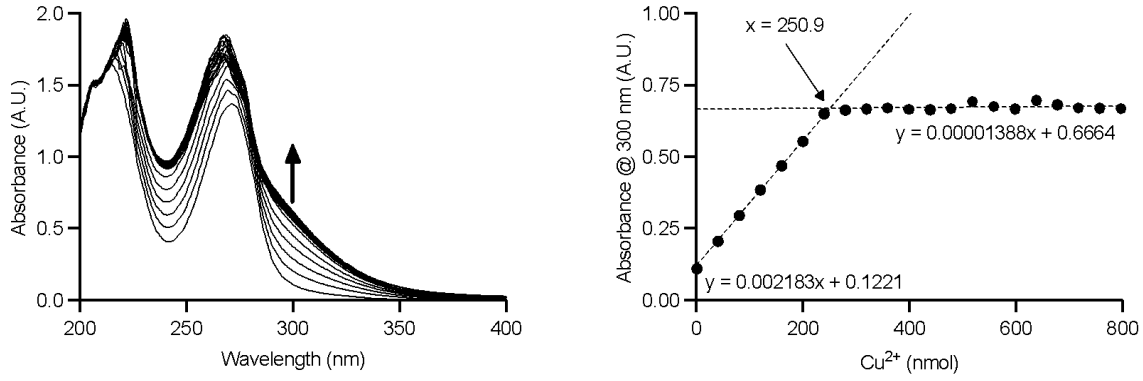


Figure S11. Spectrophotometric titration of $H_3\mathbf{L}^{\mathbf{201}}$ (H_3mpatcn) with Cu^{2+}. UV-vis absorbance spectra of $H_3\mathbf{L}^{\mathbf{201}}$ (H_3mpatcn) upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

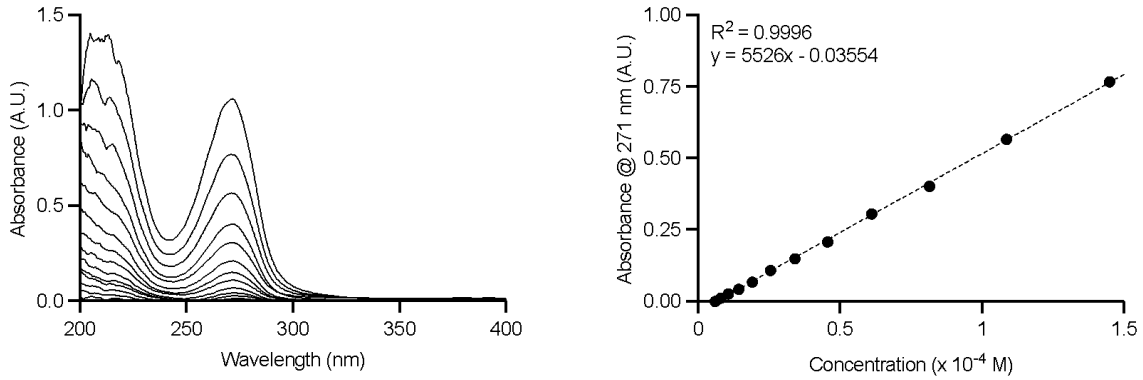


Figure S12. UV-vis analysis of $H_3\mathbf{L}^{201}$ (H_3mpatcn) to determine molar extinction coefficient. UV-vis absorbance spectra of $H_3\mathbf{L}^{201}$ (H_3mpatcn) at decreasing concentration (left) and analysis of spectra at 271 nm used to determine the molar extinction coefficient (right).

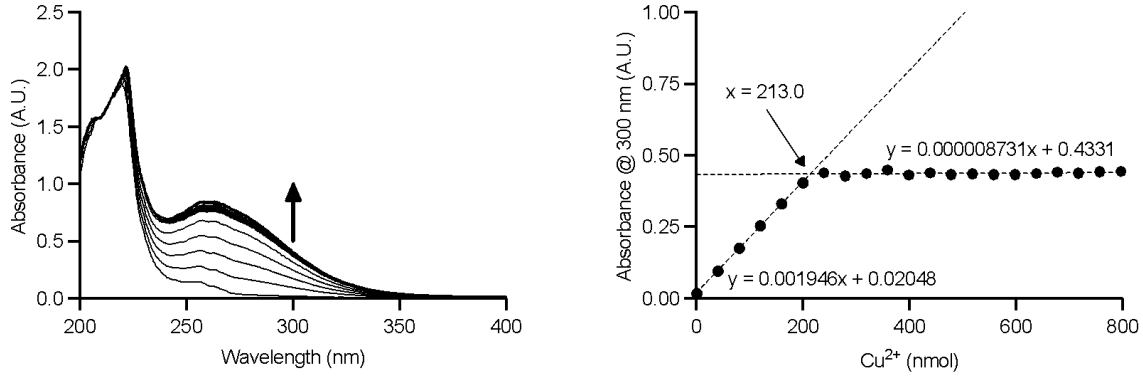


Figure S13. Spectrophotometric titration of H$\mathbf{L}^{120}$ with Cu^{2+}. UV-vis absorbance spectra of H$\mathbf{L}^{120}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

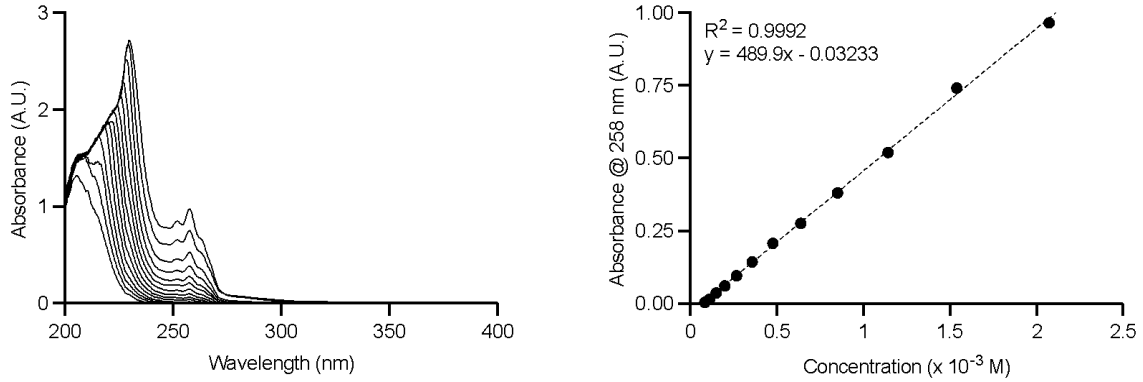


Figure S14. UV-vis analysis of H$\mathbf{L}^{120}$ to determine molar extinction coefficient. UV-vis absorbance spectra of H$\mathbf{L}^{120}$ at decreasing concentration (left) and analysis of spectra at 258 nm used to determine the molar extinction coefficient (right).

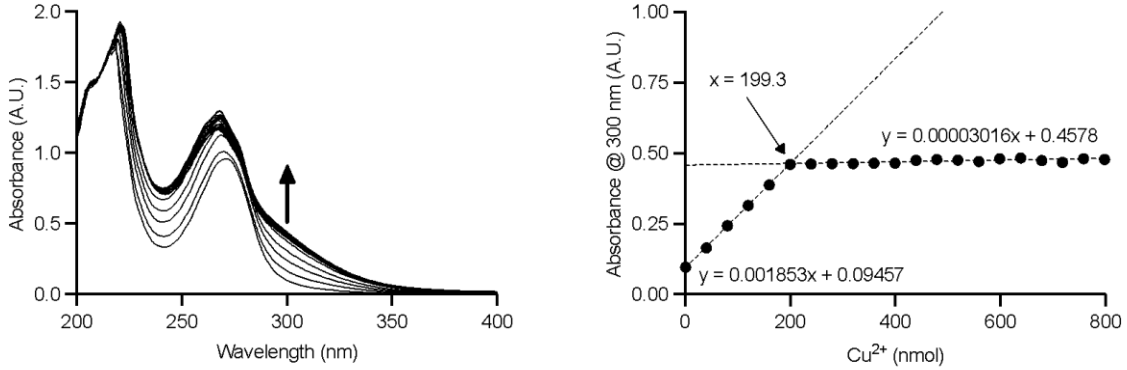


Figure S15. Spectrophotometric titration of $H_2\mathbf{L}^{111}$ with Cu^{2+}. UV-vis absorbance spectra of $H_2\mathbf{L}^{111}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

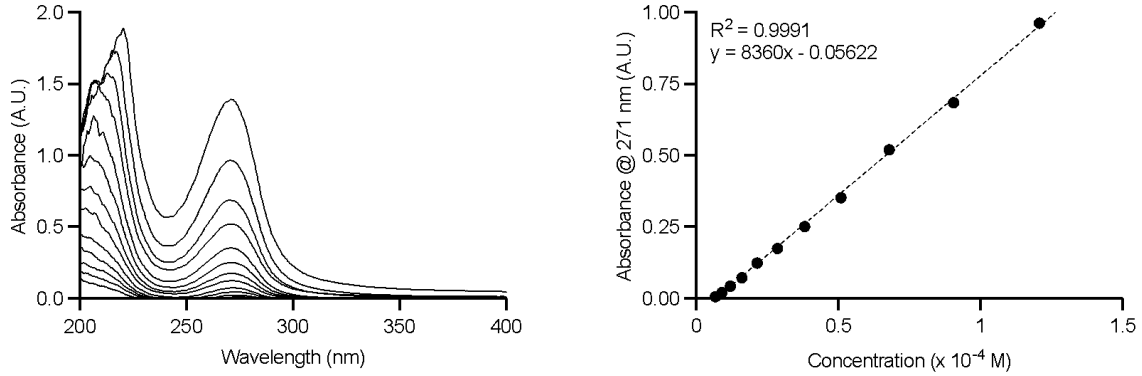


Figure S16. UV-vis analysis of $H_2\mathbf{L}^{111}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H_2\mathbf{L}^{111}$ at decreasing concentration (left) and analysis of spectra at 271 nm used to determine the molar extinction coefficient (right).

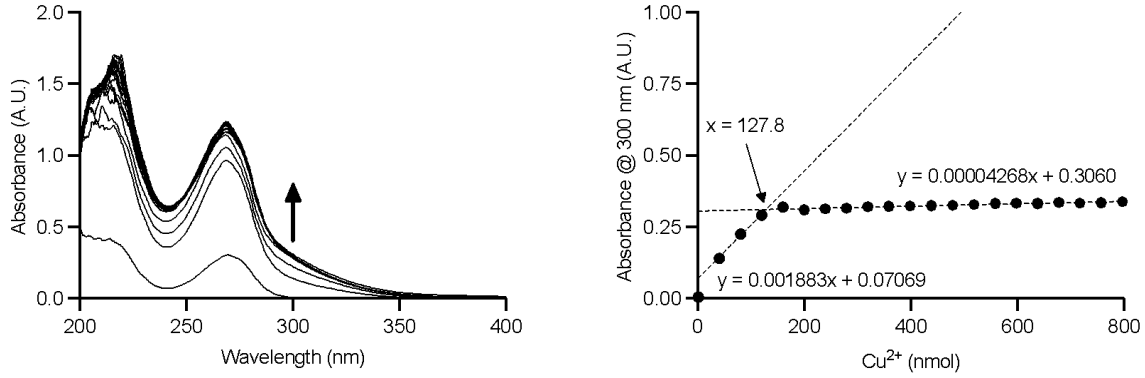


Figure S17. Spectrophotometric titration of $H_3\mathbf{L}^{102}$ with Cu^{2+}. UV-vis absorbance spectra of $H_3\mathbf{L}^{102}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

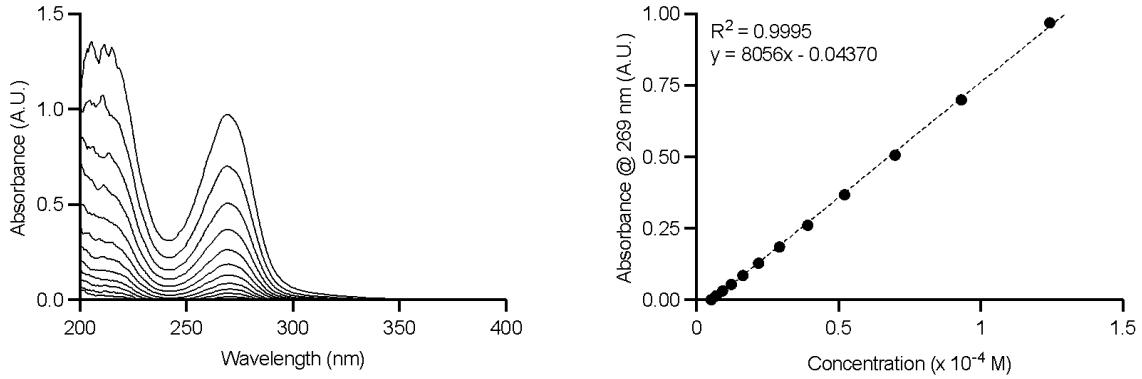


Figure S18. UV-vis analysis of $H_3\mathbf{L}^{102}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H_3\mathbf{L}^{102}$ at decreasing concentration (left) and analysis of spectra at 269 nm used to determine the molar extinction coefficient (right).

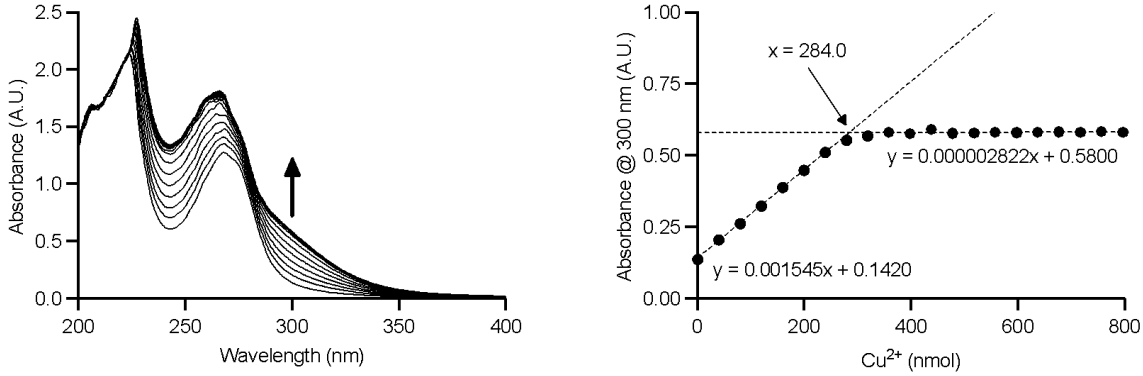


Figure S19. Spectrophotometric titration of $H\mathbf{L}^{021}$ with Cu^{2+}. UV-vis absorbance spectra of $H\mathbf{L}^{021}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

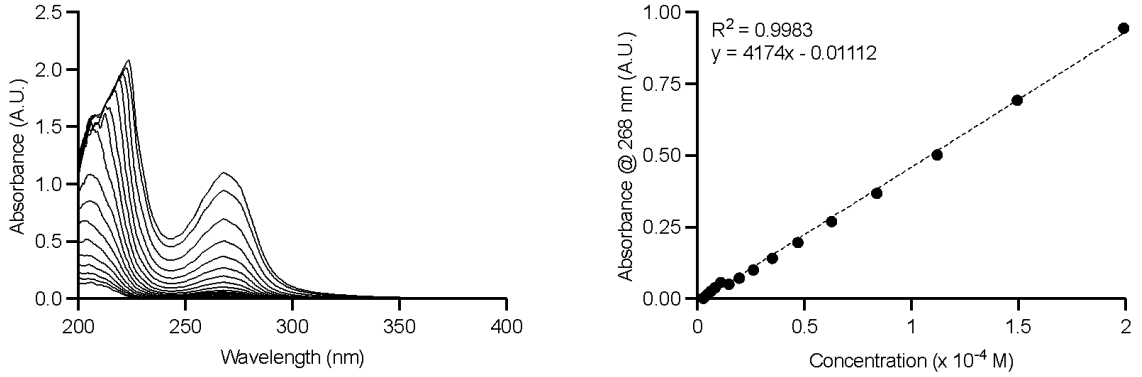


Figure S20. UV-vis analysis of $H\mathbf{L}^{021}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H\mathbf{L}^{021}$ at decreasing concentration (left) and analysis of spectra at 268 nm used to determine the molar extinction coefficient (right).

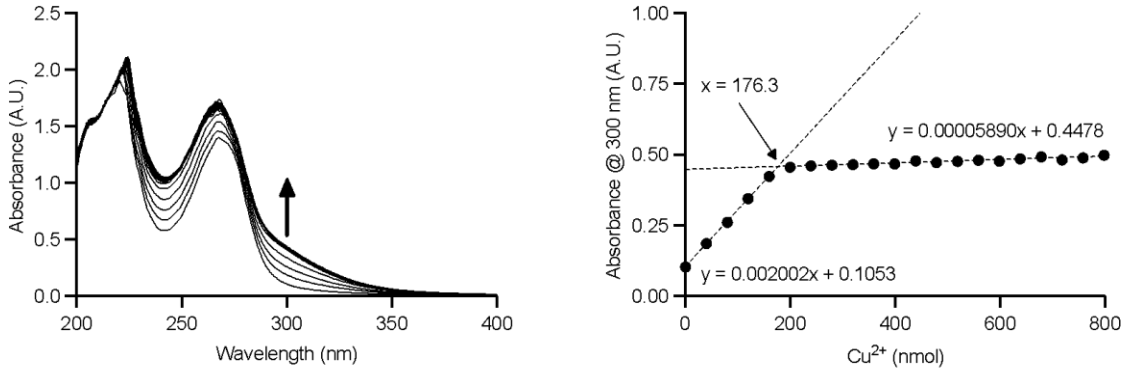


Figure S21. Spectrophotometric titration of $H_2\mathbf{L}^{012}$ with Cu^{2+}. UV-vis absorbance spectra of $H_2\mathbf{L}^{012}$ upon Cu^{2+} addition (left) and UV-vis titration to endpoint to determine ligand concentration (right).

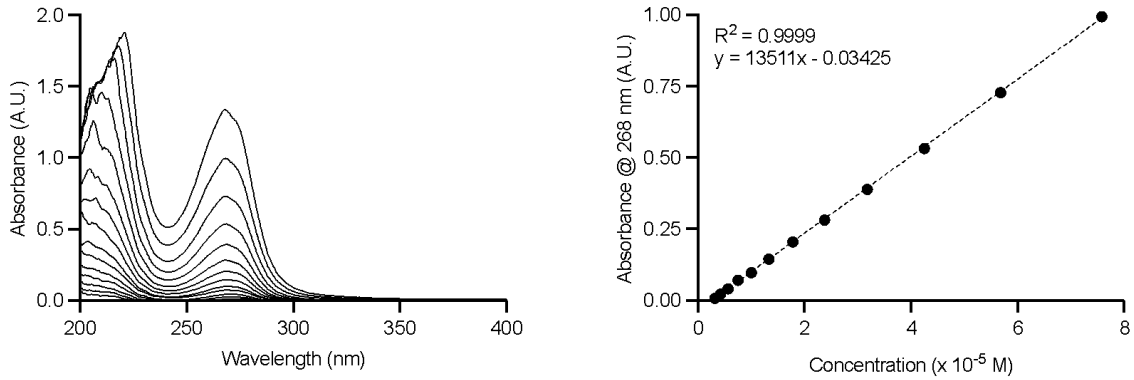


Figure S22. UV-vis analysis of $H_2\mathbf{L}^{012}$ to determine molar extinction coefficient. UV-vis absorbance spectra of $H_2\mathbf{L}^{012}$ at decreasing concentration (left) and analysis of spectra at 268 nm used to determine the molar extinction coefficient (right).

1.5 Computational Chemistry

Density Functional Theory calculations were performed using the *Gaussian16*, Revision A.03 software package. Computations were performed with the B3LYP-D3(BJ) functional and cc-pVDZ basis set. Calculations were performed using the SMD implicit solvation model (water), and structures for refinement were derived from crystal structures where available.

Calculations were performed without symmetry constraints as geometry optimizations with frequency calculations (OPT FREQ) using the B3LYP-D3(BJ) functional and cc-PVDZ basis set with SMD integral equation formalism polarizable continuum model (IEFPCM) solvation.

Sc-L and ScF-L interaction energies were calculated using the following formula.

Enthalpy of Sc(**L**)/ScF(**L**) – Enthalpy of constrained **L** – Enthalpy of constrained Sc^{3+}/ScF^{2+}

Sc-X (X = OH_2, OH^-, or F^-) bond dissociation energies were calculated using the following formula.

Enthalpy of Sc(**L**) + Enthalpy of X – Enthalpy of ScX(**L**)

Table S1. DFT calculated enthalpies and interaction energies of all ligand systems investigated.

	Enthalpy (kJ/mol)				Interaction Energy (kJ/mol)	
Complex	X = Φ	X = OH_2	X = OH^-	X = F^-	ScF-L	Sc-L
Δ-ScX**L**^{300}	-4843096	-5043757	-5042533	-5105694	-726	-
Δ-ScX**L**^{300}	-4843095	-5043757	-5042533	-5105694	-725	-
Δ-ScX**L**^{210}	-4998324	-5198992	-5197779	-5260937	-664	-
Λ- ScX**L**^{210}	-4998324	-5198992	-5197779	-5260937	-664	-
Δ-ScX**L**^{120}	-5153553	-5354221	-5353019	-5416177	-611	-
Λ-ScX**L**^{120}	-5153553	-5354221	-5353019	-5416177	-611	-
Δ-ScX**L**^{030}	-5308772	-5509447	-5508260	-5571414	-537	-
Δ-ScX**L**^{030}	-5308773	-5509457	-5508258	-5571414	-543	-
Δ-ScX**L**^{201}	-5491780	-5692415	-5691188	-5754337	-713	-
Λ- ScX**L**^{201}	-5491780	-5692415	-5691188	-5754337	-713	-
M-Δ-ScX**L**^{111}	-5647010	-5847653	-5846435	-5909588	-667	-889
M-Λ-ScX**L**^{111}	-5647018	-5847659	-5846436	-5909590	-648	-886
P-Δ-ScX**L**^{111}	-5647018	-5847660	-5846436	-5909590	-648	-886
P-Λ-ScX**L**^{111}	-5647010	-5847653	-5846435	-5909588	-667	-889
Δ-ScX**L**^{021}	-5802244	-6002892	-6001682	-6064835	-608	-
Λ-ScX**L**^{021}	-5802246	-6002892	-6001682	-6064835	-605	-
Δ-ScX**L**^{102}	-6140453	-6341116	-6339859	-6403015	-719	-
Λ-ScX**L**^{102}	-6140453	-6341116	-6339859	-6403015	-719	-
Δ-ScX**L**^{012}	-6295693	-6496350	-6495155	-6558305	-688	-
Λ-ScX**L**^{012}	-6295693	-6496351	-6495155	-6558305	-688	-
Δ-ScX**L**^{003}	-6789144	-6989741	-6988540	-7051679	-627	-
Λ-ScX**L**^{003}	-6789144	-6989735	-6988525	-7051682	-622	-

Table S2. DFT calculated bond dissociation energies and relevant bond lengths of all ligand systems investigated.

	BDE (kJ/mol)			Bond Lengths (Å)	
Complex	X = OH_2	X = OH^-	X = F^-	Sc-OH_2	Sc-F
Δ-Sc**X**$\mathbf{L^{300}}$	54	219	270	2.349	1.967
Δ-Sc**X**$\mathbf{L^{300}}$	54	218	271	2.350	1.967
Δ-Sc**X**$\mathbf{L^{210}}$	60	236	285	2.334	1.957
Λ- Sc**X**$\mathbf{L^{210}}$	60	236	285	2.334	1.957
Δ-Sc**X**$\mathbf{L^{120}}$	63	250	299	2.322	1.952
Λ-Sc**X**$\mathbf{L^{120}}$	60	247	296	2.324	1.952
Δ-Sc**X**$\mathbf{L^{030}}$	67	269	314	2.285	1.941
Δ-Sc**X**$\mathbf{L^{030}}$	77	266	313	2.247	1.940
Δ-Sc**X**$\mathbf{L^{201}}$	27	189	229	2.354	1.958
Λ- Sc**X**$\mathbf{L^{201}}$	27	189	229	2.354	1.958
M-Δ-Sc**X**$\mathbf{L^{111}}$	34	206	250	2.311	1.951
M-Λ-Sc**X**$\mathbf{L^{111}}$	34	199	244	2.337	1.954
P-Δ-Sc**X**$\mathbf{L^{111}}$	34	199	244	2.337	1.954
P-Λ-Sc**X**$\mathbf{L^{111}}$	35	206	251	2.311	1.951
Δ-Sc**X**$\mathbf{L^{021}}$	40	219	263	2.324	1.949
Λ-Sc**X**$\mathbf{L^{021}}$	39	218	262	2.324	1.948
Δ-Sc**X**$\mathbf{L^{102}}$	-	186	234	-	1.963
Λ-Sc**X**$\mathbf{L^{102}}$	-	186	234	-	1.964
Δ-Sc**X**$\mathbf{L^{012}}$	-	243	284	-	1.937
Λ-Sc**X**$\mathbf{L^{012}}$	-	243	284	-	1.937
Δ-Sc**X**$\mathbf{L^{003}}$	-	177	207	-	1.927
Λ-Sc**X**$\mathbf{L^{003}}$	-	162	210	-	1.924

Table S3. RMSD analysis comparing the XRD and DFT optimized structures of [Sc($\mathbf{L}^{003}$)].

	XRD	DFT
Mean Bond Distances [Å]		
M-N_{tacn}	2.564	2.659
M-N_{py}	2.426	2.412
M-O	2.206	2.212
Mean Plane Distances [Å]		
N_{tacn}-N_{py}	2.014	2.067
N_{tacn}-O	3.401	3.538
N_{py}-O	1.387	1.471
N_{tacn}-M	1.960	2.072
Mean Torsion [°]		
N_{tacn}-N_{tacn}	-45.95	-46.15
N_{tacn}-N_{py}	43.70	44.19
N_{tacn}-O	103.83	103.73
N_{py}-O	60.15	59.54
RMSD = 0.1946 Å		

1.6 Chiral Separation

[Sc(**L**^{111})]$^{+}$ was prepared as described in section **1.3**. The complex was then redissolved in MeOH to prepare the final solution that was used for chiral separation. Separations were performed using analytical HPLC method E.

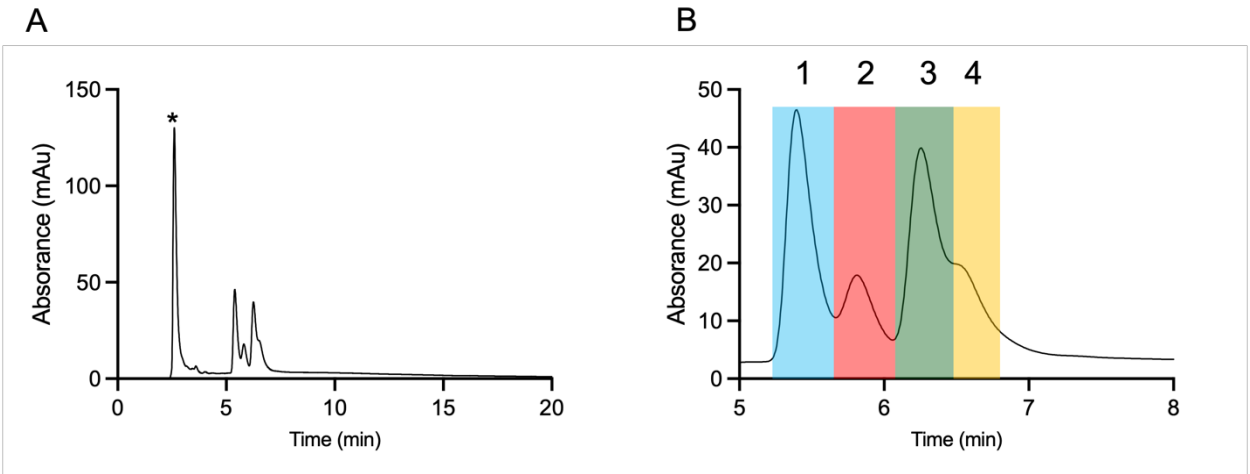


Figure S23. A) Chiral analytical HPLC trace of [Sc(**L**^{111})]$^{+}$ (Method E). B) Enhanced portion of HPLC trace to highlight the 4 metallo-atropoisomers.

Table S4. Tabulated % isomer present of the 4 [Sc(**L**^{111})]$^{+}$ isomers observed.

Species	**% isomer present**
Metallo-atropoisomer 1 (Blue)	~34%
Metallo-atropoisomer 2 (Red)	~14%
Metallo-atropoisomer 3 (Green)	~34%
Metallo-atropoisomer 4 (Yellow)	~18%

1.7 Radiolabeling Data

1.7.1 General ^{18}F Radiolabeling Procedure

Radiolabeling was conducted following a literature procedure.[2] To an aqueous solution of ammonium acetate (50 µL, 1 M, pH 4.8) was added an aliquot of unprocessed [^{18}F]F^- stock (110-143 µL, ~1 mCi) followed by an aliquot of a $ScCl_3 \cdot 6H_2O$ stock solution (2-20 µL, 20 nmol) of known concentration as determined by ICP-OES or MP-AES. Following incubation at room temperature for 10 minutes, an aliquot of a ligand stock solution (5-20 µL, 100 nmol), of known concentration as determined UV-vis spectroscopy, was added. Total reaction volume = 200 µL. The mixtures were incubated at 80 °C for 30 min prior to radioHPLC analysis (Method C). The same procedure was used for animal studies.

1.7.2 General $^{44}Sc/^{177}Lu$ Radiolabeling Procedure

Radiolabeling was conducted following a literature procedure.[2] To an aqueous solution of ammonium acetate (10 µL, 1 M, pH 4.8) was added ligand stock solution (16-54 µL, 10 nmol), of known concentration as determined UV-vis spectroscopy, followed by an aliquot of the [^{44}Sc]$ScCl_3$ or [^{177}Lu]$LuCl_3$ stock (36-74 µL, ~0.1 mCi). Total reaction volume = 100 µL. The mixtures were incubated at 80 °C for 30 min prior to radioTLC (developed with 50 mM Na_2EDTA) and radioHPLC analyses (^{44}Sc: Method B; ^{177}Lu: Method A). For radioTLC, activity with an R_f of ~0 was considered to be the desired radiolabeled complex, and activity with a R_f of ~1 was considered to be free $^{44}Sc^{3+}$ or $^{177}Lu^{3+}$ respectively.

1.7.3 $^{44}Sc/^{177}Lu$ Animal Studies Radiolabeling Procedure

To an aqueous solution of ammonium acetate (20 µL, 1 M, pH 4.8) was added ligand stock solution (2-17 µL, 100 nmol), of known concentration as determined UV-vis spectroscopy, followed by an aliquot of the [^{44}Sc]$ScCl_3$ or [^{177}Lu]$LuCl_3$ stock (163-178 µL, ~1 mCi). Total reaction volume = 200 µL. The mixtures were incubated at 80 °C for 30 min prior to radioTLC (developed with 50 mM Na_2EDTA) and radioHPLC analyses (^{44}Sc: Method B; ^{177}Lu: Method A).

1.7.4 Metabolite Analysis

Metabolite analysis was performed by analyzing 100 µL of mouse urine collected during biodistribution studies via radioHPLC. In cases where less than 100 µL of urine was collected, the urine was diluted with 1X PBS to a total volume of 100 µL. In cases where the total activity was below the sensitivity of the radio detector, fractions were collected every 30 seconds, activity in each fraction was quantified using a gamma counter, and the trace was reconstructed.

Table S5. Tabulated radiochemical conversion values for the radiochemical syntheses performed in this research. Data are represented at mean and standard deviation of triplicate results from radioTLC or radioHPLC analyses. *Triplicate results gave the same value. **Duplicate results

Ligand	**^{18}F**	**^{44}Sc**	**^{177}Lu**
H_3**L**^{300}	-	98.6 ± 0.3	81.3 ± 4.9
H_3**L**$^{300\text{-}BzNH2}$	2.1 ± 0.2	95.4 ± 4.1**	99.0*
L^{030}	-	81.4 ± 2.0	8.8 ± 0.5
H_3**L**^{003}	-	95.6 ± 3.0	97.5 ± 2.2
H_2**L**^{210}	7.9 ± 0.3	91.5 ± 2.3	62.0 ± 1.3
H_3**L**^{201}	33.3 ± 0.8	99.1 ± 0.4	99.3 ± 0.6
H**L**^{120}	13.0 ± 1.2	96.7 ± 0.2	94.8 ± 1.3
H_2**L**^{111}	36.7 ± 3.3	97.5 ± 0.4	90.2 ± 0.9
H_3**L**^{102}	-	95.1 ± 0.7	99.0 ± 1.8
H**L**^{021}	19.0 ± 0.6	96.0 ± 1.9	83.0 ± 1.0
H_2**L**^{012}	-	92.5 ± 3.6	98.9 ± 0.7

Table S6. Biodistributions of [^{18}F]F$^-$ and [^{18}F]ScF-acetate as measured by % ID/g in BALB/c mice (n = 3-5) at 1 hour post-injection (mean % ID/g ± standard deviation). Outliers removed using a Grubb's test with 95% confidence interval. *Duplicate results gave the same value.

	[^{18}F]F$^-$	**[^{18}F]ScF-acetate**
urine	-	-
blood	0.30 ± 0.14	0.58 ± 0.08
heart	0.28 ± 0.04	0.59 ± 0.08
lungs	0.19 ± 0.06	0.69*
liver	0.17*	4.6 ± 0.50
spleen	0.16 ± 0.02	2.49 ± 0.40
kidneys	0.38 ± 0.04	0.97 ± 0.11
stomach	0.09 ± 0.02	0.18*
small intestine	0.58 ± 0.30	0.61 ± 0.01
large intestine	1.77 ± 0.57	1.76 ± 0.72
muscle	0.32 ± 0.18	0.52 ± 0.17
bone	11.97 ± 3.51	17.60 ± 3.81
brain	0.13 ± 0.06	0.22 ± 0.14

Table S7. Biodistributions of $[^{18}F][ScF(\mathbf{L^{201}})]^-$, $[^{18}F][ScF(\mathbf{L^{111}})]$, $[^{18}F][ScF(\mathbf{L^{210}})]$, and $[^{18}F][ScF(\mathbf{L^{120}})]^+$ as measured by % ID/g in BALB/c mice (n = 3-5) at 1 hour post-injection (mean % ID/g ± standard deviation). Outliers removed using a Grubb's test with 95% confidence interval. *Duplicate results gave the same value.

	$[^{18}F][ScF(L^{201})]^-$	$[^{18}F][ScF(L^{111})]$	$[^{18}F][ScF(L^{210})]$	$[^{18}F][ScF(L^{120})]^+$
urine	-	219.50 ± 56.42	-	-
blood	0.64 ± 0.29	0.35 ± 0.13	0.34 ± 0.33	0.11 ± 0.03
heart	0.26 ± 0.06	0.10 ± 0.04	0.11 ± 0.04	0.12 ± 0.03
lungs	0.25 ± 0.03	0.23 ± 0.06	0.18 ± 0.1	0.18 ± 0.02
liver	0.48 ± 0.06	0.85 ± 0.31	2.53 ± 0.63	0.62 ± 0.24
spleen	0.09 ± 0.03	0.98 ± 0.39	0.17 ± 0.07	0.15 ± 0.02
kidneys	3.16 ± 0.85	1.47 ± 0.32	1.90 ± 0.91	0.43 ± 0.06
stomach	0.09 ± 0.05	0.08 ± 0.02	0.10 ± 0.04	0.06 ± 0.03
small intestine	0.44 ± 0.12	0.60 ± 0.11	7.09 ± 5.9	15.93 ± 7.20
large intestine	0.10 ± 0.02	0.07 ± 0.01	0.31 ± 0.22	0.30 ± 0.02
muscle	0.06 ± 0.05	0.04 ± 0.01	0.11 ± 0.05	0.11 ± 0.05
bone	0.20 ± 0.16	0.27 ± 0.20	1.50 ± 0.37	2.48 ± 0.31
brain	-	0.03 ± 0.01	0.06 ± 0.04	0.03 ± 0.01

Table S8. Biodistributions of [^{44}Sc]Sc-acetate, [^{44}Sc][Sc(**L**$^{\mathbf{201}}$)], [^{44}Sc][Sc(**L**$^{\mathbf{111}}$)]$^{+}$, and [^{44}Sc][Sc(**L**$^{\mathbf{021}}$)]$^{2+}$ as measured by % ID/g in BALB/c mice (n = 3-5) at 1 hour post-injection (mean % ID/g ± standard deviation). Outliers removed using a Grubb's test with 95% confidence interval.

	[^{44}Sc]Sc-acetate	[^{44}Sc] [Sc(**L**$^{\mathbf{201}}$)]	[^{44}Sc][Sc(**L**$^{\mathbf{111}}$)]$^{+}$	[^{44}Sc][Sc(**L**$^{\mathbf{021}}$)]$^{+}$
urine	4.82 ± 0.70	1456.72 ± 466.15	1536.91 ± 199.86	561.04 ± 316.95
blood	17.04 ± 0.85	0.57 ± 0.08	0.39 ± 0.03	2.17 ± 0.68
heart	5.13 ± 0.11	0.41 ± 0.11	0.21 ± 0.02	0.68 ± 0.09
lungs	8.72 ± 1.46	1.06 ± 0.27	0.88 ± 0.08	1.39 ± 0.20
liver	24.51 ± 3.13	0.75 ± 0.09	2.00 ± 0.17	6.24 ± 2.37
spleen	8.56 ± 0.43	0.69 ± 0.09	0.47 ± 0.07	0.69 ± 0.06
kidneys	6.53 ± 0.01	3.48 ± 1.29	2.85 ± 0.82	2.72 ± 0.36
stomach	1.85 ± 0.08	0.27 ± 0.05	0.50 ± 0.52	1.09 ± 0.50
small intestine	2.45 ± 0.27	0.38 ± 0.08	2.28 ± 0.44	35.09 ± 14.76
large intestine	1.00 ± 0.08	0.20 ± 0.05	0.19 ± 0.04	1.53 ± 0.66
muscle	0.70 ± 0.06	0.25 ± 0.07	0.20 ± 0.03	0.28 ± 0.06
bone	2.36 ± 0.78	1.17 ± 0.33	0.49 ± 0.05	0.68 ± 0.22
brain	0.60 ± 0.06	0.14 ± 0.08	0.06 ± 0.01	0.08 ± 0.03

Table S9. Biodistributions of [^{44}Sc][Sc(**L**^{300})], [^{44}Sc][Sc(**L**^{210})]$^{+}$, and [^{44}Sc][Sc(**L**^{120})]$^{2+}$ as measured by % ID/g in BALB/c mice (n = 5) at 1 hour post-injection (mean % ID/g ± standard deviation). Outliers removed using a Grubb's test with 95% confidence interval.

	[^{44}Sc][Sc(**L**^{300})]	[^{44}Sc][Sc(**L**^{210})]$^{+}$	[^{44}Sc][Sc(**L**^{120})]$^{2+}$
urine	195.09 ± 273.27	356.34 ± 247.69	153.37 ± 103.81
blood	0.28 ± 0.05	3.22 ± 0.11	1.45 ± 0.45
heart	0.10 ± 0.02	1.12 ± 0.23	0.49 ± 0.05
lungs	0.22 ± 0.04	1.69 ± 0.14	1.23 ± 0.19
liver	0.21 ± 0.03	2.34 ± 0.20	9.75 ± 1.23
spleen	0.09 ± 0.02	0.94 ± 0.11	2.62 ± 0.31
kidneys	1.54 ± 0.38	3.58 ± 0.24	6.14 ± 1.03
stomach	0.80 ± 1.01	1.06 ± 0.38	2.61 ± 0.80
small intestine	0.17 ± 0.08	1.54 ± 0.18	8.56 ± 0.97
large intestine	0.06 ± 0.01	0.31 ± 0.06	0.26 ± 0.04
muscle	0.07 ± 0.02	0.22 ± 0.03	0.17 ± 0.03
bone	0.26 ± 0.08	0.69 ± 0.01	0.42 ± 0.15
brain	0.04 ± 0.02	0.13 ± 0.01	0.09 ± 0.03

Table S10. Biodistributions of [^{177}Lu]Lu-acetate, [^{177}Lu][Lu(**L**$^{\mathbf{201}}$)], and [^{177}Lu][Lu(**L**$^{\mathbf{111}}$)]$^{+}$ as measured by % ID/g in BALB/c mice (n = 3-5) at 1 hour post-injection (mean % ID/g ± standard deviation). Outliers removed using a Grubb's test with 95% confidence interval.

	[^{177}Lu]Lu-acetate	[^{177}Lu]Lu(**L**$^{\mathbf{201}}$)	[^{177}Lu][Lu(**L**$^{\mathbf{111}}$)]$^{+}$
urine	33.17 ± 15.41	836.64 ± 217.87	151.35 ± 98.05
blood	3.11 ± 0.61	0.47 ± 0.19	0.68 ± 0.08
heart	1.92 ± 0.29	0.22 ± 0.09	0.26 ± 0.03
lungs	4.36 ± 0.40	0.49 ± 0.14	0.91 ± 0.07
liver	68.53 ± 9.08	0.72 ± 0.11	2.37 ± 0.11
spleen	16.89 ± 3.73	0.24 ± 0.06	0.33 ± 0.01
kidneys	3.42 ± 0.28	7.14 ± 1.65	10.69 ± 2.05
stomach	1.29 ± 0.63	0.36 ± 0.06	0.73 ± 0.17
small intestine	1.16 ± 0.06	0.49 ± 0.3	1.82 ± 0.06
large intestine	0.42 ± 0.05	0.17 ± 0.06	0.22 ± 0.03
muscle	0.53 ± 0.04	0.18 ± 0.05	0.18 ± 0.02
bone	4.07 ± 1.52	0.51 ± 0.22	0.43 ± 0.05
brain	0.10 ± 0.01	0.04 ± 0.01	0.08 ± 0.05

1.7.5 HPLC Chromatograms

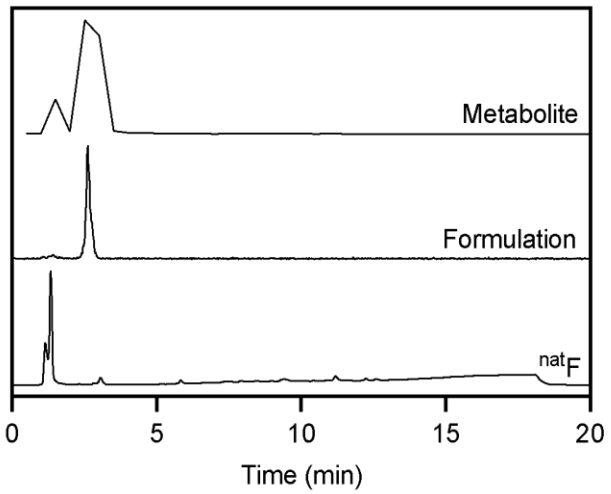


Figure S24. The RP-HPLC (Method A) analyses of [^{nat}F][ScF(**L^{201}**)]$^{-}$, [^{18}F][ScF(**L^{201}**)]$^{-}$ formulation, and urine metabolite.

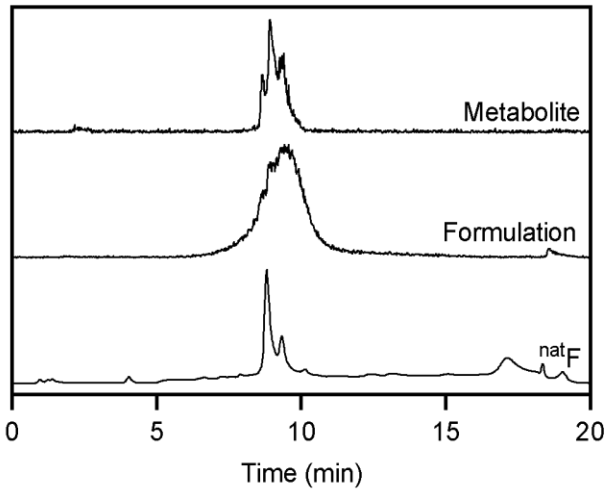


Figure S25. The RP-HPLC (Method C) analyses of [^{nat}F][ScF(**L^{111}**)], [^{18}F][ScF(**L^{111}**)], formulation, and urine metabolite.

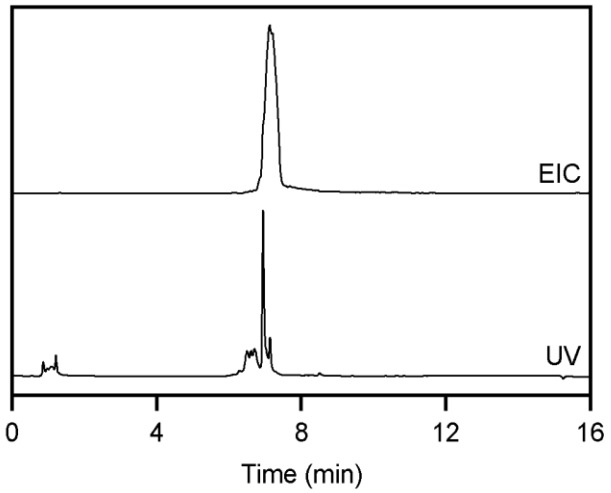


Figure S26. The UV (254 nm) and extracted ion (m/z = 545-547) LCMS (Method G) chromatograms of [ScF(**L**^{111})].

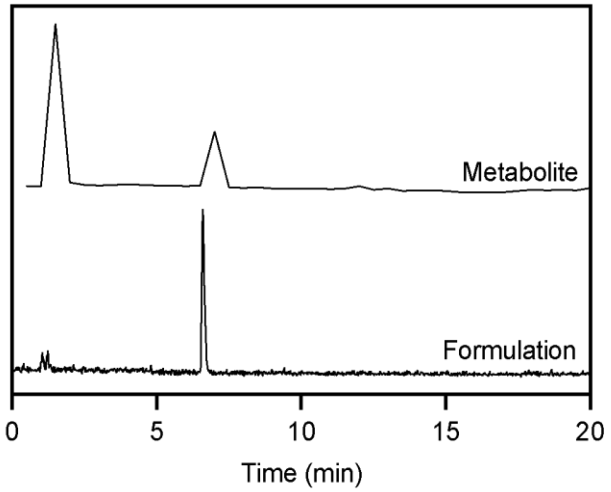


Figure S27. The RP-radioHPLC (Method A) analyses of the [^{18}F][ScF(**L**^{210})] formulation and urine metabolite.

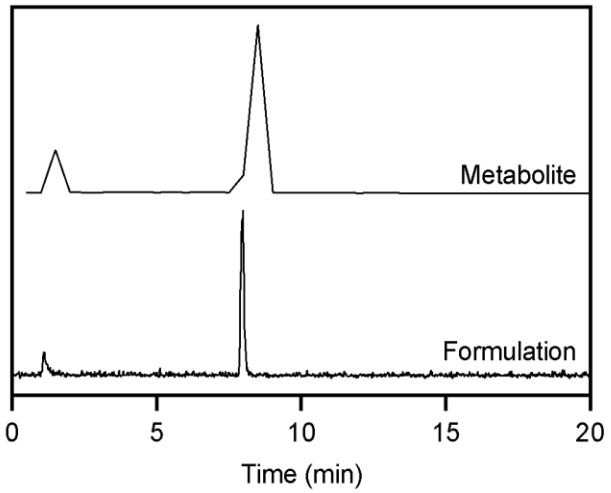


Figure S28. The RP-radioHPLC (Method A) analyses of the $[^{18}F][ScF(\mathbf{L^{120}})]^+$ formulation and urine metabolite.

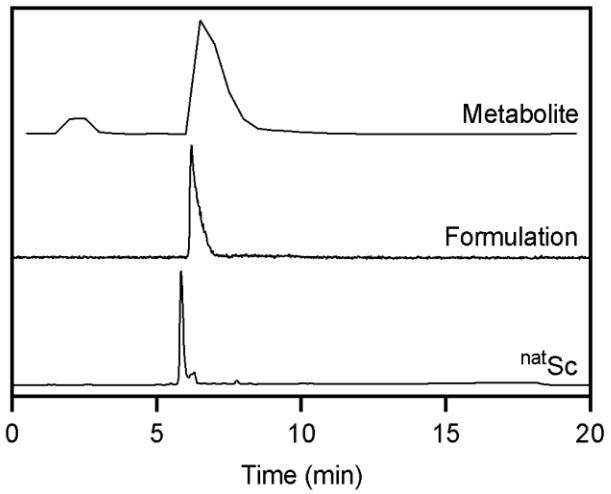


Figure S29. The RP-HPLC (Method B) analyses of $[^{nat}Sc][\ Sc(\mathbf{L^{201}})]$, $[^{44}Sc][Sc(\mathbf{L^{201}})]$ formulation, and urine metabolite.

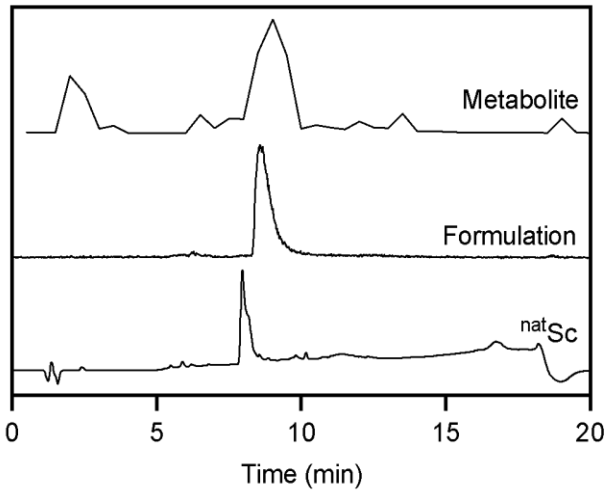


Figure S30. The RP-HPLC (Method B) analyses of [^{nat}Sc][Sc(**L**^{111})]$^+$, [^{44}Sc][Sc(**L**^{111})]$^+$ formulation, and urine metabolite.

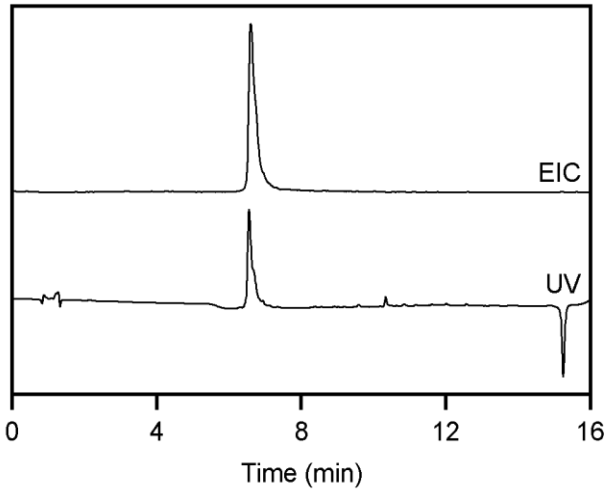


Figure S31. The UV (280 nm) and extracted ion (m/z = 525-527) LCMS (Method G) chromatograms of [Sc(**L**^{111})]$^+$.

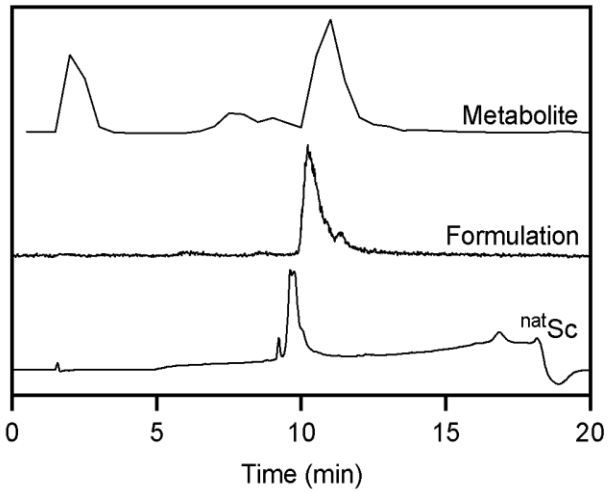


Figure S32. The RP-HPLC (Method B) analyses of $[^{nat}Sc][Sc(\mathbf{L^{021}})]^{2+}$, $[^{44}Sc][Sc(\mathbf{L^{021}})]^{2+}$ formulation, and urine metabolite.

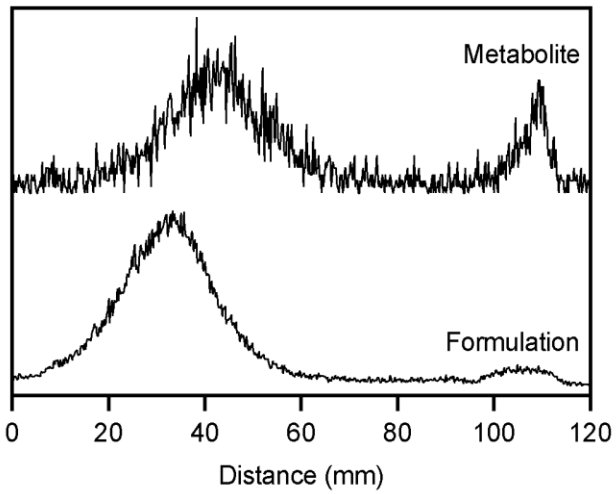


Figure S33. The iTLC (right) analyses of the $[^{44}Sc][Sc(\mathbf{L^{300}})]$ formulation and urine metabolite.

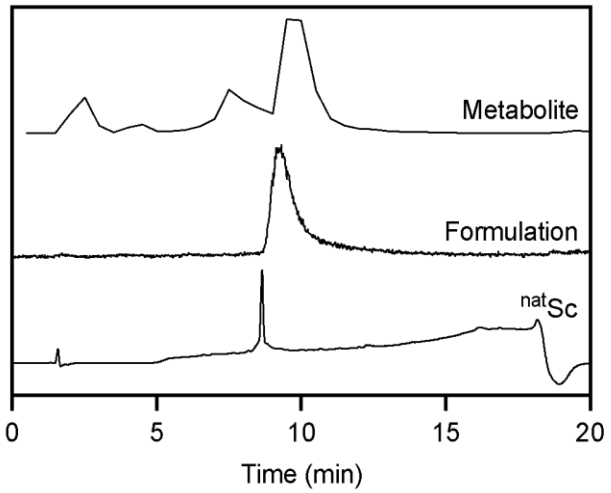


Figure S34. The RP-HPLC (Method B) analyses of $[^{nat}Sc][Sc(\mathbf{L^{210}})]^{+}$, the $[^{44}Sc][Sc(\mathbf{L^{210}})]^{+}$ formulation, and urine metabolite.

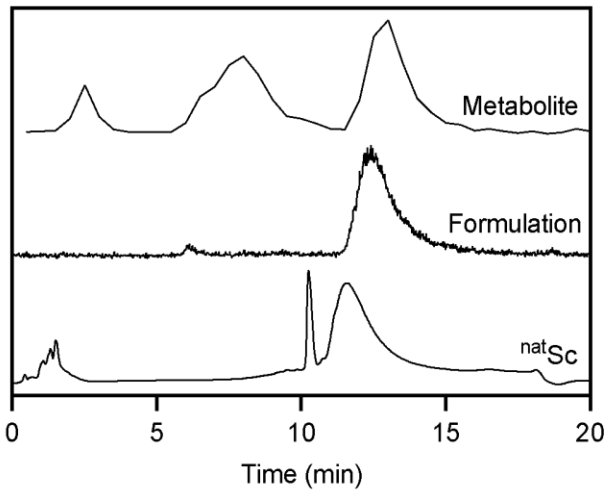


Figure S35. The RP-HPLC (Method B) analyses of $[^{nat}Sc][Sc(\mathbf{L^{120}})]^{2+}$, the $[^{44}Sc][Sc(\mathbf{L^{120}})]^{2+}$ formulation, and urine metabolite. Decomplexation of $[^{nat}Sc][Sc(\mathbf{L^{120}})]^{2+}$ was observed when using HPLC mobile phases containing TFA.

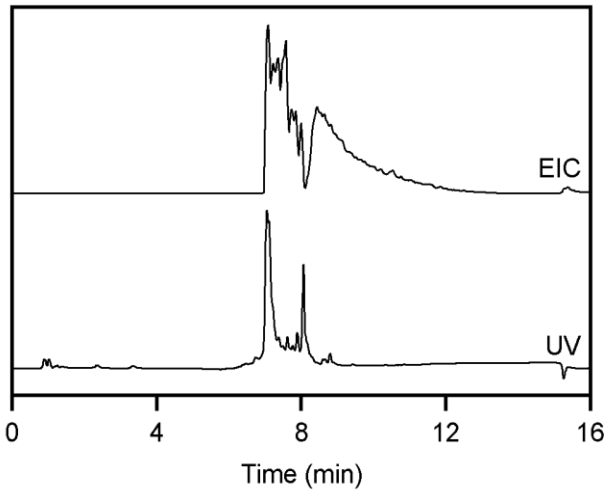


Figure S36. The UV (254 nm) and extracted ion (m/z = 597-599) LCMS (Method G) chromatograms of $[^{nat}Sc][Sc(\mathbf{L^{120}})]^{2+}$.

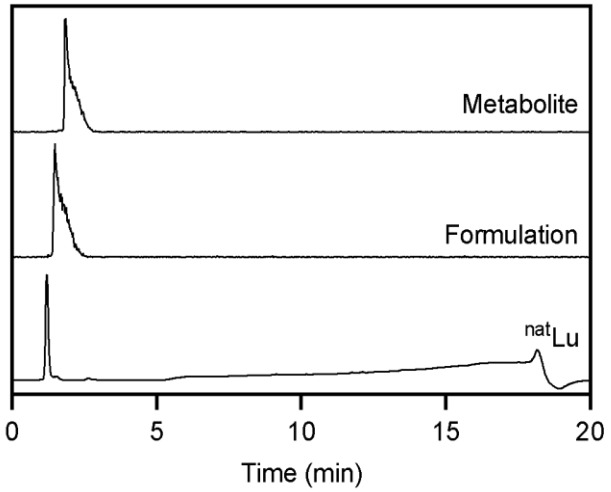


Figure S37. The RP-HPLC (Method A) analyses of $[^{nat}Lu]Lu(\mathbf{L^{201}})$, $[^{177}Lu]Lu(\mathbf{L^{201}})$ formulation, and urine metabolite.

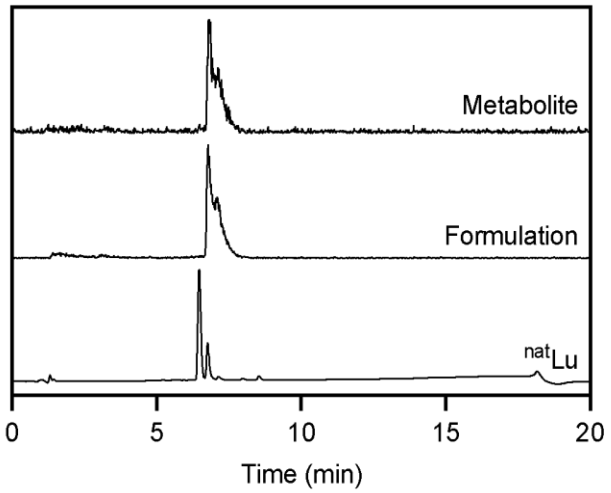


Figure S38. The RP-HPLC (Method A) analyses of $[^{nat}Lu][Lu(\mathbf{L^{111}})]^+$, $[^{177}Lu][Lu(\mathbf{L^{111}})]^+$ formulation, and urine metabolite.

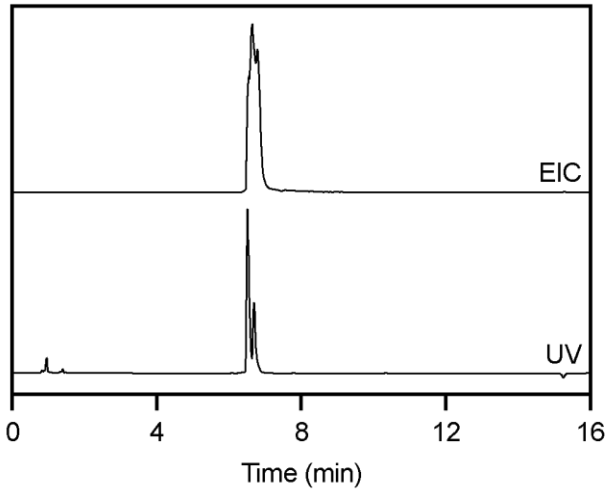


Figure S39. The UV (280 nm) and extracted ion (m/z = 655-657) LCMS (Method G) chromatograms of $[Lu(\mathbf{L^{111}})]^+$.

1.8 Speciation Studies

1.8.1 Speciation of $H_2\mathbf{L^{111}}$

L^{111} (130 µL, 19.23 mM, 0.0025 mmol), KCl (0.1888 g, 2.5 mmol), and HCl (0.2600g, 1 M, 0.25 mmol) were combined and diluted to 25.0 mL total volume to create the initial stock L^{111} solution at approximately pH 2 (0.1 mM H_2**L**^{111}, 0.1 M KCl, 0.01M HCl). Aliquots of 1 mL of the stock solution were removed, and the pH was adjusted via addition of 0.1 M KOH. Solutions were allowed to fully equilibrate over 24 hours prior to analysis. ^{1}H NMR spectra and pH measurements were recorded for each sample and speciation calculations were performed using the HypNMR2008 program. Speciation plots were generated 23 ^{1}H NMR from pH 2-12.

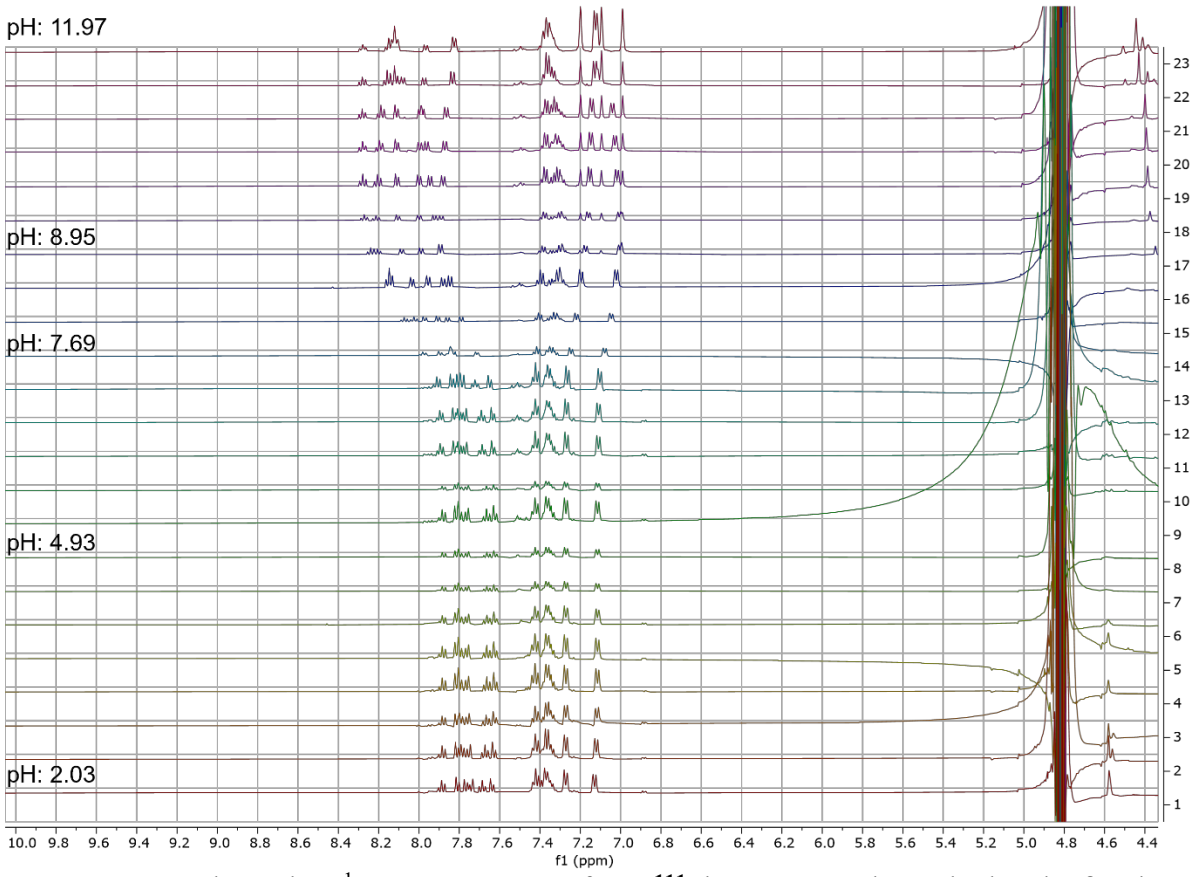


Figure S40. pH dependent ^{1}H NMR spectra of H_2**L**^{111} that were used to calculate logß values for **L**^{111}.

Table S11. Tabulated logß values for $H_2\mathbf{L}^{111}$.

Species	logß
H $\mathbf{L}^{111}$	12.97
H_2 $\mathbf{L}^{111}$	18.23
H_3 $\mathbf{L}^{111}$	22.49
H_4 $\mathbf{L}^{111}$	25.43

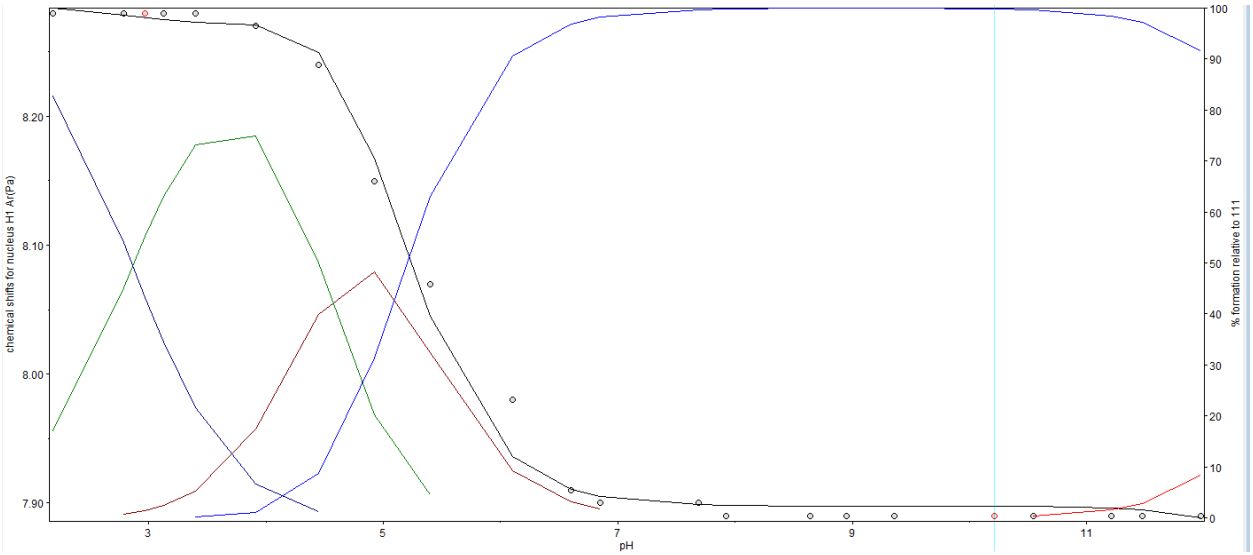


Figure S41. Representative data fit of ^{1}H NMR spectra of $H_2\mathbf{L}^{111}$in HYPNMR2008

1.8.2 Speciation of $[Sc(\mathbf{L^{111}})]^+$ and $[Lu(\mathbf{L^{111}})]^+$

$ScCl_3 \cdot 6H_2O$ (54.3 µL, 4.6 mM, 0.00025 mmol), $H_2\mathbf{L^{111}}$ (35.7 µL, 7.0 mM, 0.00025 mmol), KCl (0.1830 g, 2.5 mmol), and HCl (0.2549 g, 1 M, 0.25 mmol) were combined and diluted to 25.0 mL total volume to create the initial stock $[Sc(\mathbf{L^{111}})]^+$ solution at approximately pH 2 (0.01 mM $H_2\mathbf{L^{111}}$, 0.01 mM Sc^{3+}, 0.1 M KCl, 0.01M HCl). LuCl3·6H2O (33 µL, 7.5 mM, 0.00025 mmol), $H_2\mathbf{L^{111}}$ (33 µL, 7.6 mM, 0.00025 mmol), KCl (0.1850 g, 2.5 mmol), and HCl (0.2568 g, 1 M, 0.25 mmol) were combined and diluted to 25.0 mL total volume to create the initial $[Lu(\mathbf{L^{111}})]^+$ stock solution at approximately pH 2 (0.01 mM $H_2\mathbf{L^{111}}$, 0.01 mM Lu^{3+}, 0.1 M KCl, 0.01M HCl). Aliquots of 1 mL of the stock solution were removed, and the pH was adjusted via addition of 0.1 M KOH. Solutions were allowed to fully equilibrate over 48 hours prior to analysis. UV-visible spectra and pH measurements were recorded for each sample, and speciation calculations were performed using the HypSpec2014 program. The appearance of a peak at 280 nm in the $[Sc(\mathbf{L^{111}})]^+$ speciation was taken as the binding of Sc^{3+} to $H_2\mathbf{L^{111}}$, and an increase at 207 nm as the formation of the hydroxide species. The appearance of a peak at 280 nm in the $[Lu(\mathbf{L^{111}})]^+$ speciation was taken as the binding of Lu^{3+} to $H_2\mathbf{L^{111}}$, and an increase at 207 nm as the formation of the hydroxide species. For both systems, speciation plots were generated using 23 UV-vis spectra from pH 1.5-12.

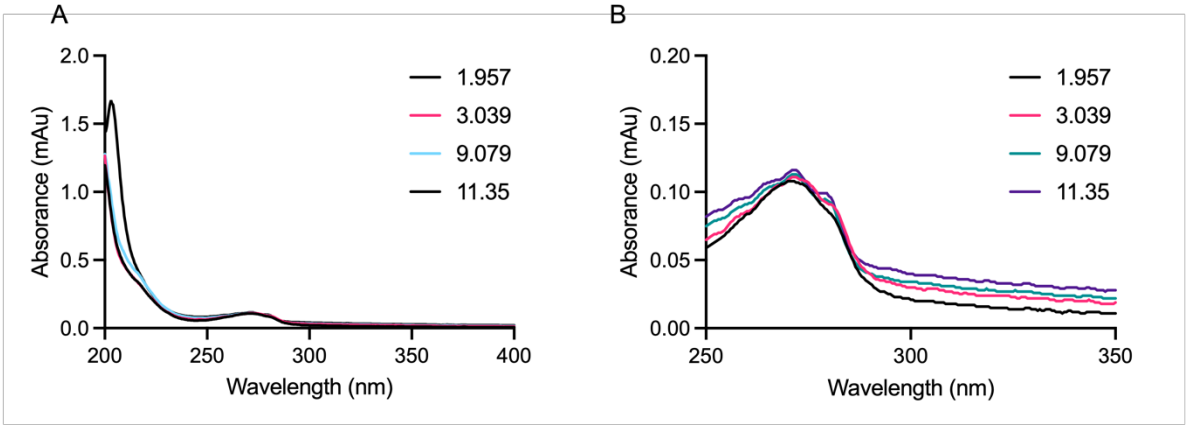


Figure S42. a) Select pH dependent UV-vis spectra of $[Sc(\mathbf{L^{111}})]^+$ that were used to calculate logß values for $[Sc(\mathbf{L^{111}})]^+$. b) Enhanced region to show subtle differences in UV-vis absorbance.

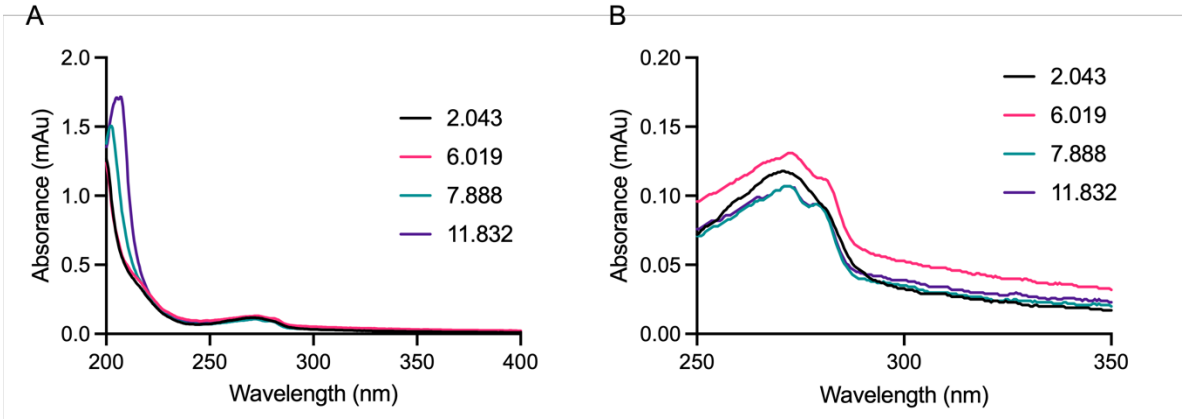


Figure S43. a) Select pH dependent UV-vis spectra of $[Lu(\mathbf{L^{111}})]^+$ that were used to calculate logß values for $[Lu(\mathbf{L^{111}})]^+$. b) Enhanced region to show subtle differences in UV-vis absorbance.

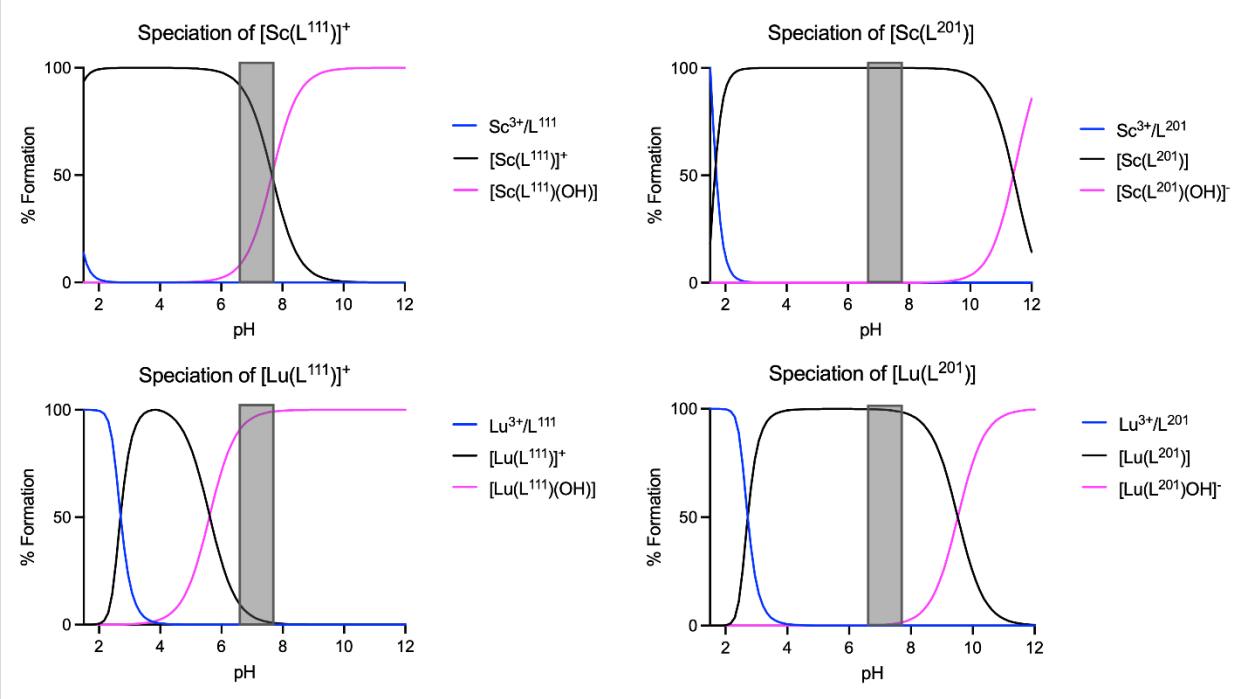


Figure S44. Speciation plots of $[M(L^{111})]^+$ and $[M(L^{201})]$ ($M = Sc^{3+}$, Lu^{3+}). The grey box denotes physiologically relevant pH (7.4).

Table S12. Thermodynamic and spectroscopic parameters for [Sc(L)] and [Lu(L)] ($ML/_{110}$ and $MLOH/_{111}$species). Values for L^{201} come from previous work.

Parameter	$M = Sc^{3+}$ $L^{xxx} = L^{111}$	$M = Lu^{3+}$ $L^{xxx} = L^{111}$	$M = Sc^{3+}$ $L^{xxx} = L^{201}$	$M = Lu^{3+}$ $L^{xxx} = L^{201}$
$\log \beta_{110/} \log K_{ML}$	26.8	20.1	21.3	17.5
$\log \beta_{111/} \log K_{MLOH}$	19.1	14.5	9.8	8
pM	23.4	18.3	17.8	16.5
pKa_{ML}	0.74	2.6	1.6	2.5
pKa_{MLOH}	7.7	5.6	11.5	9.5

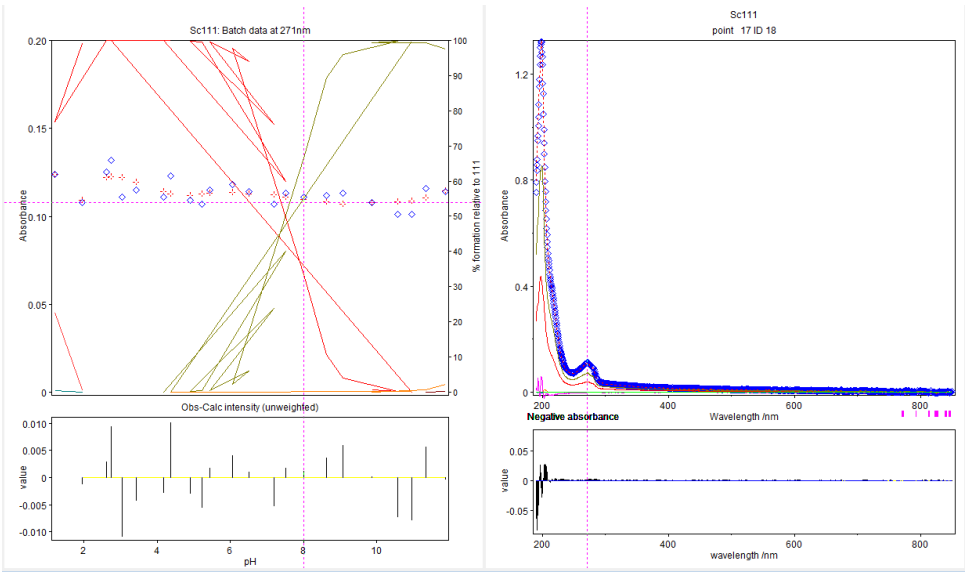


Figure S45. Representative data fit of UV-Vis spectra of $[Sc(\mathbf{L}^{\mathbf{111}})]^{+}$ in HYPSPEC2014

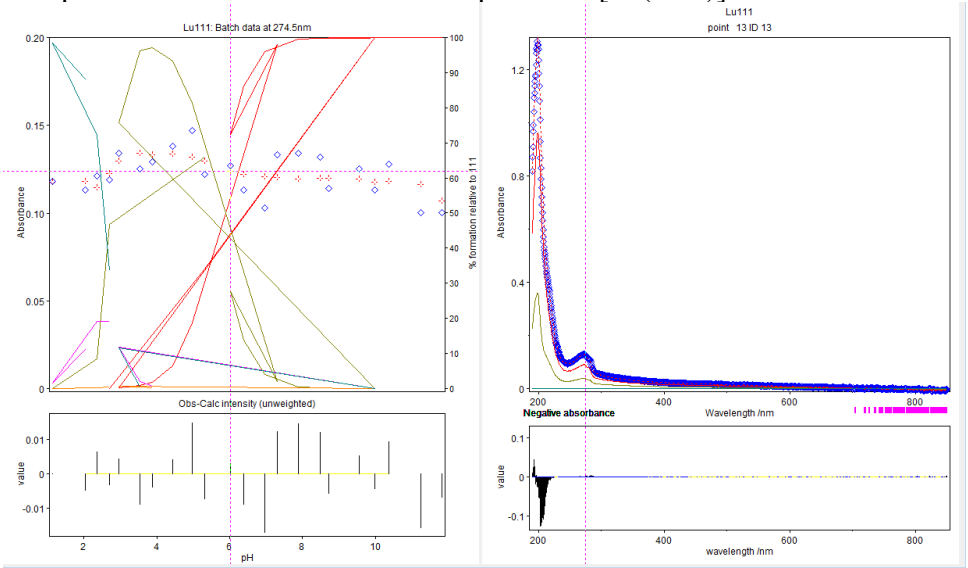


Figure S46. Representative data fit of UV-Vis spectra of $[Lu(\mathbf{L}^{\mathbf{111}})]^{+}$ in HYPSPEC2014

2 Ligand and Complex Characterization Data

2.1 NMR Characterization

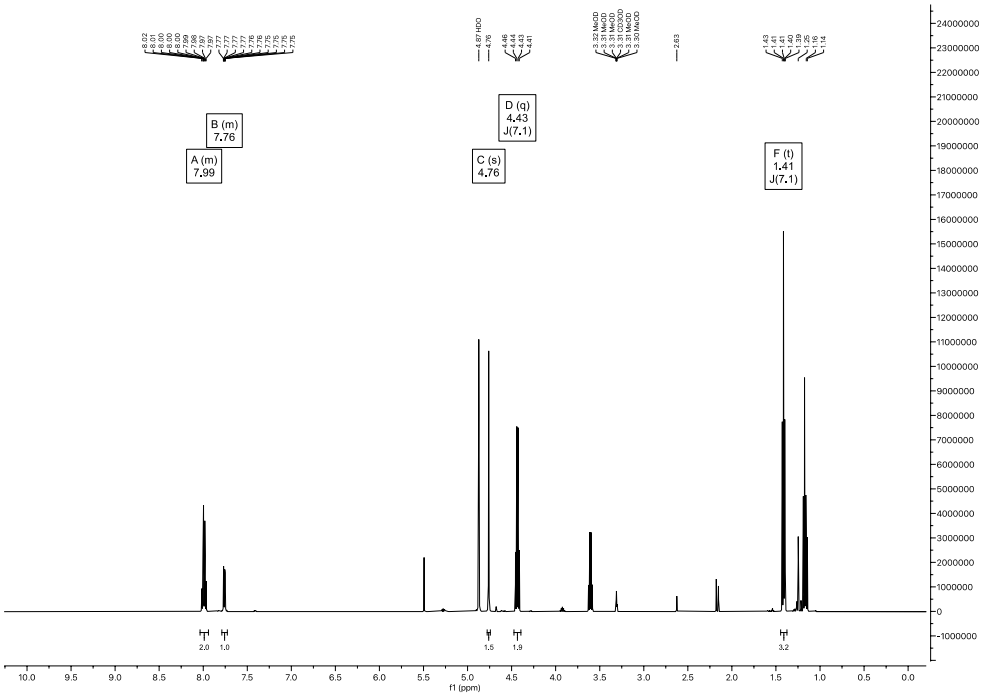


Figure S47 The ^{1}H NMR spectrum of ethyl 6-(hydroxymethyl)picolinate in MeOD.

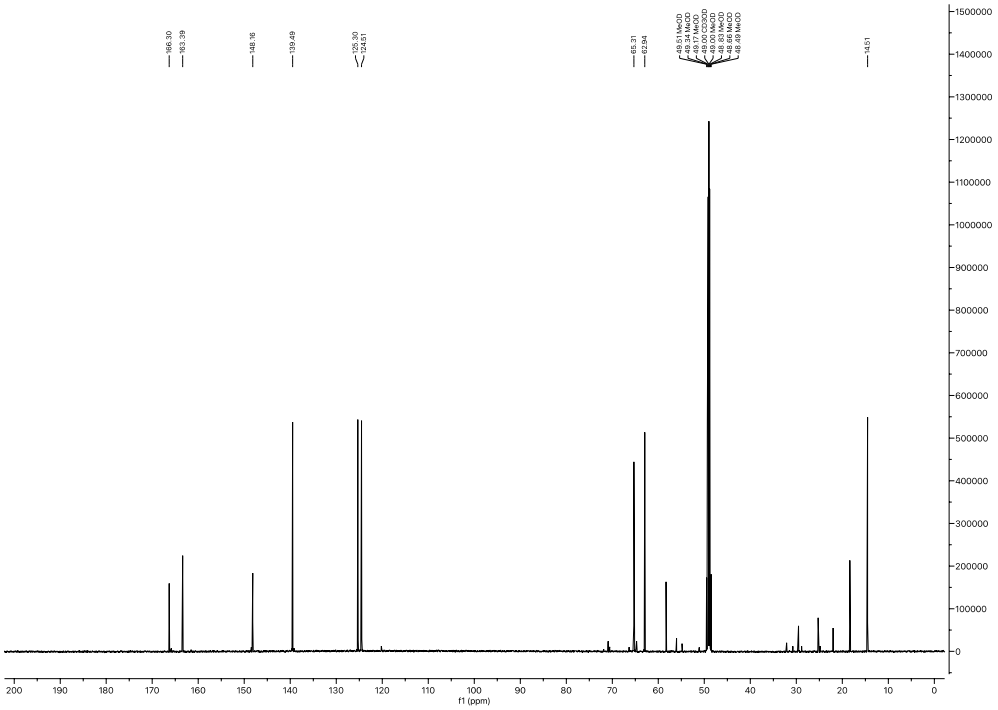


Figure S48 The $^{13}C\{^{1}H\}$ NMR spectrum of ethyl 6-(hydroxymethyl)picolinate in MeOD.

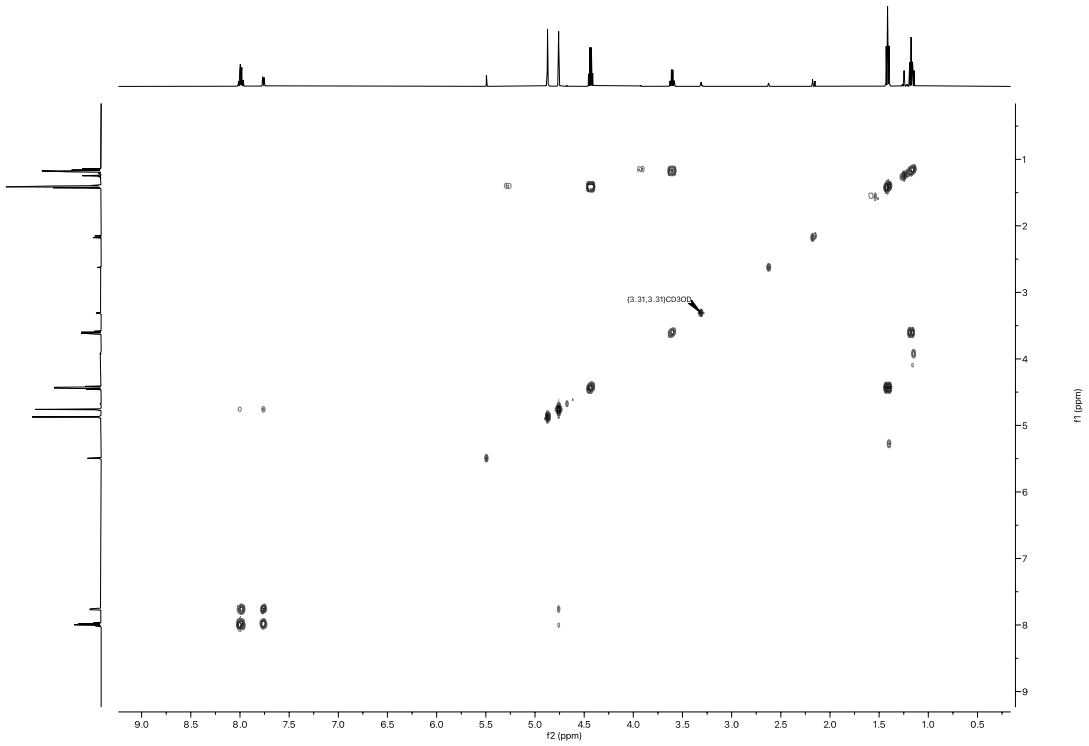


Figure S49 The ^{1}H-^{1}H COSY NMR spectrum of ethyl 6-(hydroxymethyl)picolinate in MeOD.

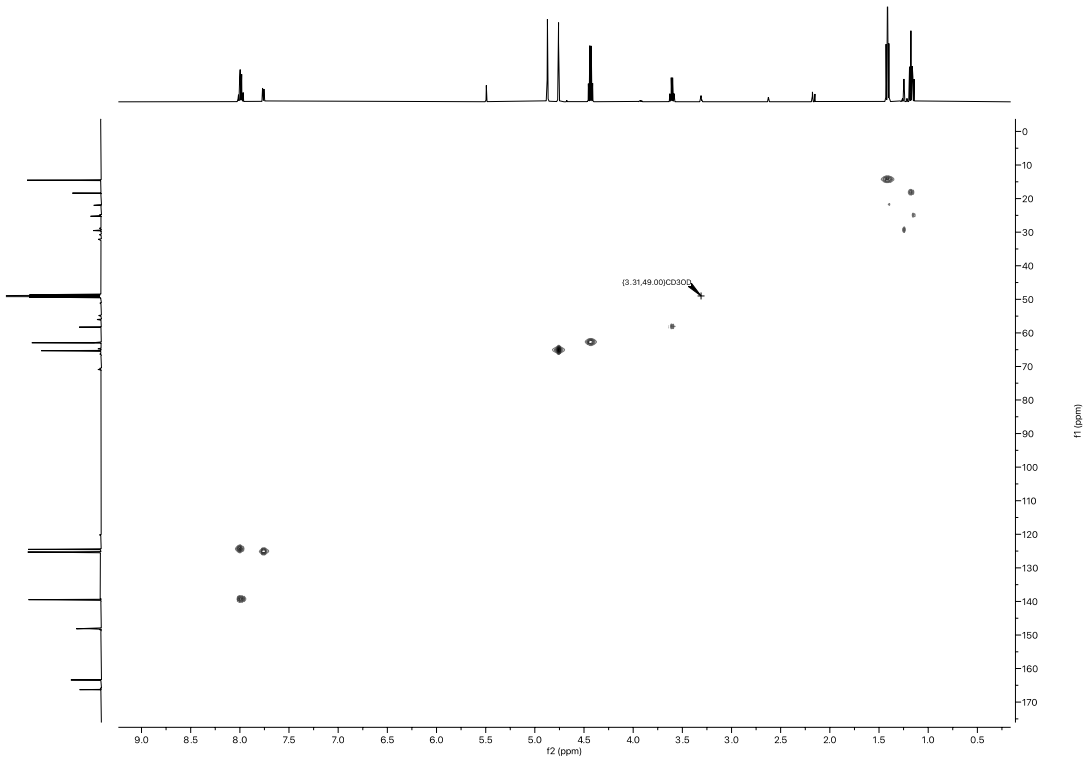


Figure S50 The ^{1}H-^{13}C HSQC NMR spectrum of ethyl 6-(hydroxymethyl)picolinate in MeOD.

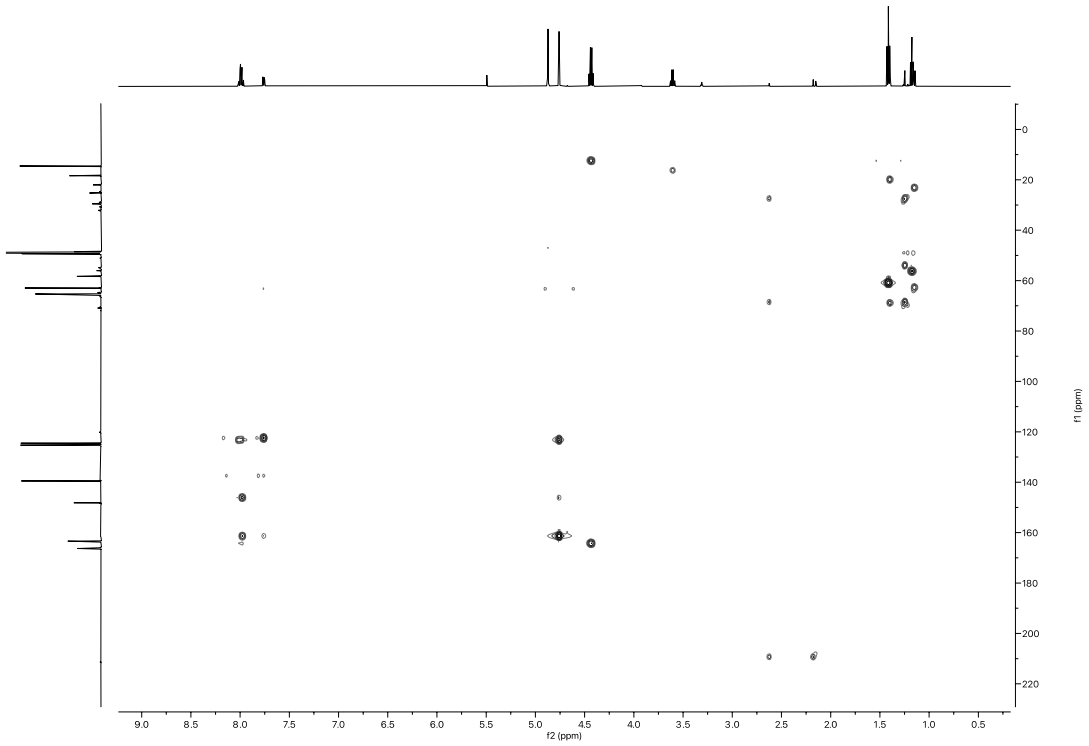


Figure S51 The ^{1}H-^{13}C HMBC NMR spectrum of ethyl 6-(hydroxymethyl)picolinate in MeOD.

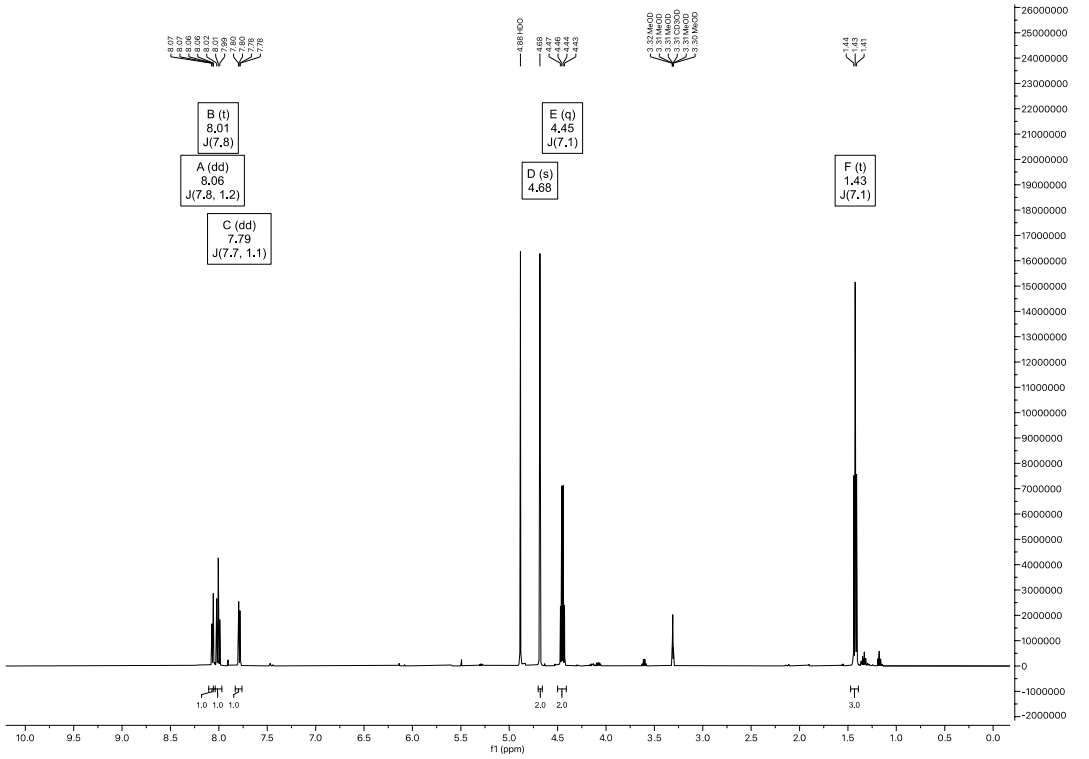


Figure S52 The ^{1}H NMR spectrum of ethyl 6-(bromomethyl)picolinate in MeOD.

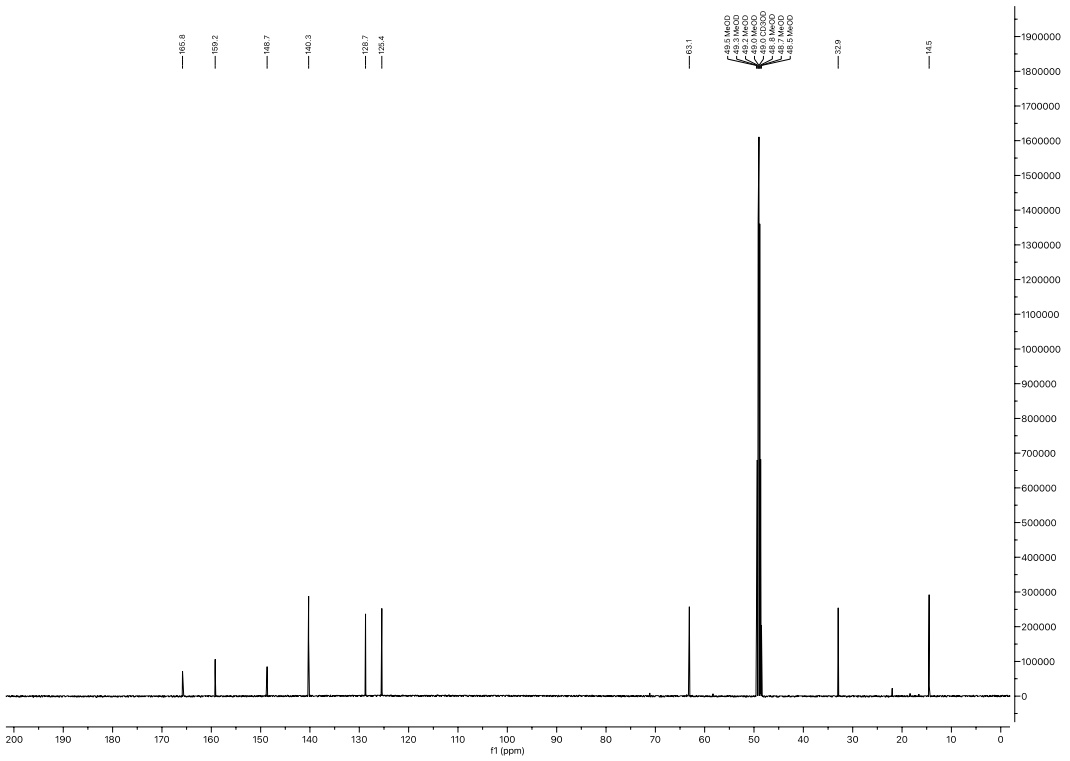


Figure S53 The $^{13}C\{^{1}H\}$ NMR spectrum of ethyl 6-(bromomethyl)picolinate in MeOD.

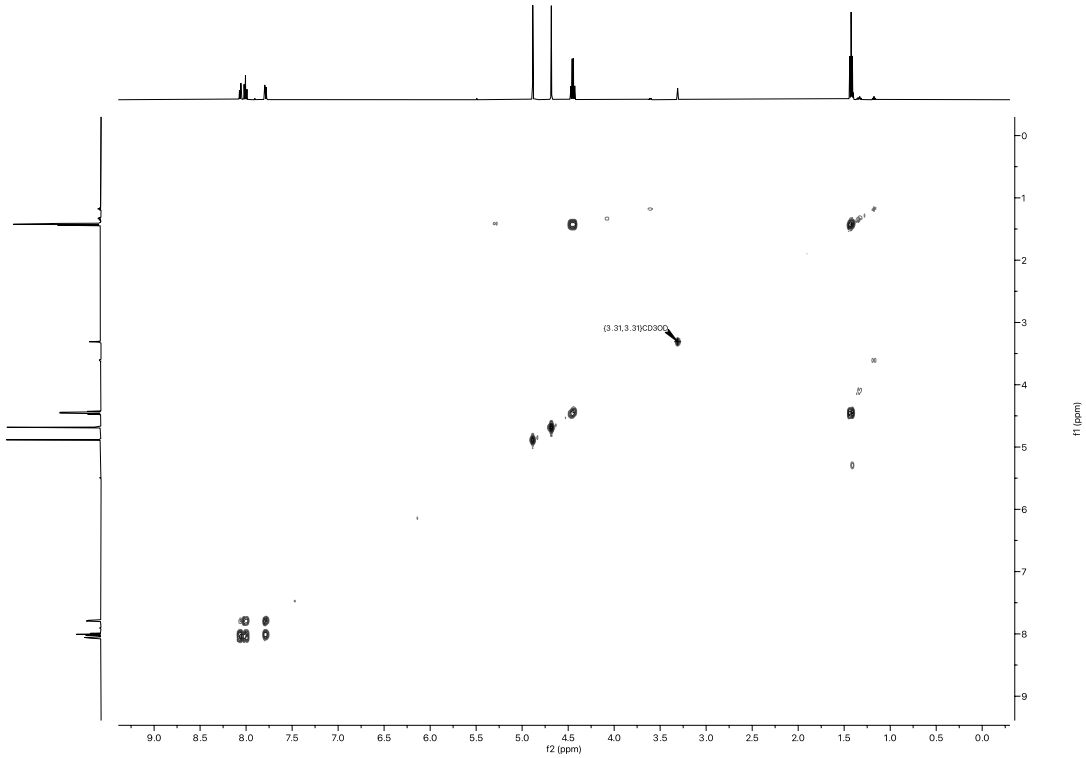


Figure S54 The ^{1}H-^{1}H COSY NMR spectrum of ethyl 6-(bromomethyl)picolinate in MeOD.

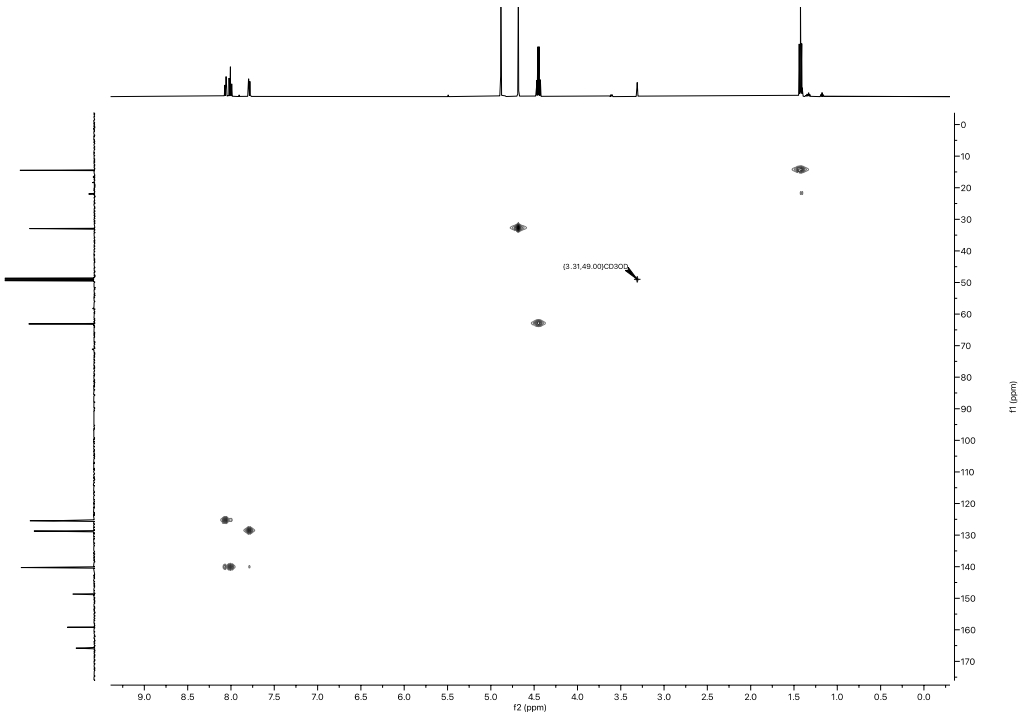


Figure S55 The ^{1}H-^{13}C HSQC NMR spectrum of ethyl 6-(bromomethyl)picolinate in MeOD.

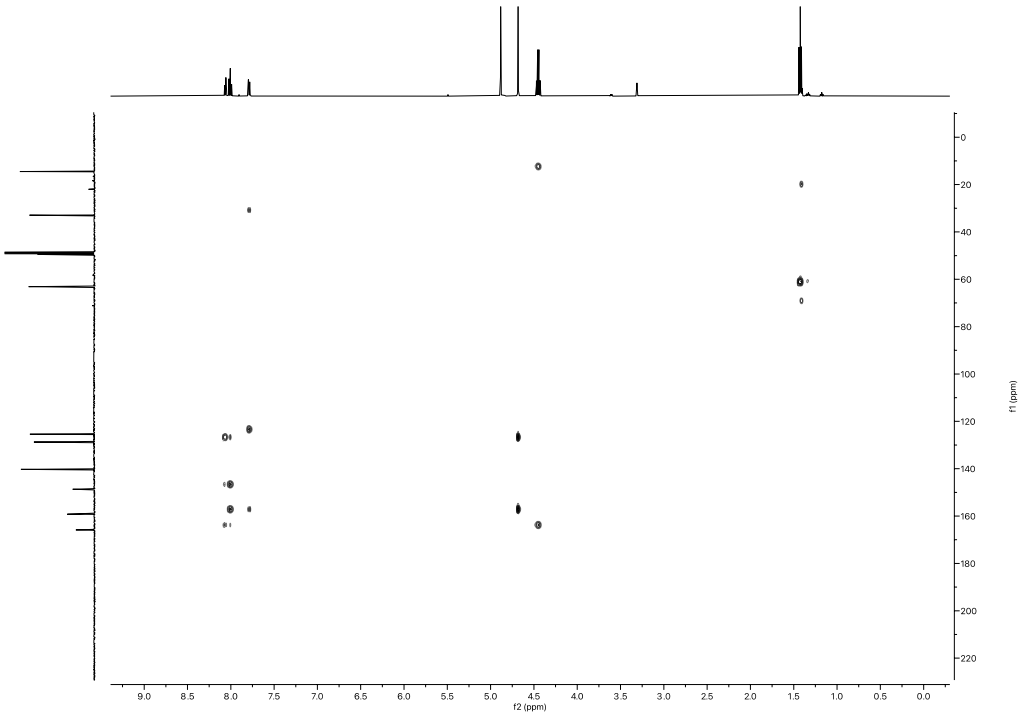


Figure S56 The ^{1}H-^{13}C HMBC NMR spectrum of ethyl 6-(bromomethyl)picolinate in MeOD.

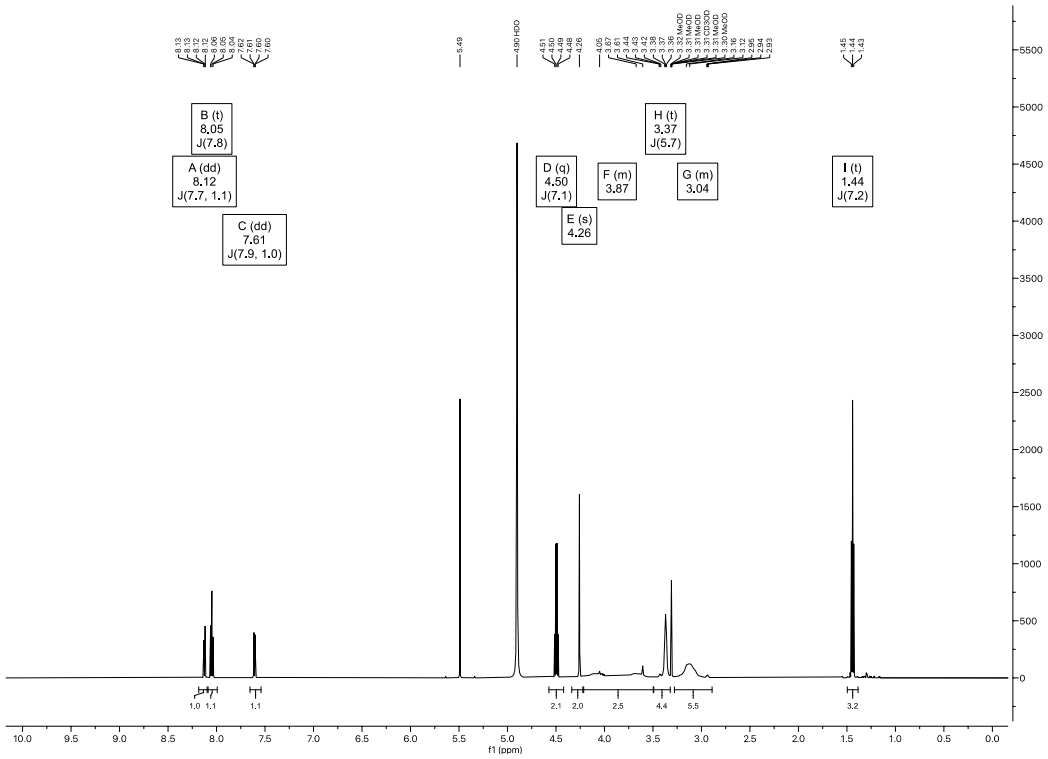


Figure S57 The ^{1}H NMR spectrum of monoPic in MeOD.

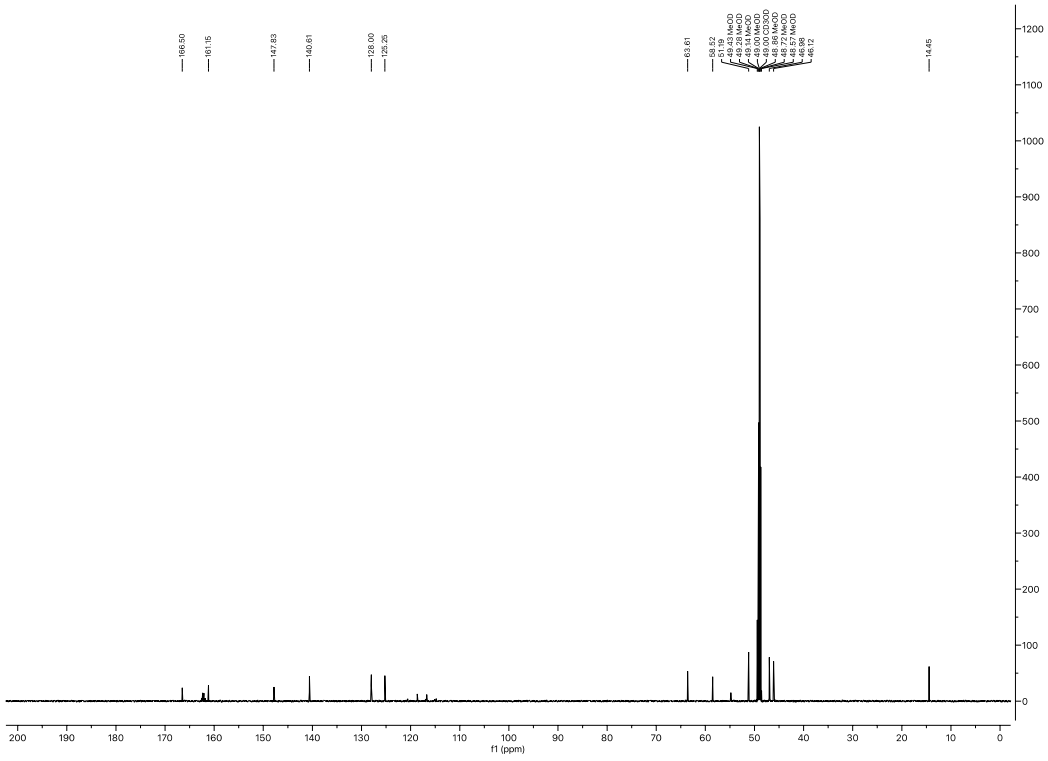


Figure S58 The ^{13}C{^{1}H} NMR spectrum of monoPic in MeOD.

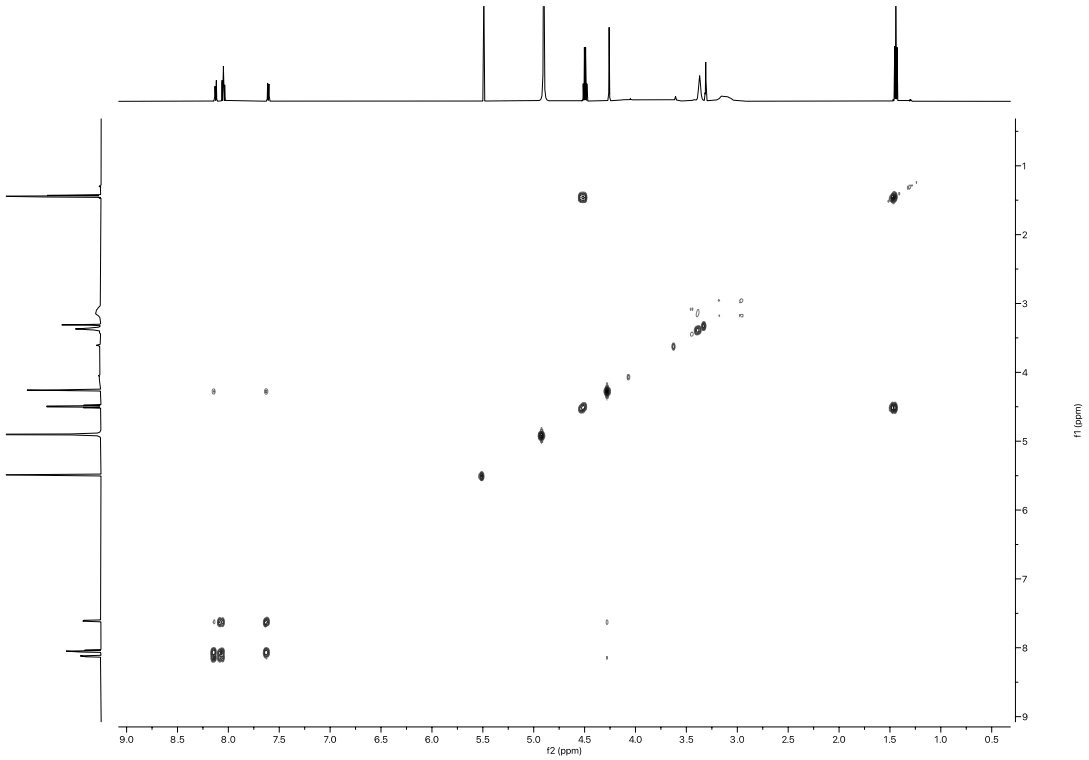


Figure S59 The ^{1}H-^{1}H COSY NMR spectrum of monoPic in MeOD.

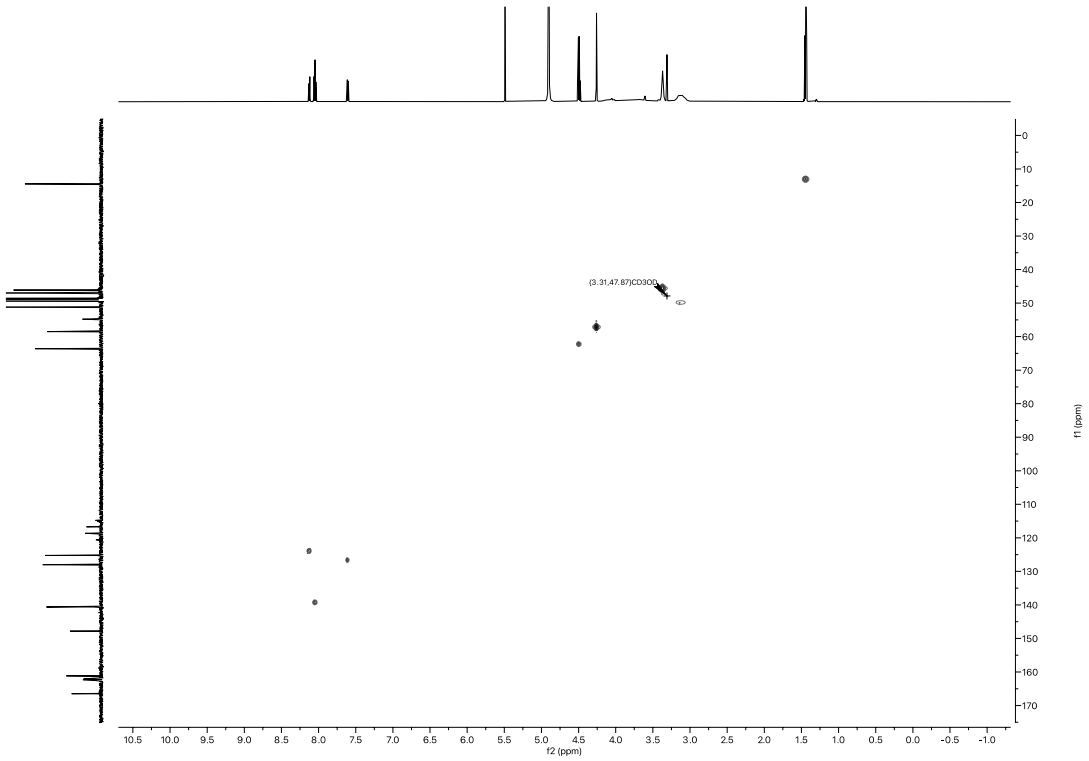


Figure S60 The ^{1}H-^{13}C HSQC NMR spectrum of monoPic in MeOD.

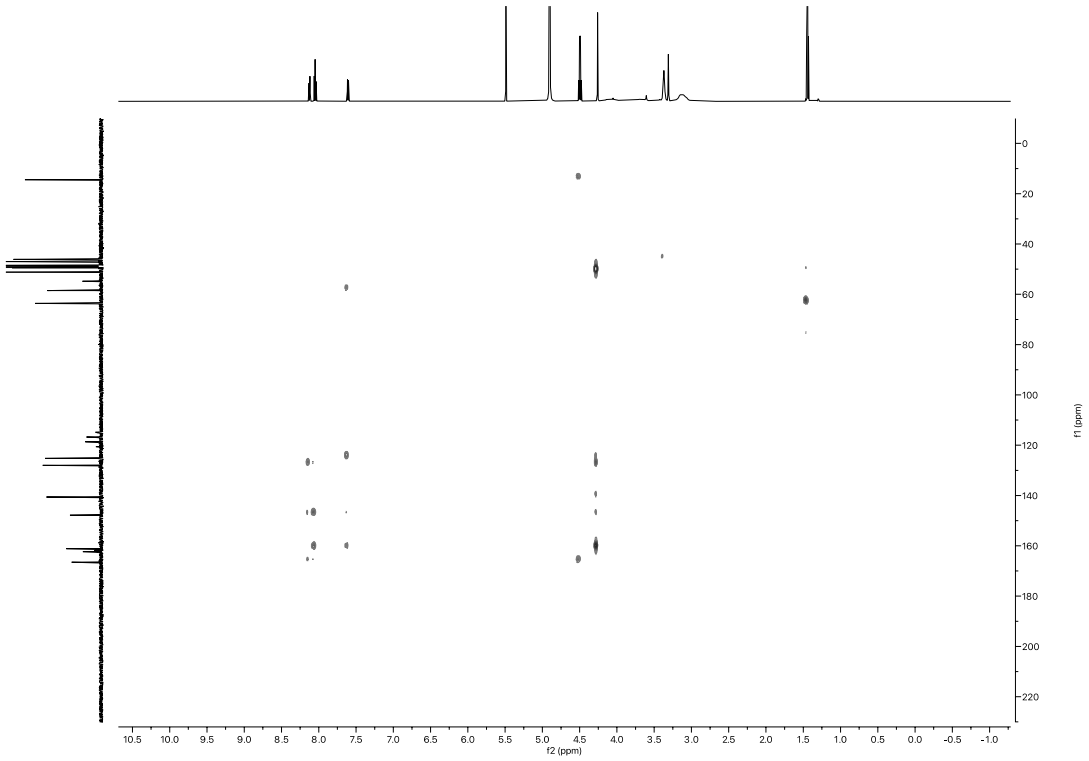


Figure S61 The ^{1}H-^{13}C HMBC NMR spectrum of monoPic in MeOD.

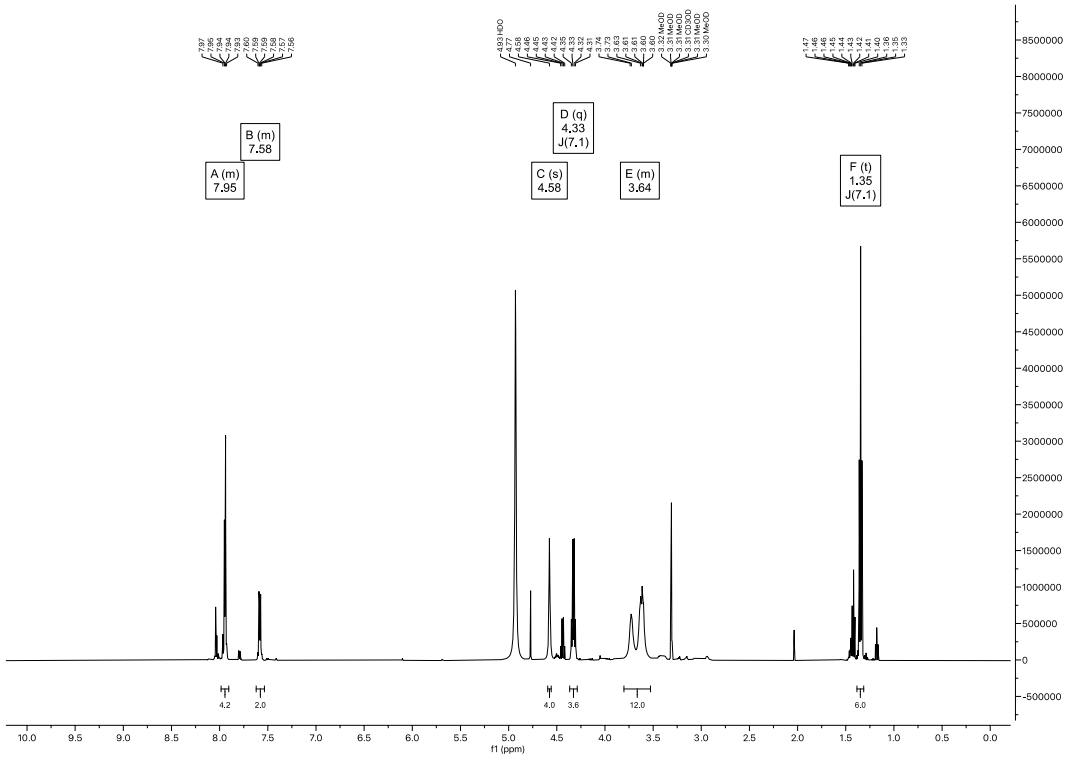


Figure S62 The ^{1}H NMR spectrum of diPic in MeOD.

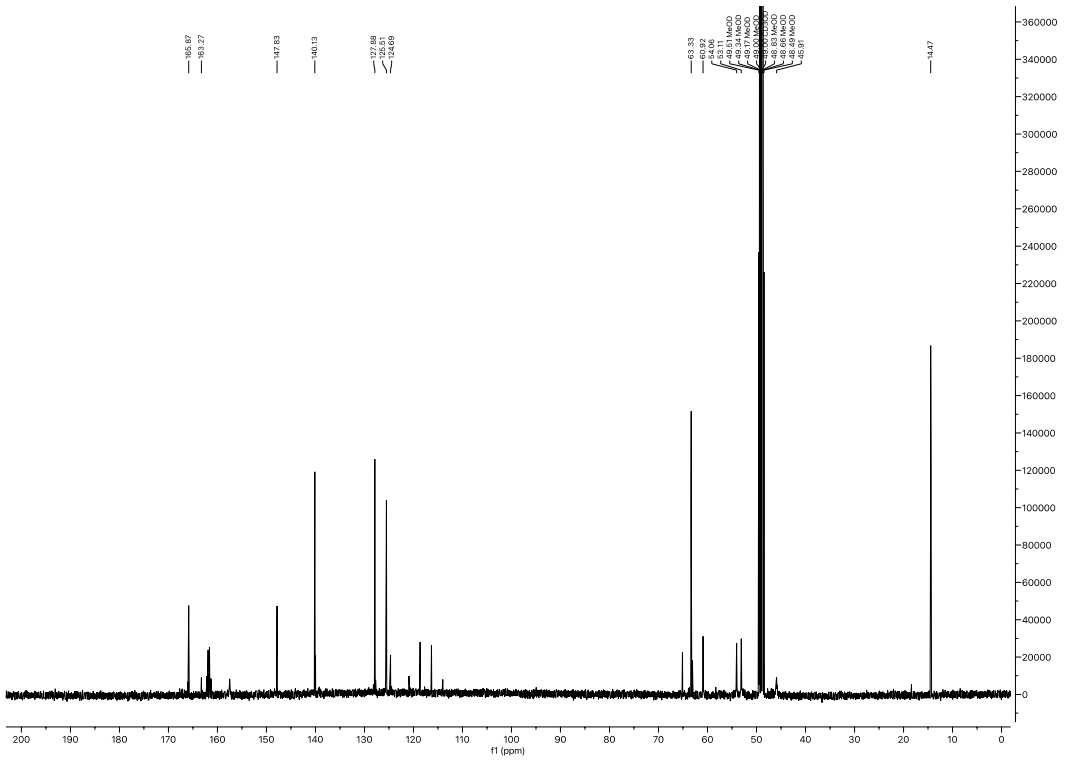


Figure S63 The $^{13}C\{^{1}H\}$ NMR spectrum of diPic in MeOD.

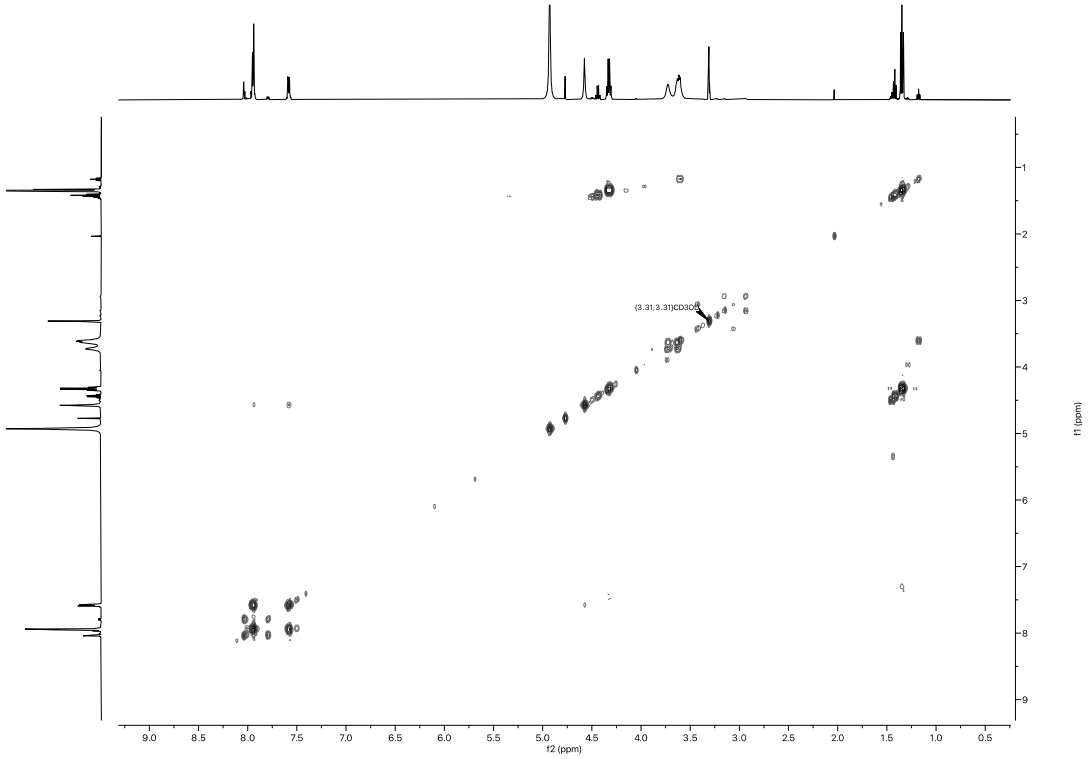


Figure S64 The ^{1}H-^{1}H COSY NMR spectrum of diPic in MeOD.

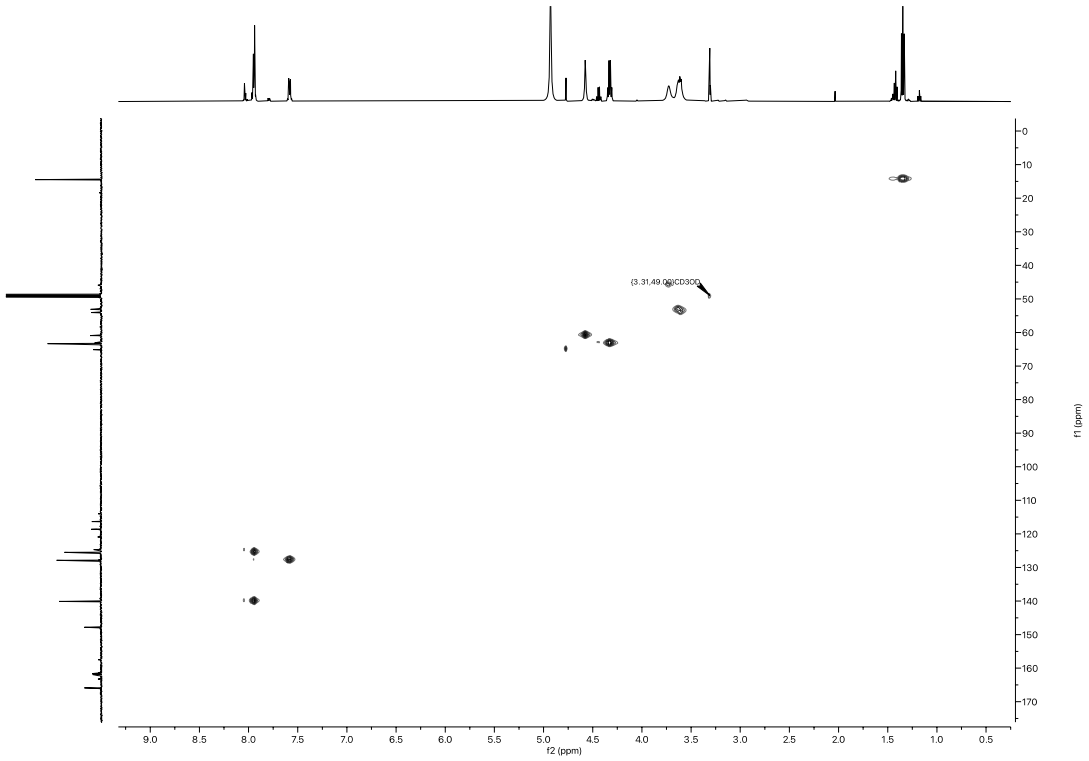


Figure S65 The ^{1}H-^{13}C HSQC NMR spectrum of diPic in MeOD.

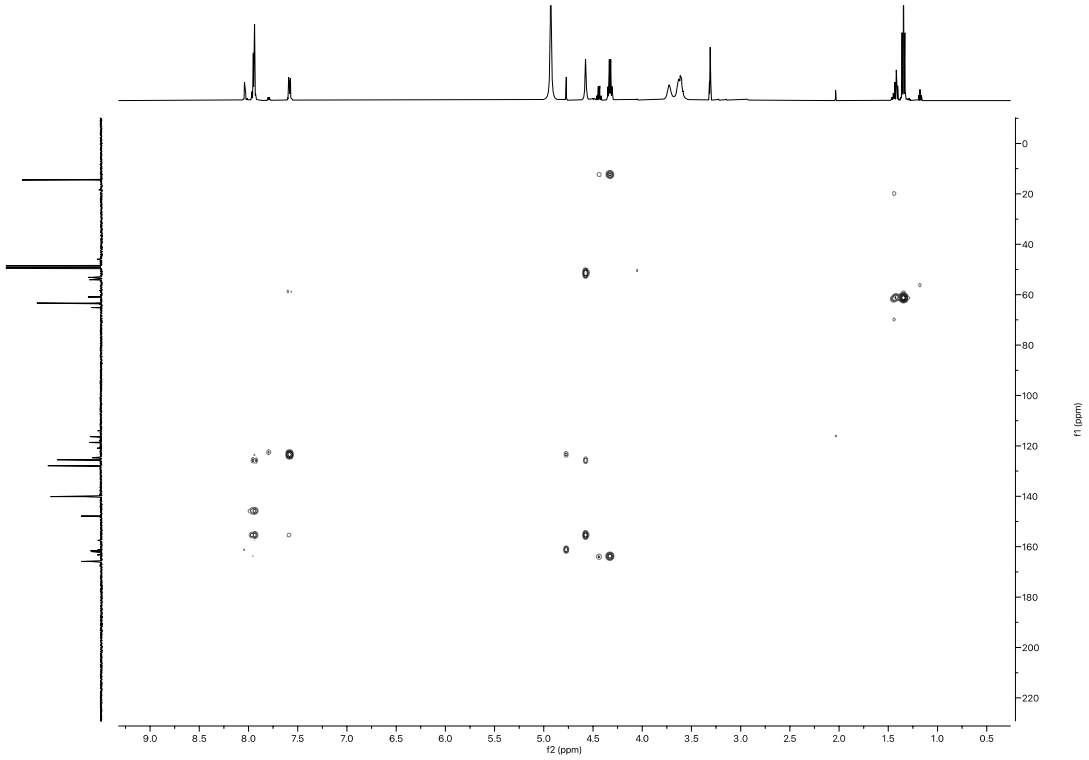


Figure S66 The ^{1}H-^{13}C HMBC NMR spectrum of diPic in MeOD.

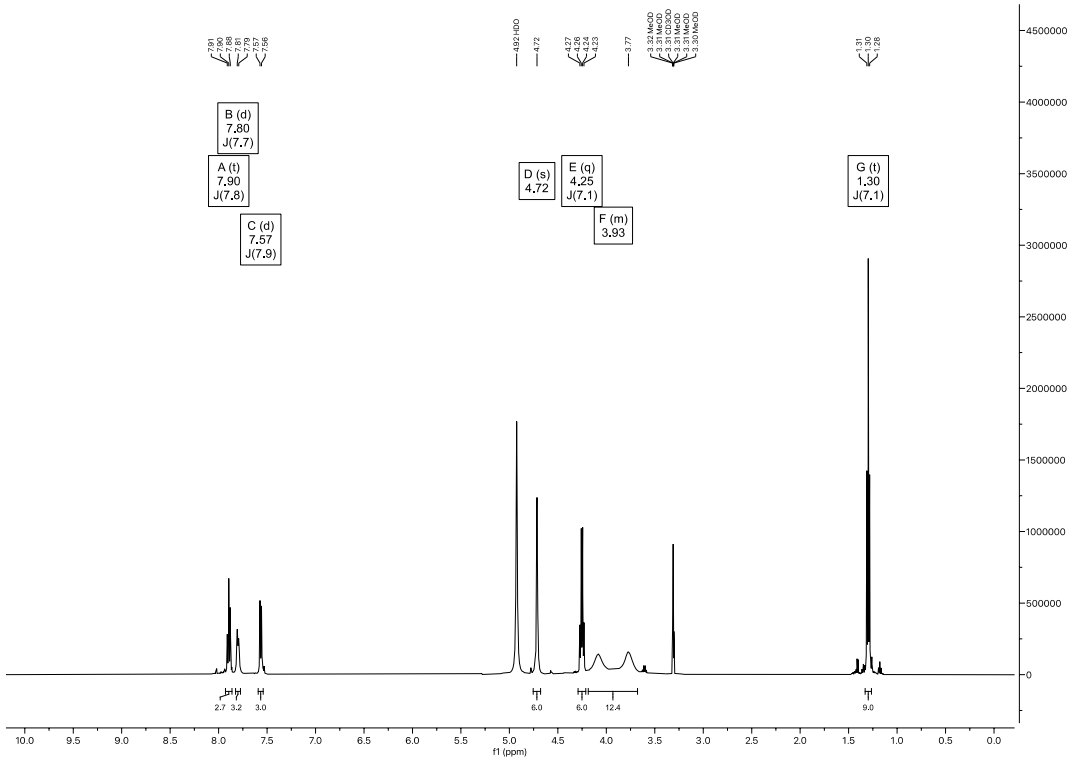


Figure S67 The ^{1}H NMR spectrum of triPic in MeOD.

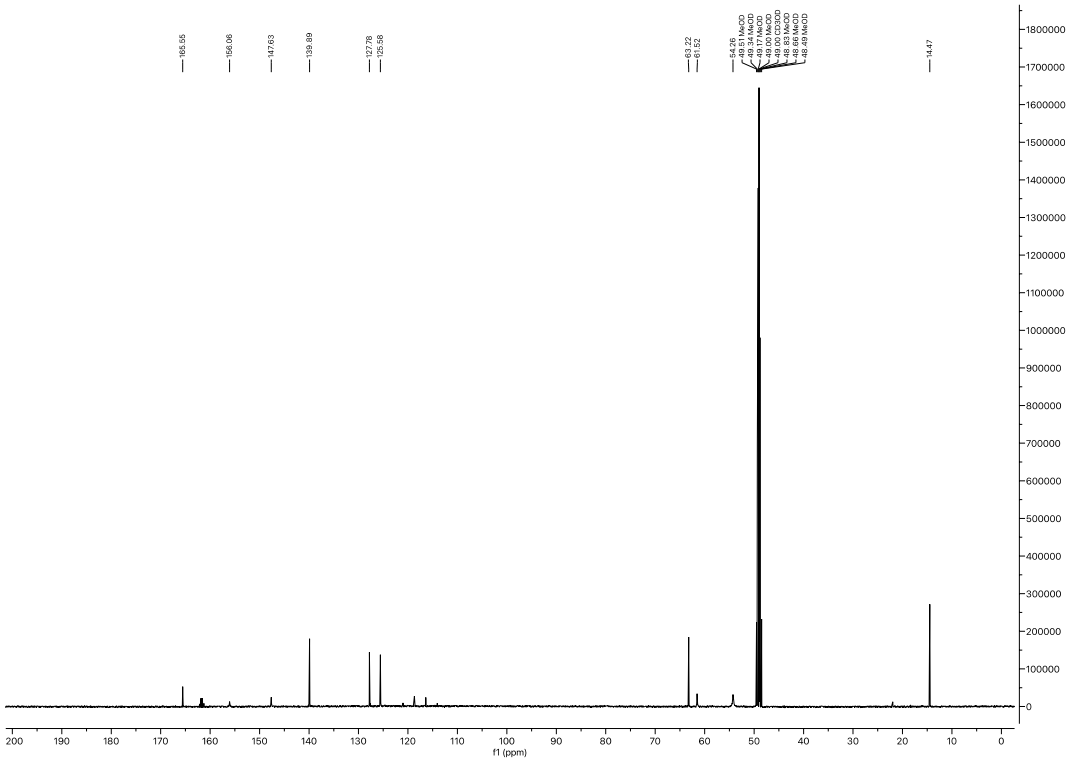


Figure S68 The ^{13}C{^{1}H} NMR spectrum of triPic in MeOD

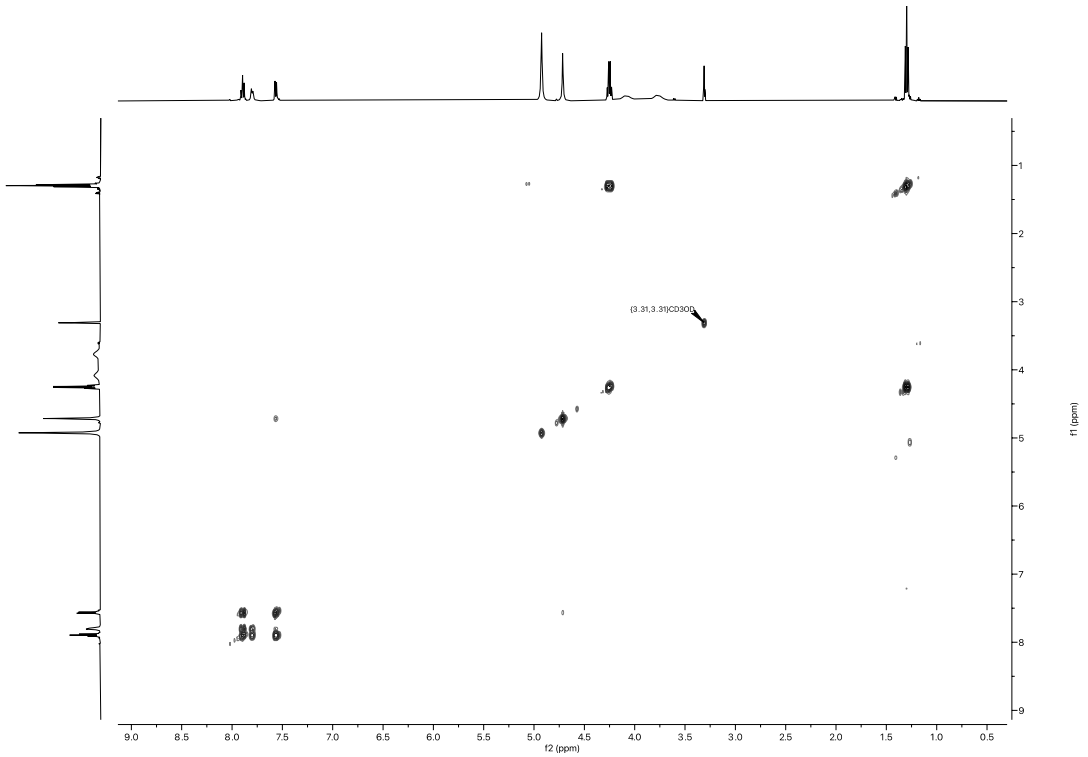


Figure S69 The ^{1}H-^{1}H COSY NMR spectrum of triPic in MeOD.

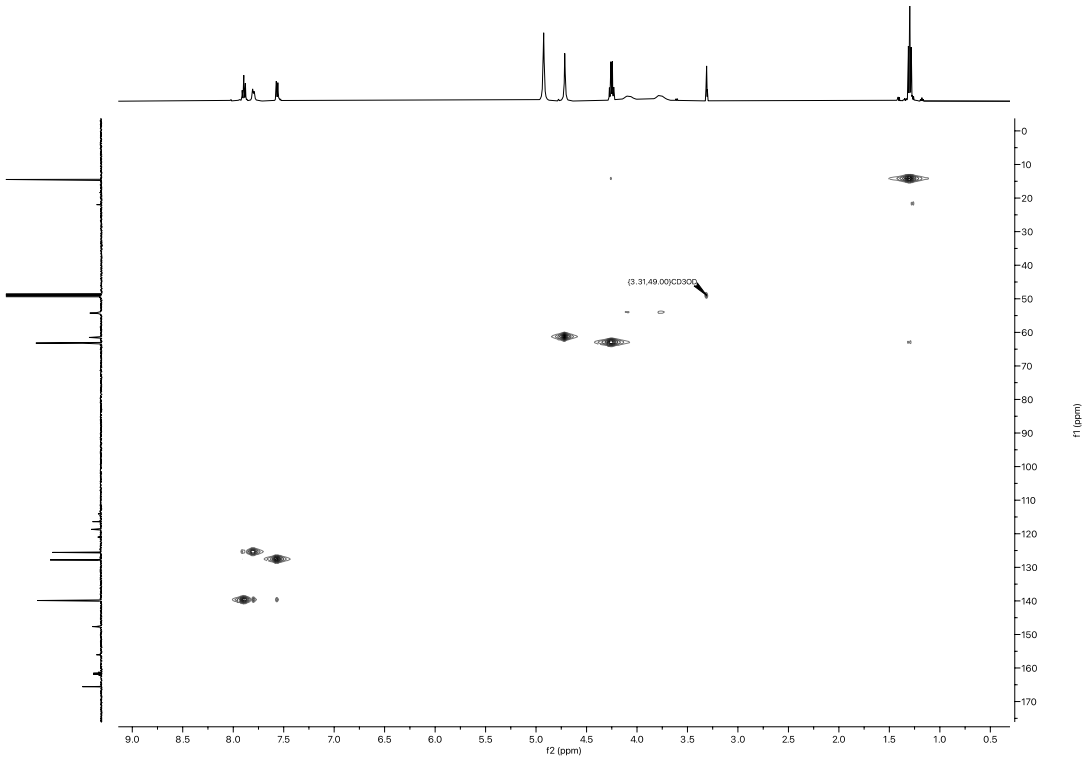


Figure S70 The ^{1}H-^{13}C HSQC NMR spectrum of triPic in MeOD.

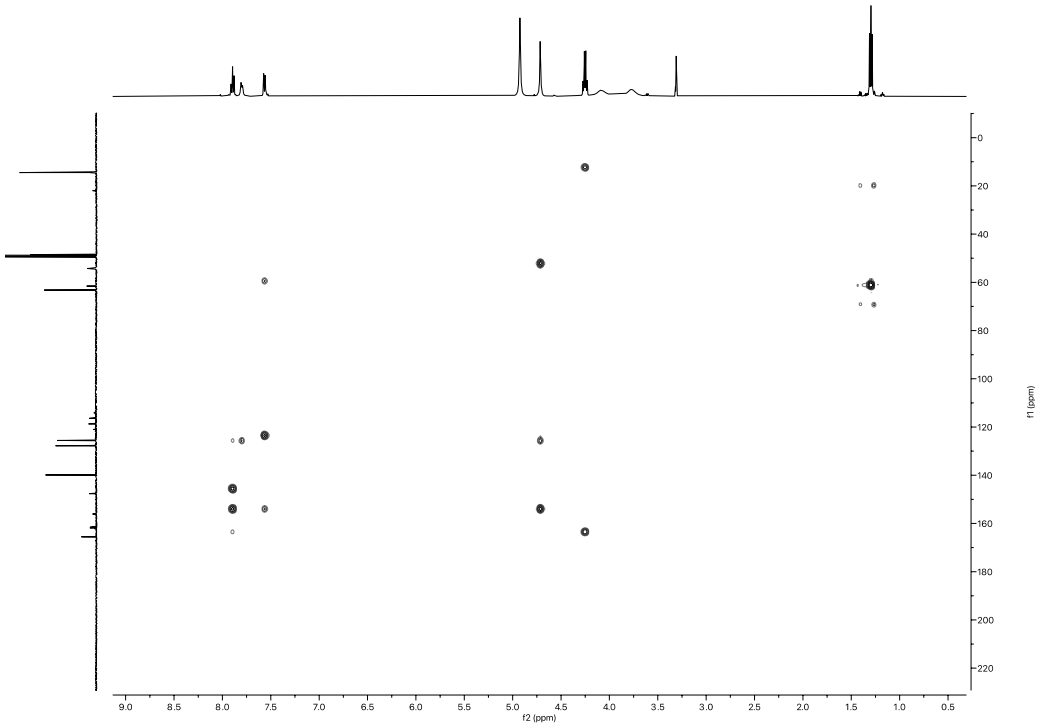


Figure S71 The ^{1}H-^{13}C HMBC NMR spectrum of triPic in MeOD.

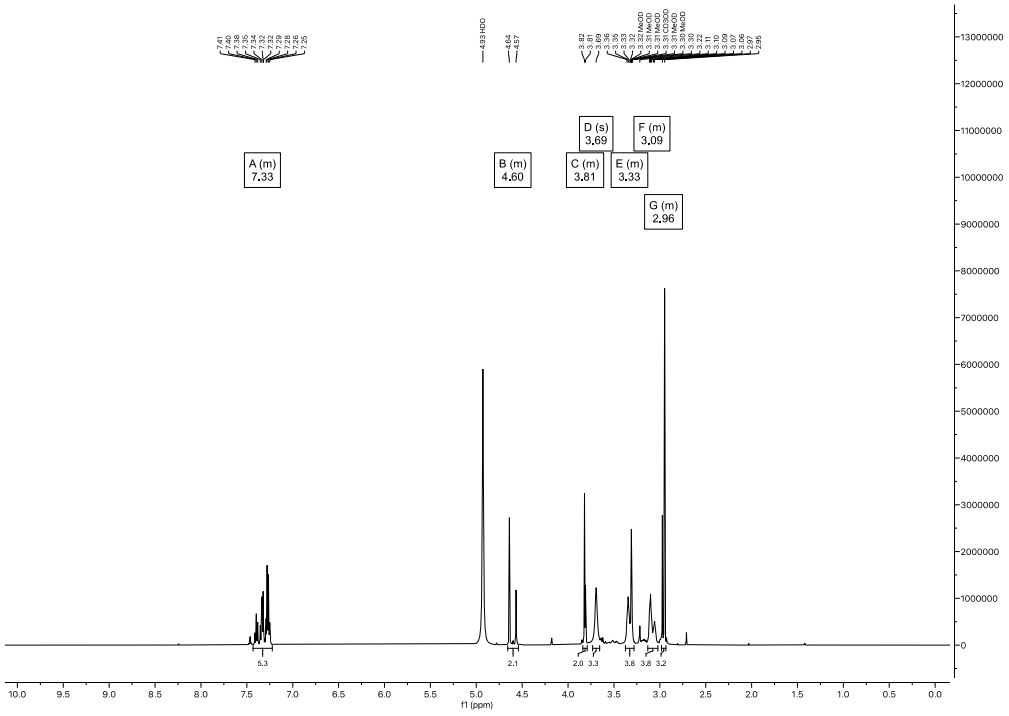


Figure S72 The ^{1}H NMR spectrum of monoAm in MeOD.

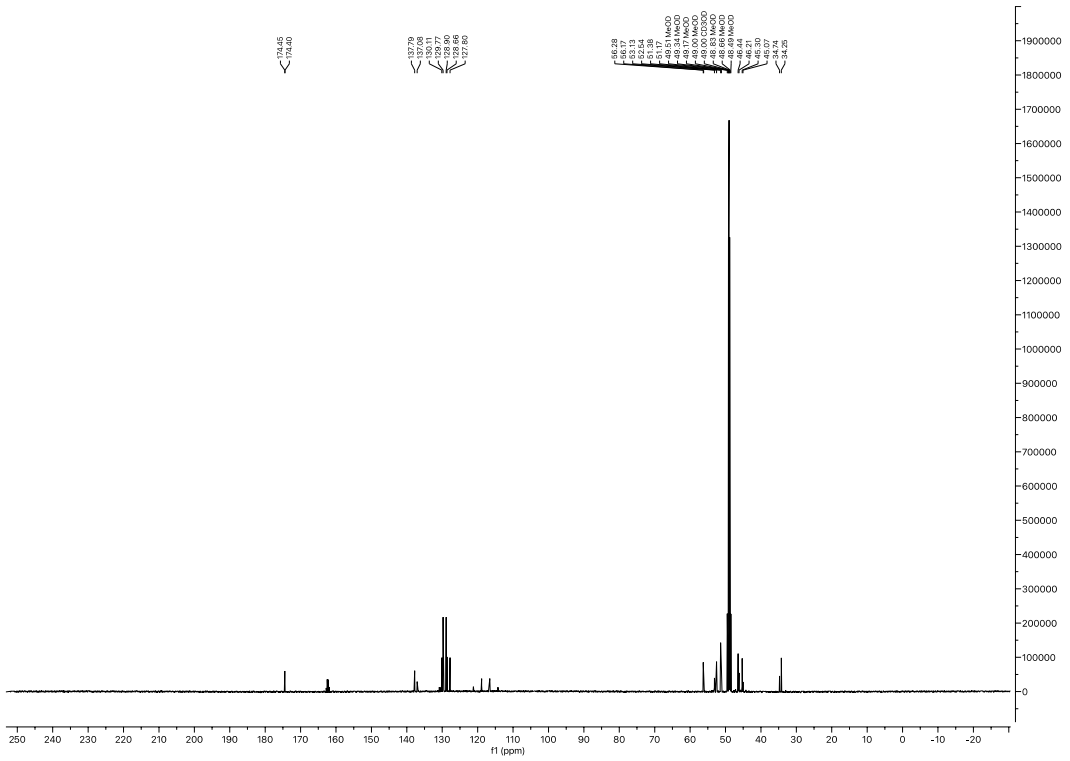


Figure S73 The $^{13}C\{^{1}H\}$ NMR spectrum of monoAm in MeOD.

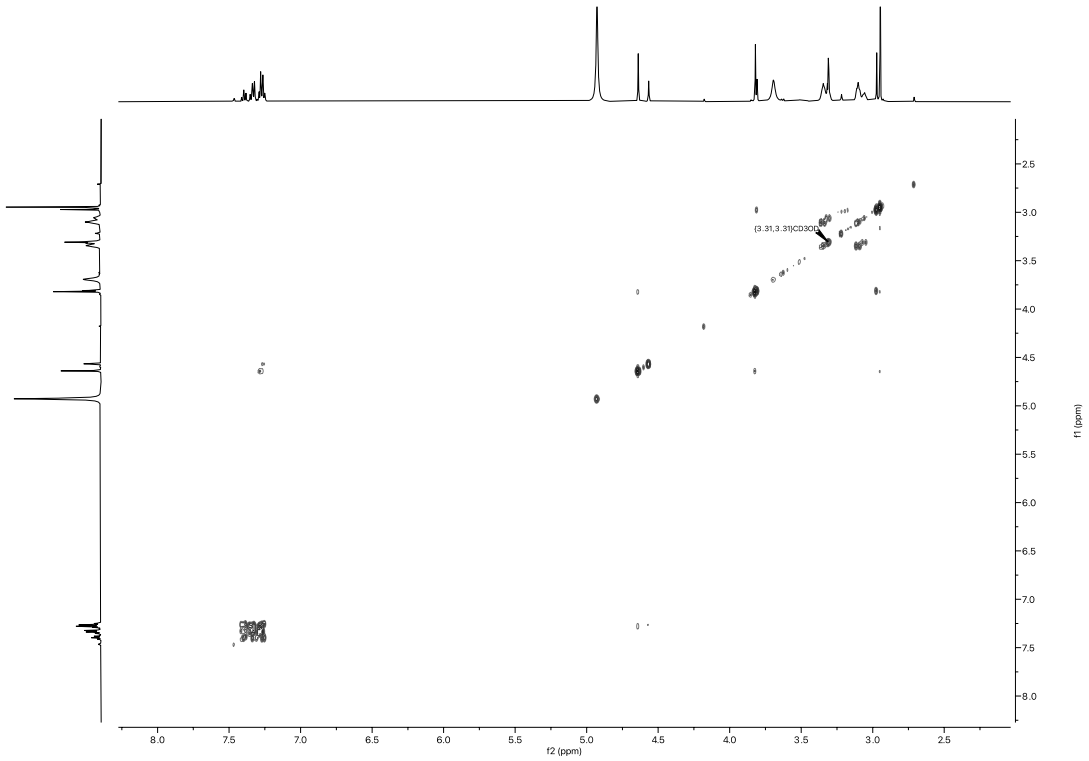


Figure S74 The ^{1}H-^{1}H COSY NMR spectrum of monoAm in MeOD.

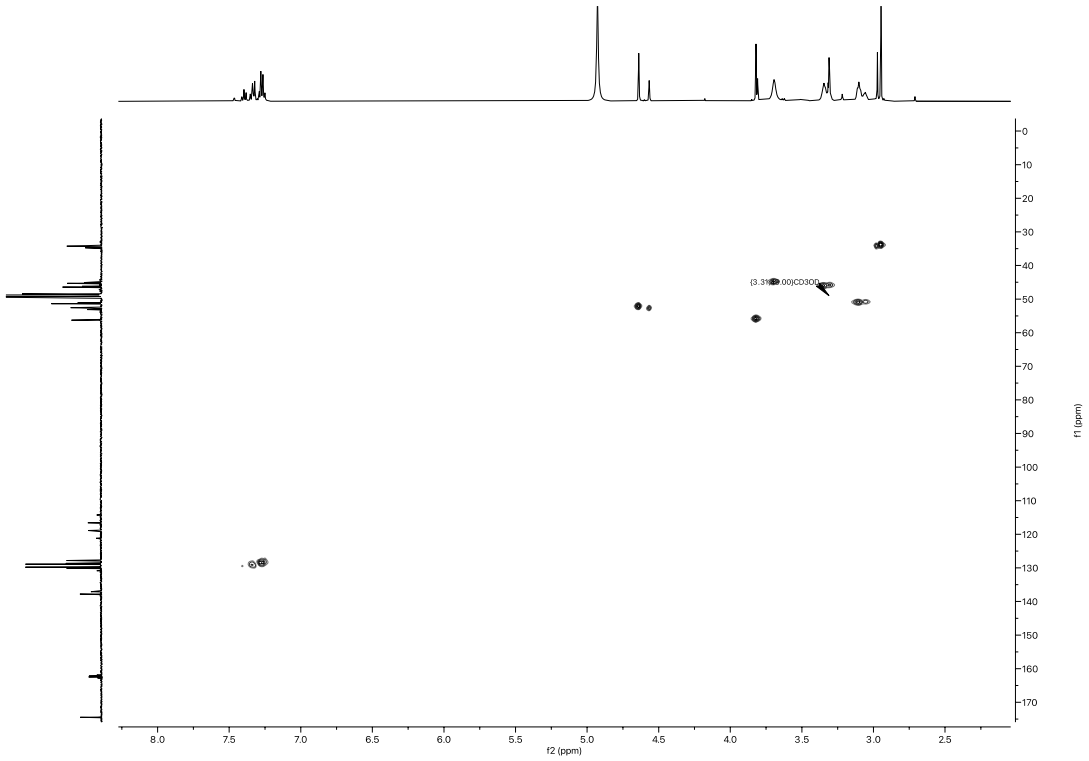


Figure S75 The ^{1}H-^{13}C HSQC NMR spectrum of monoAm in MeOD.

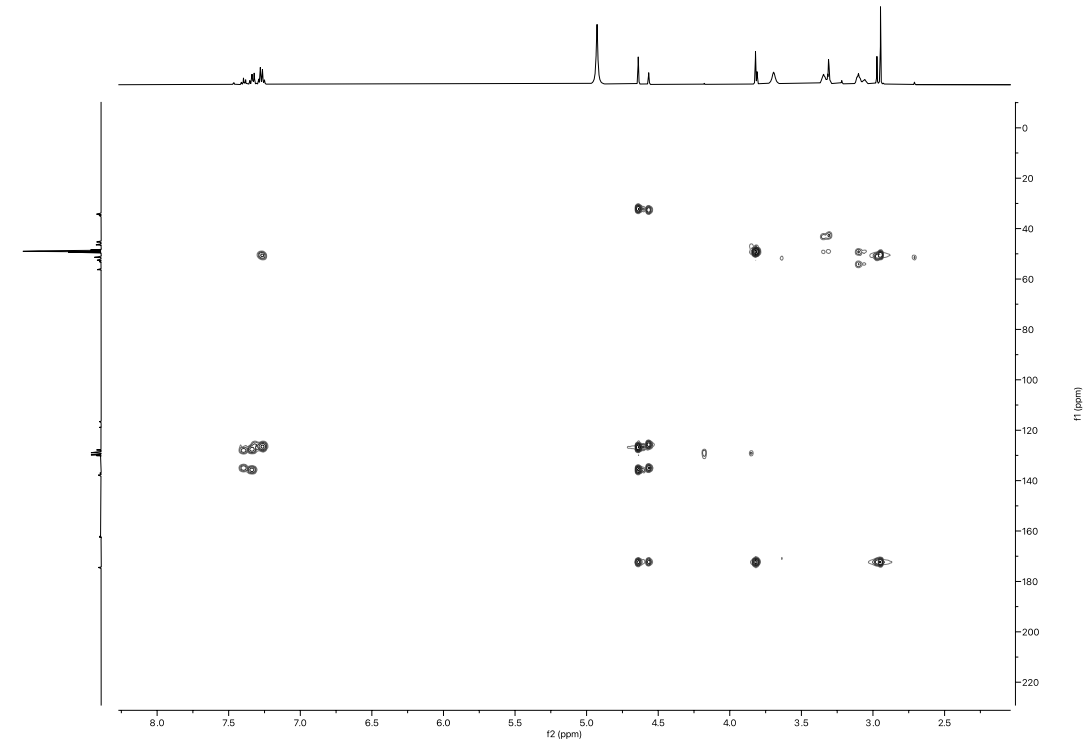


Figure S76 The ^{1}H-^{13}C HMBC NMR spectrum of monoAm in MeOD.

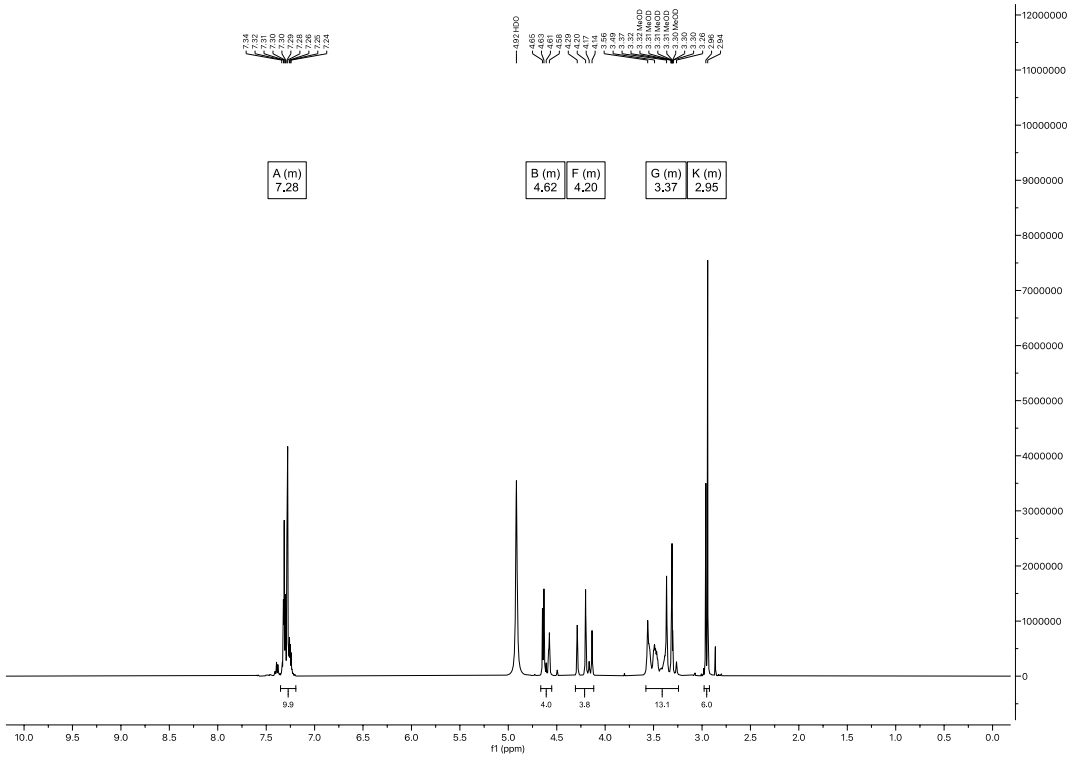


Figure S77 The ^{1}H NMR spectrum of diAm in MeOD.

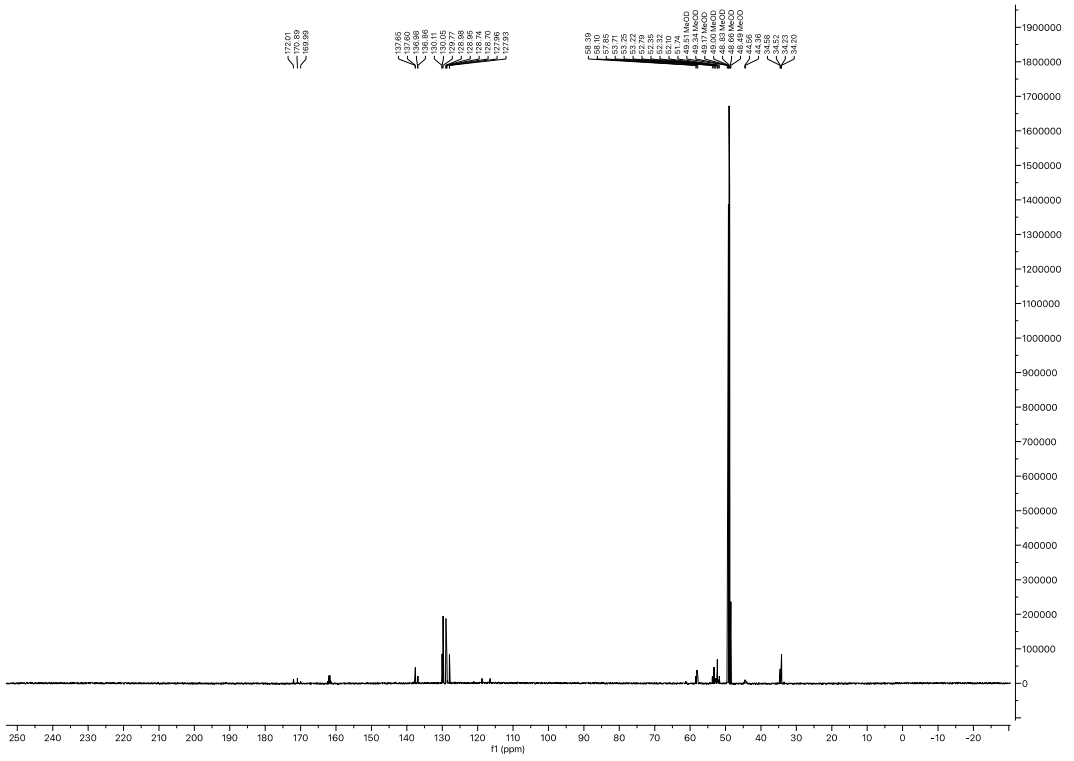


Figure S78 The ^{13}C{^{1}H} NMR spectrum of diAm in MeOD.

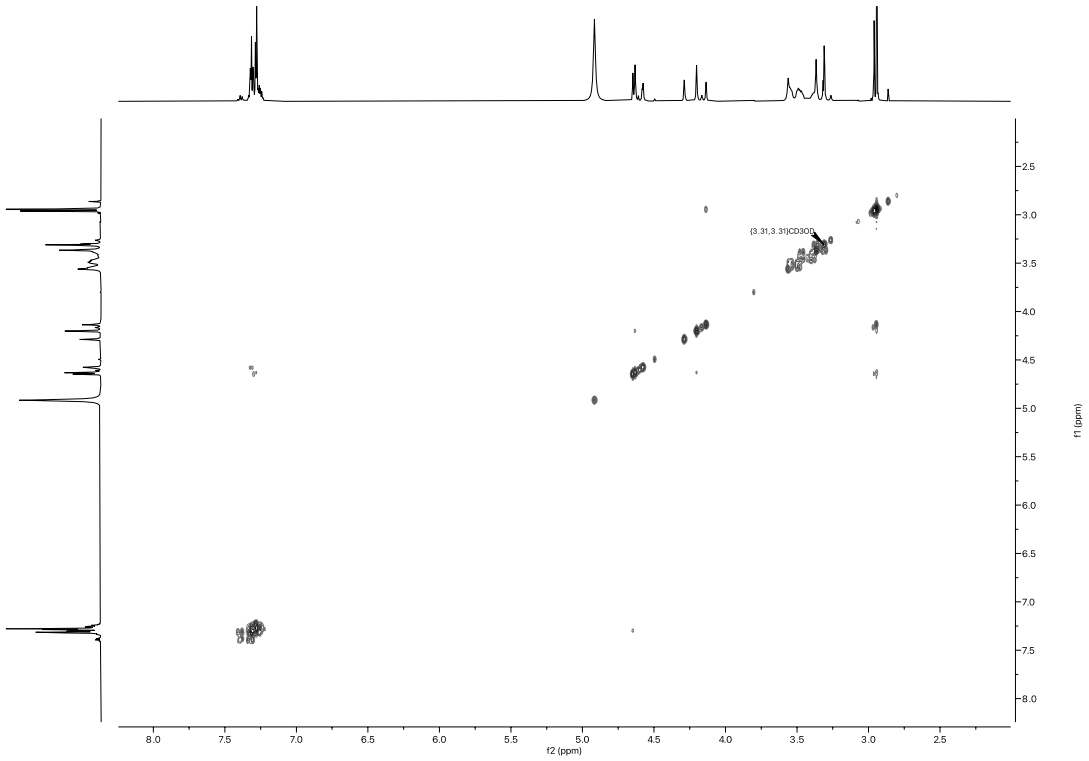


Figure S79 The ^{1}H-^{1}H COSY NMR spectrum of diAm in MeOD.

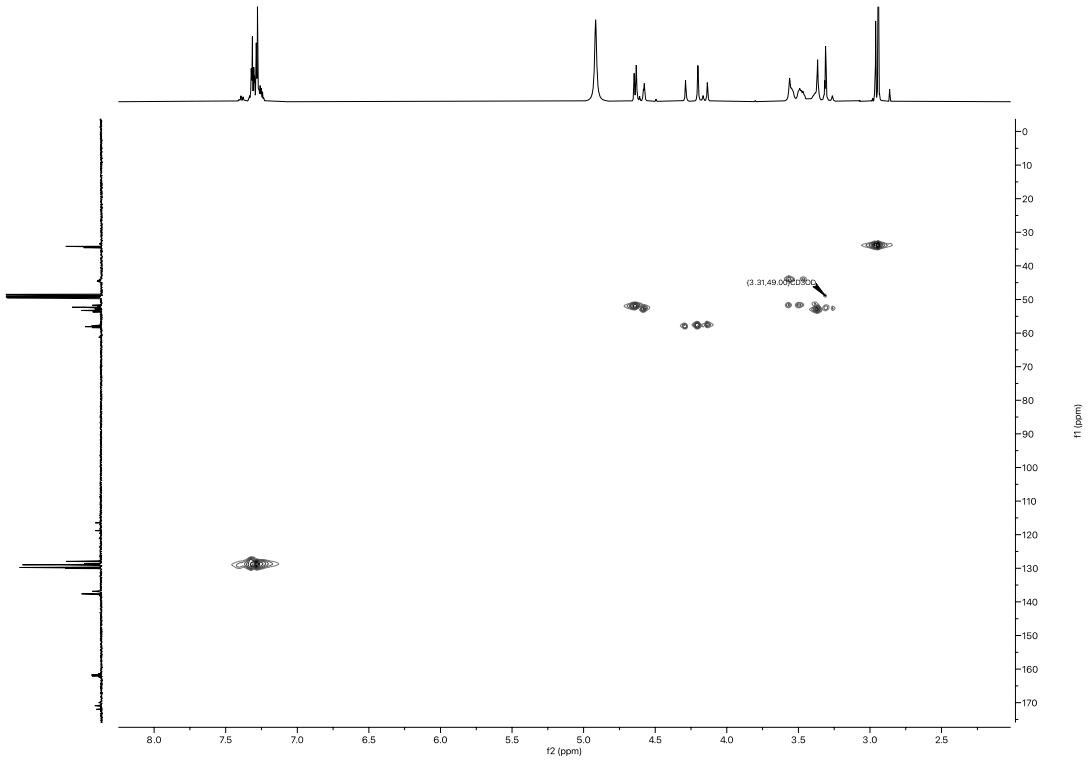


Figure S80 The ^{1}H-^{13}C HSQC NMR spectrum of diAm in MeOD.

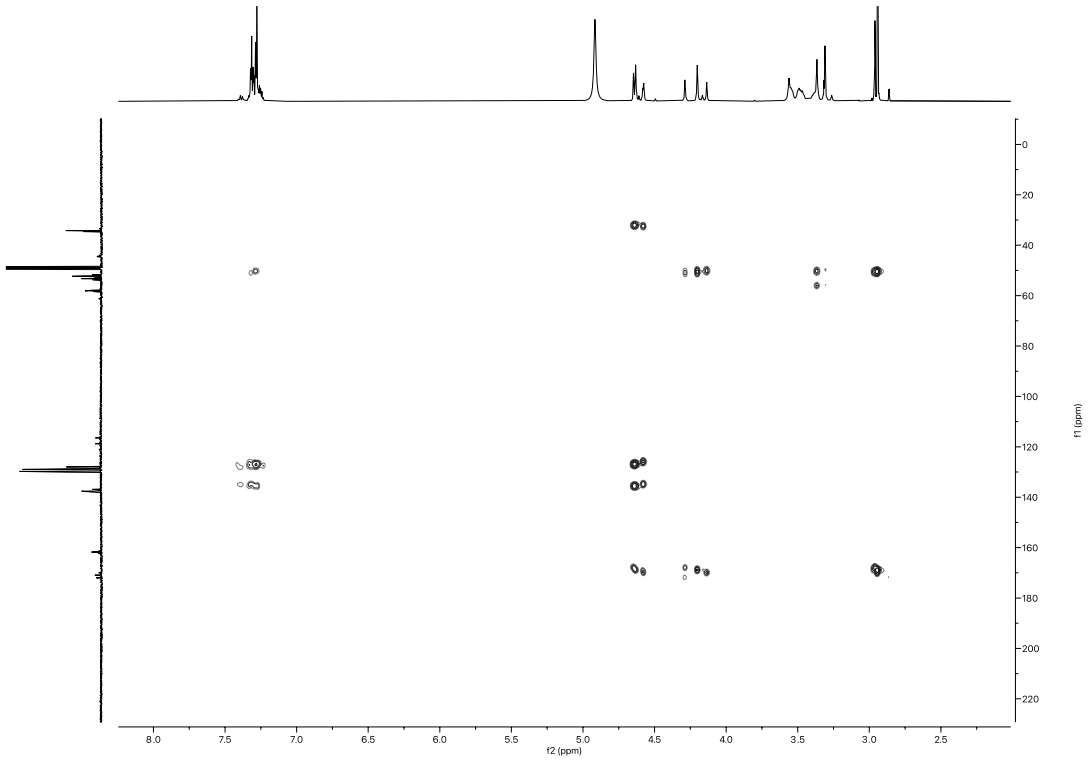


Figure S81 The ^{1}H-^{13}C HMBC NMR spectrum of diAm in MeOD.

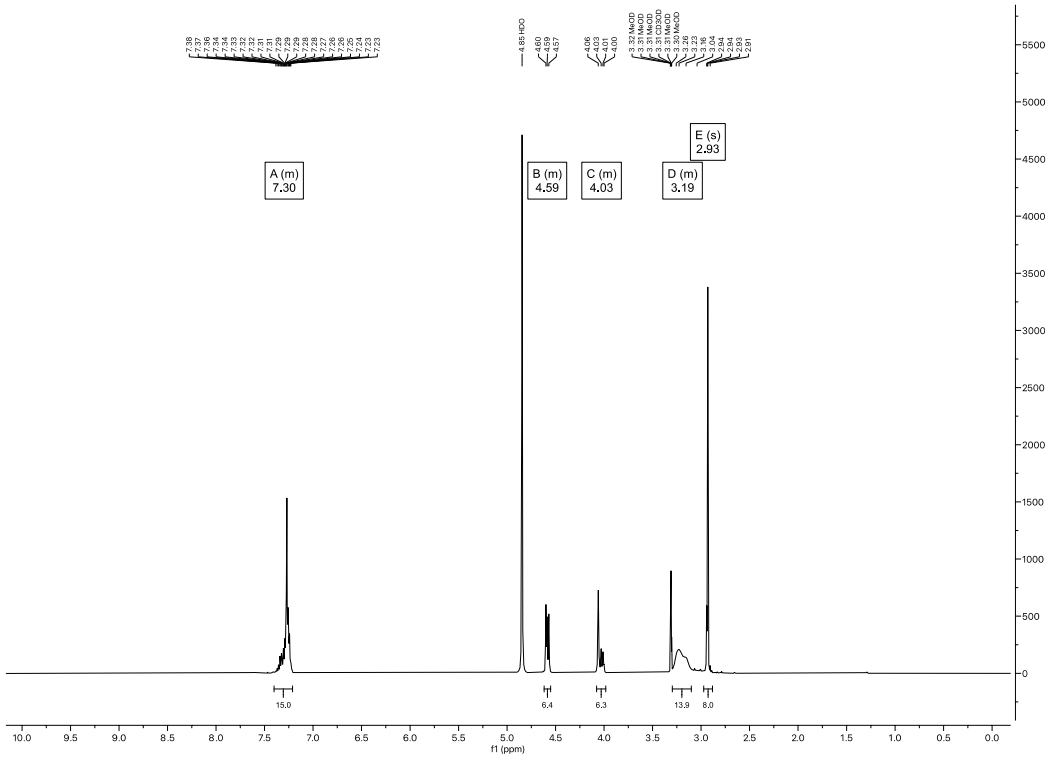


Figure S82 The ^{1}H NMR spectrum of **L^{030}** in MeOD.

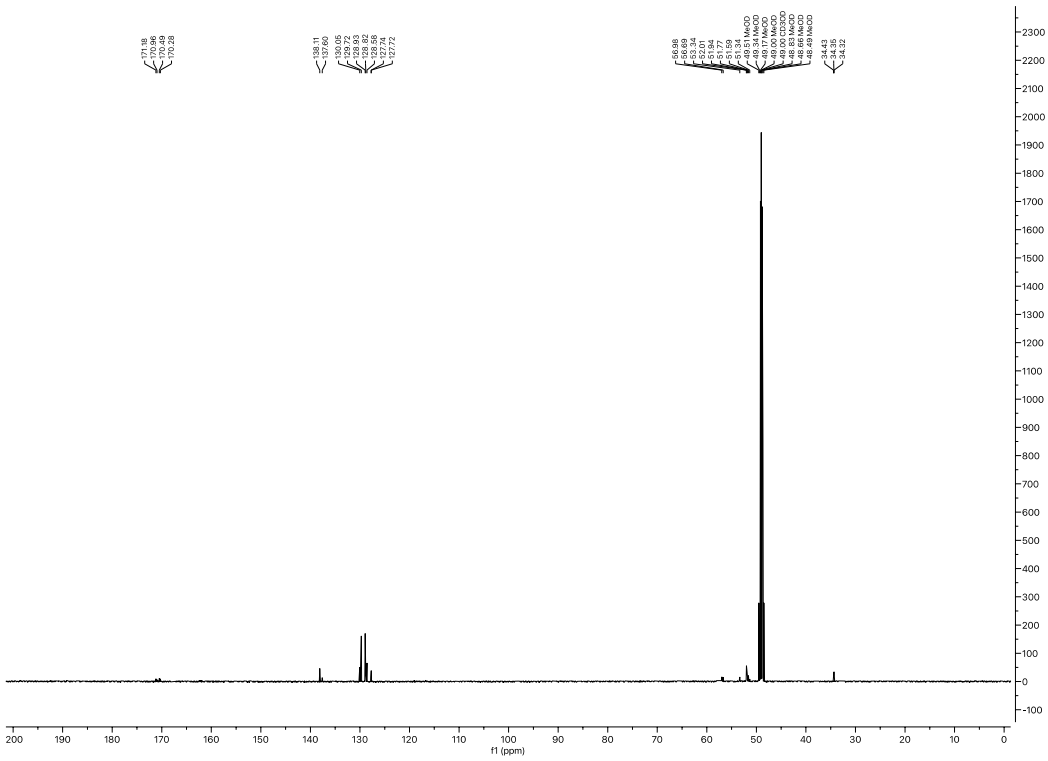


Figure S83 The $^{13}C\{^{1}H\}$ NMR spectrum of **L^{030}** in MeOD.

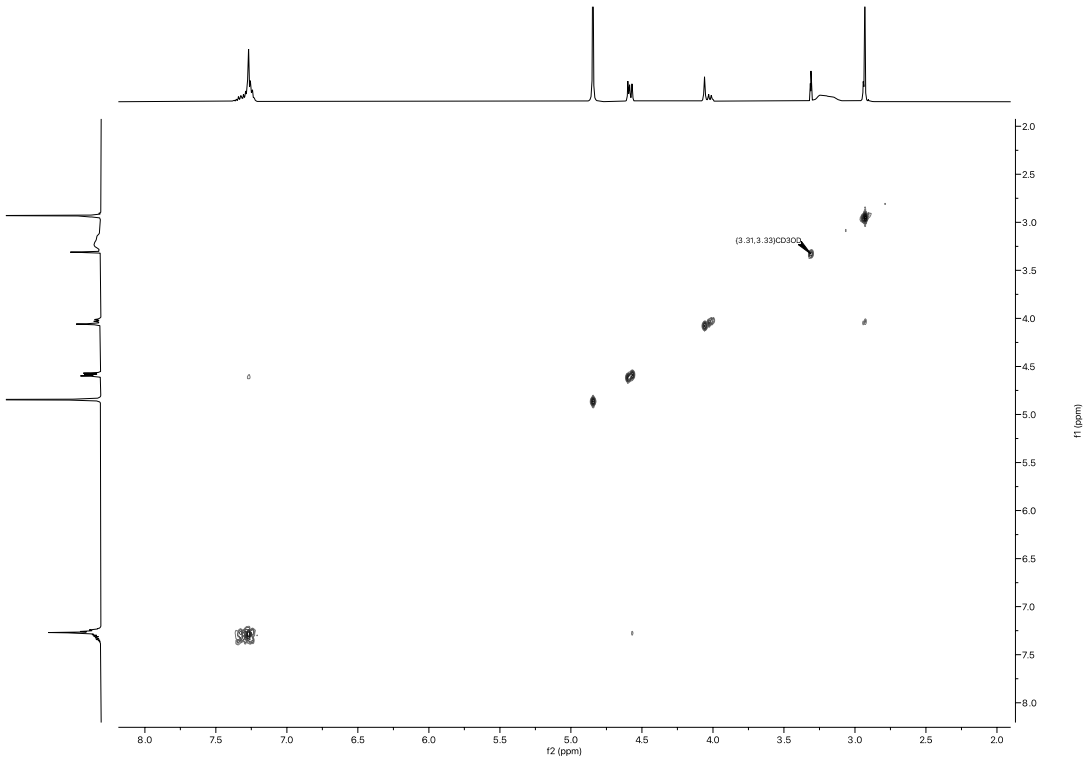


Figure S84 The ^{1}H-^{1}H COSY NMR spectrum of **L^{030}** in MeOD.

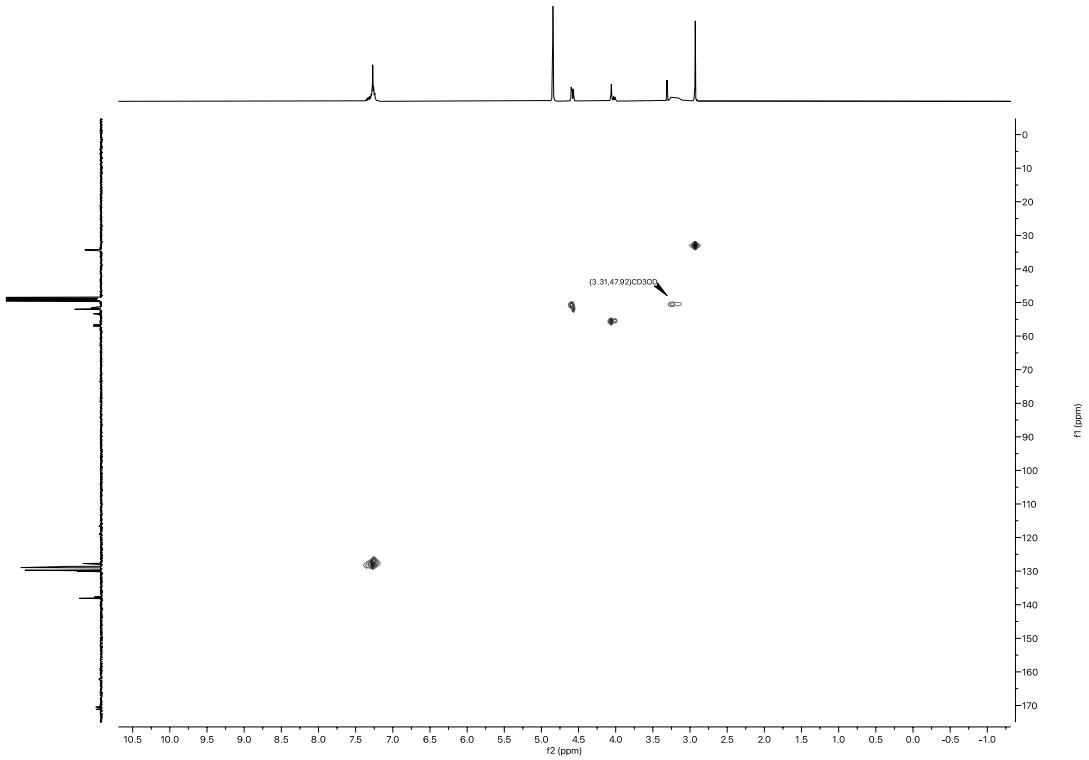


Figure S85 The ^{1}H-^{13}C HSQC NMR spectrum of $\mathbf{L^{030}}$ in MeOD.

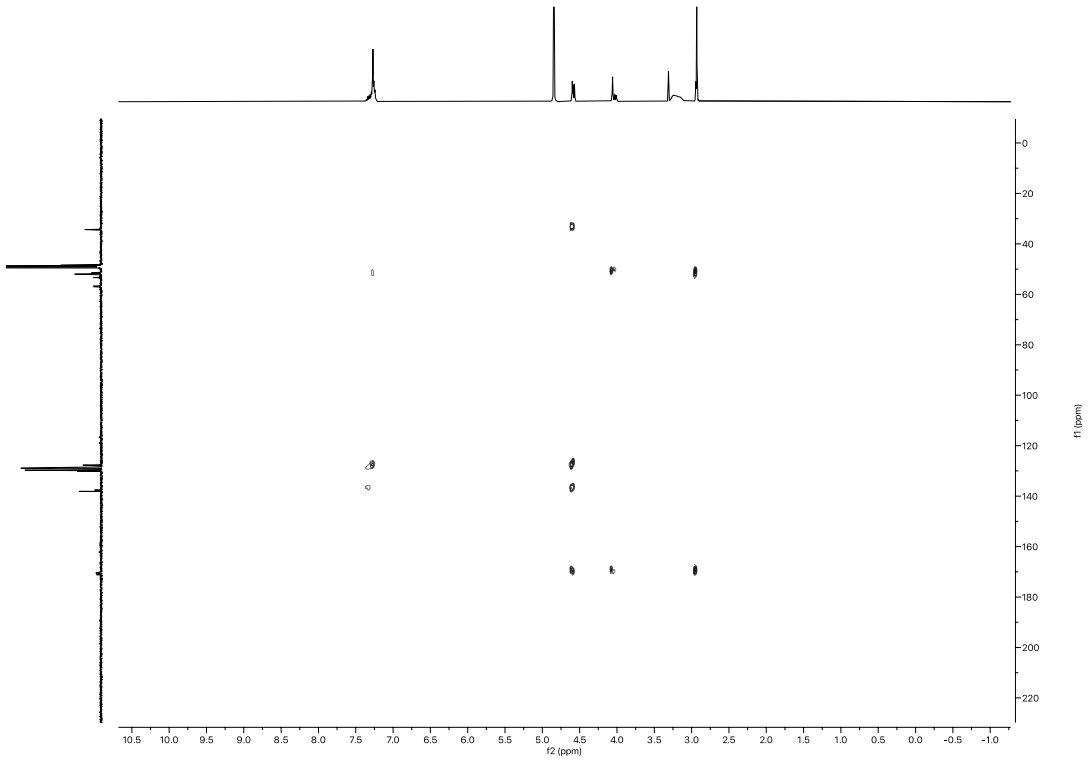


Figure S86 The ^{1}H-^{13}C HMBC NMR spectrum of $\mathbf{L^{030}}$ in MeOD.

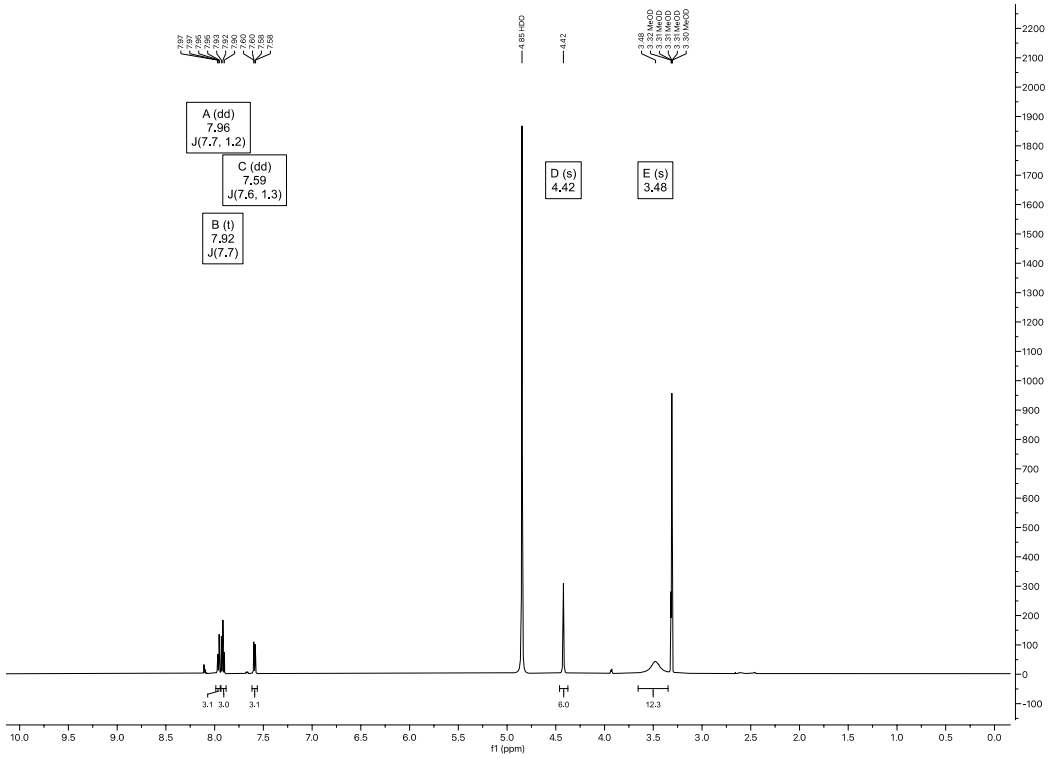


Figure S87 The ^{1}H NMR spectrum of $H_3\mathbf{L}^{\mathbf{003}}$ in MeOD.

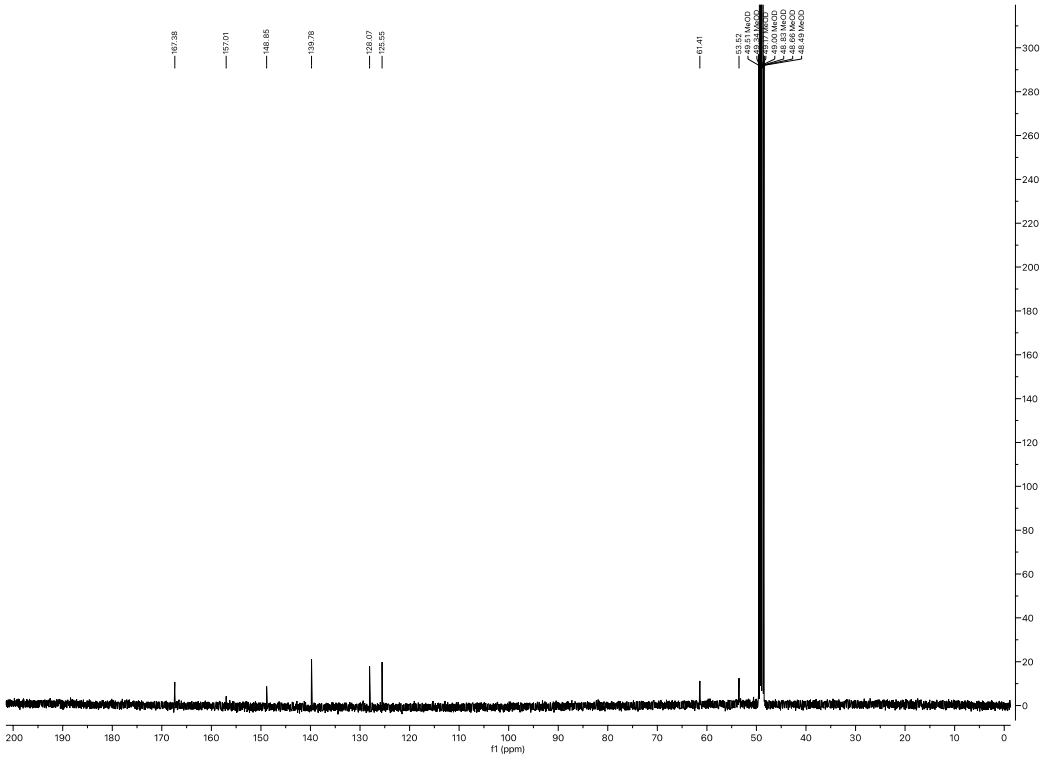


Figure S88 The $^{13}C\{^{1}H\}$ NMR spectrum of $H_3\mathbf{L}^{\mathbf{003}}$ in MeOD.

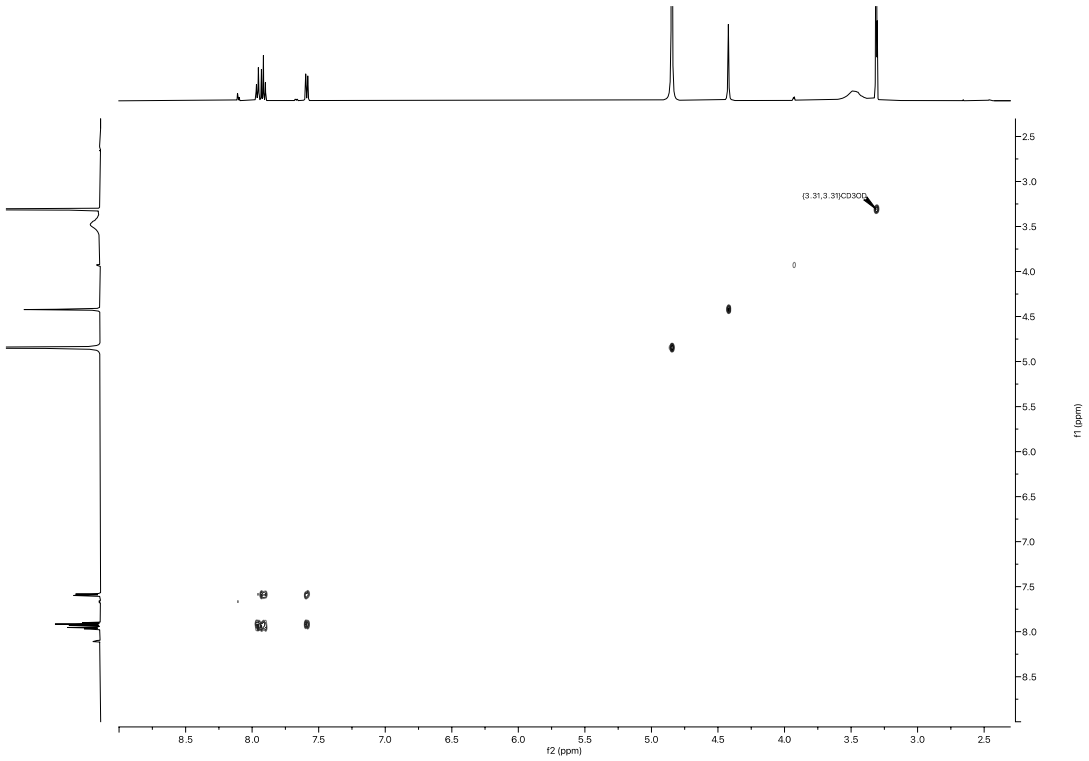


Figure S89 The ^{1}H-^{1}H COSY NMR spectrum of H_3**L**^{003} in MeOD.

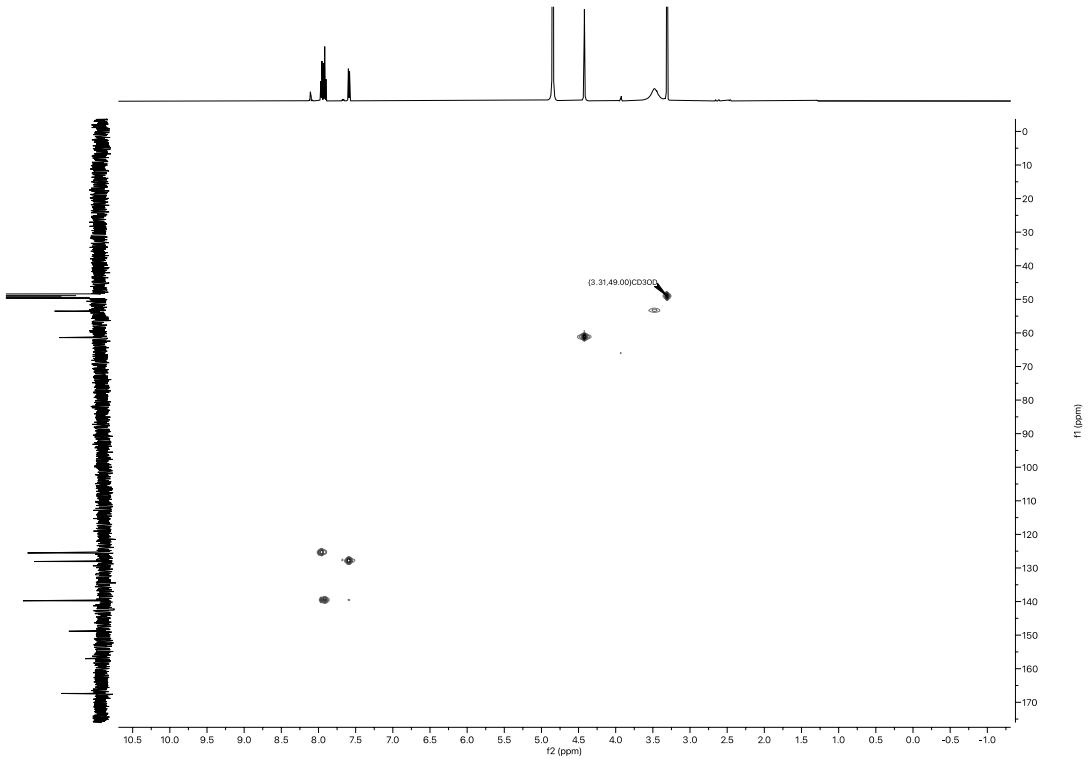


Figure S90 The ^{1}H-^{13}C HSQC NMR spectrum of H_3**L**^{003} in MeOD.

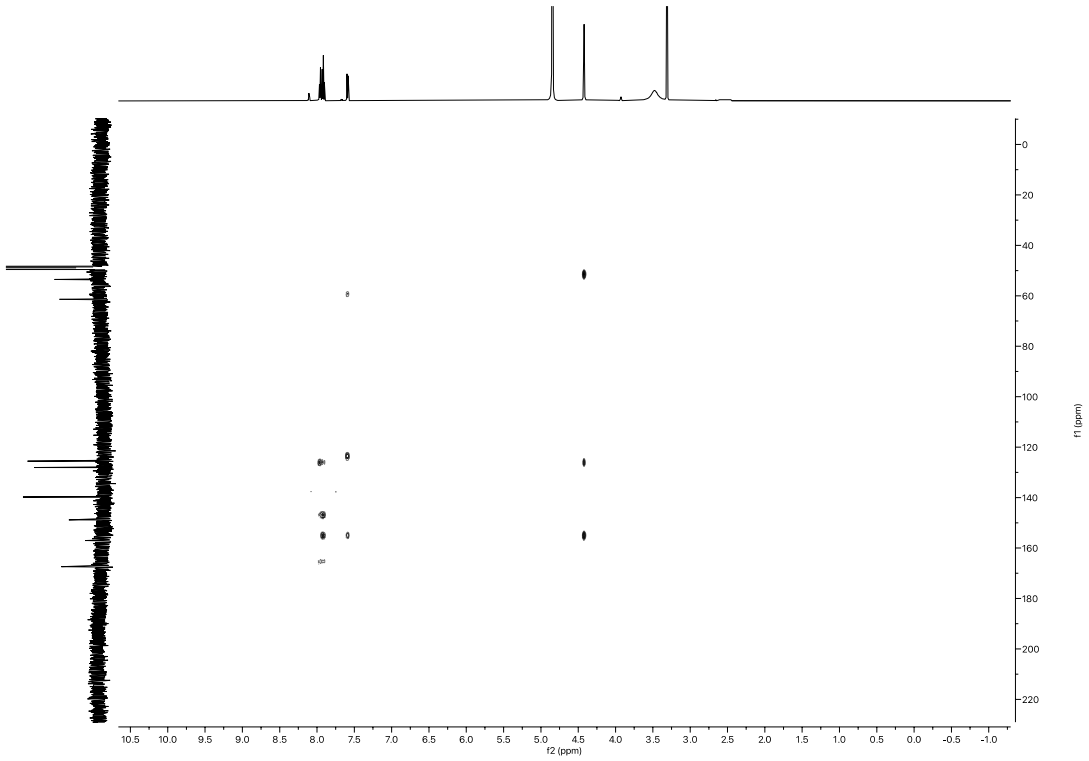


Figure S91 The ^{1}H-^{13}C HMBC NMR spectrum of H_3**L**^{003} in MeOD.

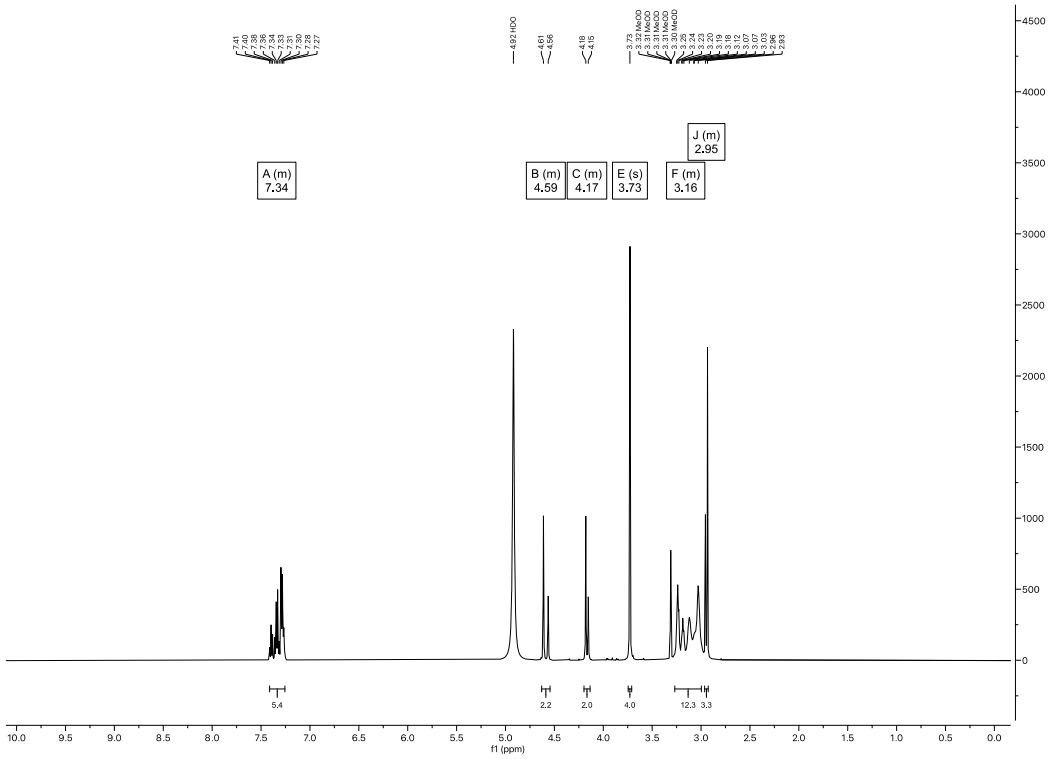


Figure S92 The ^{1}H NMR spectrum of H_2**L**^{210} in MeOD.

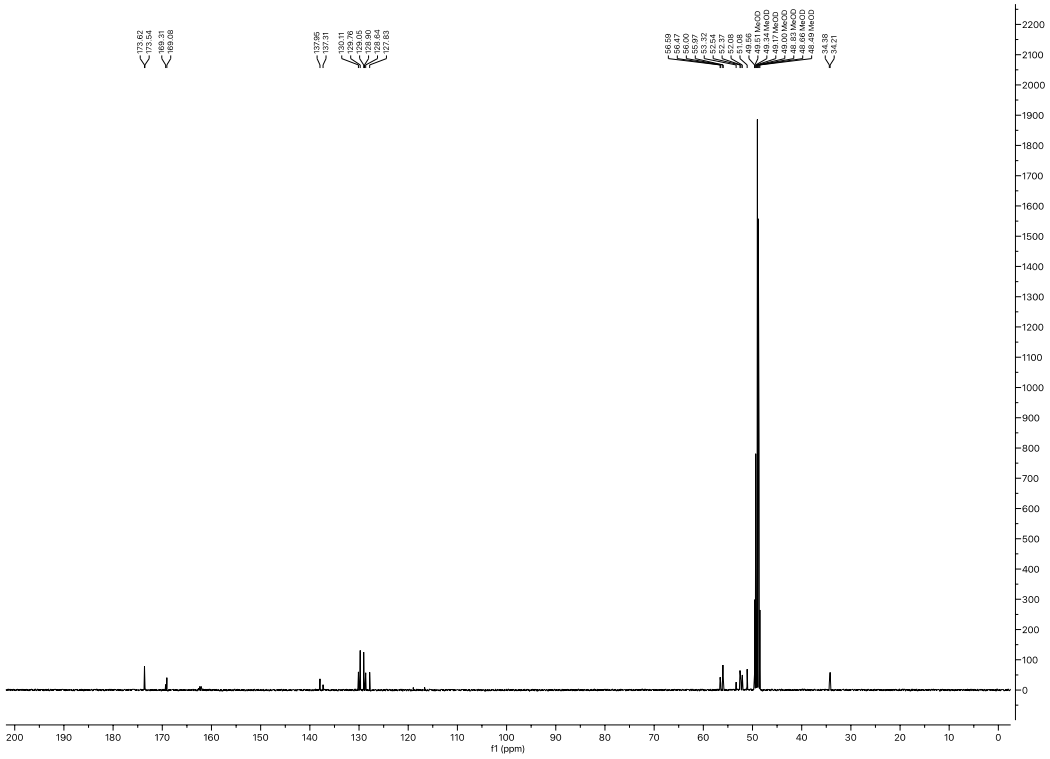


Figure S93 The $^{13}C\{^{1}H\}$ NMR spectrum of $H_2\mathbf{L}^{\mathbf{210}}$ in MeOD.

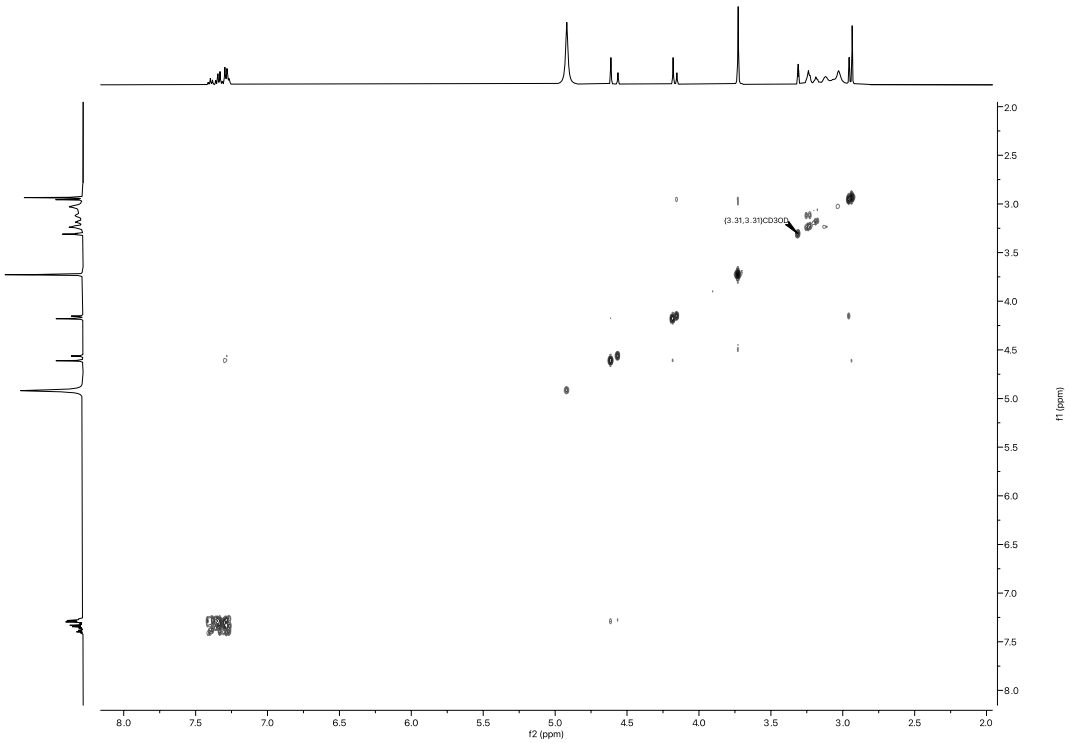


Figure S94 The ^{1}H-^{1}H COSY NMR spectrum of $H_2\mathbf{L}^{\mathbf{210}}$ in MeOD.

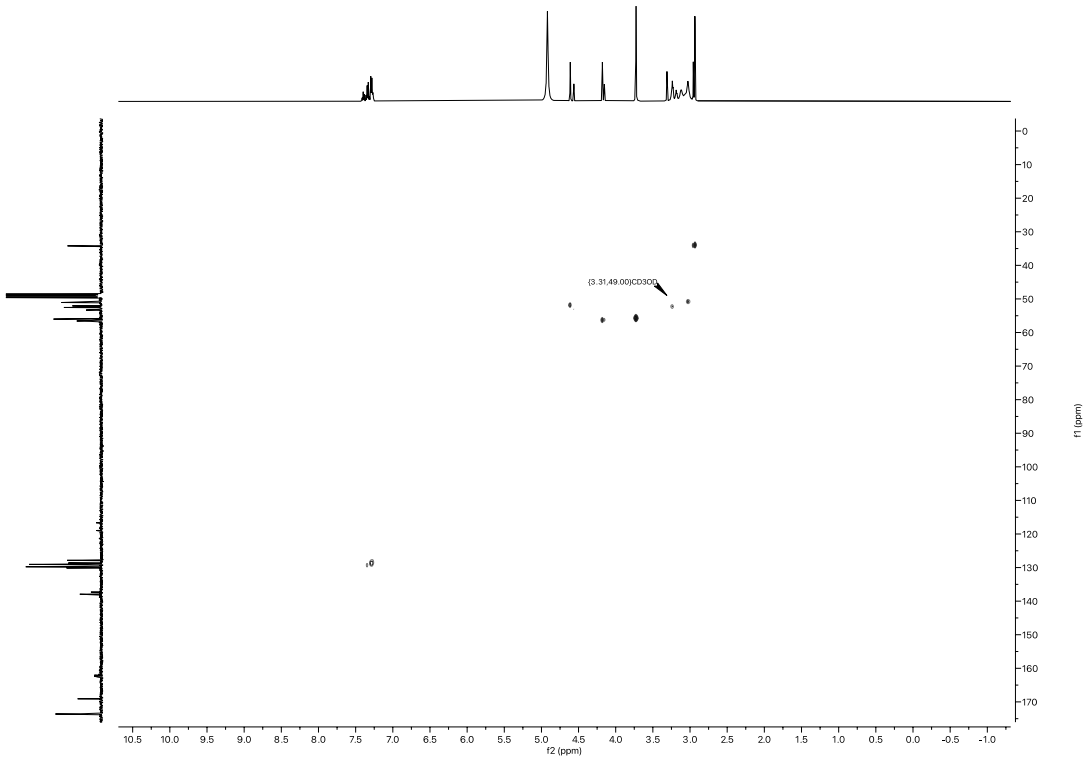


Figure S95 The ^{1}H-^{13}C HSQC NMR spectrum of $H_2\mathbf{L^{210}}$ in MeOD.

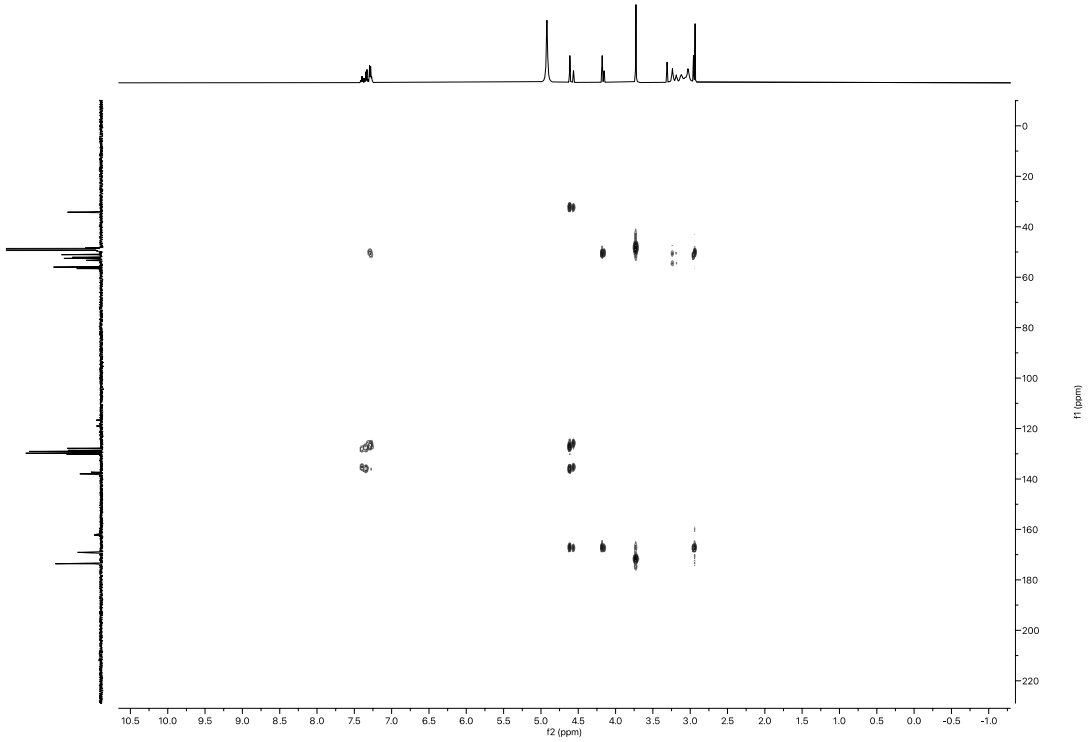


Figure S96 The ^{1}H-^{13}C HMBC NMR spectrum of $H_2\mathbf{L^{210}}$ in MeOD.

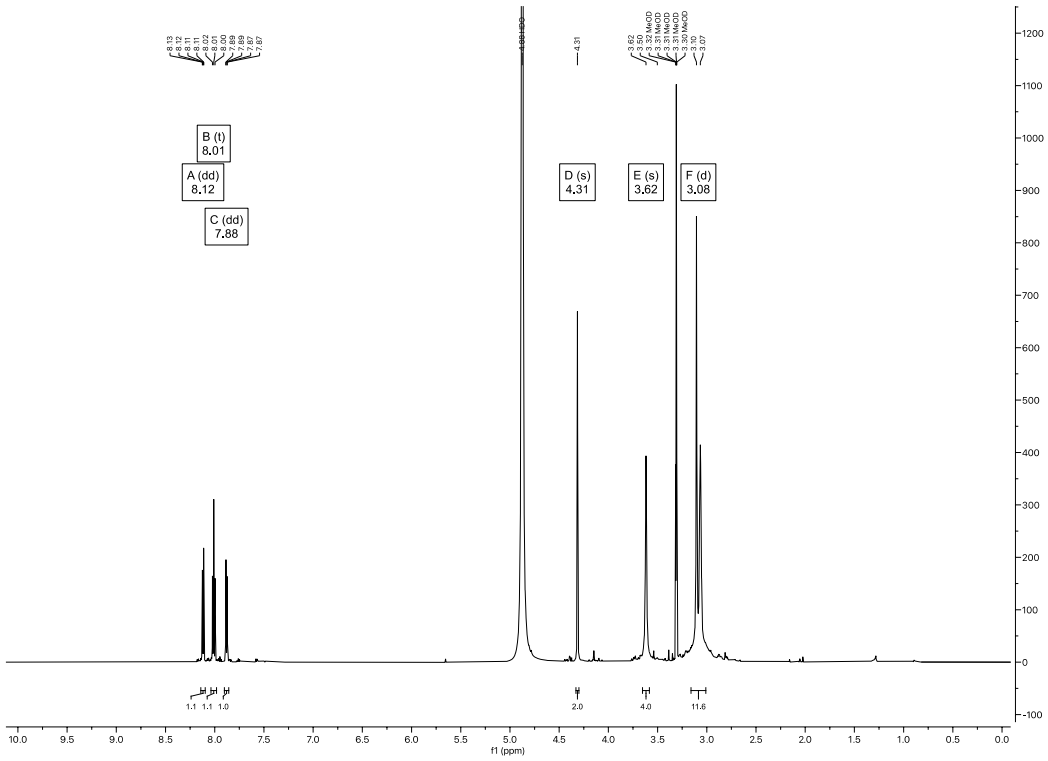


Figure S97 The ^{1}H NMR spectrum of H_3**L**^{201} in MeOD.

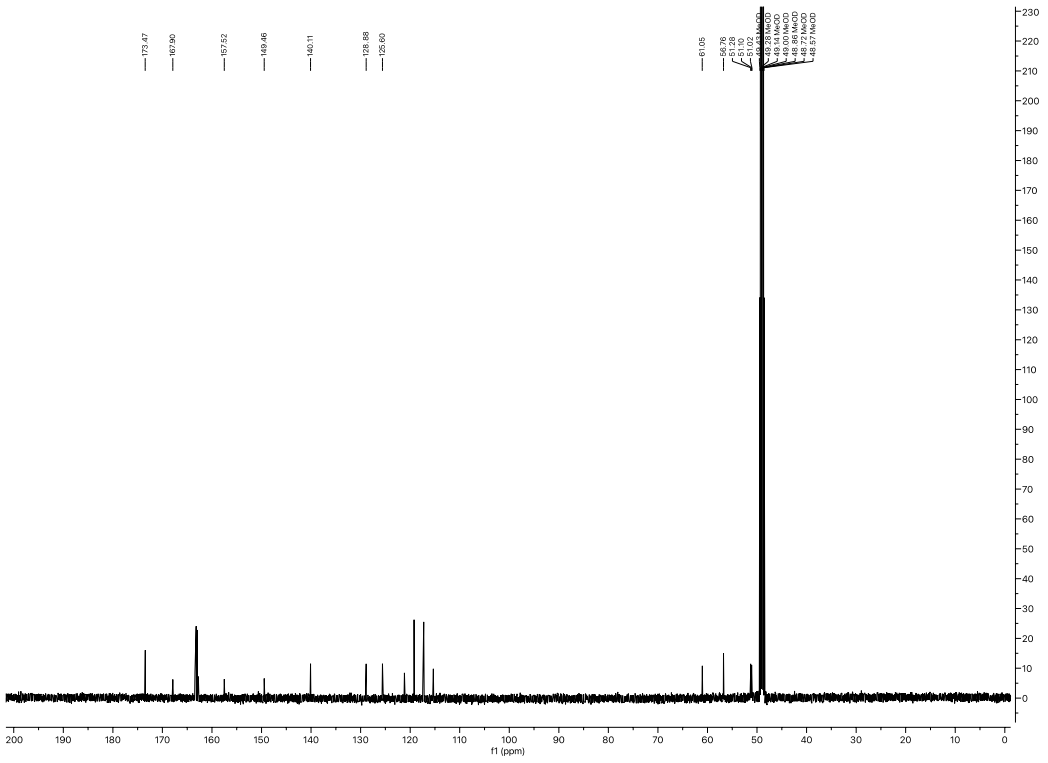


Figure S98 The ^{13}C{^{1}H} NMR spectrum of H_3**L**^{201} in MeOD.

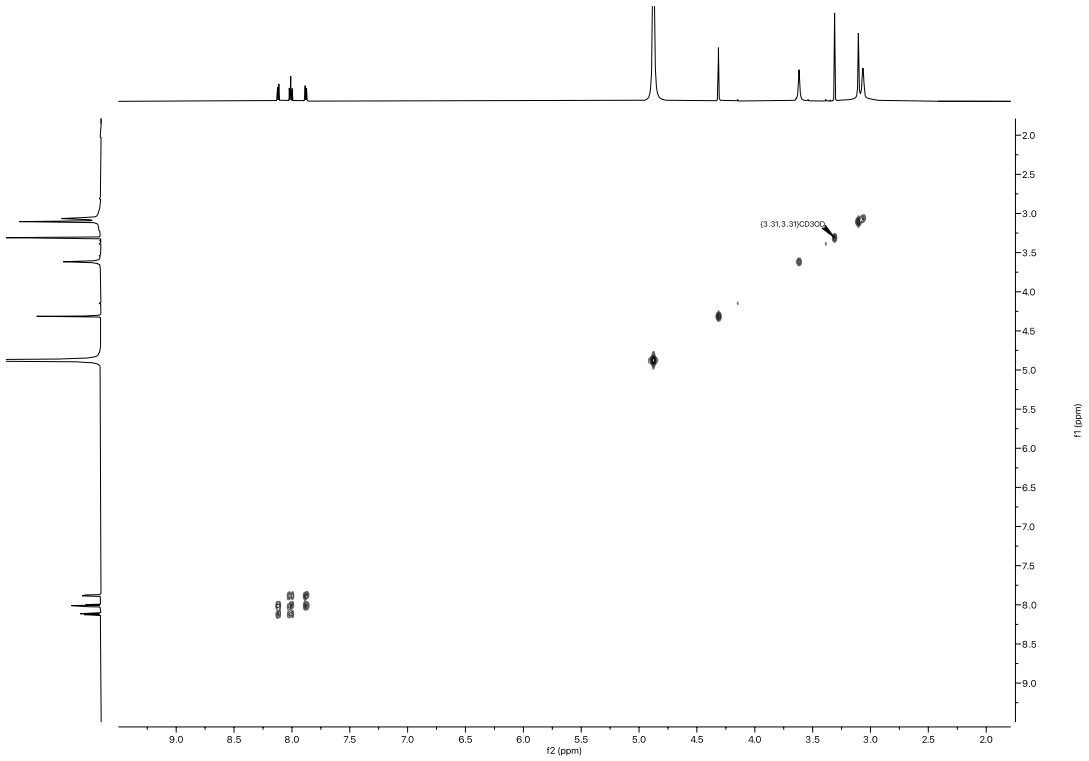


Figure S99 The ^{1}H-^{1}H COSY NMR spectrum of H_3**L**^{201} in MeOD.

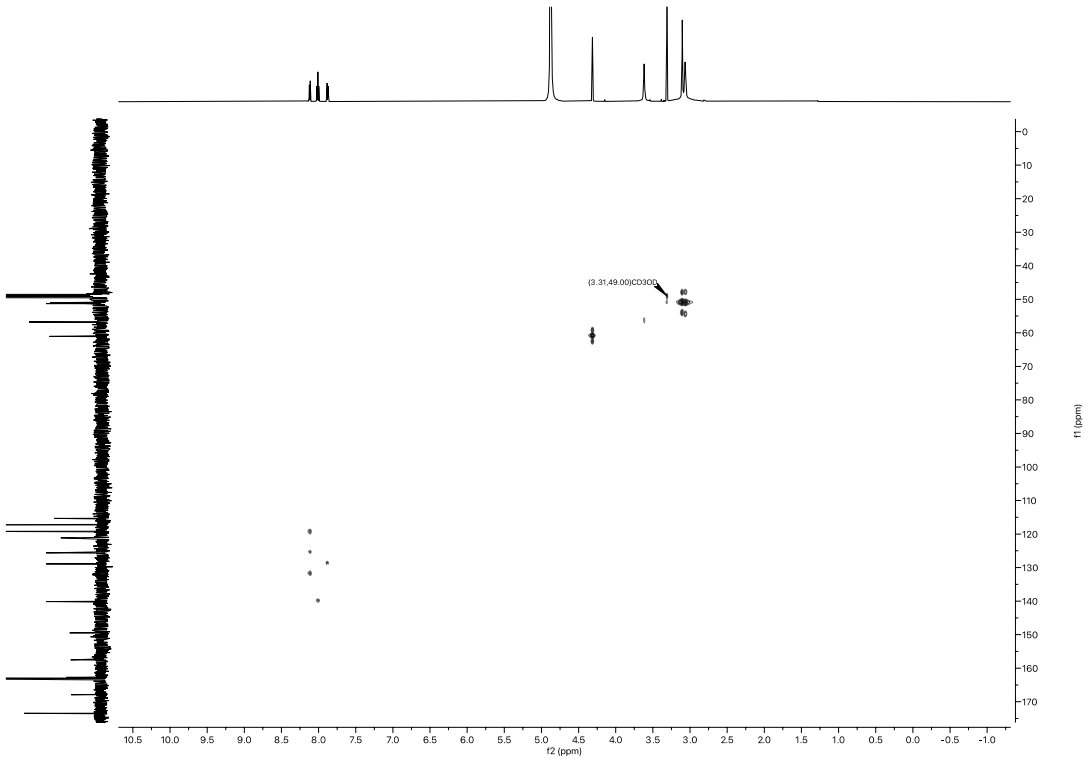


Figure S100 The ^{1}H-^{13}C HSQC NMR spectrum of H_3**L**^{201} in MeOD.

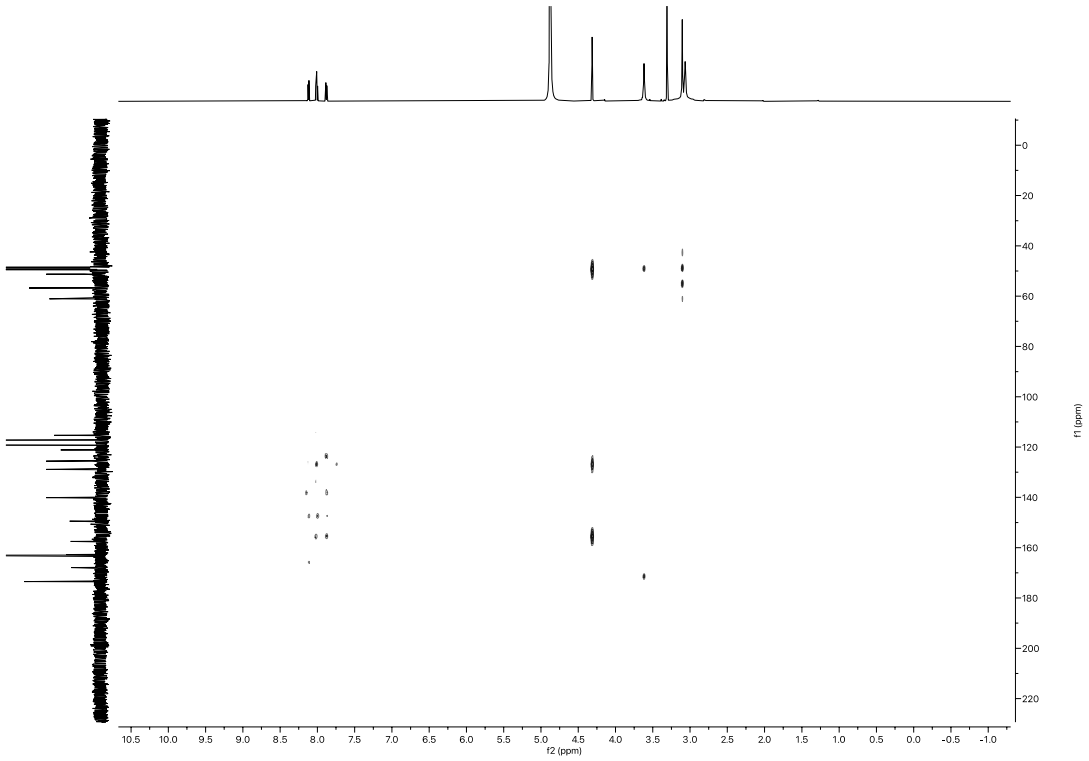


Figure S101 The ^{1}H-^{13}C HMBC NMR spectrum of H_3**L**^{201} in MeOD.

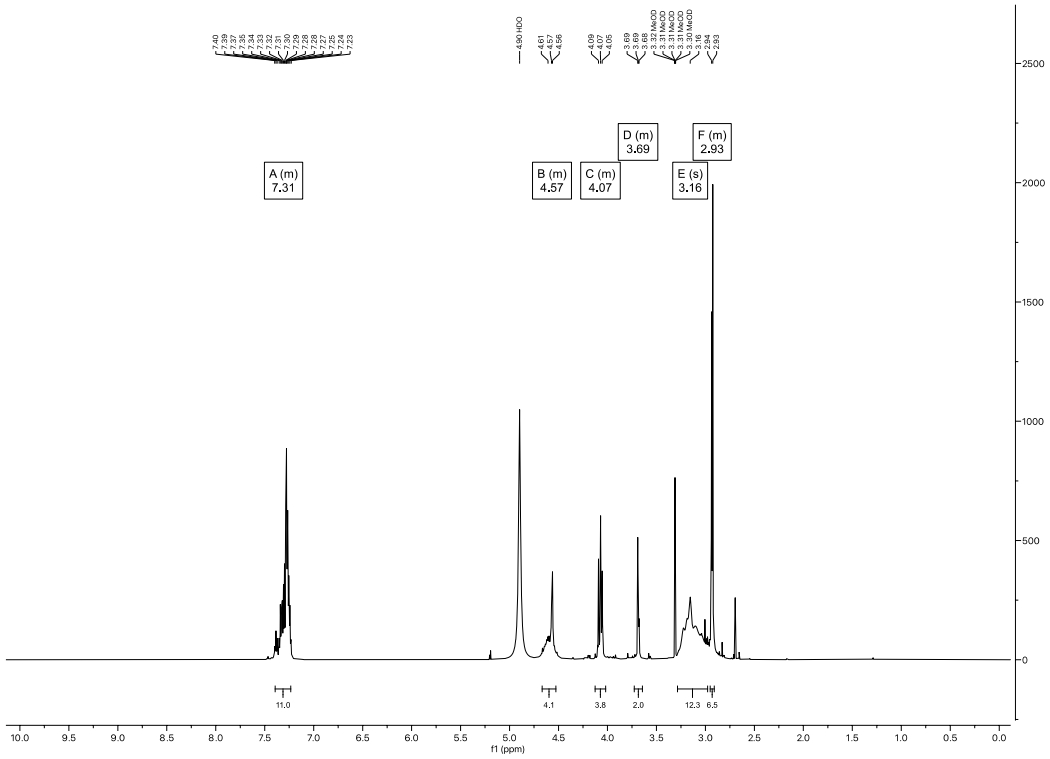


Figure S102 The ^{1}H NMR spectrum of H**L**^{120} in MeOD.

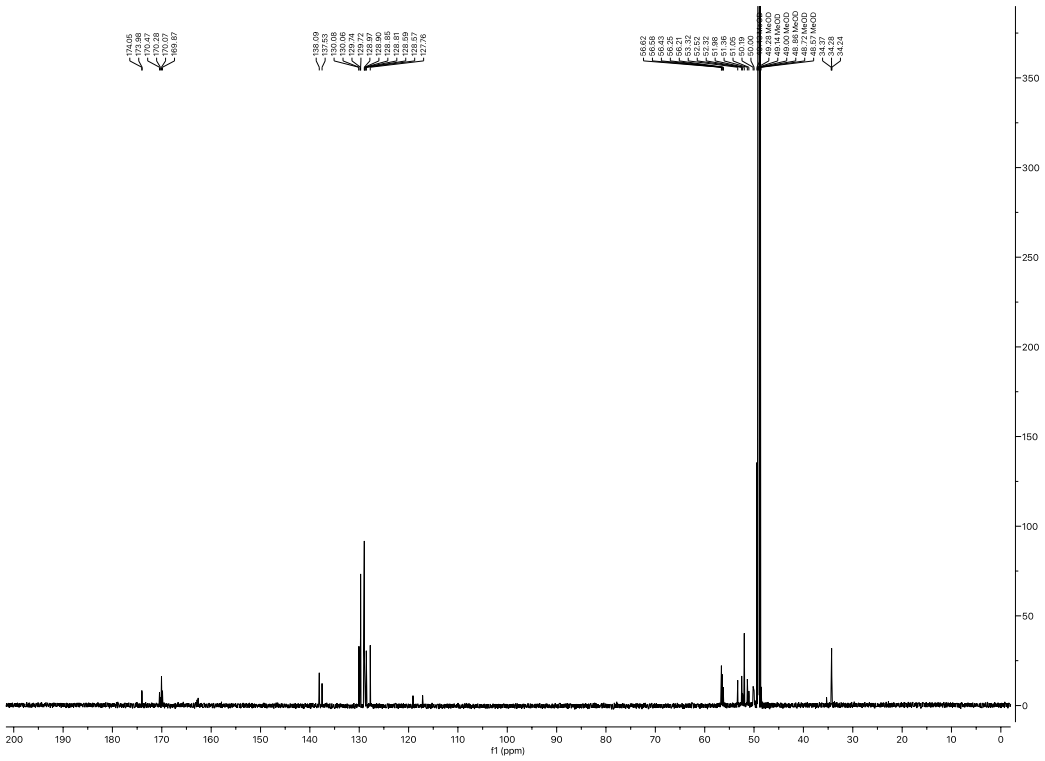


Figure S103 The $^{13}C\{^{1}H\}$ NMR spectrum of H**L**^{120} in MeOD.

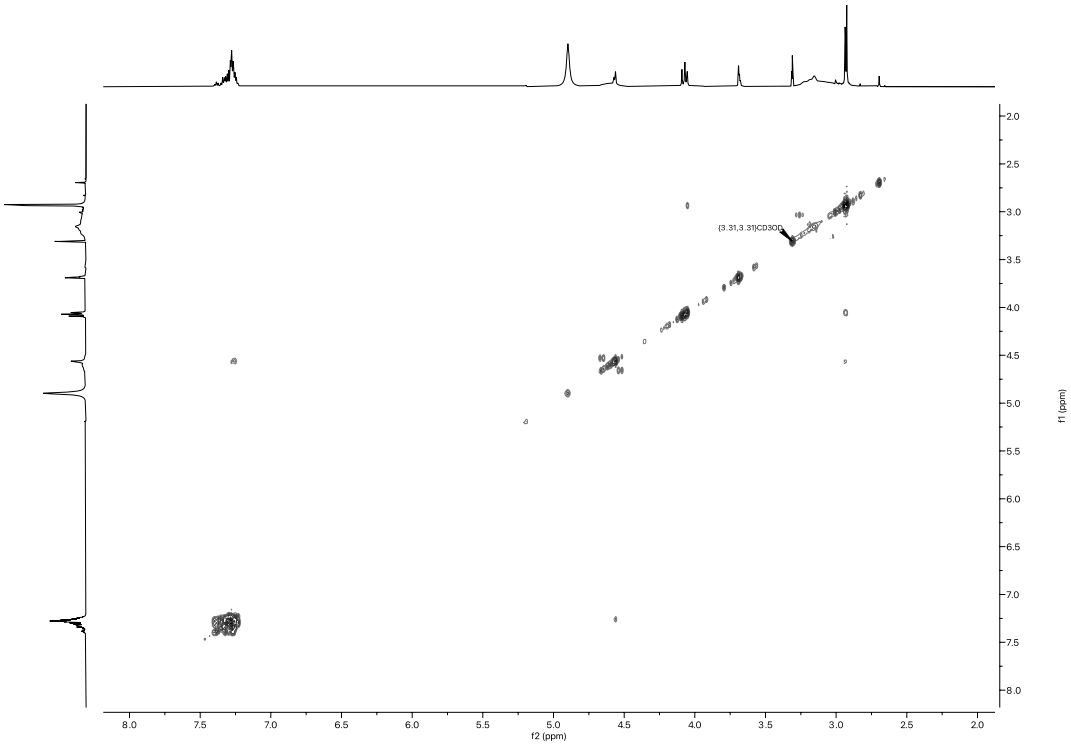


Figure S104 The ^{1}H-^{1}H COSY NMR spectrum of H**L**^{120} in MeOD.

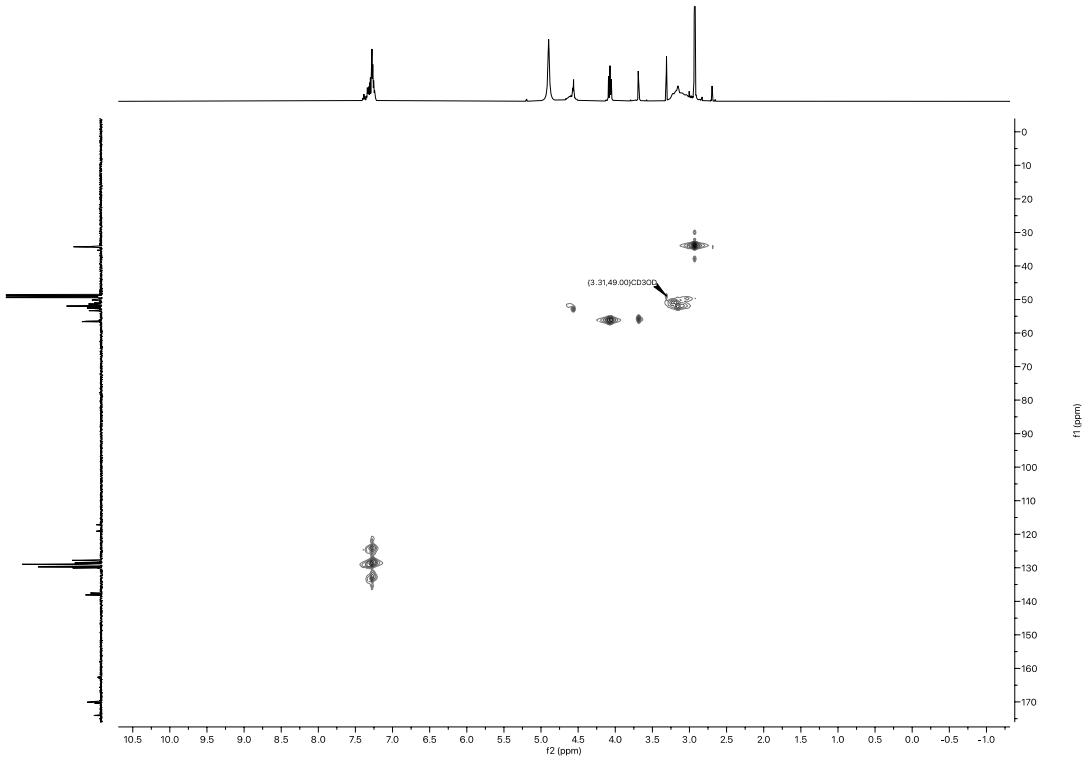


Figure S105 The ^{1}H-^{13}C HSQC NMR spectrum of H**L**^{120} in MeOD.

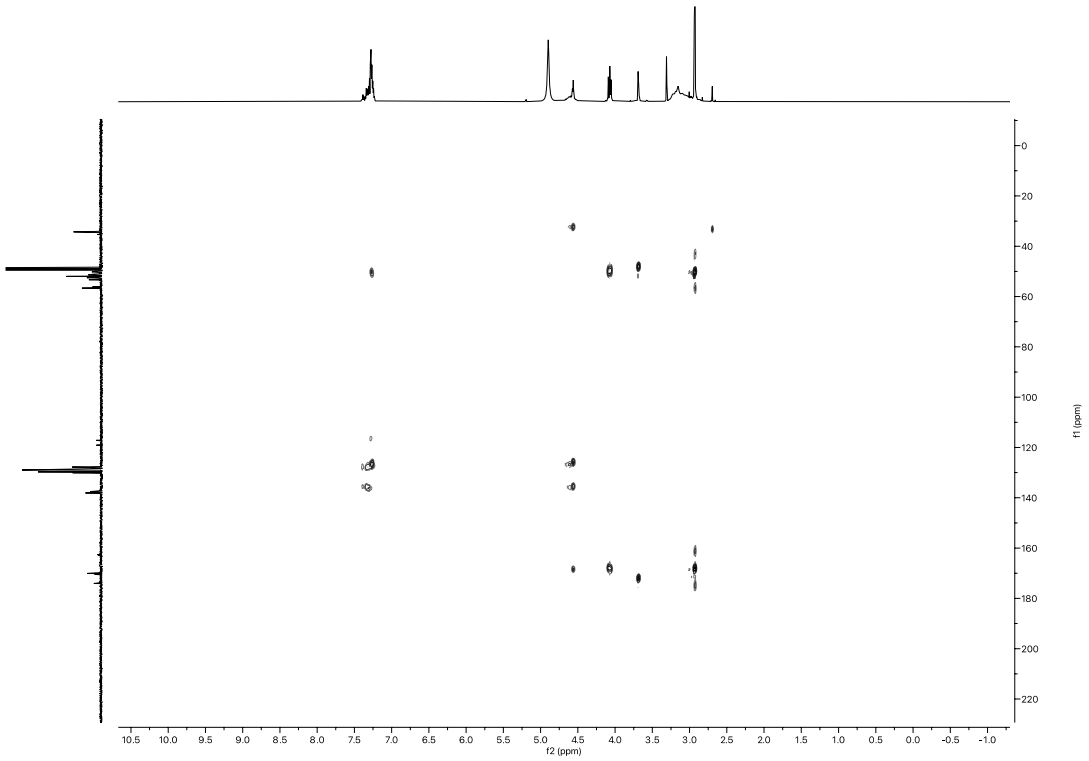


Figure S106 The ^{1}H-^{13}C HMBC NMR spectrum of H**L**^{120} in MeOD.

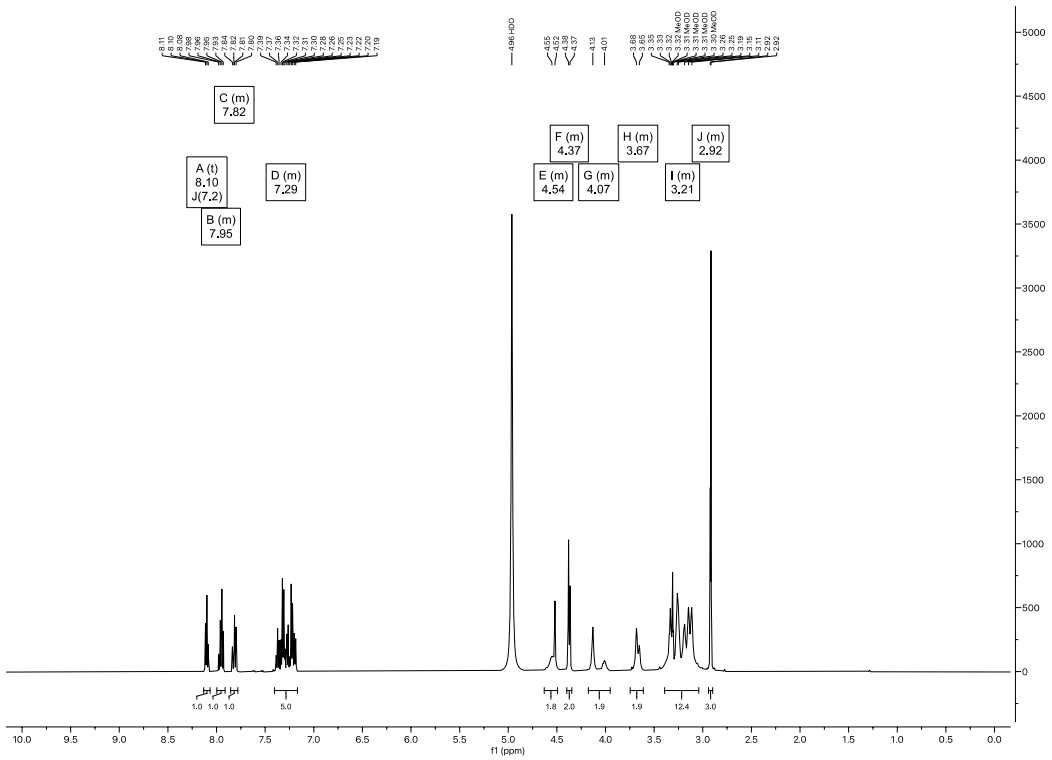


Figure S107 The ^{1}H NMR spectrum of $H_2\mathbf{L}^{111}$ in MeOD.

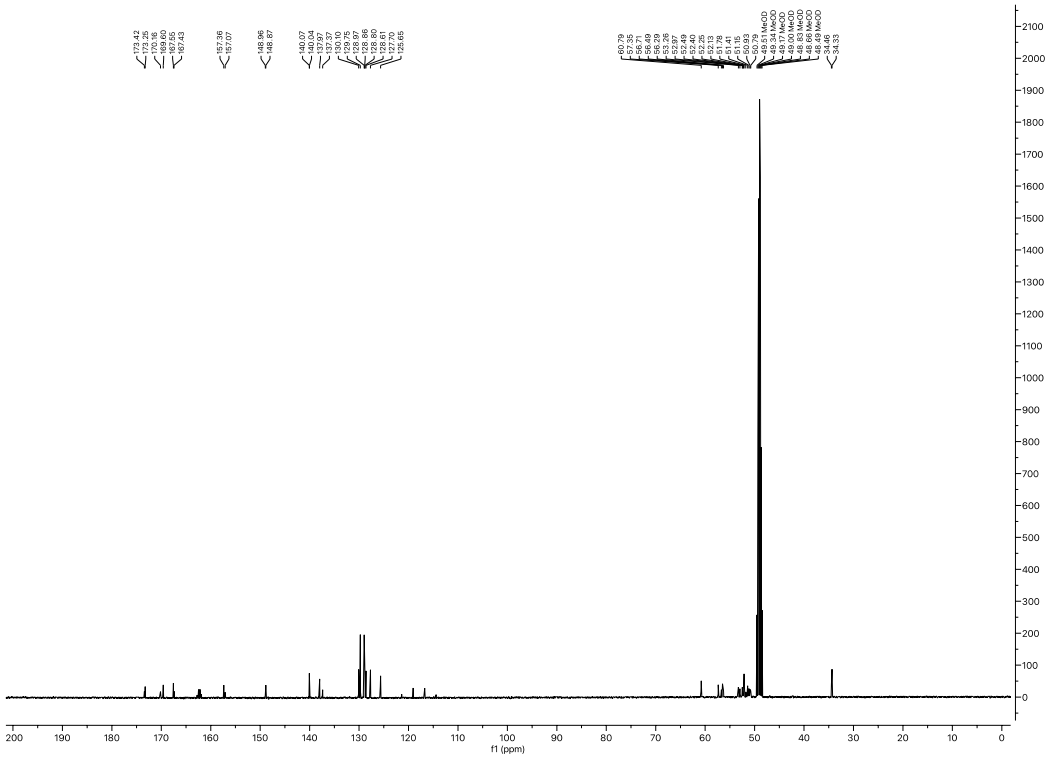


Figure S108 The $^{13}C\{^{1}H\}$ NMR spectrum of $H_2\mathbf{L}^{111}$ in MeOD.

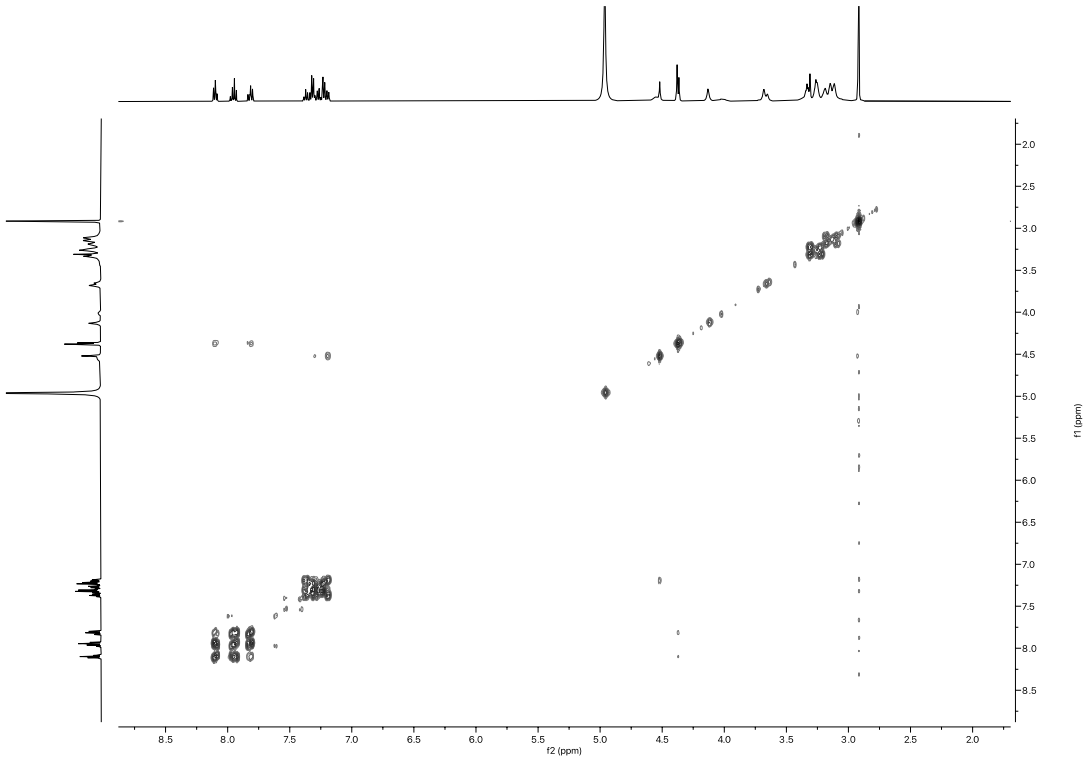


Figure S109 The ^{1}H-^{1}H COSY NMR spectrum of H_2**L**^{111} in MeOD.

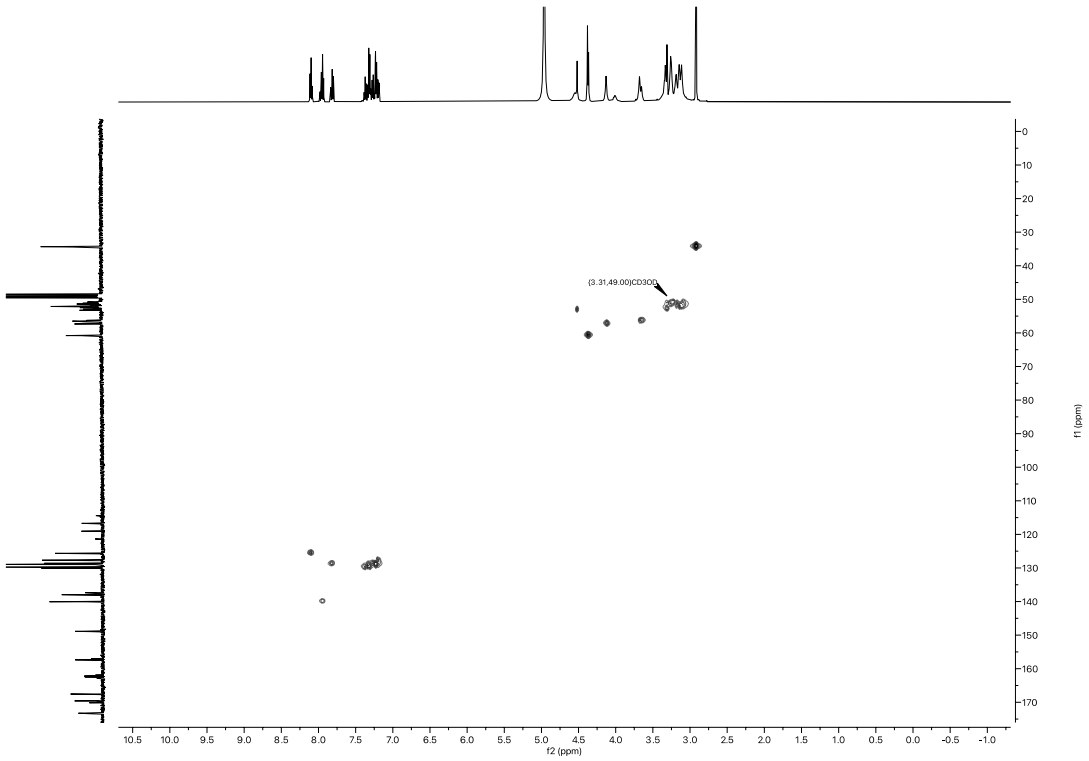


Figure S110 The ^{1}H-^{13}C HSQC NMR spectrum of H_2**L**^{111} in MeOD.

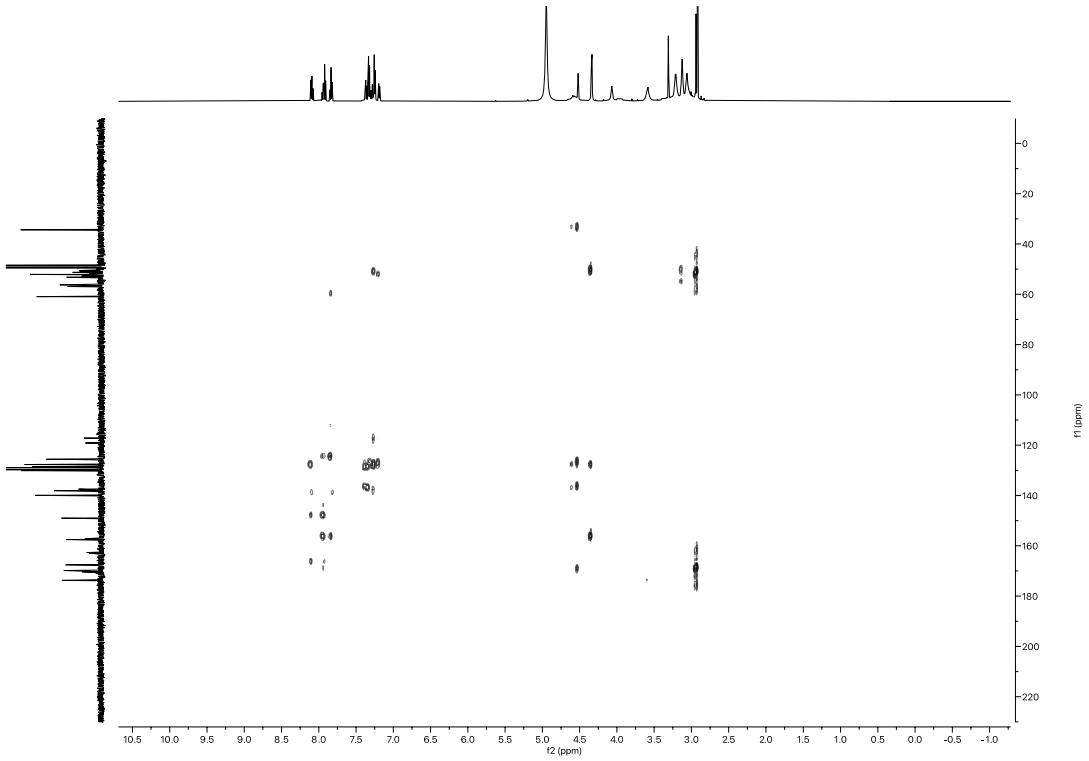


Figure S111 The ^{1}H-^{13}C HMBC NMR spectrum of $H_2\mathbf{L}^{111}$ in MeOD.

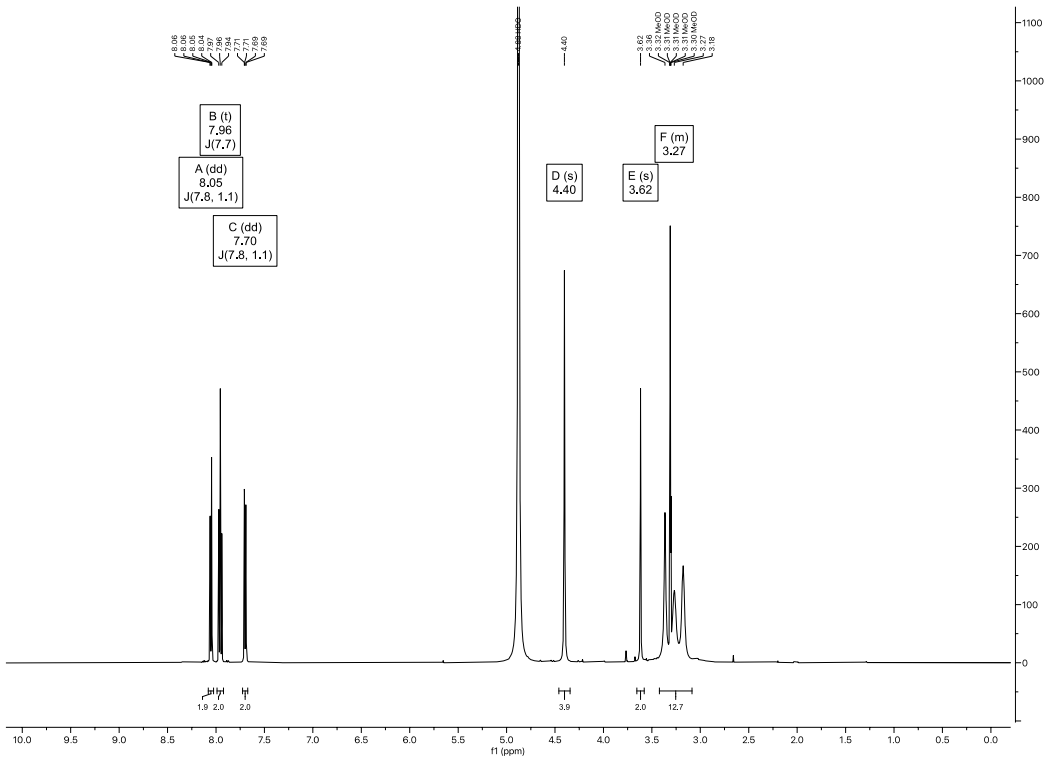


Figure S112 The ^{1}H NMR spectrum of $H_3\mathbf{L}^{102}$ in MeOD.

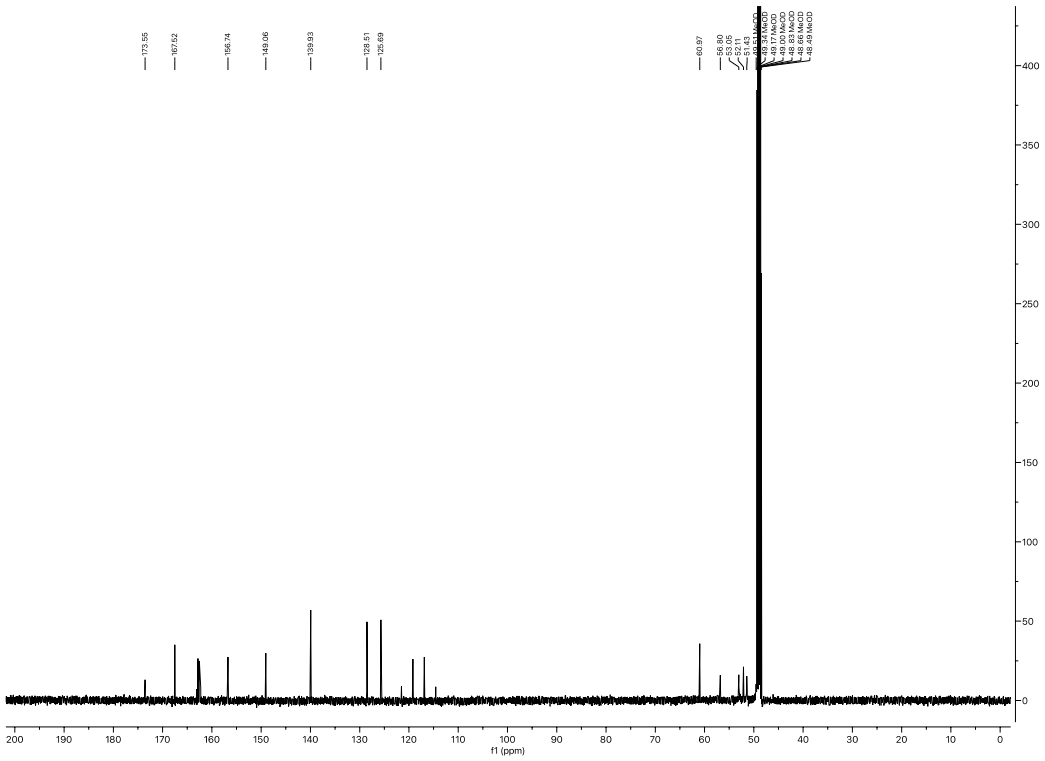


Figure S113 The $^{13}C\{^{1}H\}$ NMR spectrum of $H_3\mathbf{L^{102}}$ in MeOD.

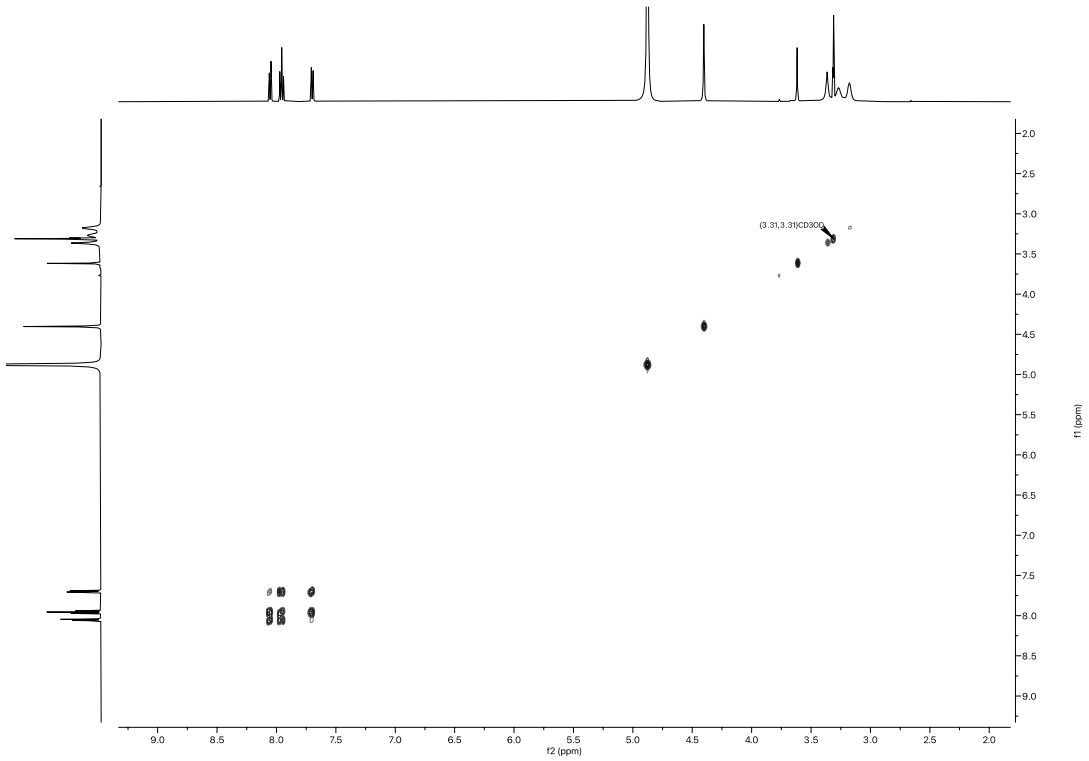


Figure S114 The ^{1}H-^{1}H COSY NMR spectrum of $H_3\mathbf{L^{102}}$ in MeOD.

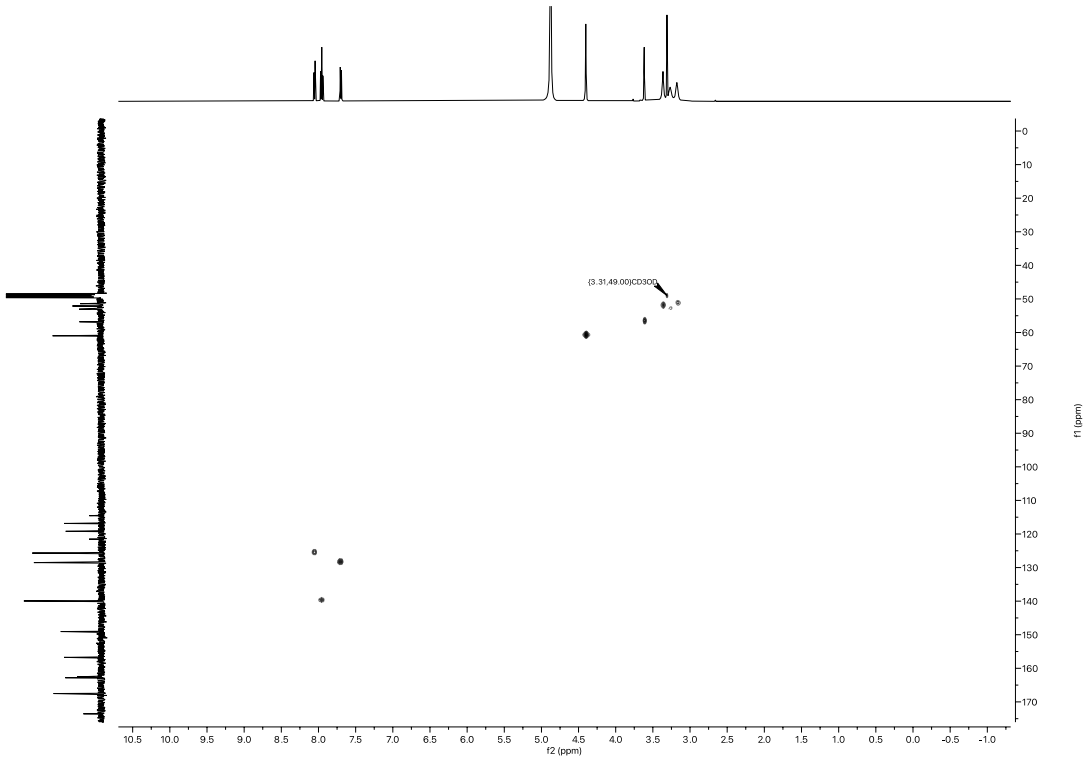


Figure S115 The ^{1}H-^{13}C HSQC NMR spectrum of $H_3\mathbf{L}^{102}$ in MeOD.

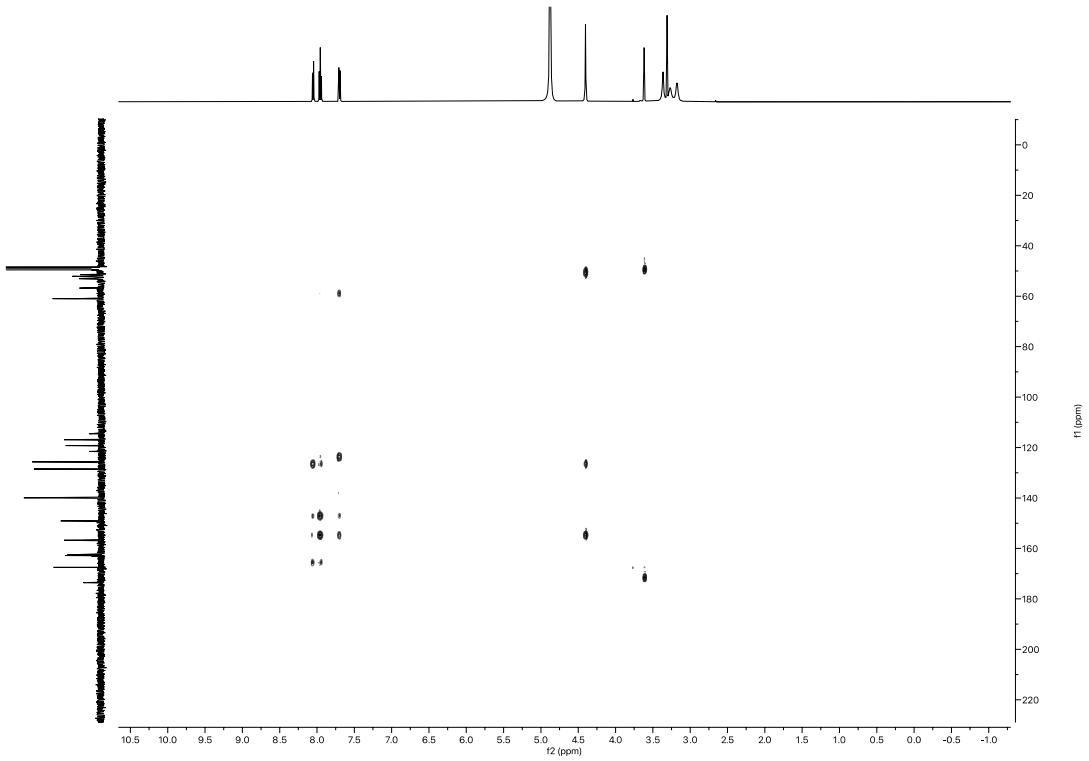


Figure S116 The ^{1}H-^{13}C HMBC NMR spectrum of $H_3\mathbf{L}^{102}$ in MeOD.

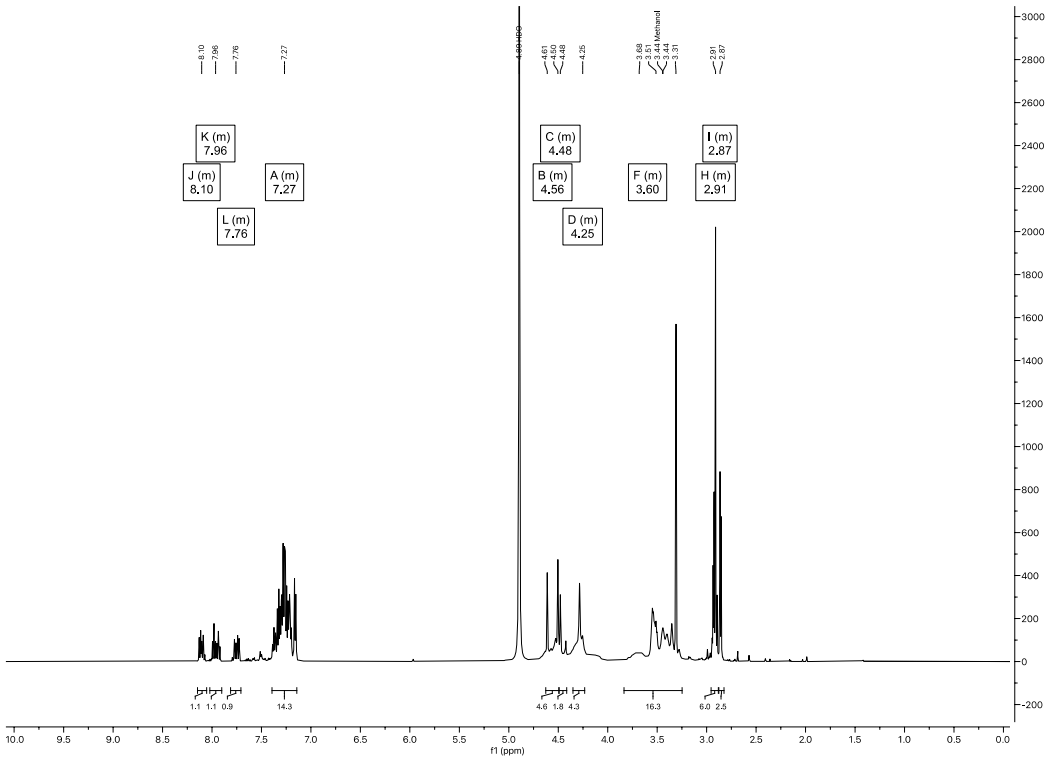


Figure S117 The ^{1}H NMR spectrum of H**L**^{021} in MeOD.

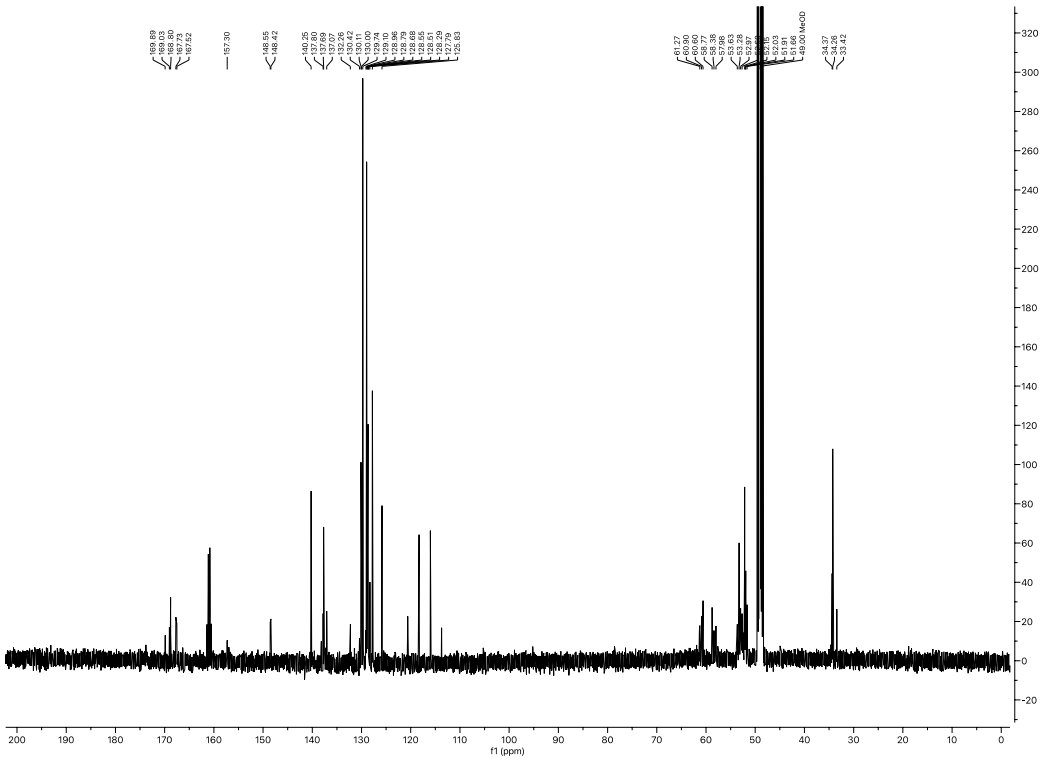


Figure S118 The ^{13}C{^{1}H} NMR spectrum of H**L**^{021} in MeOD.

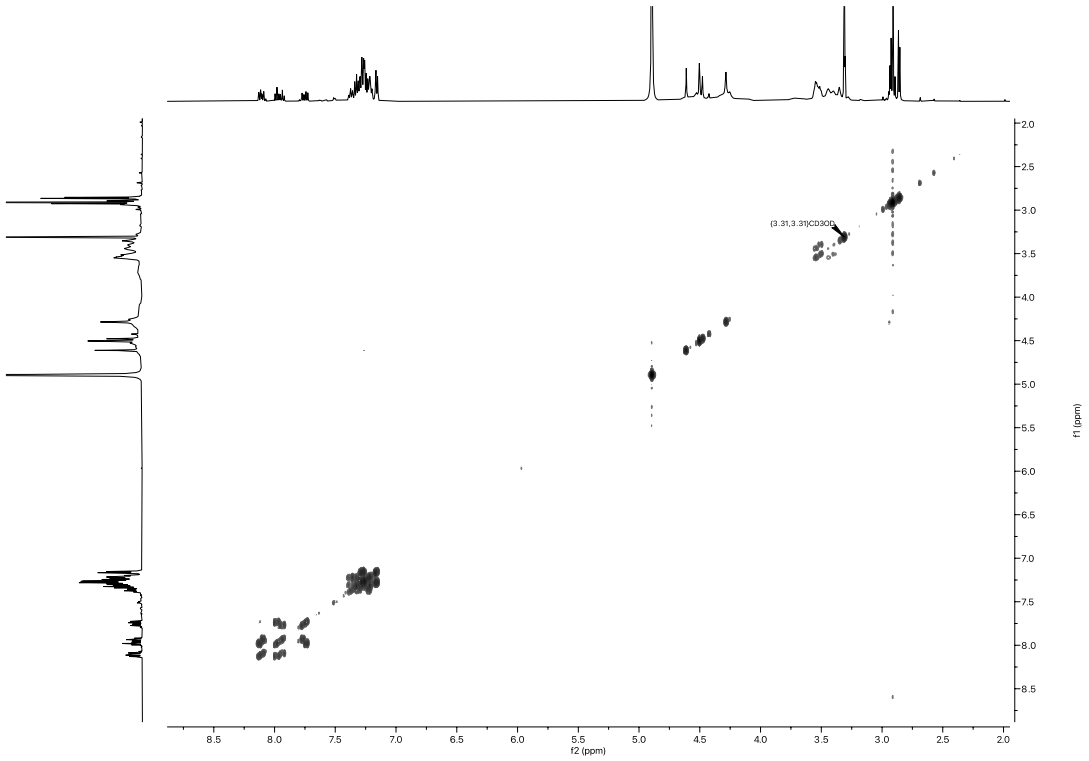


Figure S119 The ^{1}H-^{1}H COSY NMR spectrum of H**L**^{021} in MeOD.

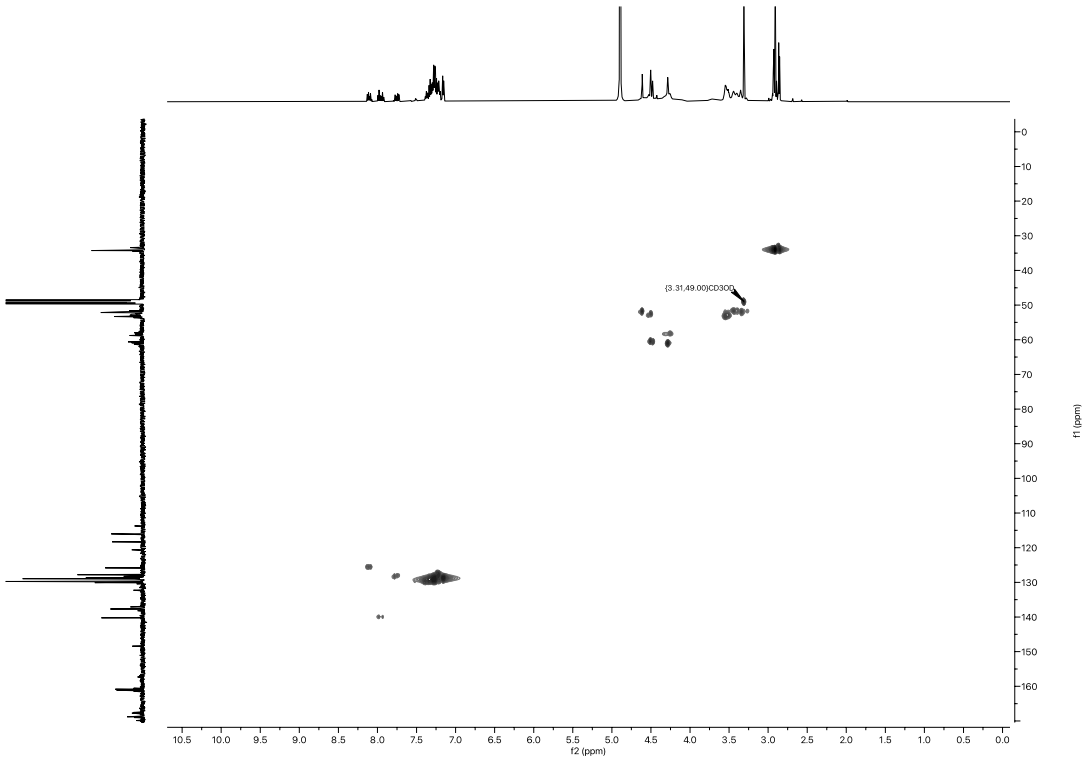


Figure S120 The ^{1}H-^{13}C HSQC NMR spectrum of H**L**^{021} in MeOD.

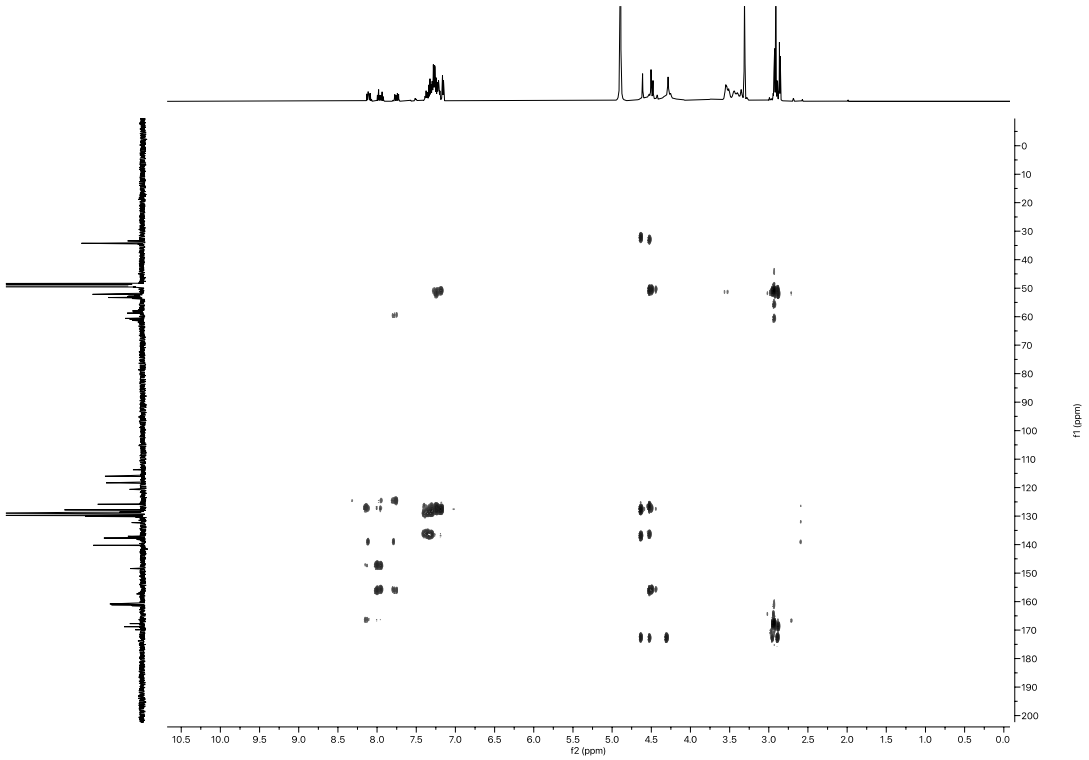


Figure S121 The ^{1}H-^{13}C HMBC NMR spectrum of H**L**^{021} in MeOD.

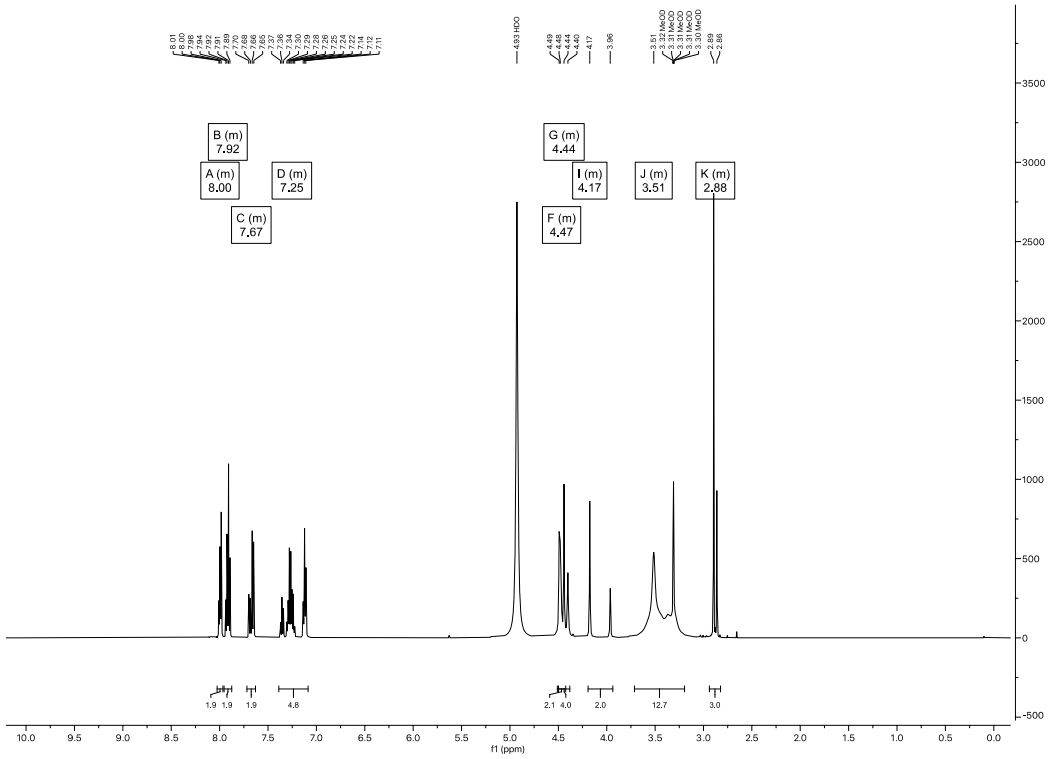


Figure S122 The ^{1}H NMR spectrum of H_2**L**^{012} in MeOD.

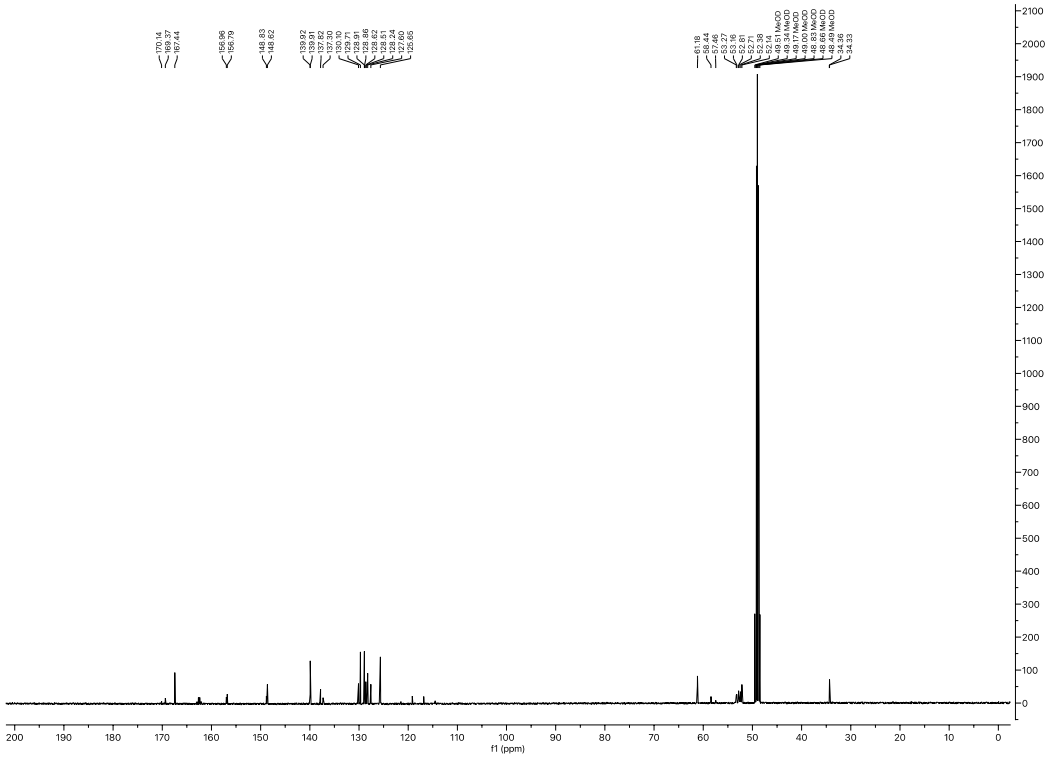


Figure S123 The $^{13}C\{^{1}H\}$ NMR spectrum of $H_2\mathbf{L^{012}}$ in MeOD.

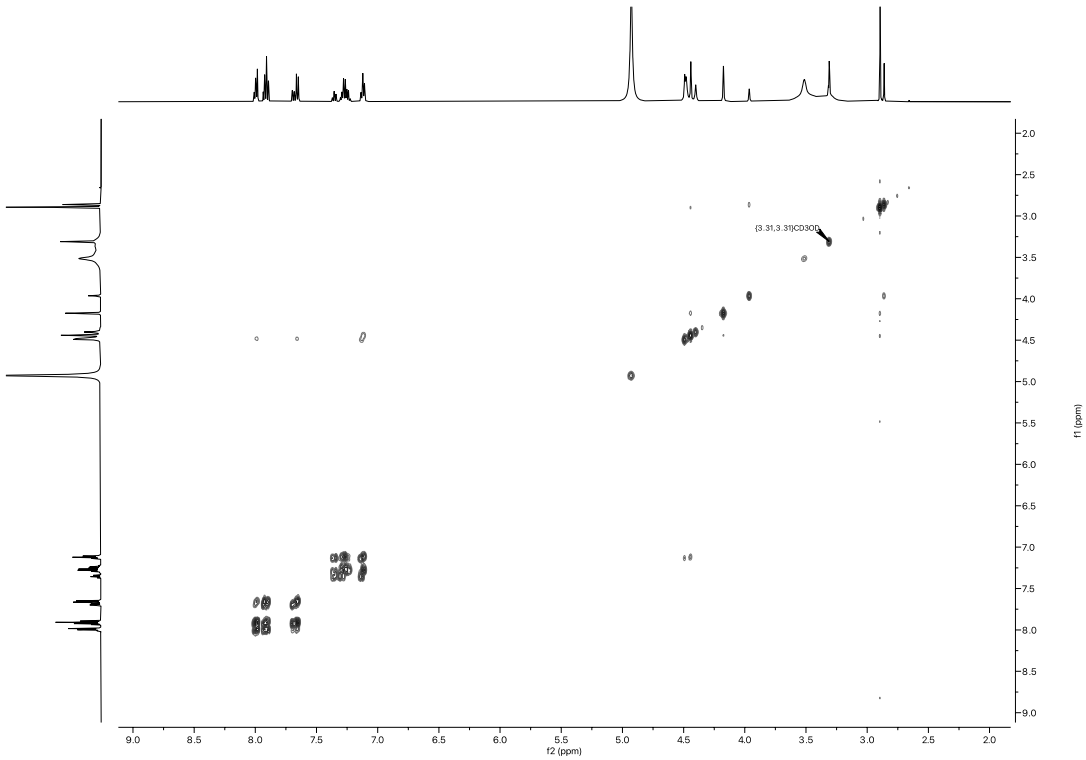


Figure S124 The ^{1}H-^{1}H COSY NMR spectrum of $H_2\mathbf{L^{012}}$ in MeOD.

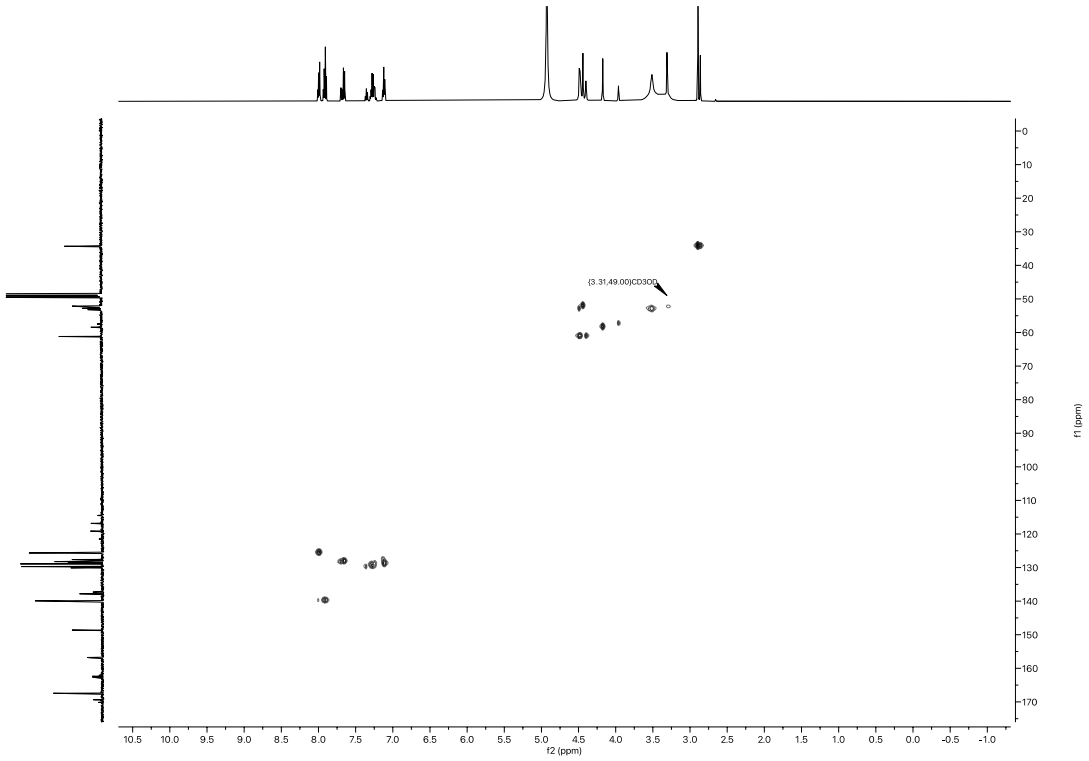


Figure S125 The ^{1}H-^{13}C HSQC NMR spectrum of H_2**L**^{012} in MeOD.

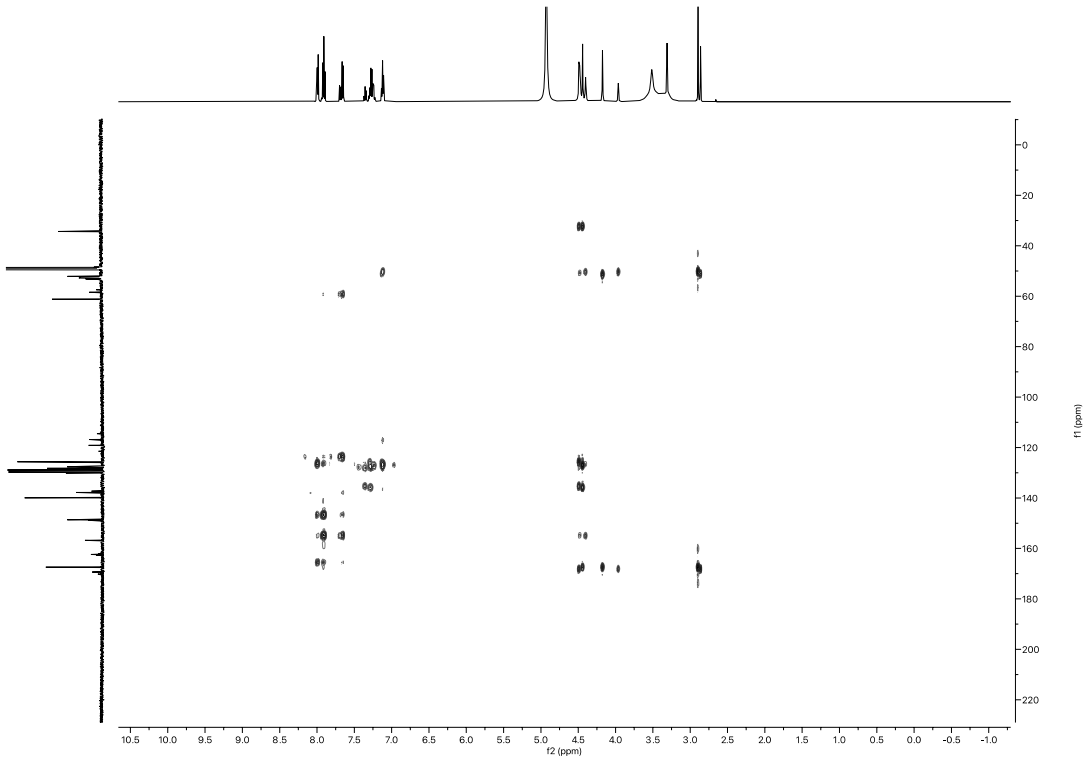


Figure S126 The ^{1}H-^{13}C HMBC NMR spectrum of H_2**L**^{012} in MeOD.

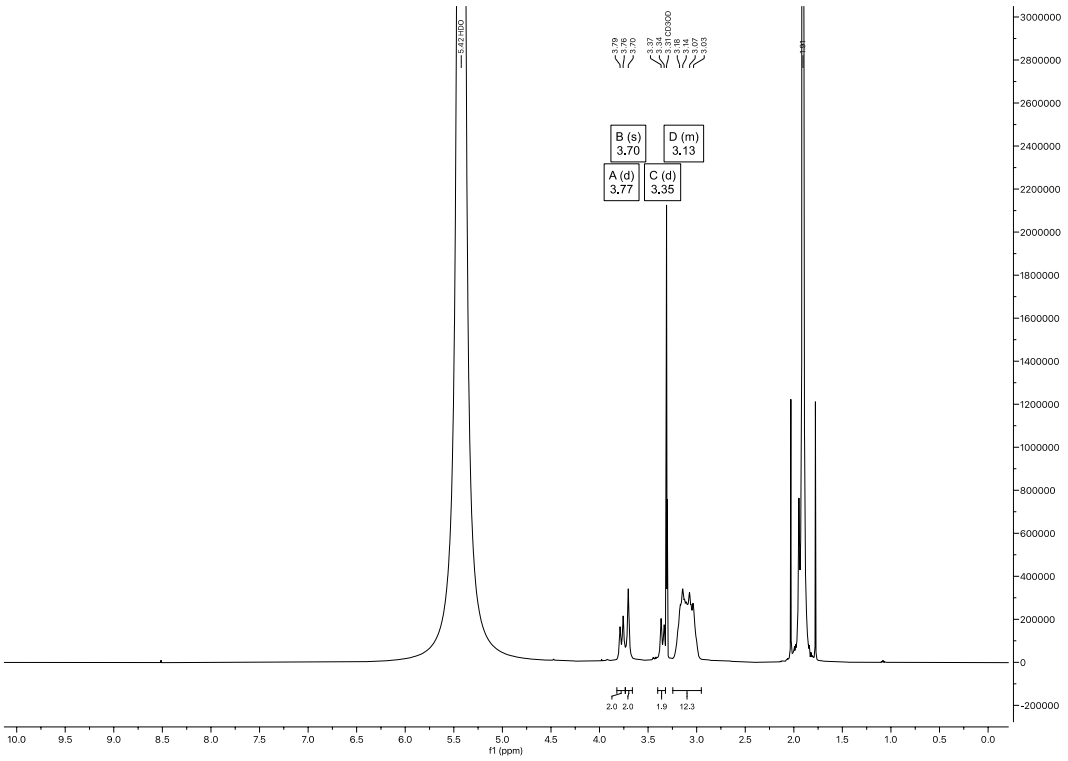


Figure S127 The ^{1}H NMR spectrum of [Sc(**L**^{300})] in MeOD.

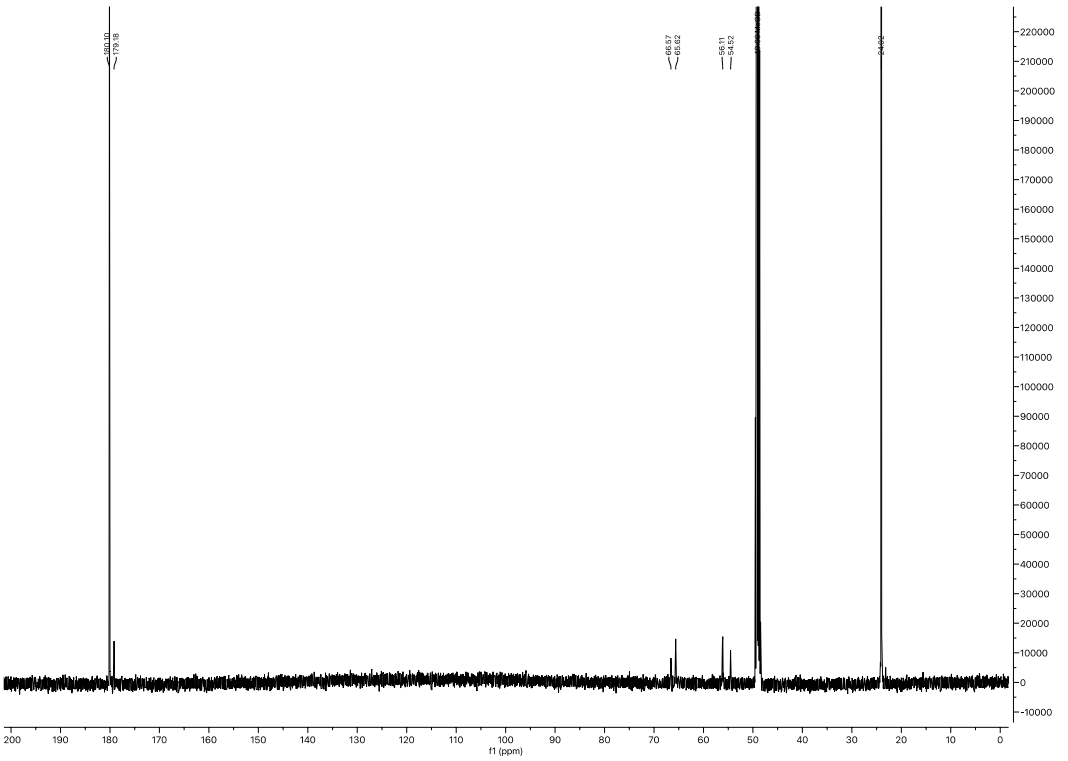


Figure S128 The $^{13}C\{^{1}H\}$ NMR spectrum of [Sc(**L**^{300})] in MeOD.

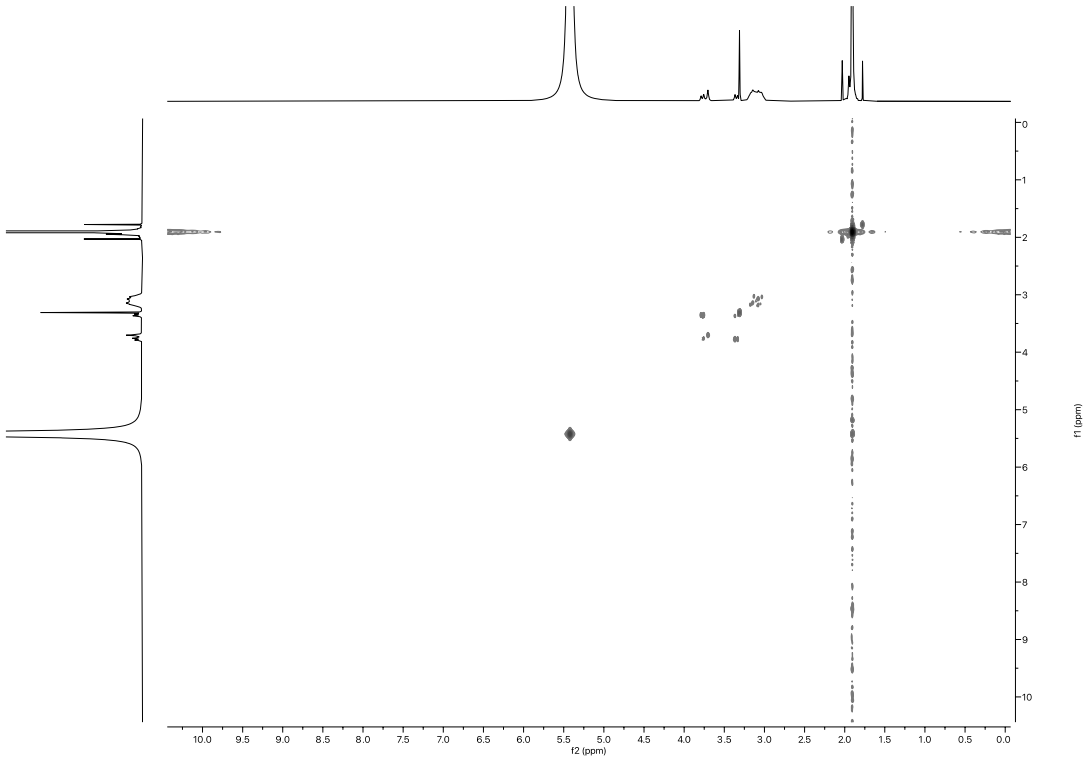


Figure S129 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**^{300})] in MeOD.

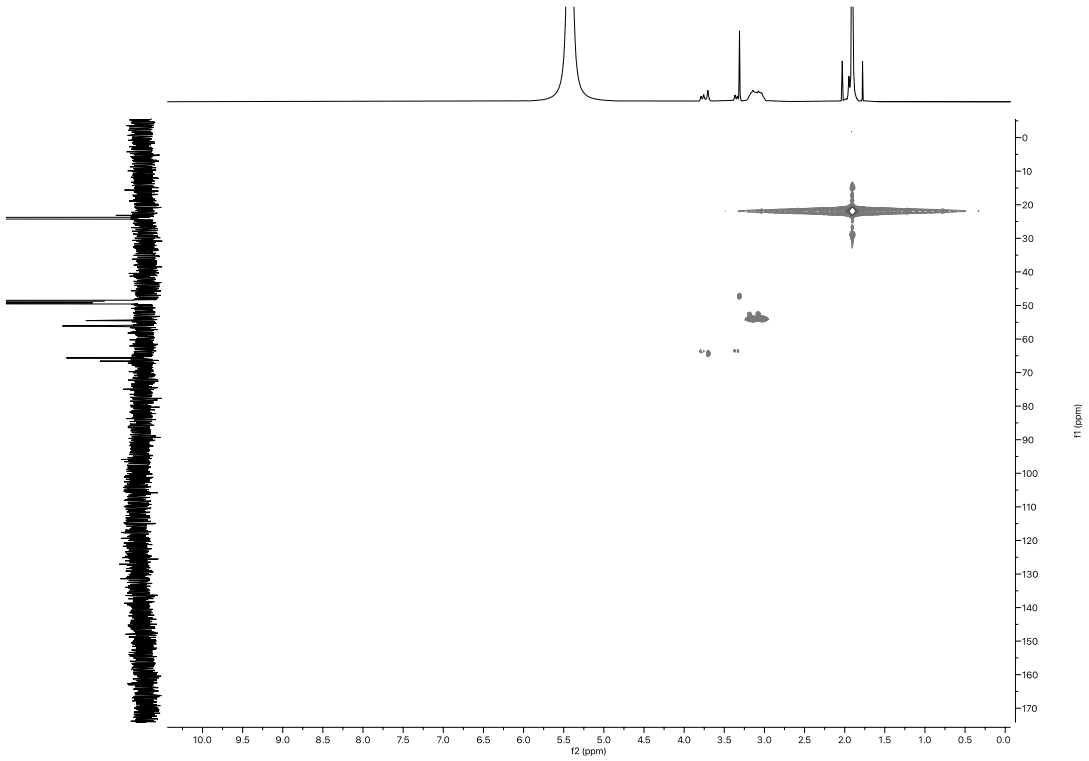


Figure S130 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**^{300})] in MeOD.

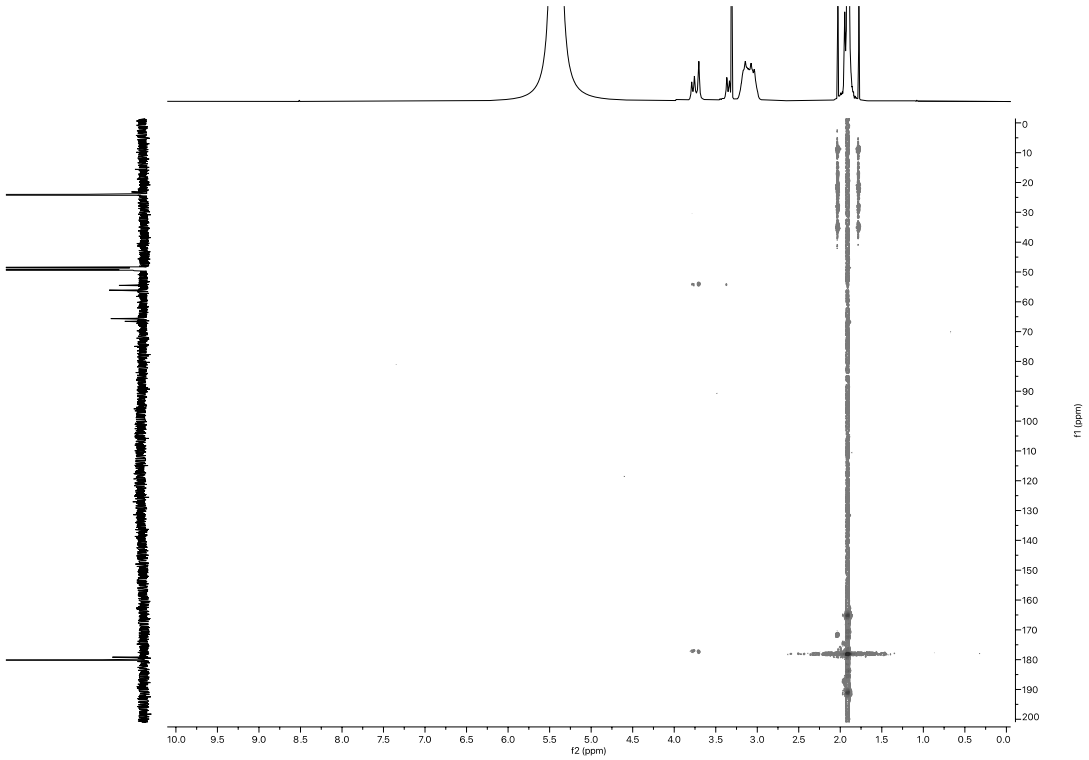


Figure S131 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**^{300})] in MeOD.

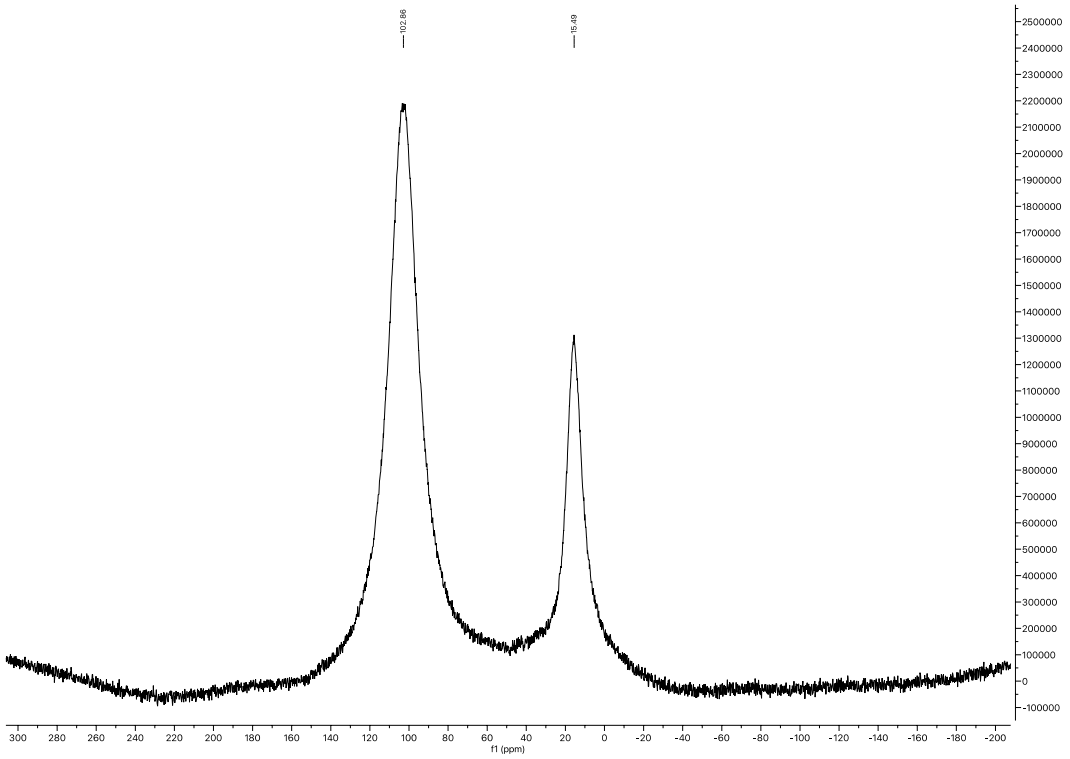


Figure S132 The ^{45}Sc NMR spectrum of [Sc(**L**^{300})] in MeOD.

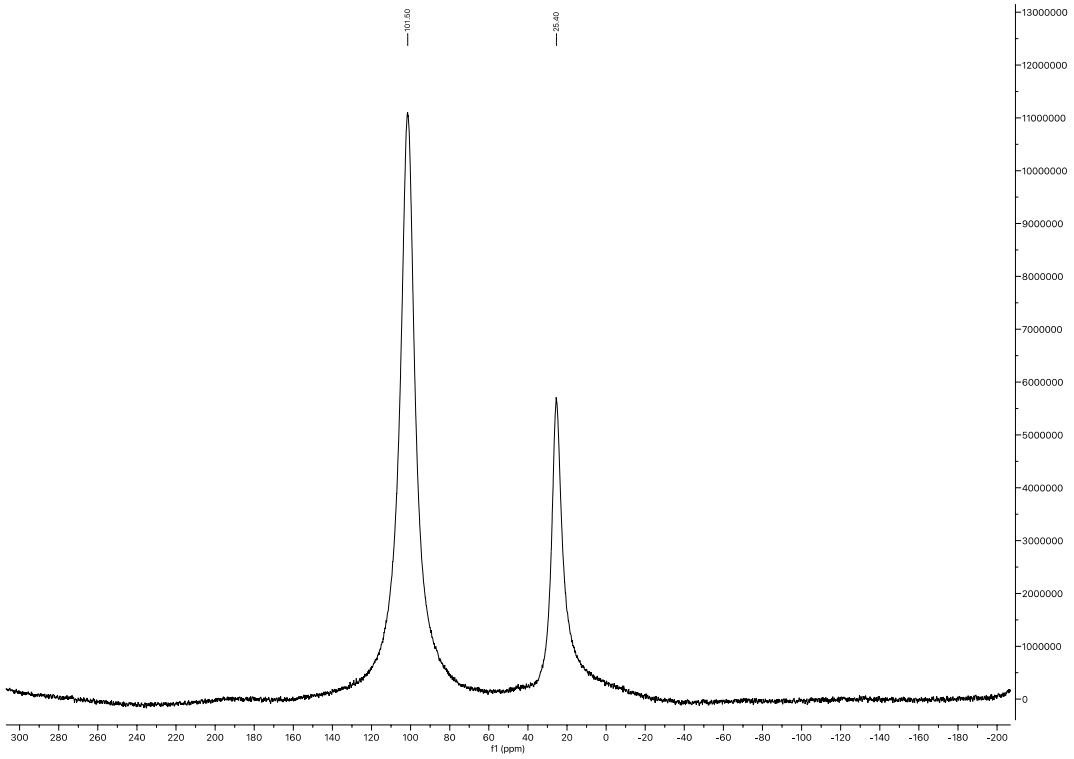


Figure S133 The ^{45}Sc NMR spectrum of [Sc(**L^{300}**)] in D_2O.

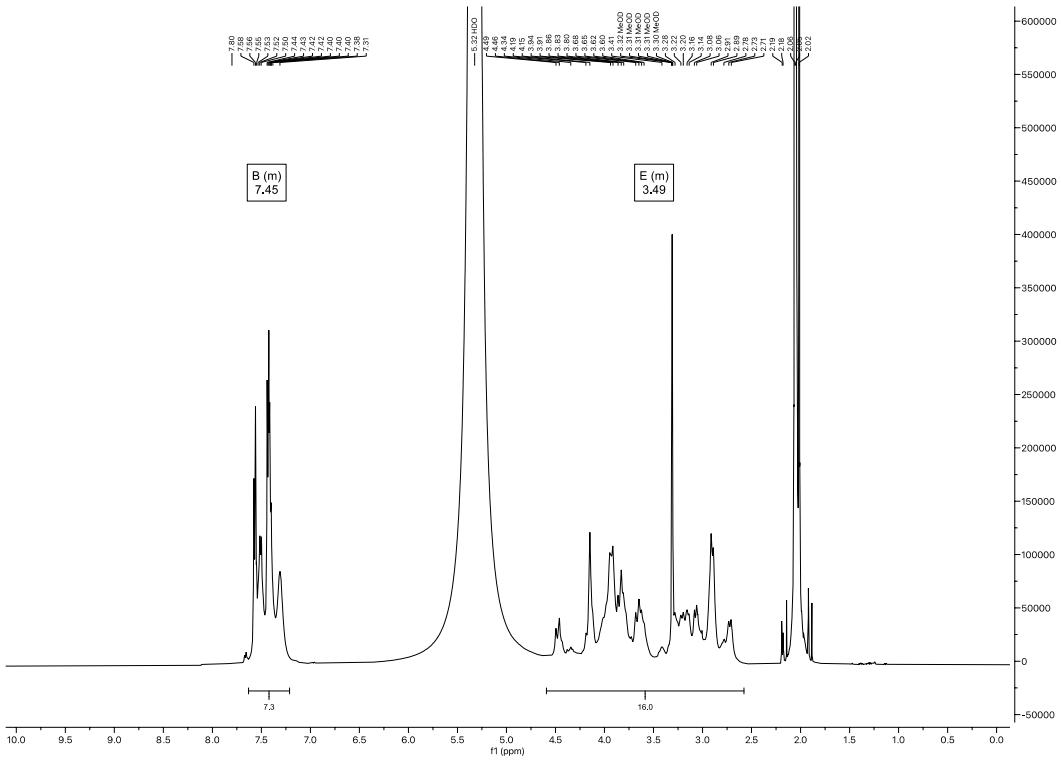


Figure S134 The ^{1}H NMR spectrum of [Sc(**L$^{300\text{-}BzNH2}$**)] in MeOD.

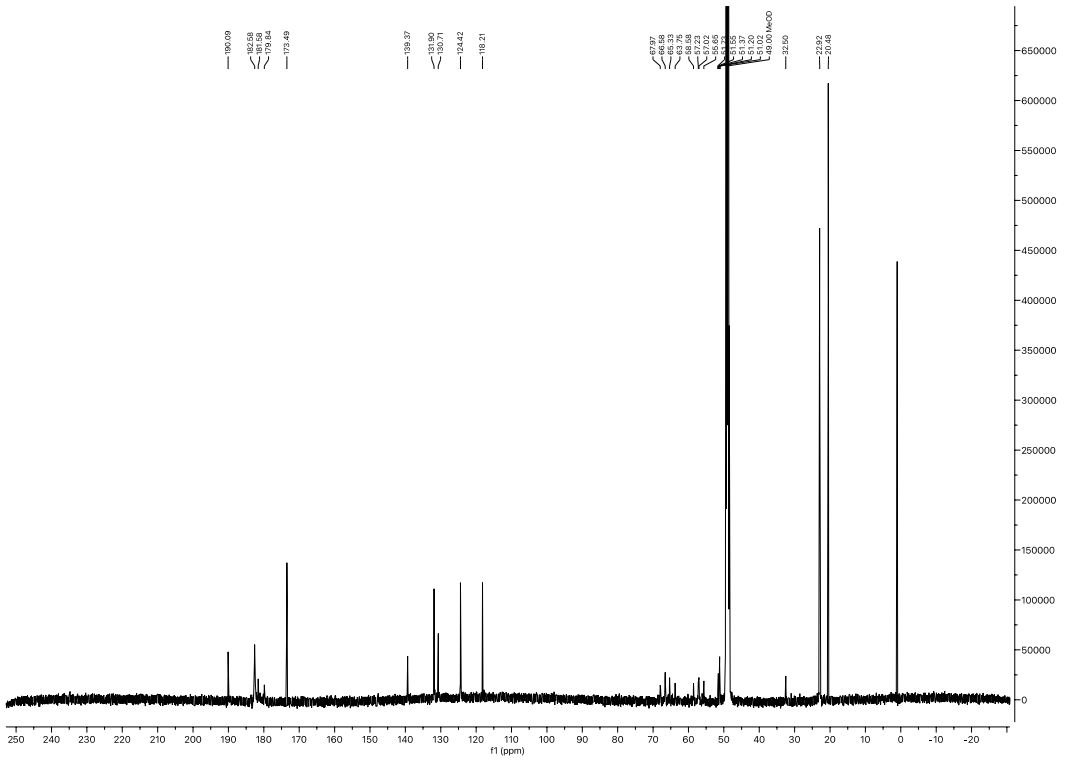


Figure S135 The $^{13}C\{^{1}H\}$ NMR spectrum of [Sc(**L**$^{\mathbf{300\text{-}BzNH2}}$)] in MeOD.

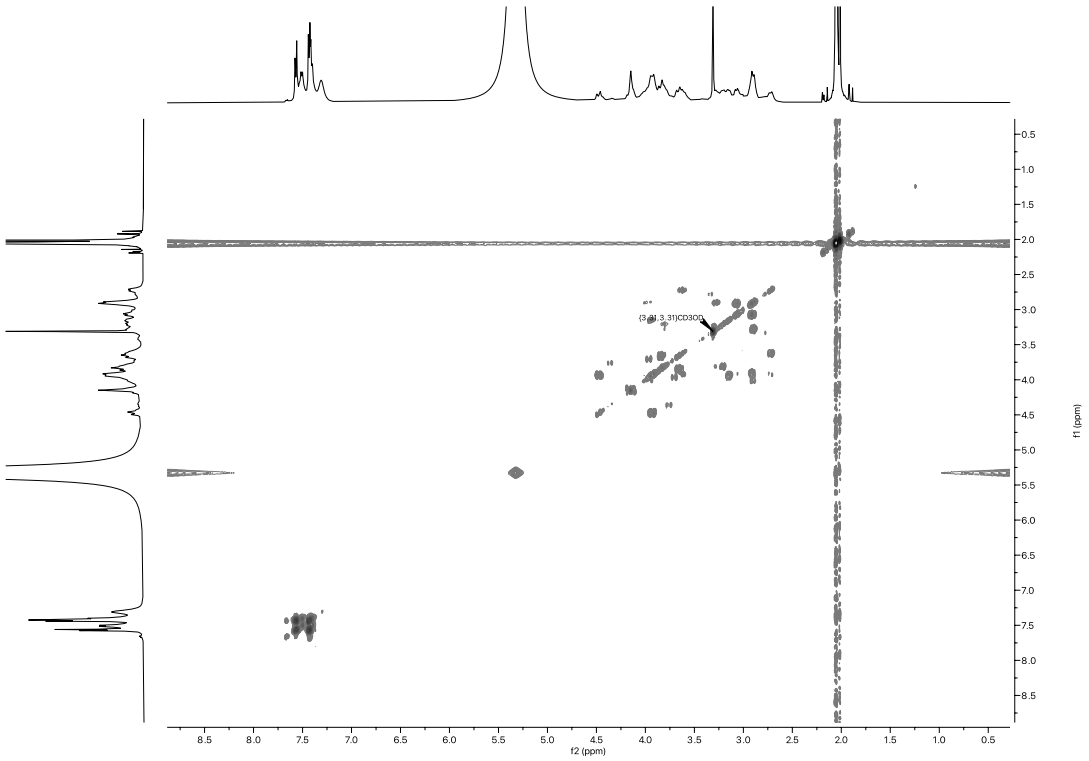


Figure S136 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**$^{\mathbf{300\text{-}BzNH2}}$)] in MeOD.

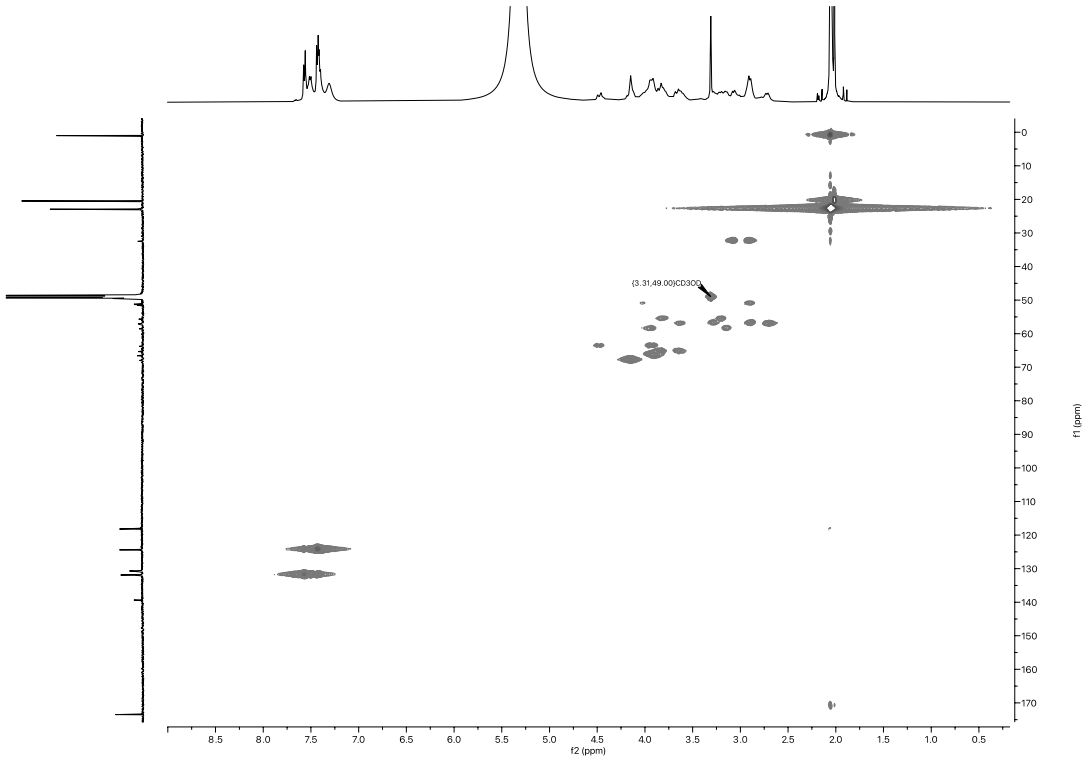


Figure S137 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**$^{\mathbf{300\text{-}BzNH2}}$)] in MeOD.

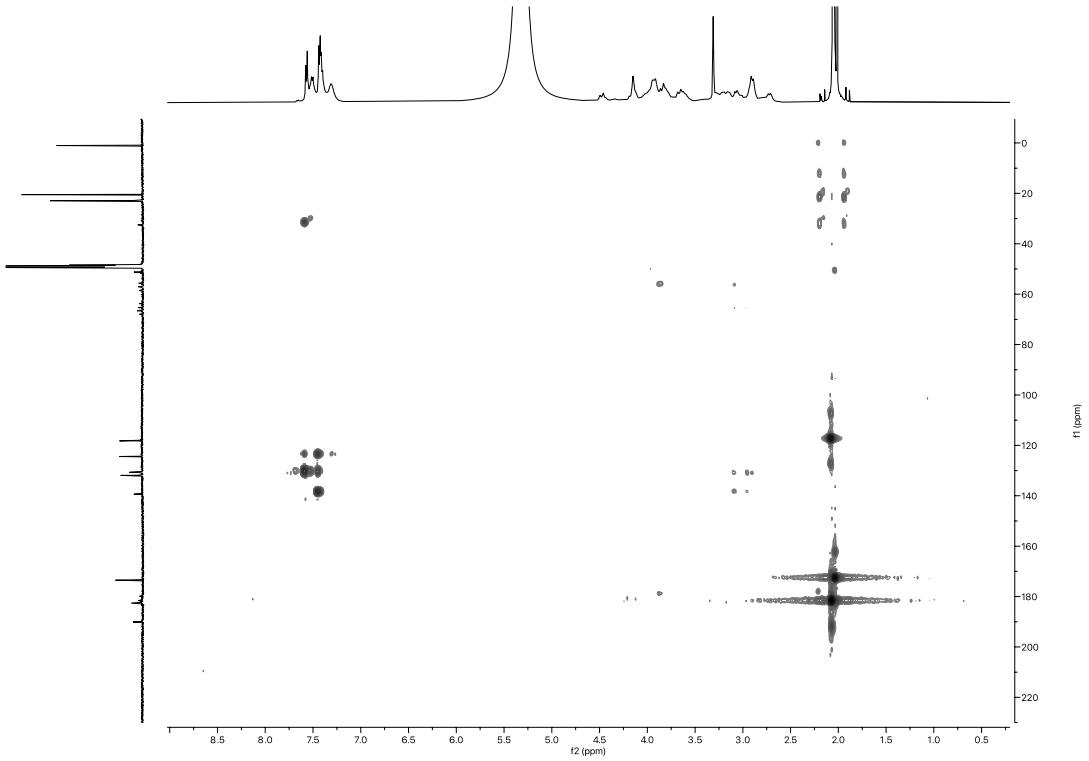


Figure S138 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**$^{\mathbf{300\text{-}BzNH2}}$)] in MeOD.

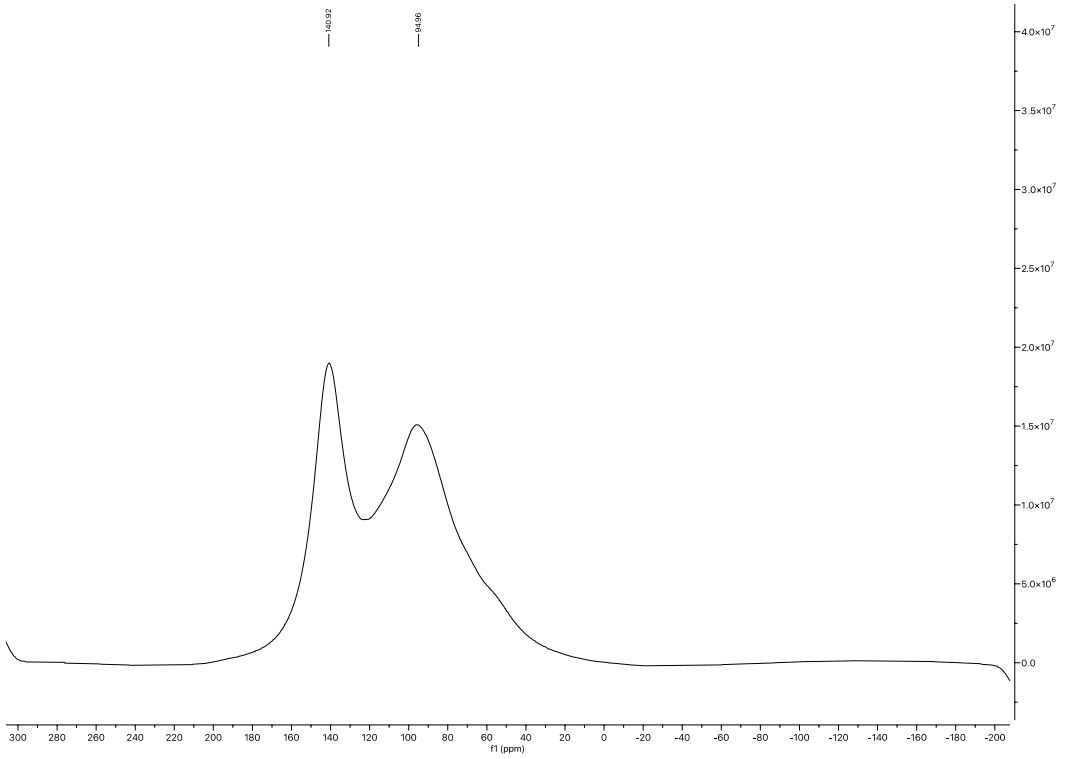


Figure S139 The ^{45}Sc NMR spectrum of [Sc(**L**$^{\mathbf{300\text{-}BzNH2}}$)] in MeOD.

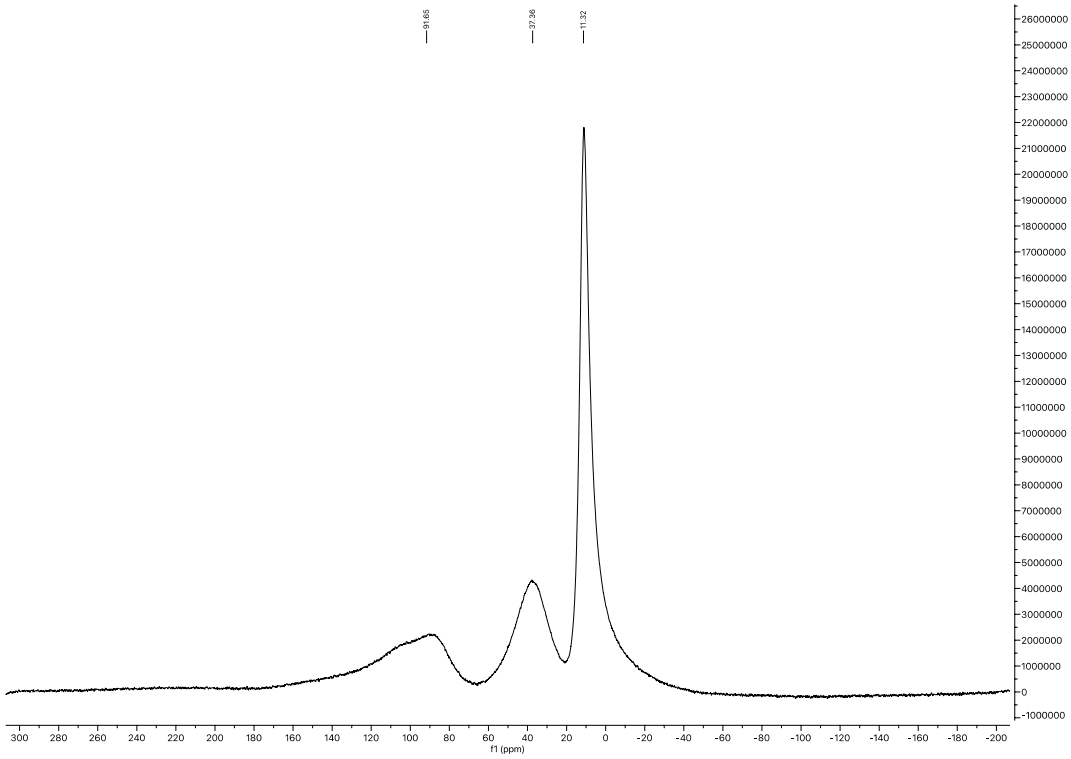


Figure S140 The ^{45}Sc NMR spectrum of [Sc(**L**$^{\mathbf{300\text{-}BzNH2}}$)] in D_2O.

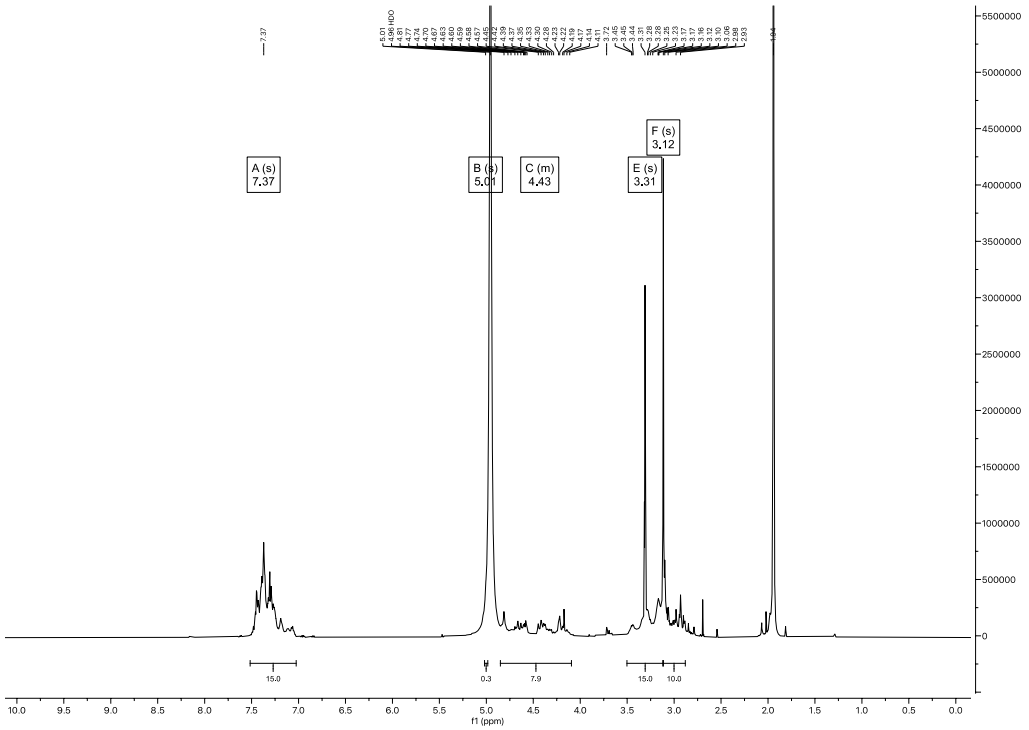


Figure S141 The ^{1}H NMR spectrum of [Sc(**L**$^{\mathbf{030}}$)]$^{3+}$ in MeOD.

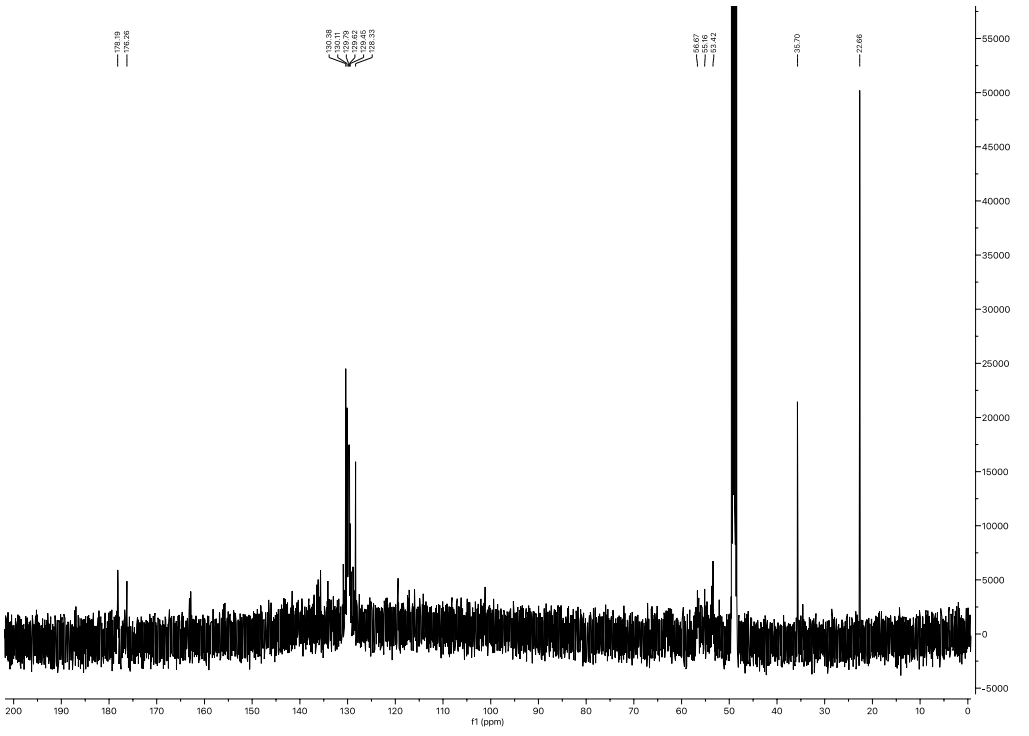


Figure S142 The ^{13}C{^{1}H} NMR spectrum of [Sc(**L**$^{\mathbf{030}}$)]$^{3+}$ in MeOD.

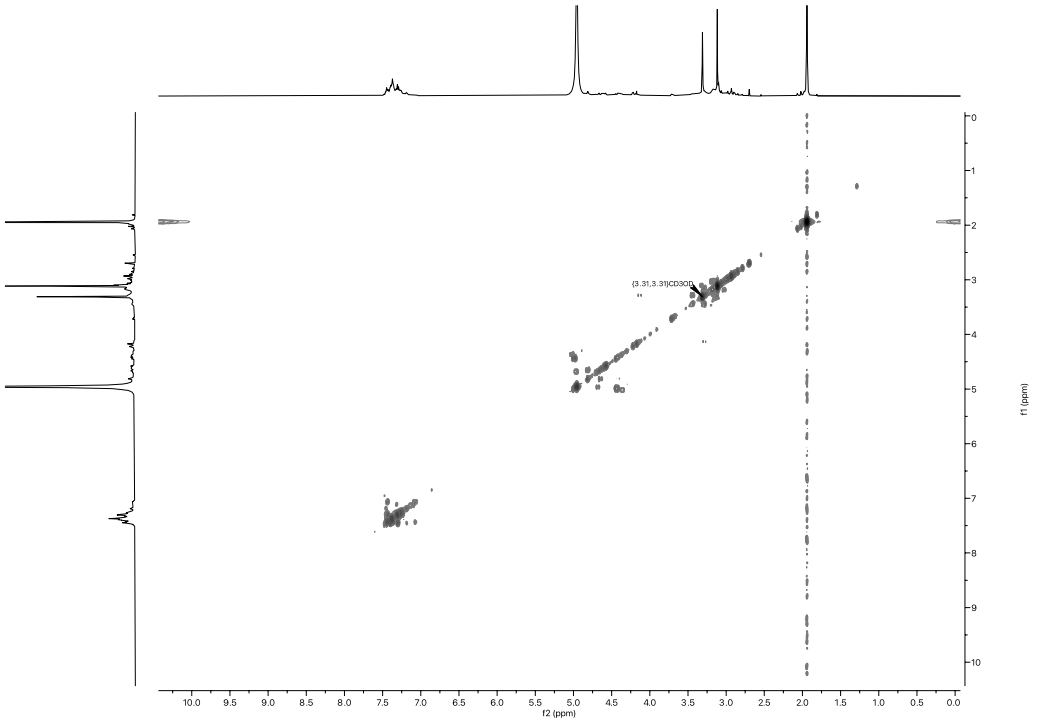


Figure S143 The ^{1}H-^{1}H COSY NMR spectrum of $[Sc(\mathbf{L^{030}})]^{3+}$ in MeOD.

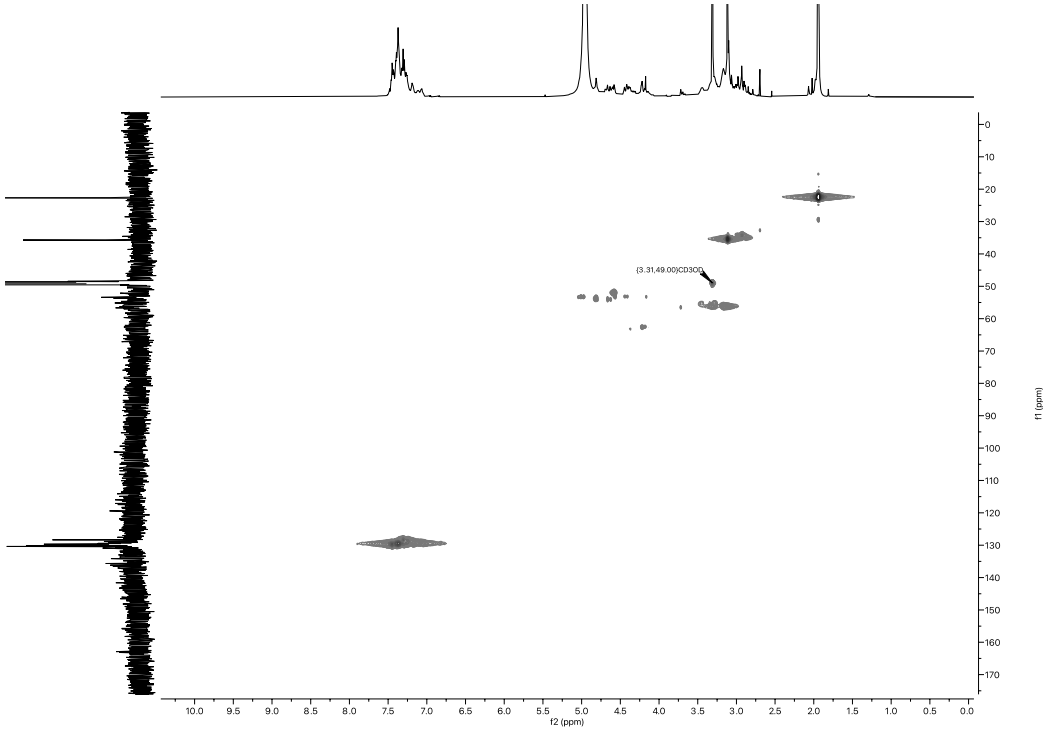


Figure S144 The ^{1}H-^{13}C HSQC NMR spectrum of $[Sc(\mathbf{L^{030}})]^{3+}$ in MeOD.

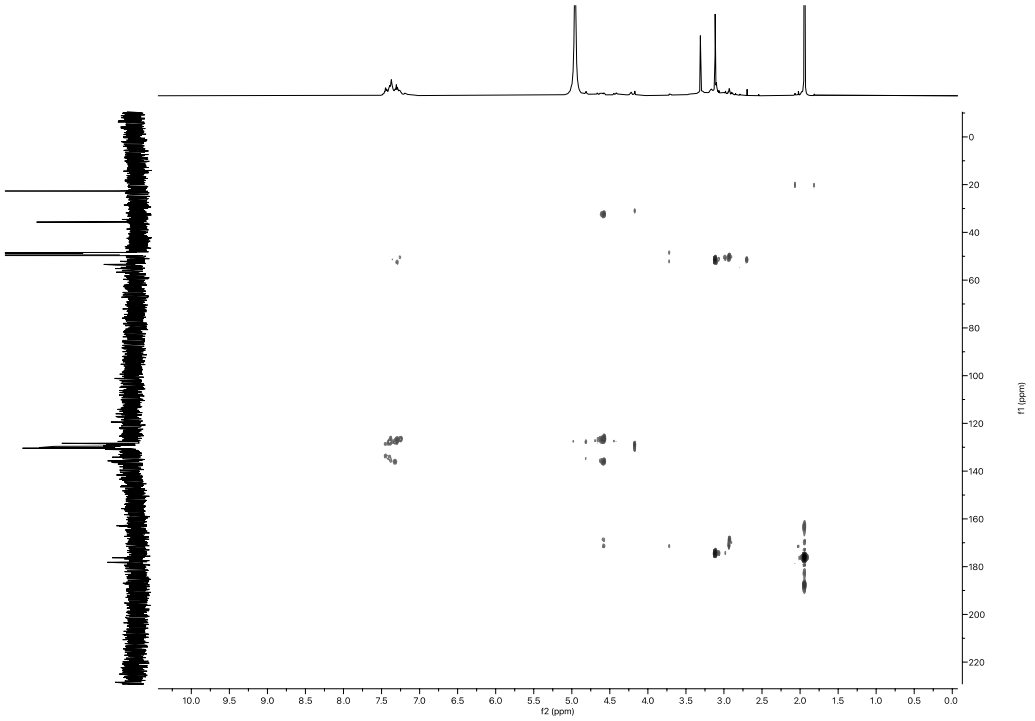


Figure S145 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**$^{\mathbf{030}}$)]$^{3+}$ in MeOD.

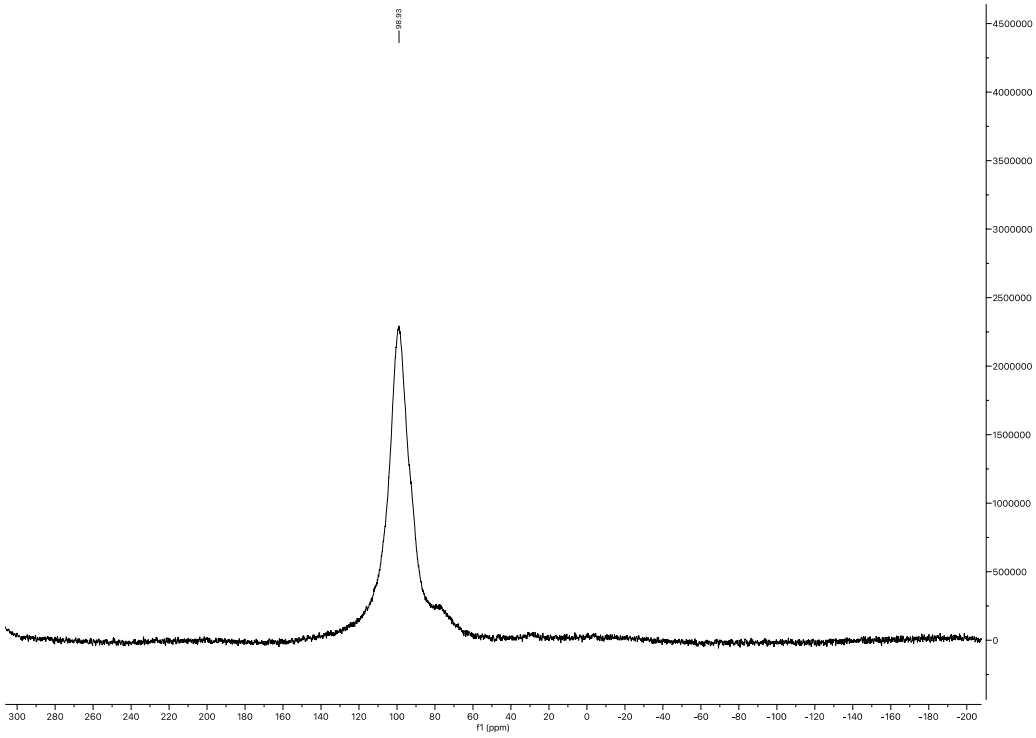


Figure S146 The ^{45}Sc NMR spectrum of [Sc(**L**$^{\mathbf{030}}$)]$^{3+}$ in MeOD.

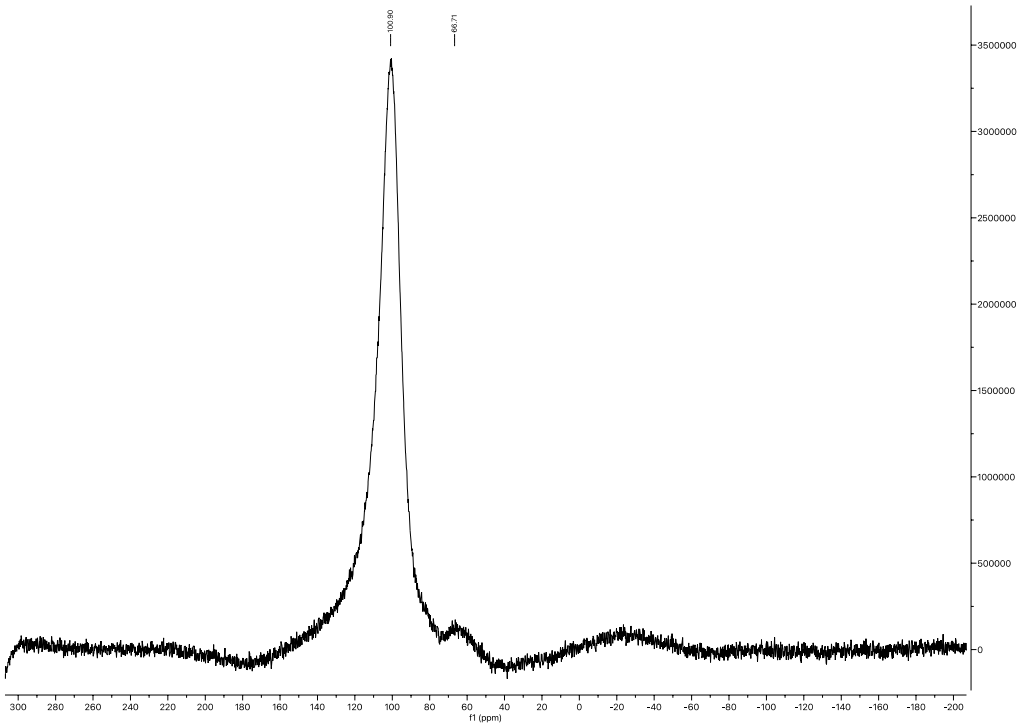


Figure S147 The ^{45}Sc NMR spectrum of [Sc(**L**^{030})]$^{3+}$ in D_2O.

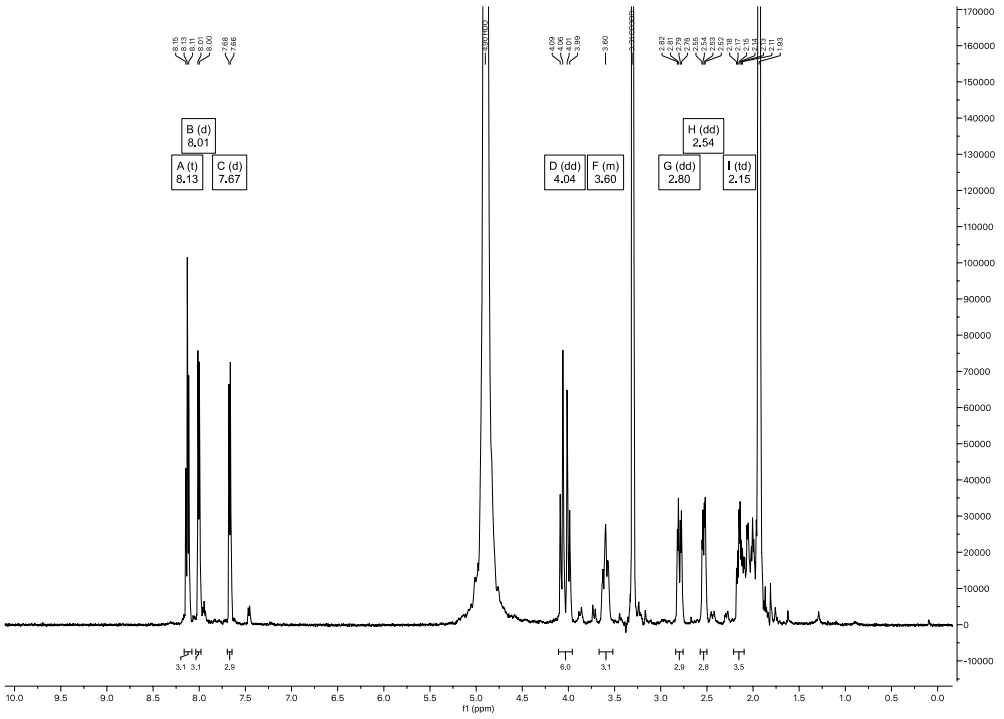


Figure S148 The ^{1}H NMR spectrum of [Sc(**L**^{003})] in MeOD.

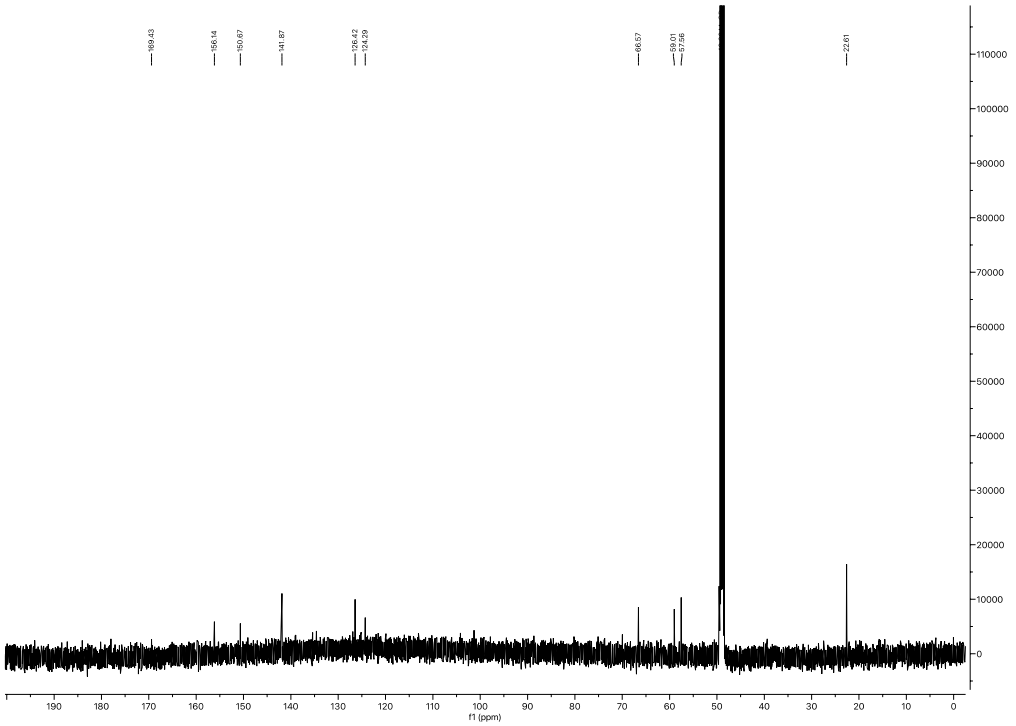


Figure S149 The $^{13}C\{^{1}H\}$ NMR spectrum of [Sc(**L**^{003})]) in MeOD.

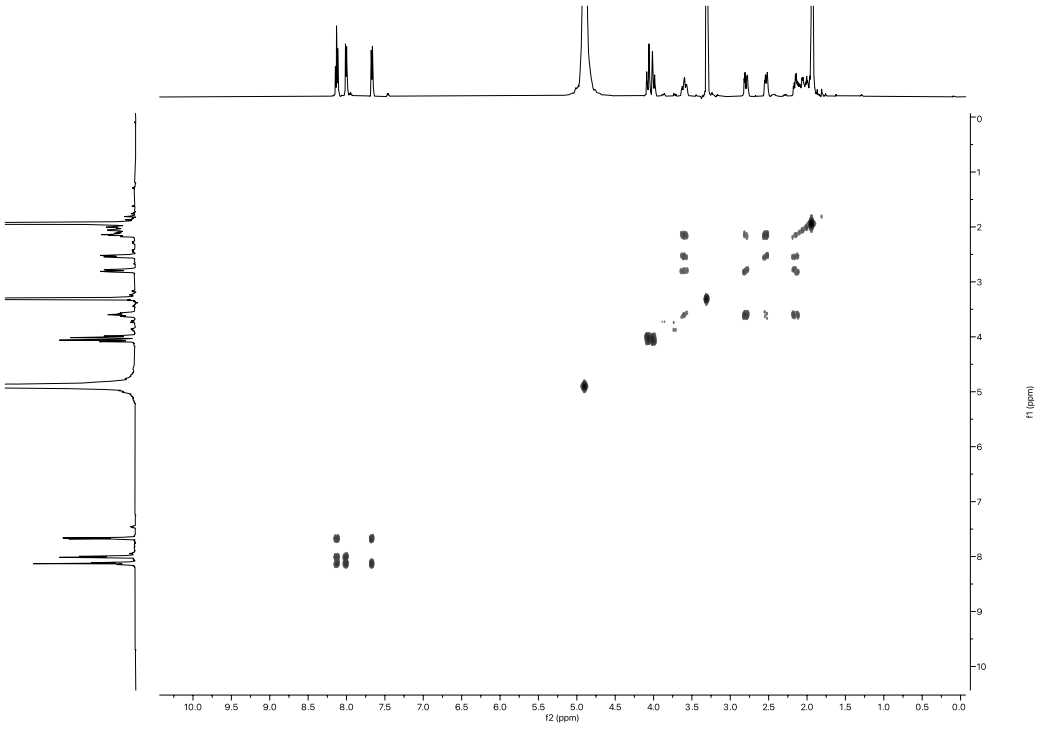


Figure S150 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**^{003})] in MeOD.

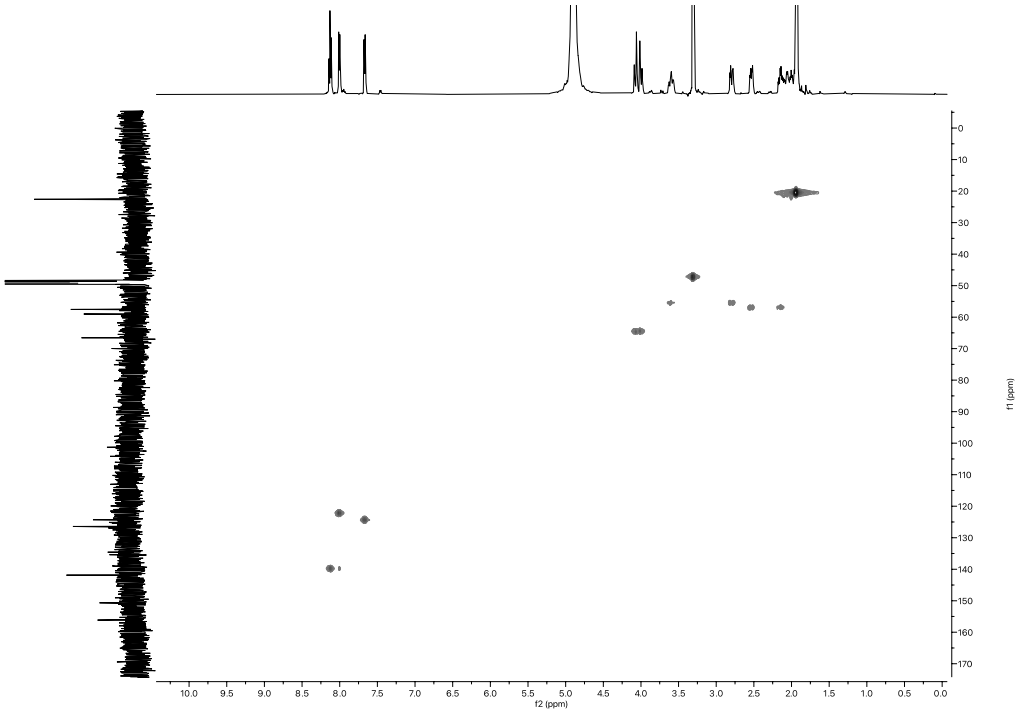


Figure S151 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**^{003})] in MeOD.

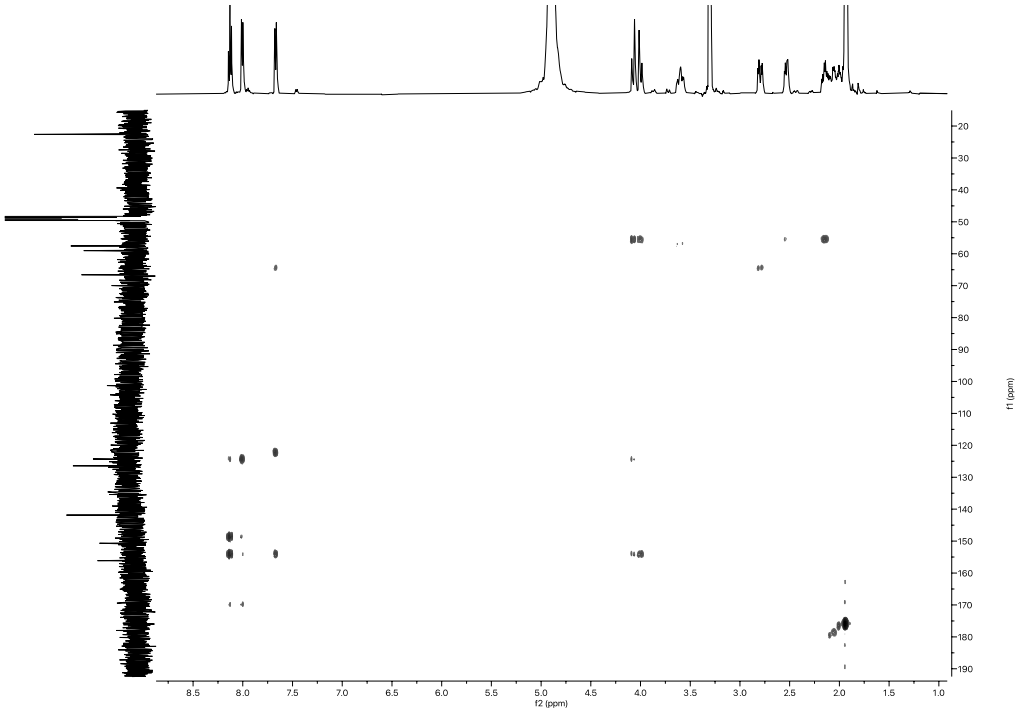


Figure S152 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**^{003})] in MeOD.

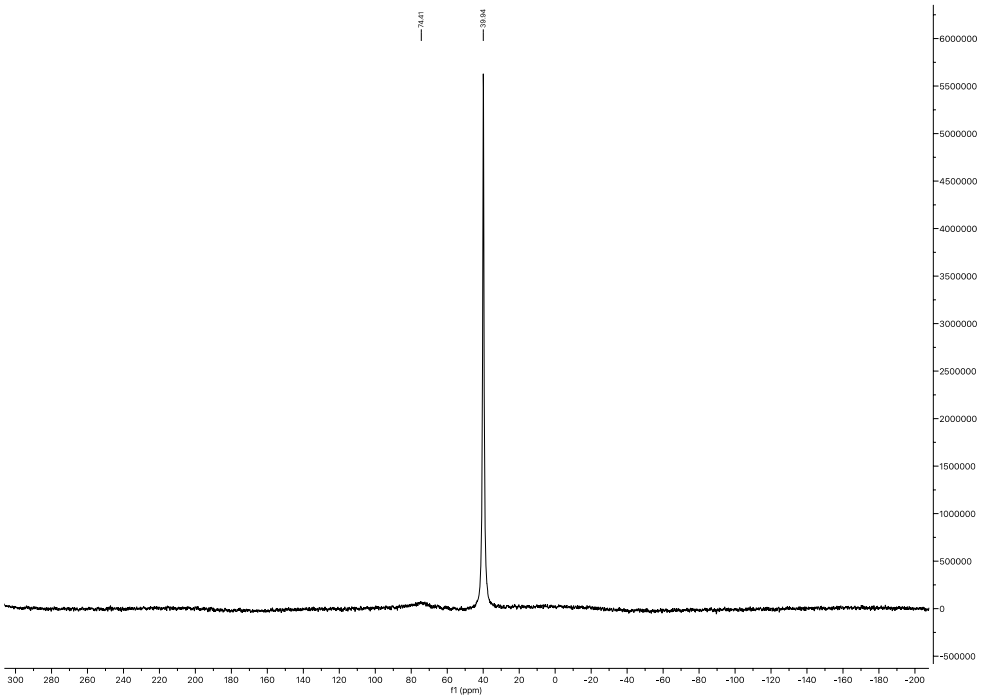


Figure S153 The ^{45}Sc NMR spectrum of [Sc(**L**^{003})] in MeOD.

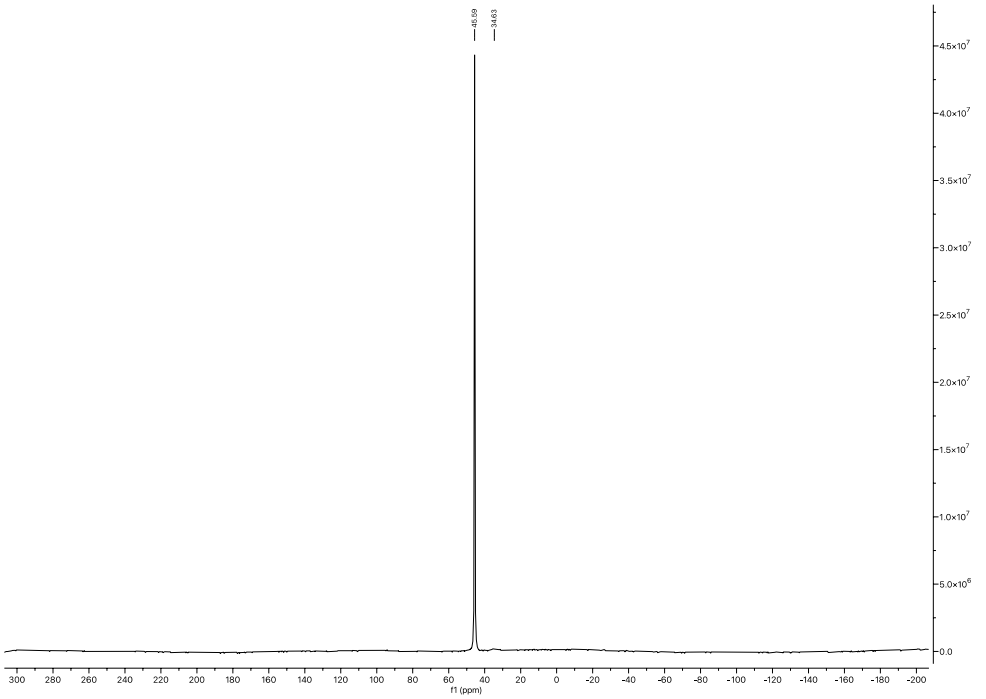


Figure S154 The ^{45}Sc NMR spectrum of [Sc(**L**^{003})] in D_2O.

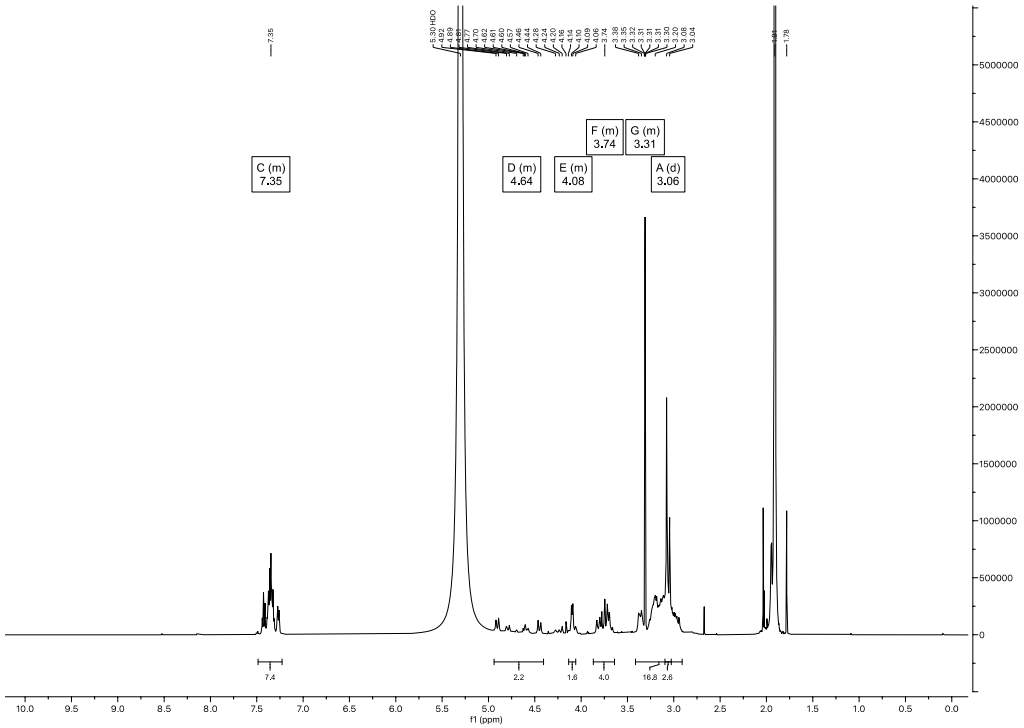


Figure S155 The ^{1}H NMR spectrum of [Sc(**L^{210}**)]$^{+}$ in MeOD.

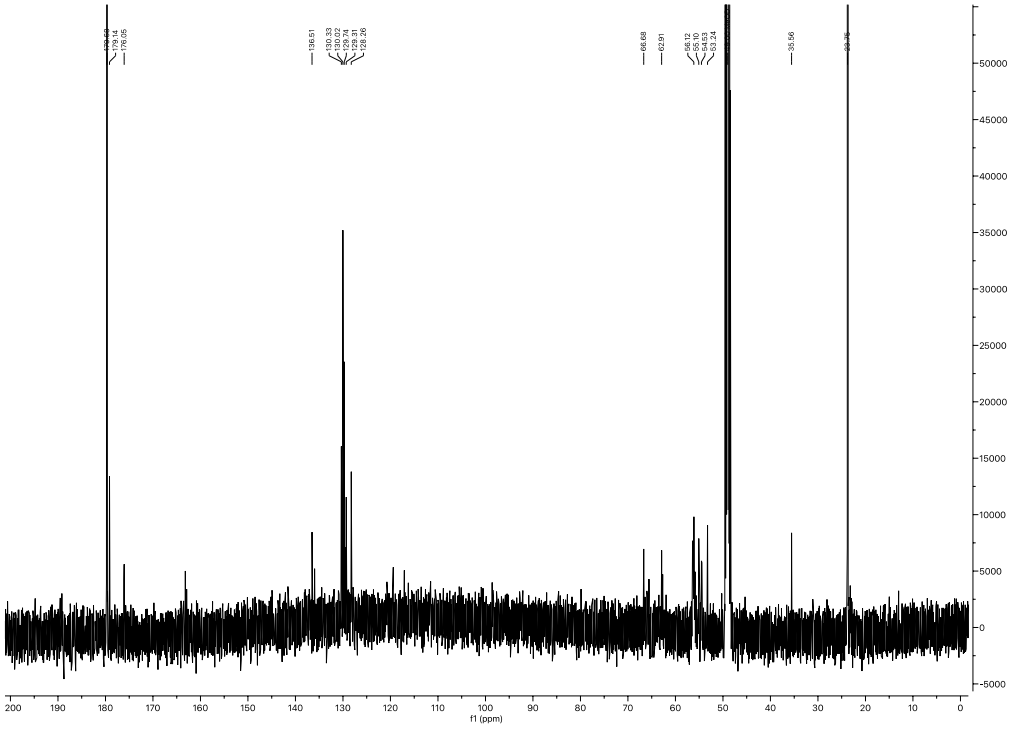


Figure S156 The ^{13}C{^{1}H} NMR spectrum of [Sc(**L^{210}**)]$^{+}$ in MeOD.

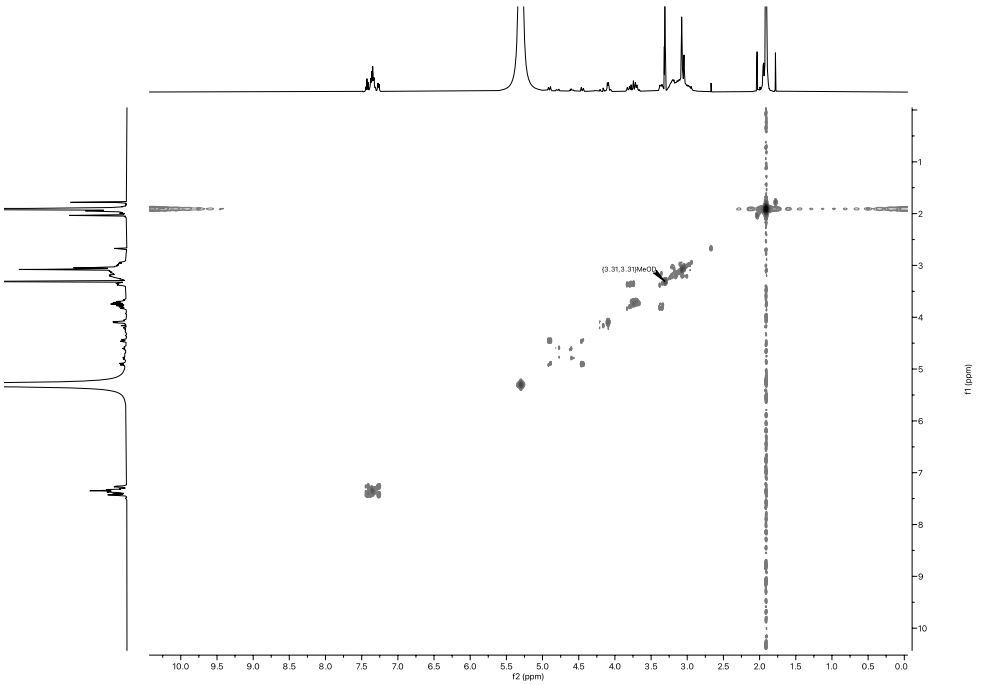


Figure S157 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**^{210})]$^{+}$ in MeOD.

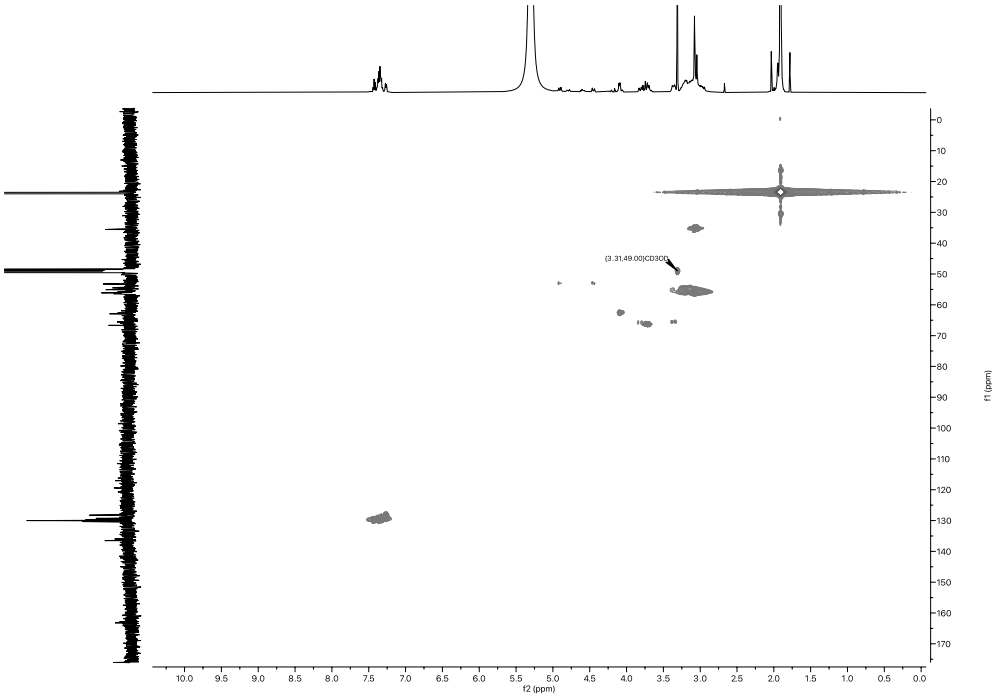


Figure S158 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**^{210})]$^{+}$ in MeOD.

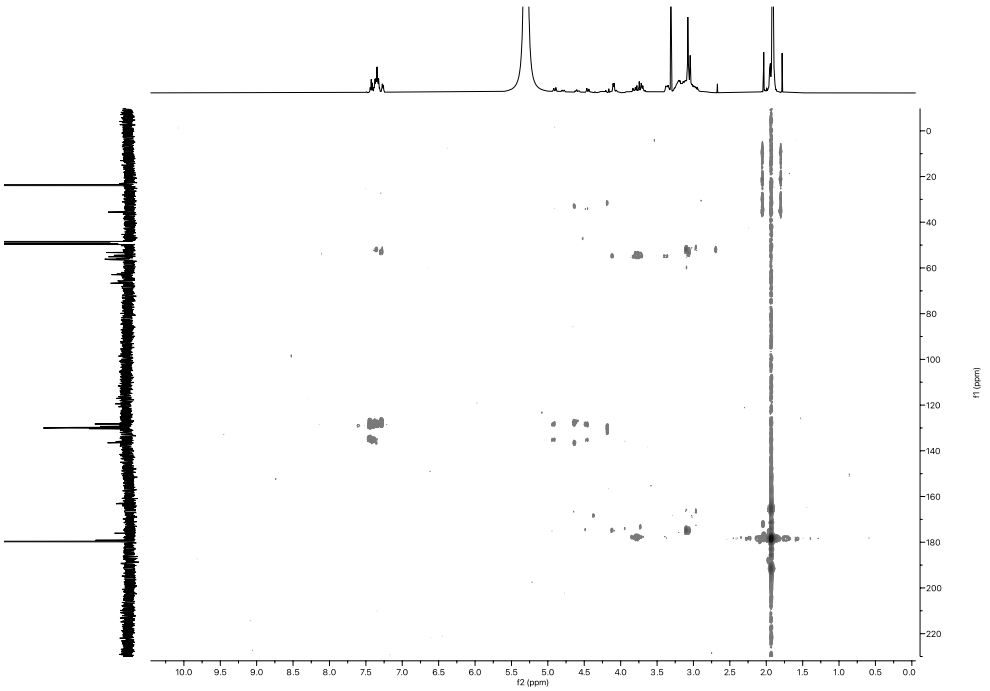


Figure S159 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**^{210})]$^{+}$ in MeOD.

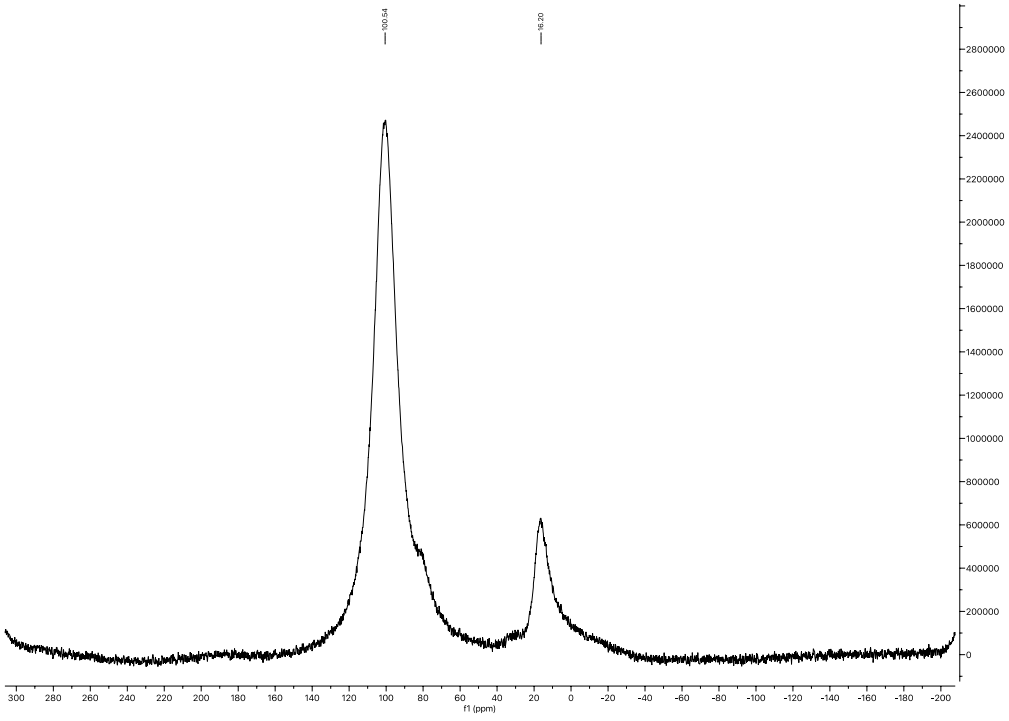


Figure S160 The ^{45}Sc NMR spectrum of [Sc(**L**^{210})]$^{+}$ in MeOD.

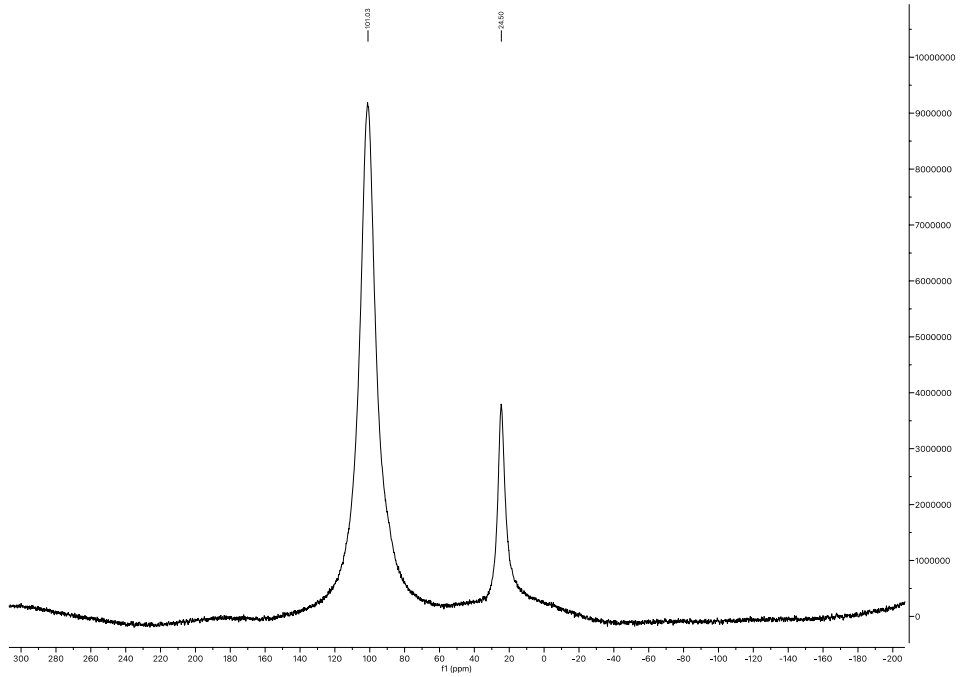


Figure S161 The ^{45}Sc NMR spectrum of [Sc(**L**^{210})]$^{+}$ in D_2O.

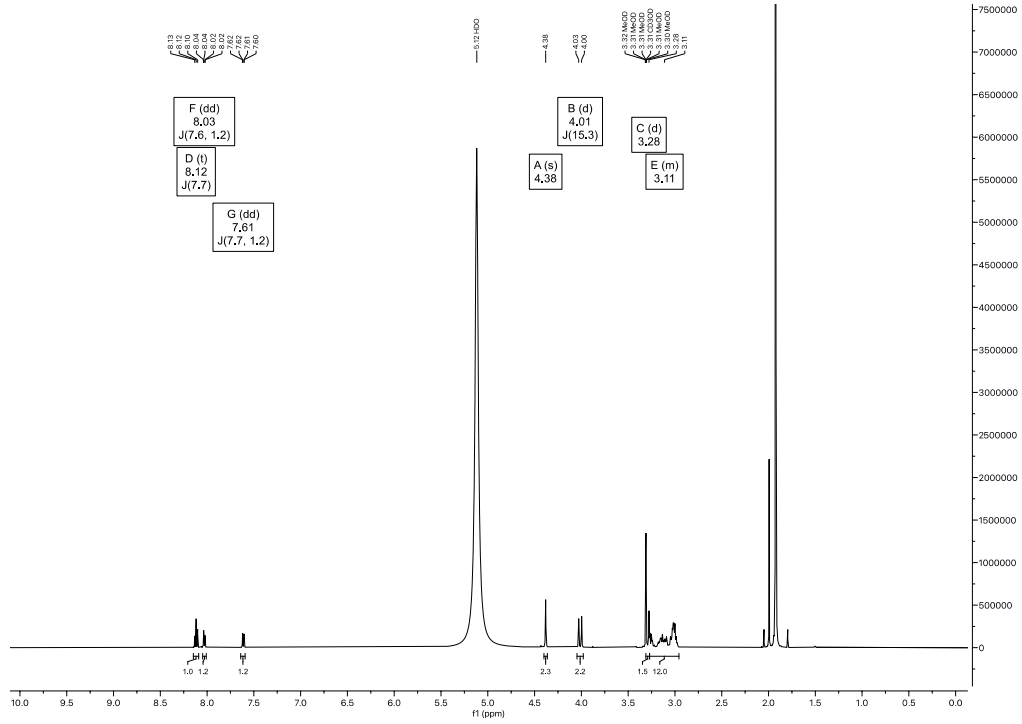


Figure S162 The ^{1}H NMR spectrum of [Sc(**L**^{201})] in MeOD.

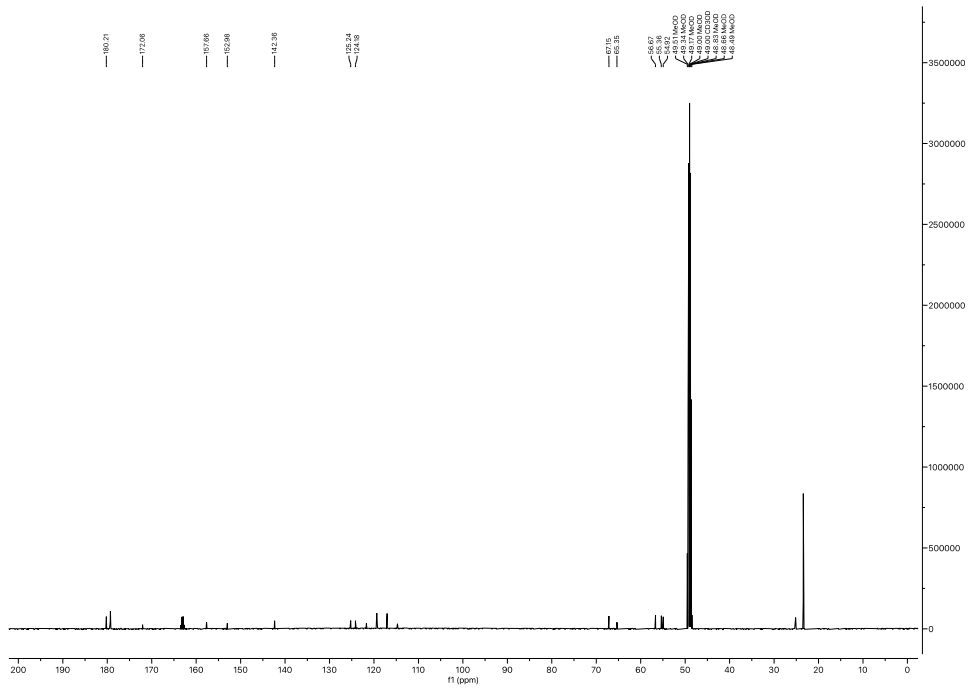


Figure S163 The $^{13}C\{^{1}H\}$ NMR spectrum of [Sc(**L**^{201})] in MeOD.

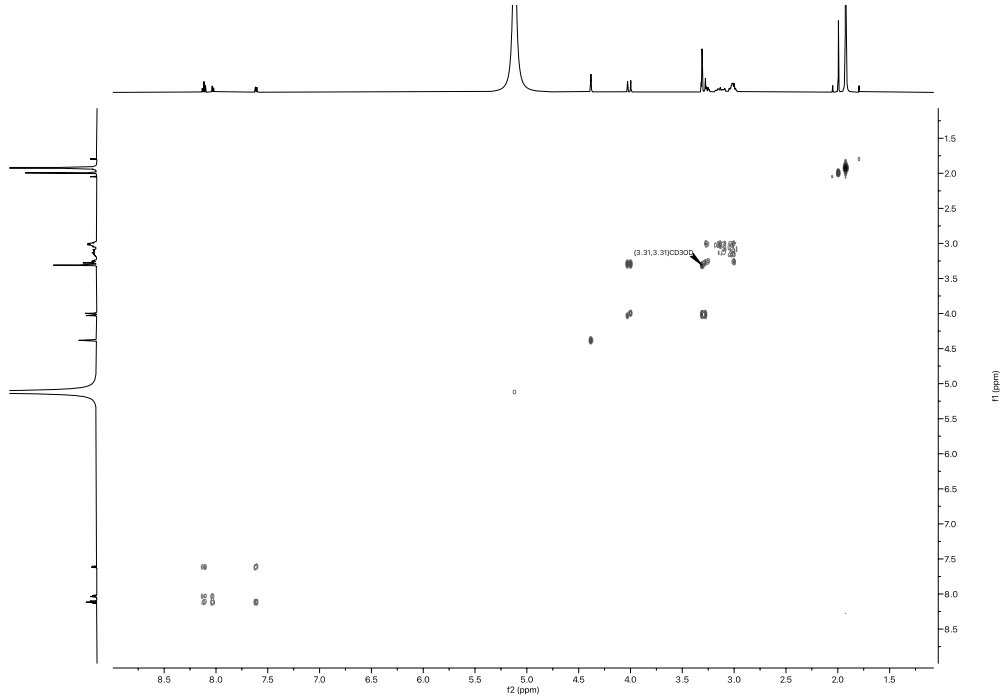


Figure S164 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**^{201})] in MeOD.

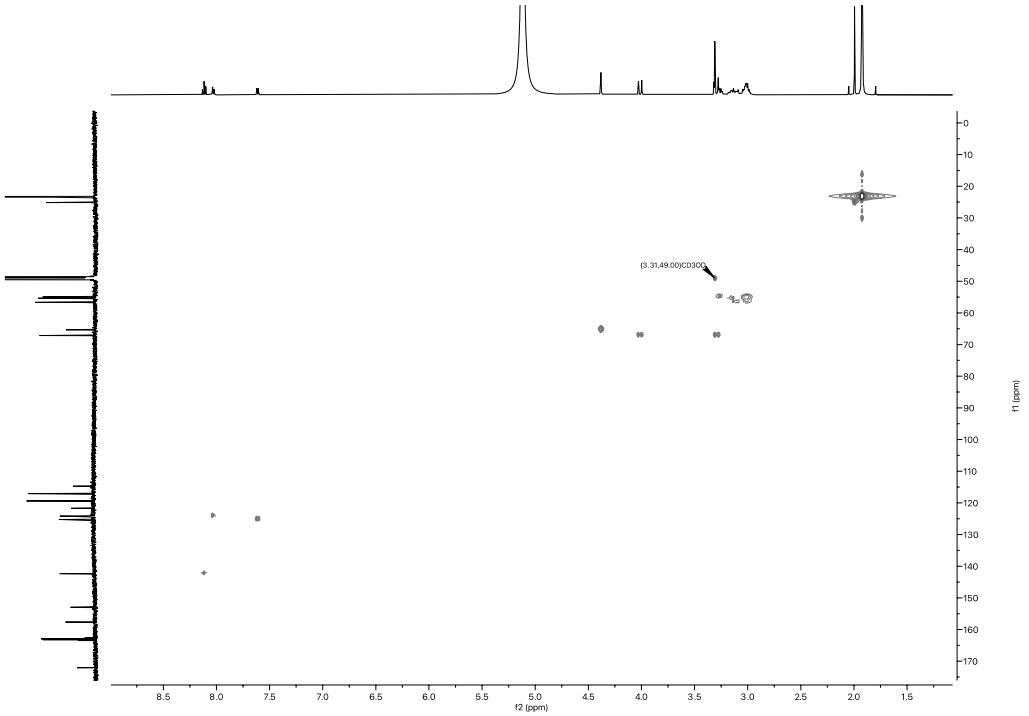


Figure S165 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**^{201})] in MeOD.

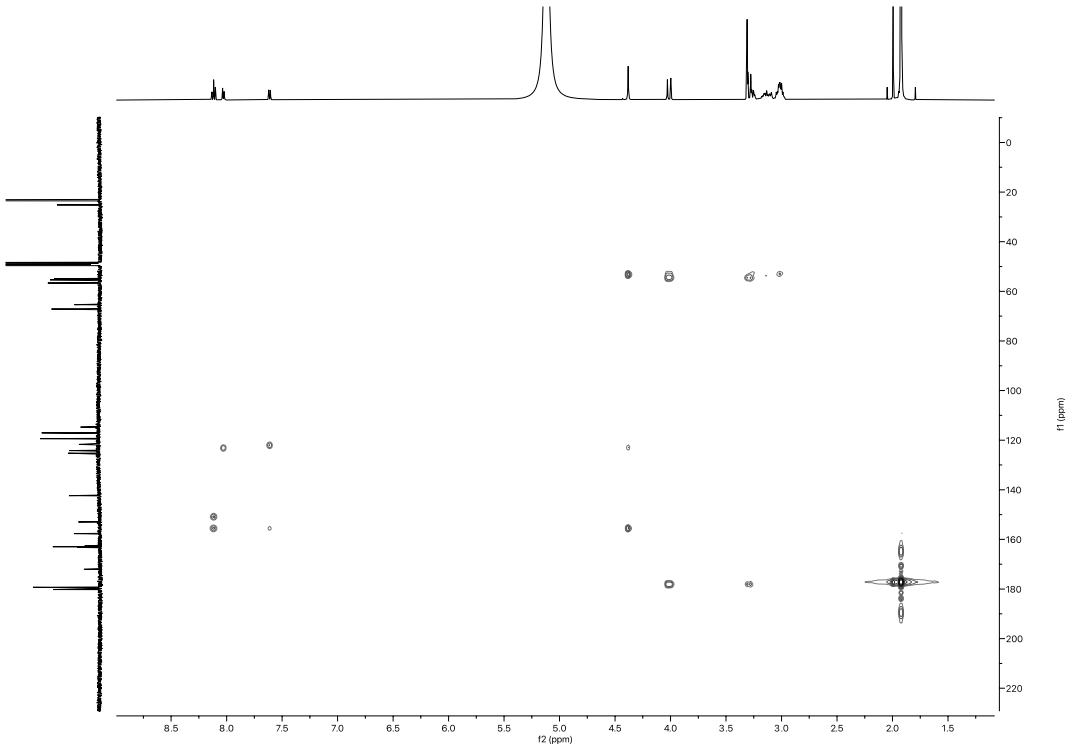


Figure S166 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**^{201})] in MeOD.

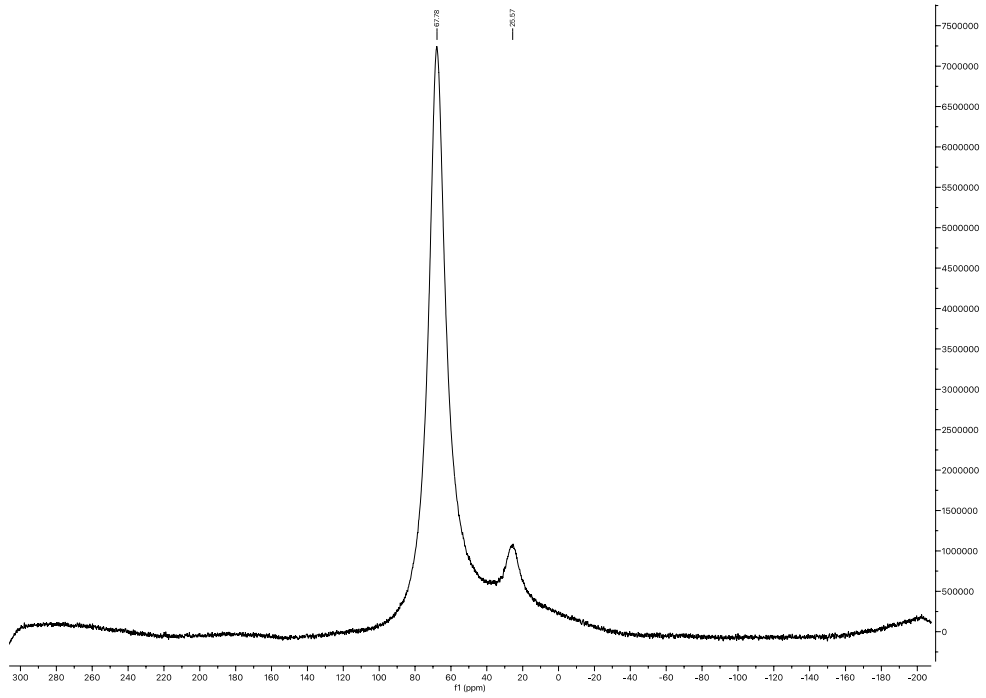


Figure S167 The ^{45}Sc NMR spectrum of [Sc(**L**^{201})] in MeOD.

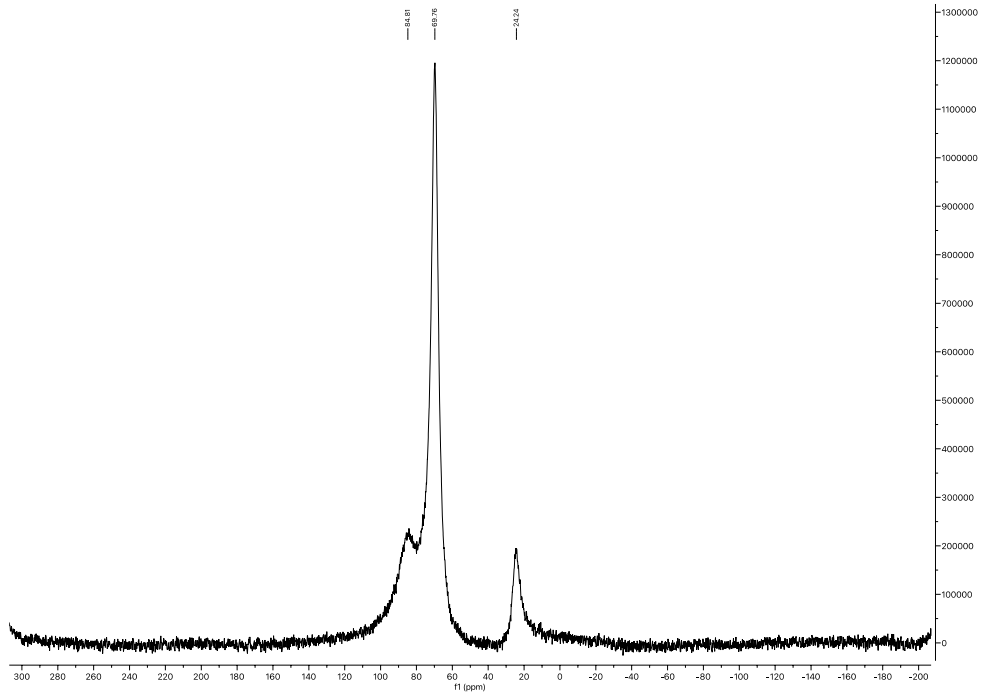


Figure S168 The ^{45}Sc NMR spectrum of [Sc(**L**^{201})] in D_2O.

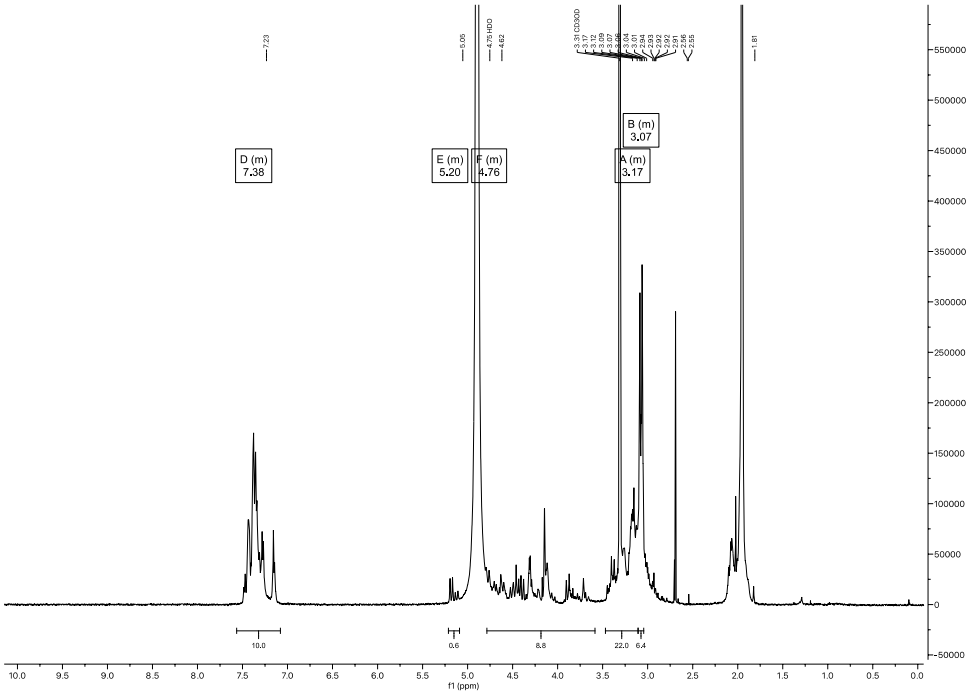


Figure S169 The ^{1}H NMR spectrum of [Sc(**L**^{120})]$^{2+}$ in MeOD.

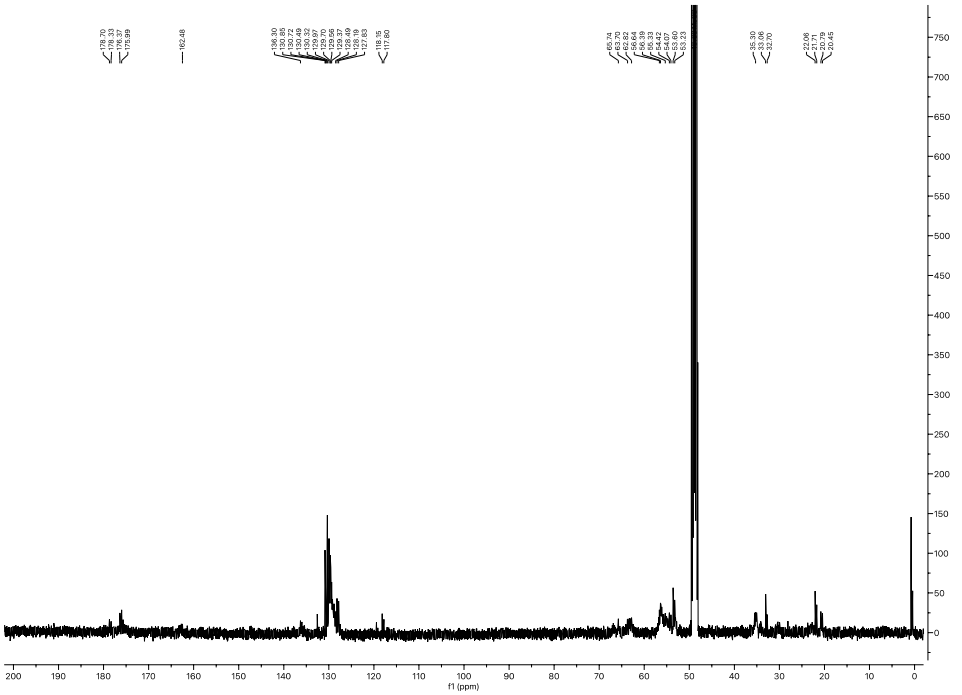


Figure S170 The ^{13}C{^{1}H} NMR spectrum of [Sc(**L**^{120})]$^{2+}$ in MeOD.

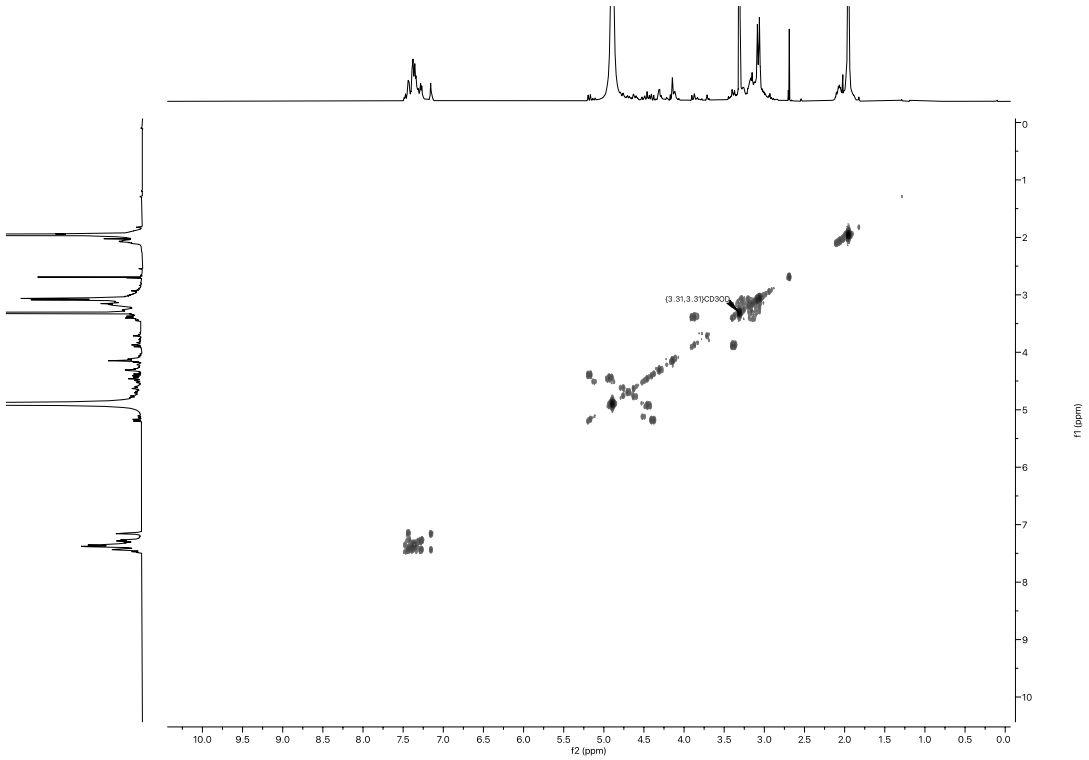


Figure S171 The ^{1}H-^{1}H COSY NMR spectrum of $[Sc(\mathbf{L^{120}})]^{2+}$ in MeOD.

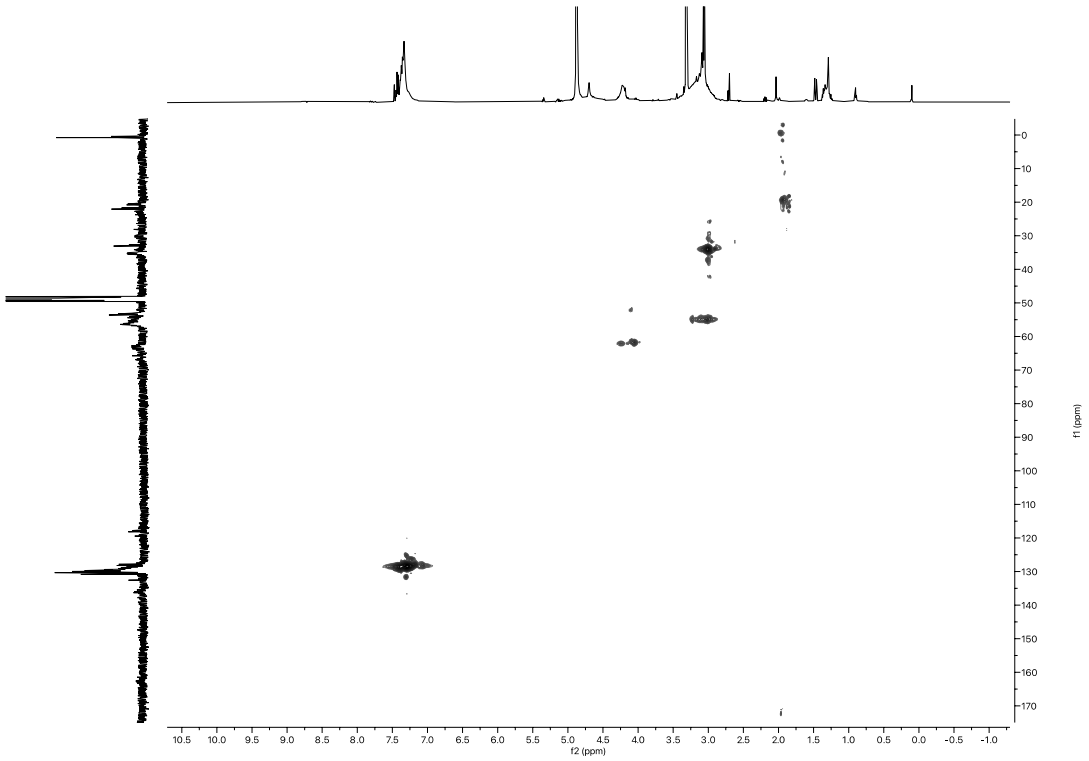


Figure S172 The ^{1}H-^{13}C HSQC NMR spectrum of $[Sc(\mathbf{L^{120}})]^{2+}$ in MeOD.

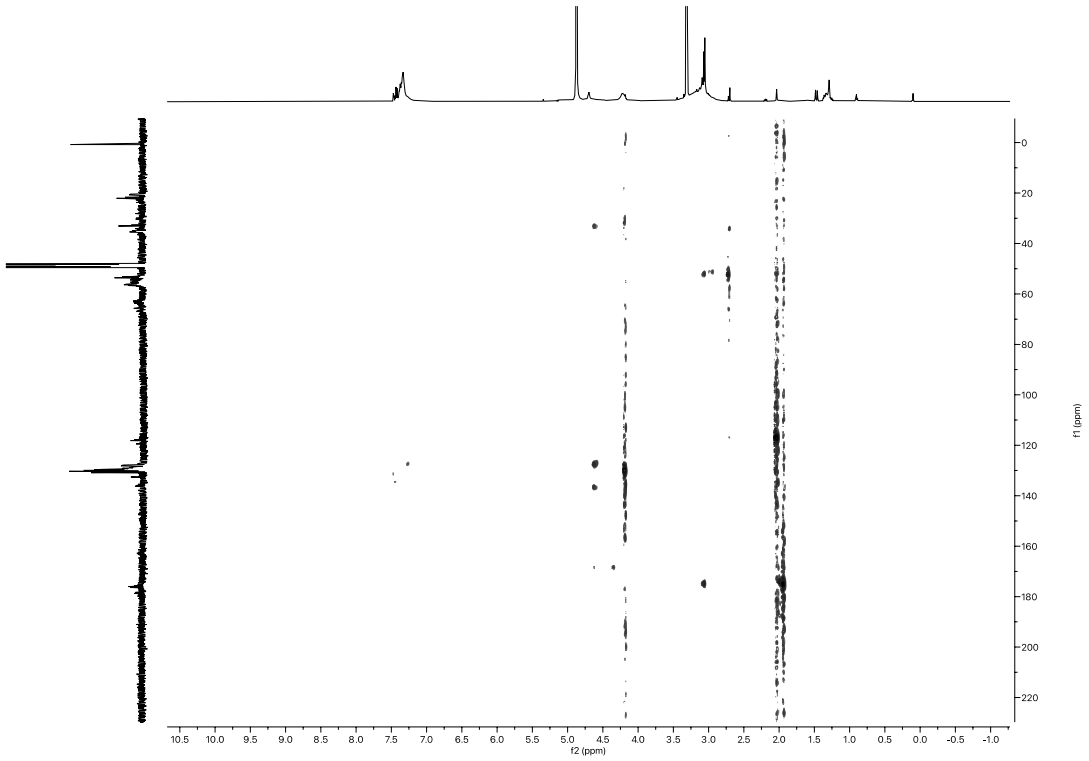


Figure S173 The ^{1}H-^{13}C HMBC NMR spectrum of $[Sc(\mathbf{L^{120}})]^{2+}$ in MeOD.

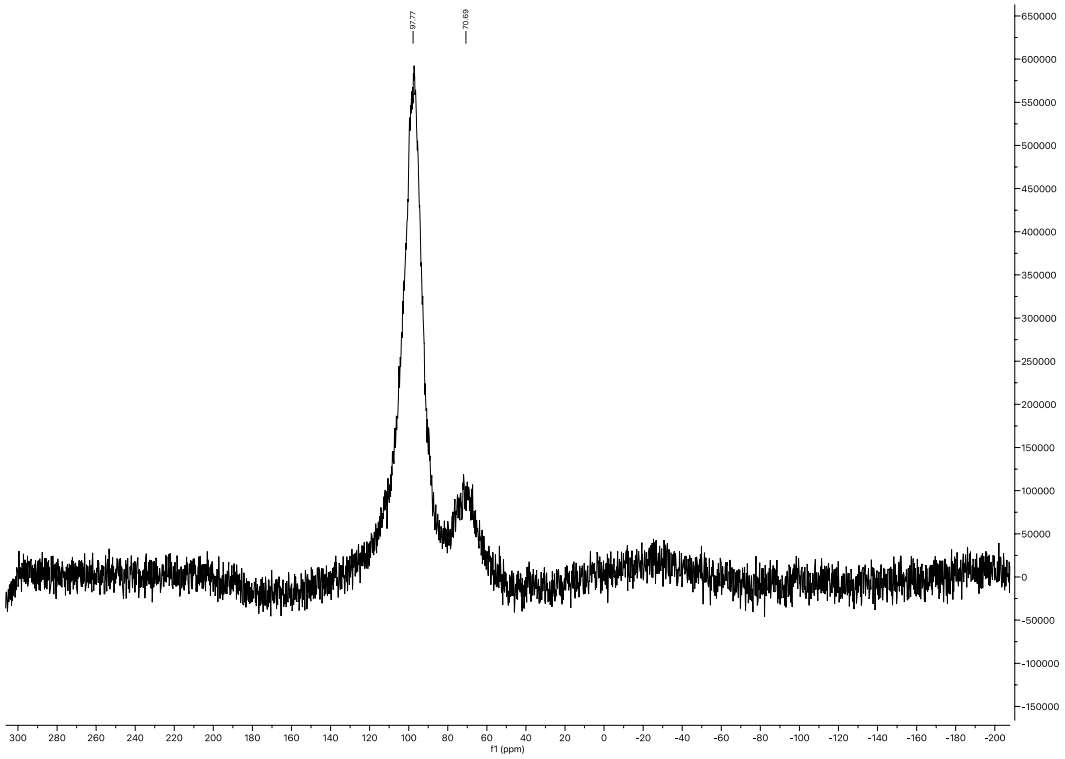


Figure S174 The ^{45}Sc NMR spectrum of $[Sc(\mathbf{L^{120}})]^{2+}$ in MeOD.

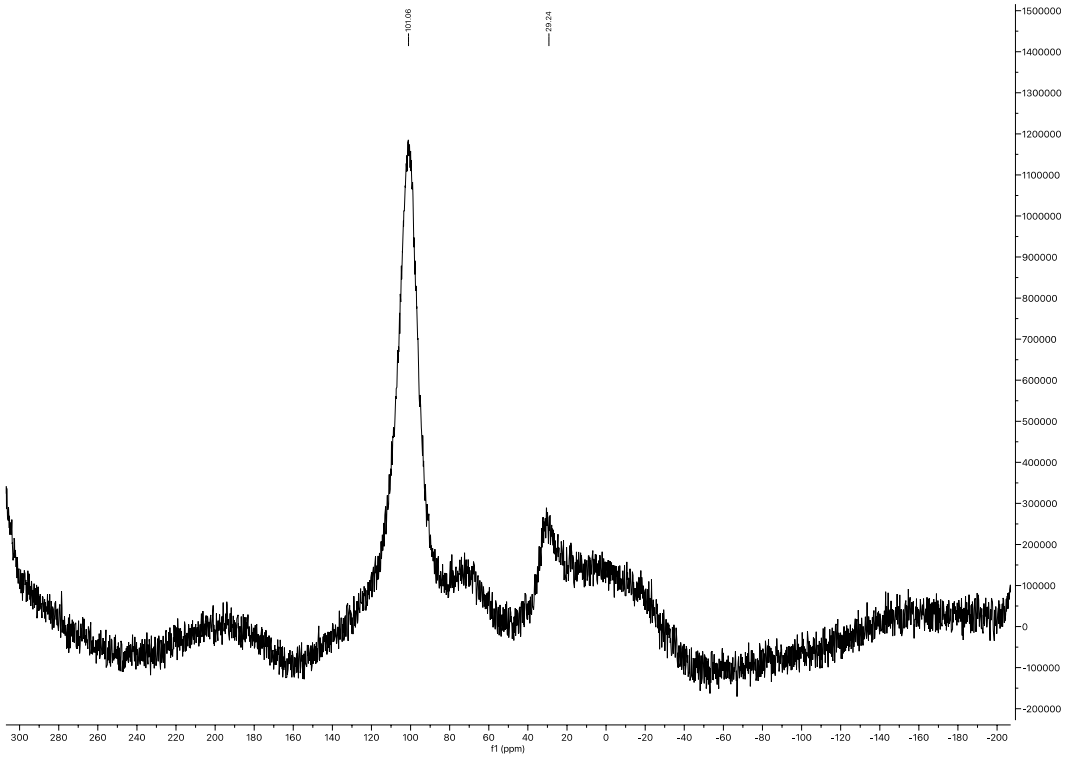


Figure S175 The ^{45}Sc NMR spectrum of $[Sc(\mathbf{L^{120}})]^{2+}$ in D_2O.

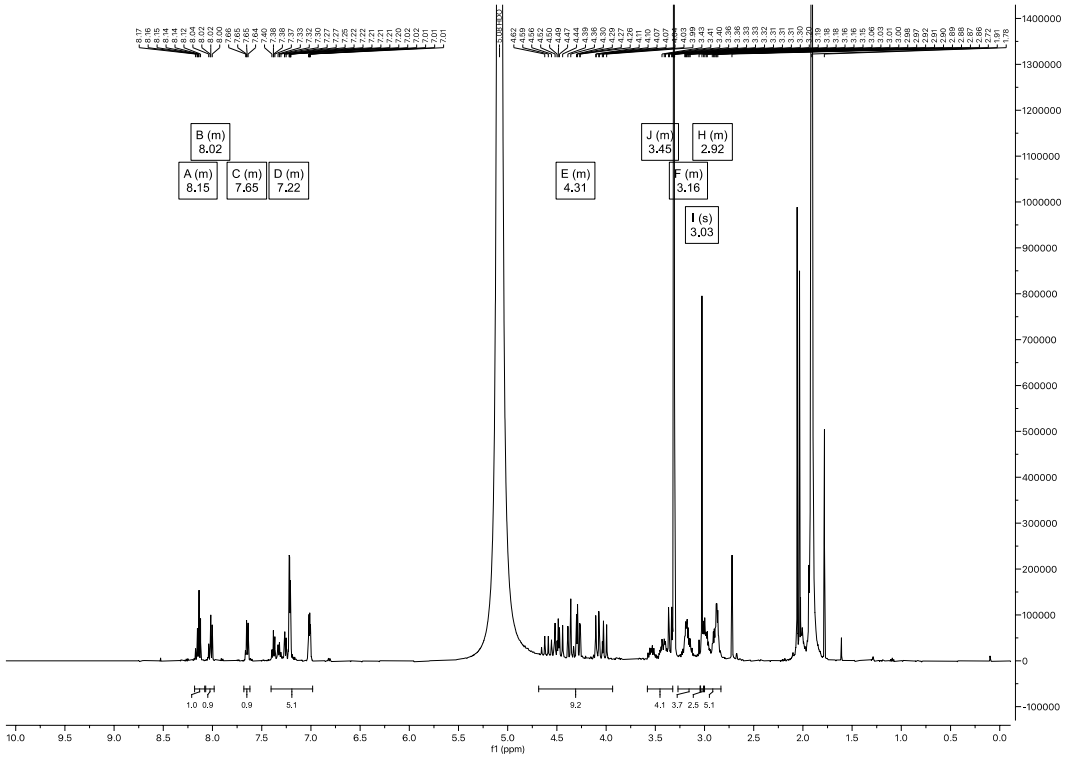


Figure S176 The ^{1}H NMR spectrum of $[Sc(\mathbf{L^{111}})]^{+}$ in MeOD.

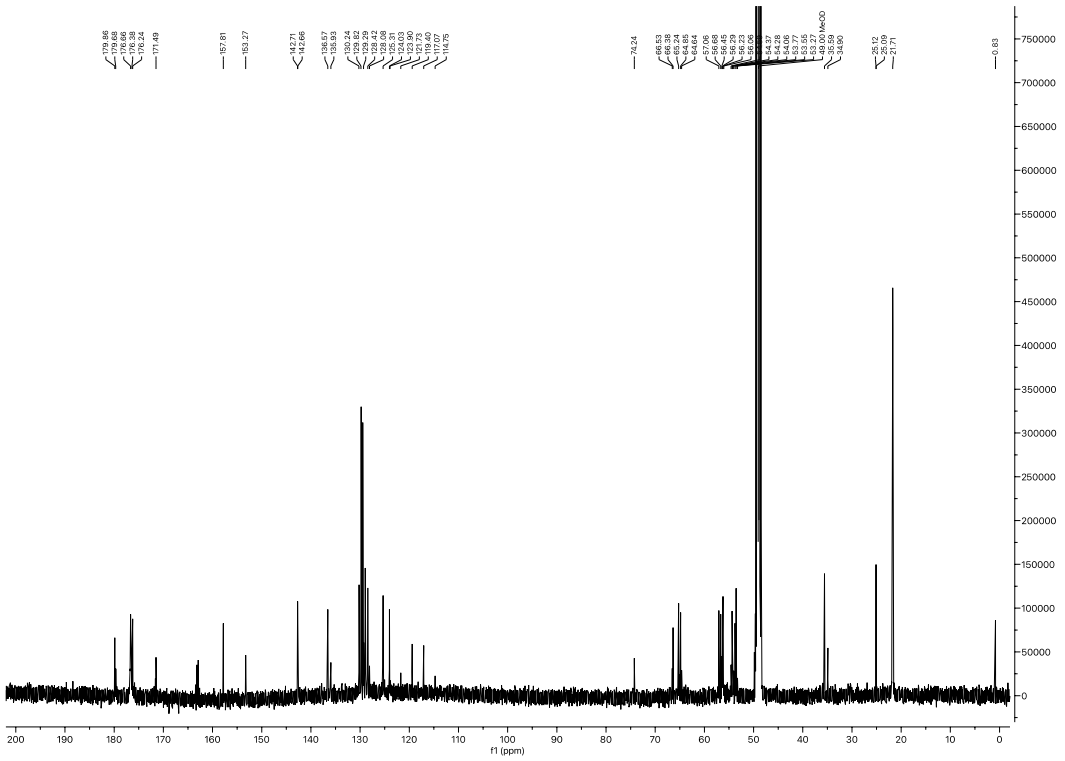


Figure S177 The $^{13}C\{^{1}H\}$ NMR spectrum of $[Sc(\mathbf{L^{111}})]^{+}$ in MeOD.

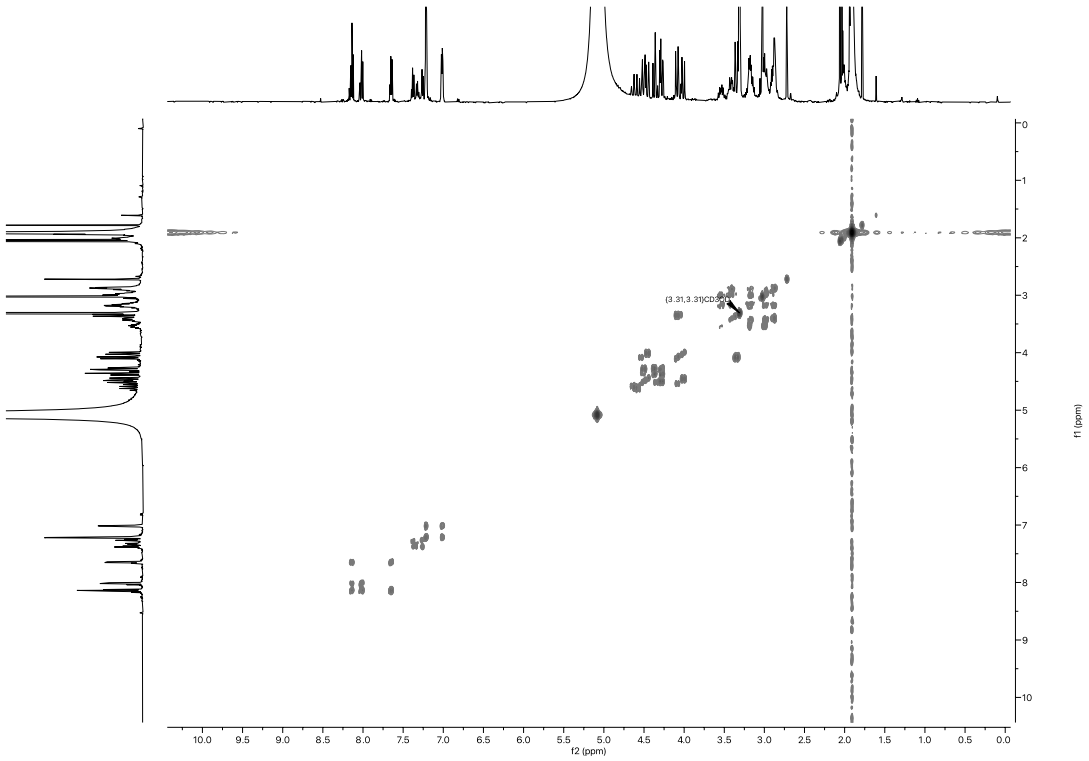


Figure S178 The ^{1}H-^{1}H COSY NMR spectrum of $[Sc(\mathbf{L^{111}})]^{+}$ in MeOD.

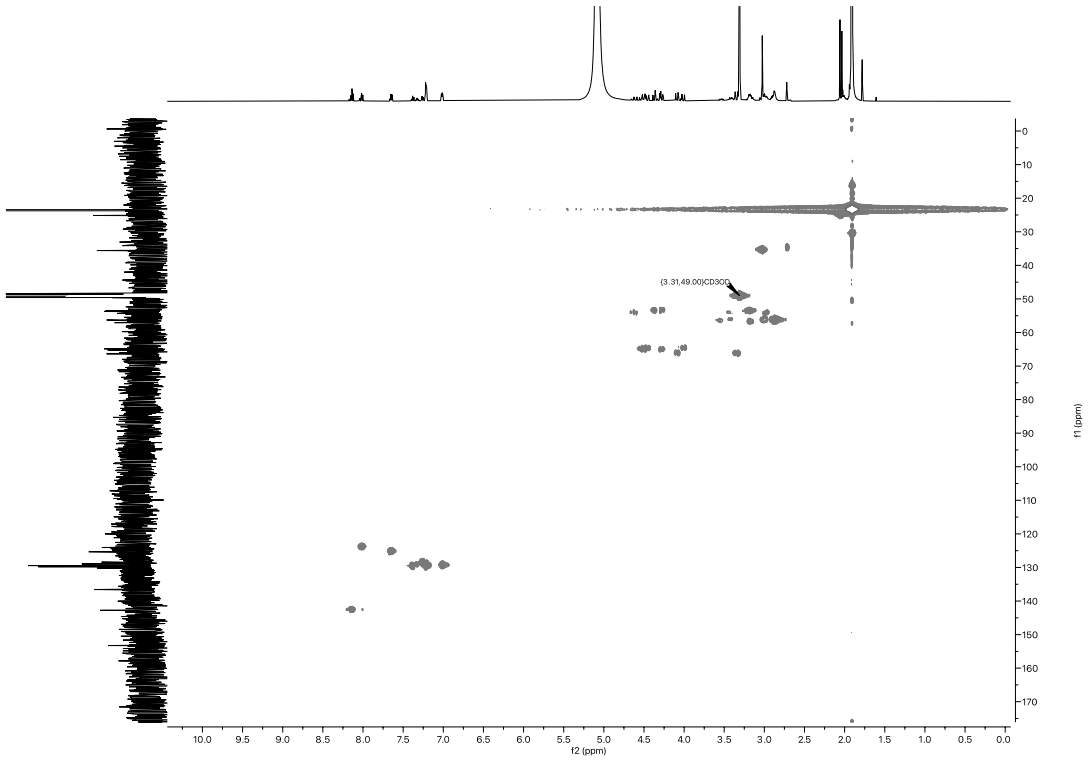


Figure S179 The ^{1}H-^{13}C HSQC NMR spectrum of $[Sc(\mathbf{L^{111}})]^{+}$ in MeOD.

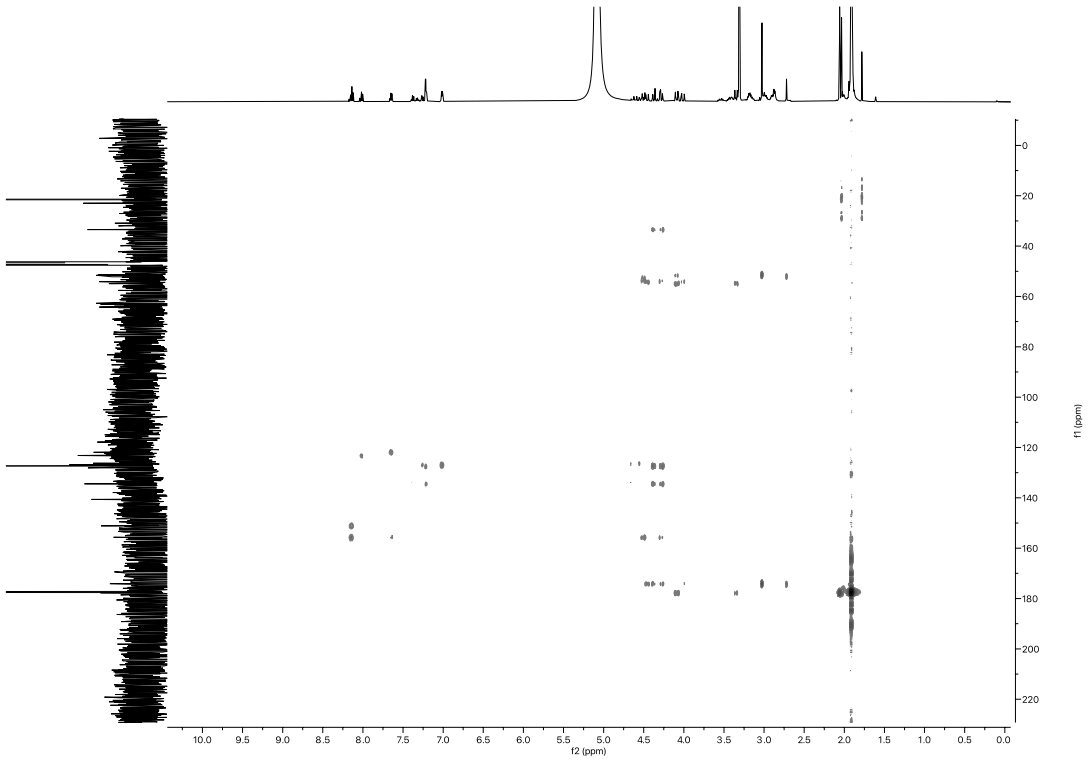


Figure S180 The ^{1}H-^{13}C HMBC NMR spectrum of $[Sc(\mathbf{L^{111}})]^{+}$ in MeOD.

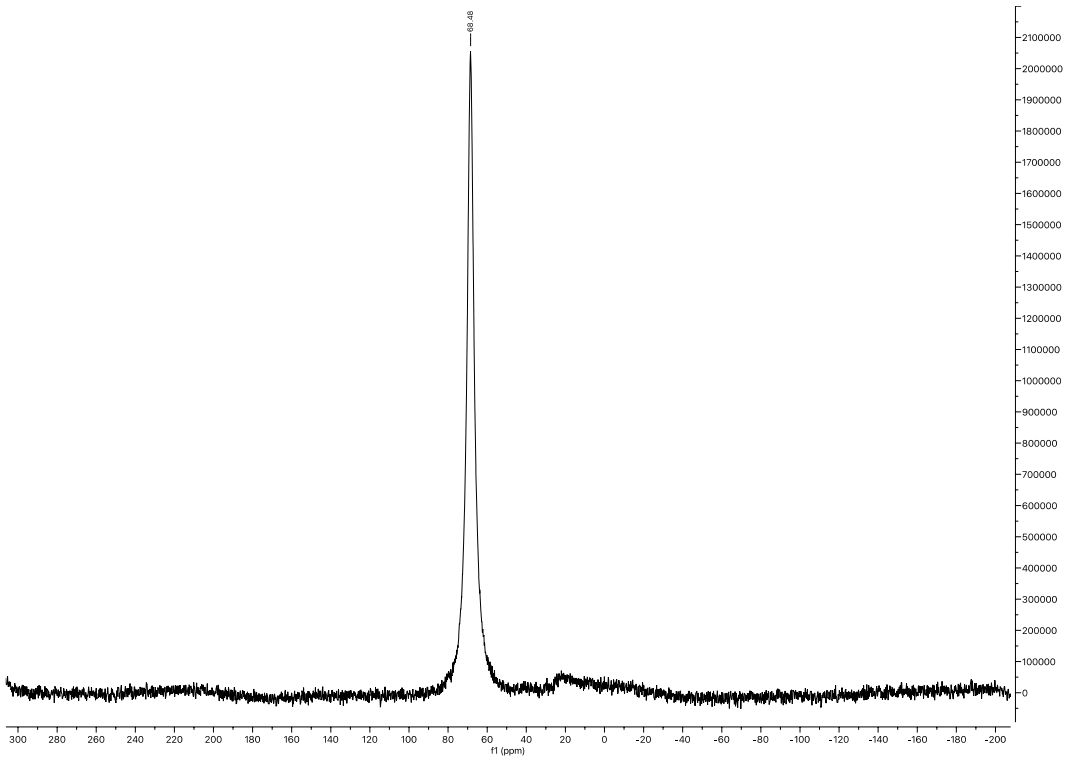


Figure S181 The ^{45}Sc NMR spectrum of [Sc(**L**^{111})]$^{+}$ in MeOD.

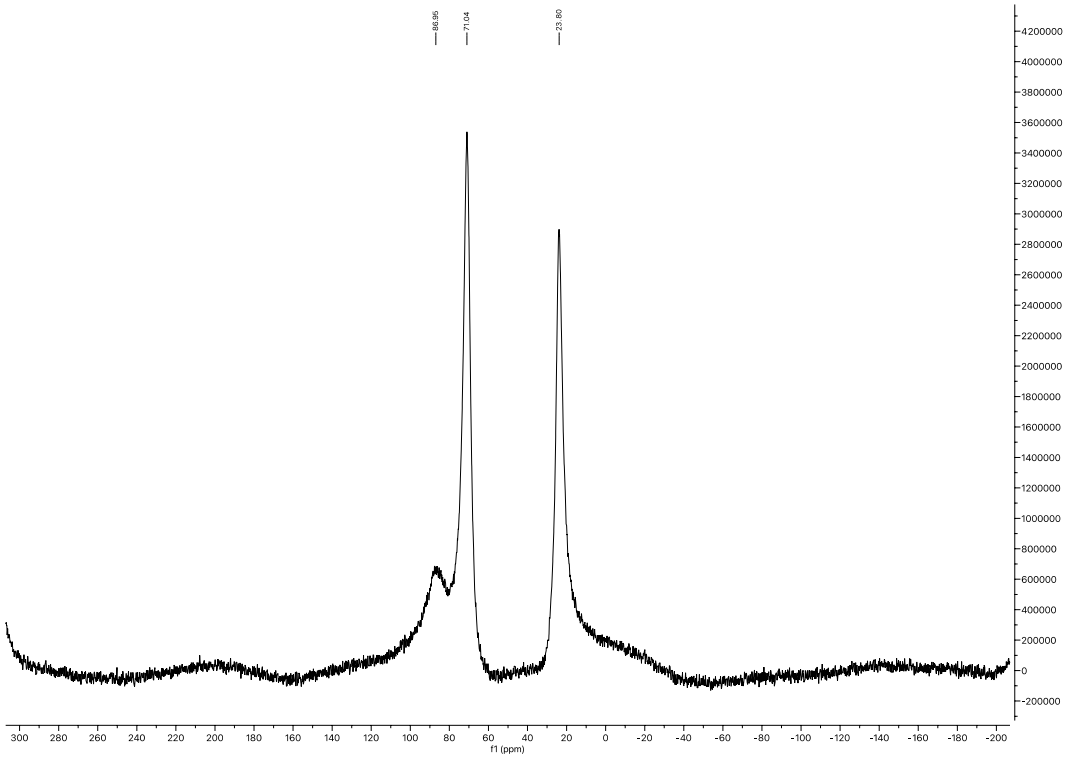


Figure S182 The ^{45}Sc NMR spectrum of [Sc(**L**^{111})]$^{+}$ in D_2O.

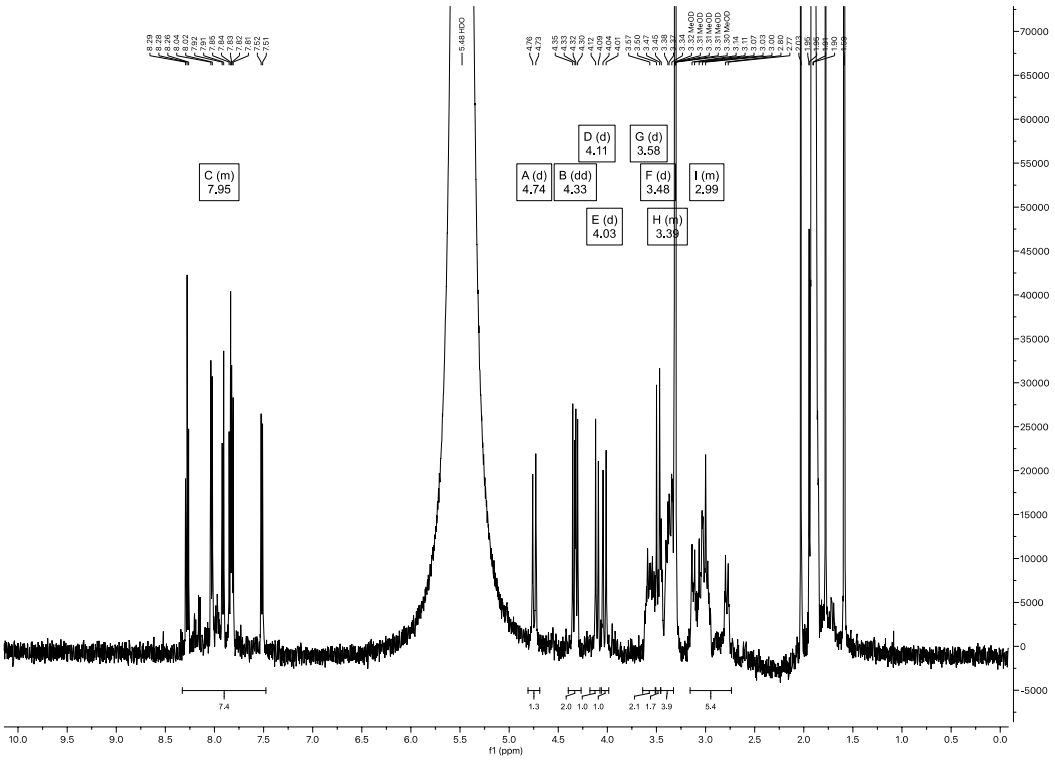


Figure S183 The ^{1}H NMR spectrum of [Sc(**L**^{102})] in MeOD.

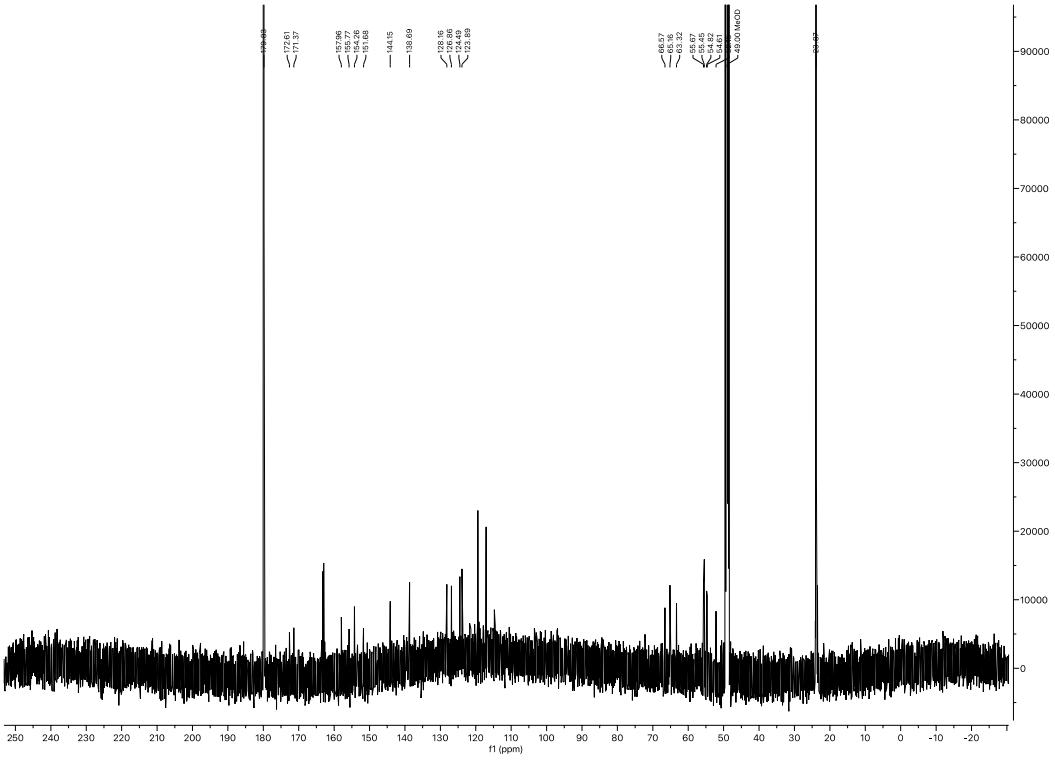


Figure S184 The $^{13}C\{^{1}H\}$ NMR spectrum of [Sc(**L**^{102})] in MeOD.

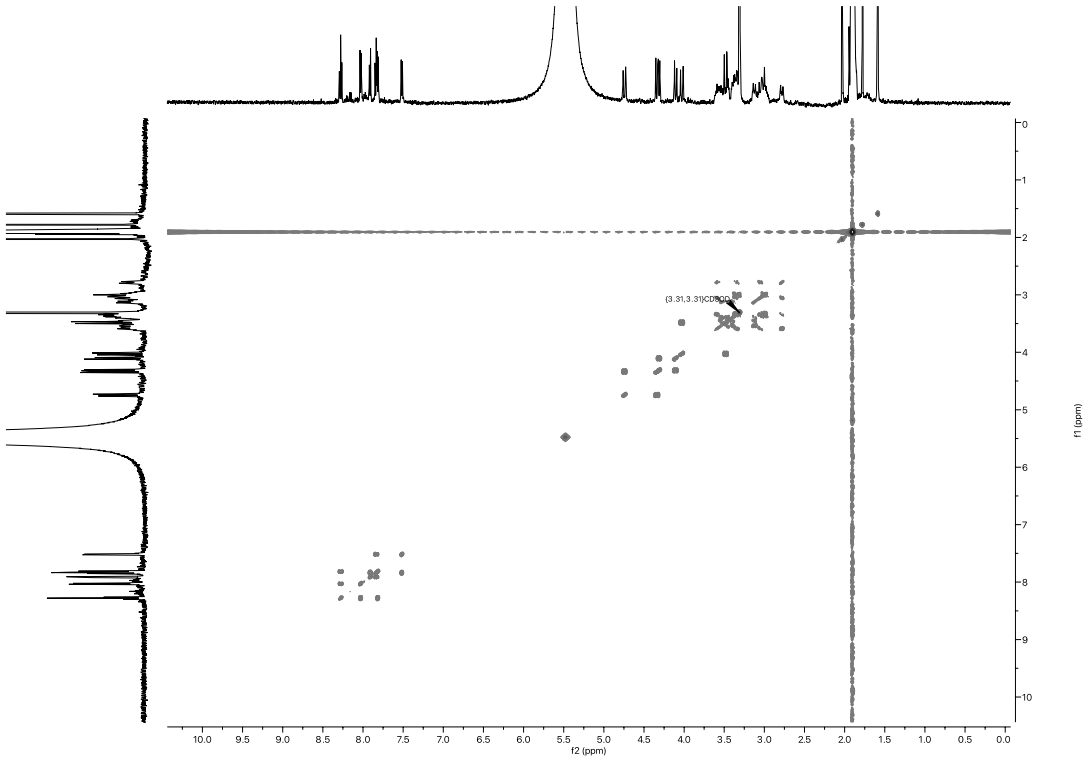


Figure S185 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**^{102})] in MeOD.

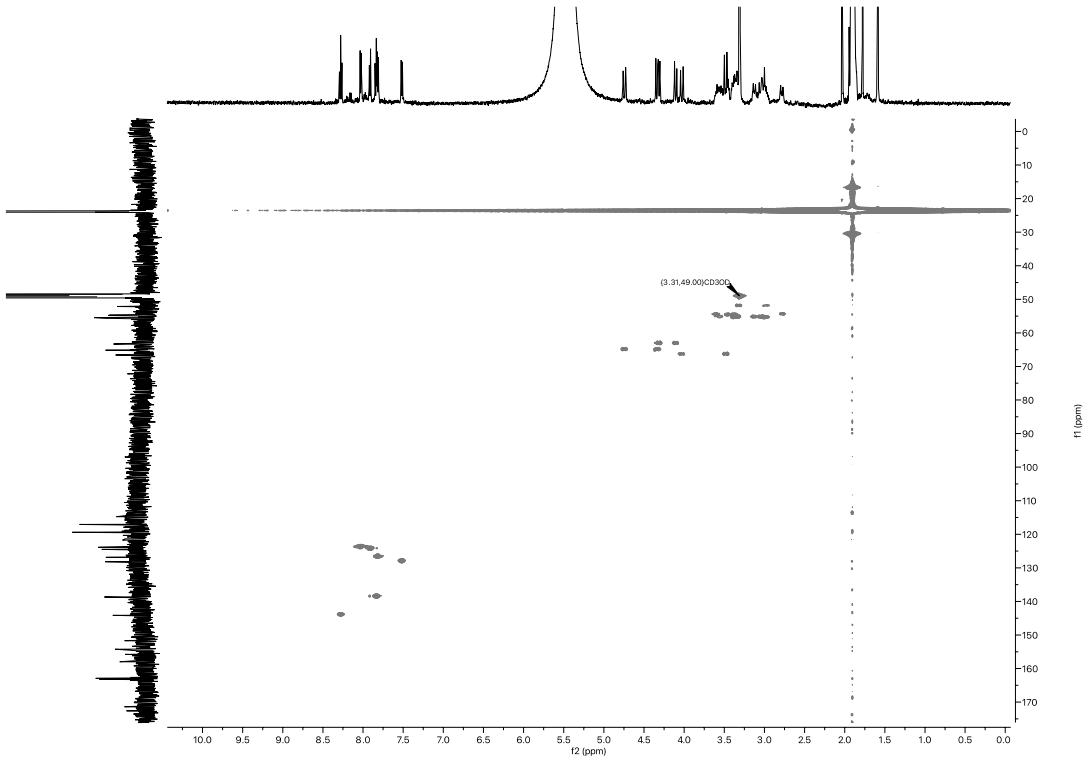


Figure S186 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**^{102})] in MeOD.

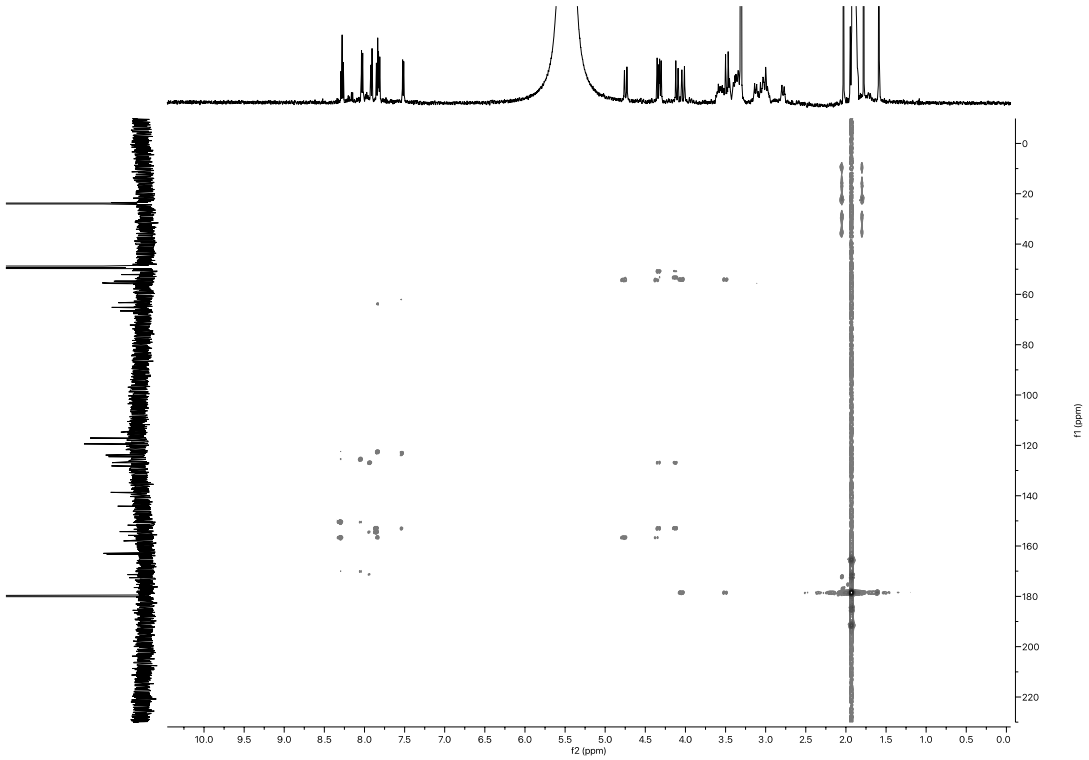


Figure S187 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**^{102})] in MeOD.

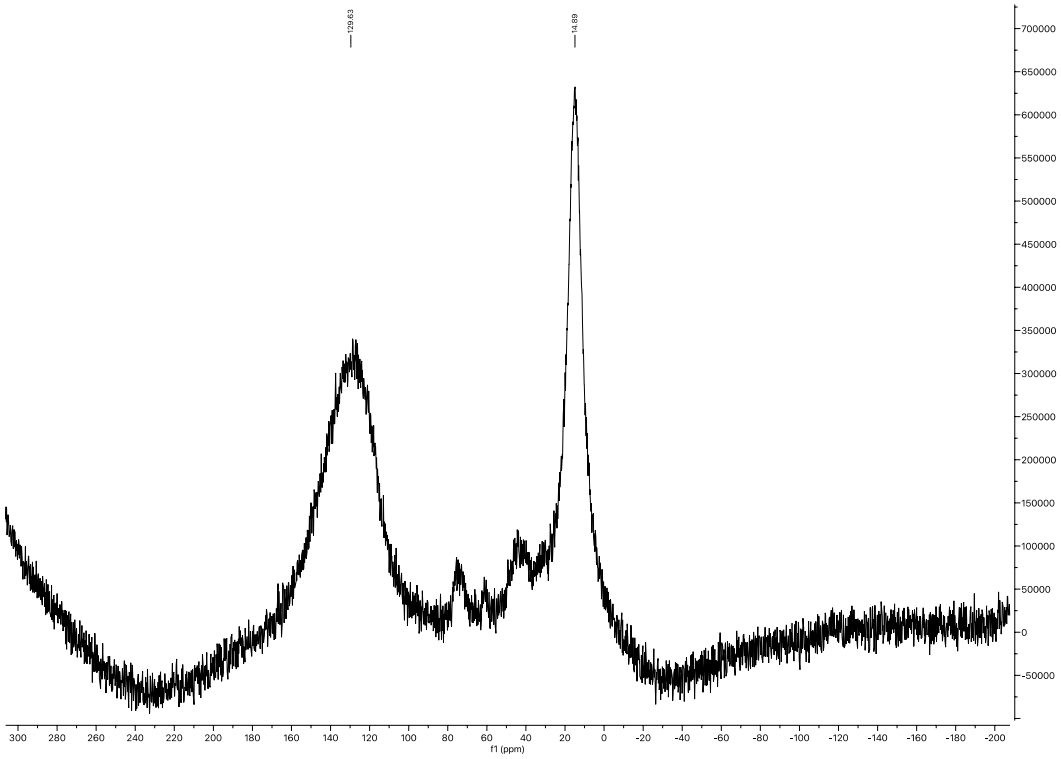


Figure S188 The ^{45}Sc NMR spectrum of [Sc(**L**^{102})] in MeOD.

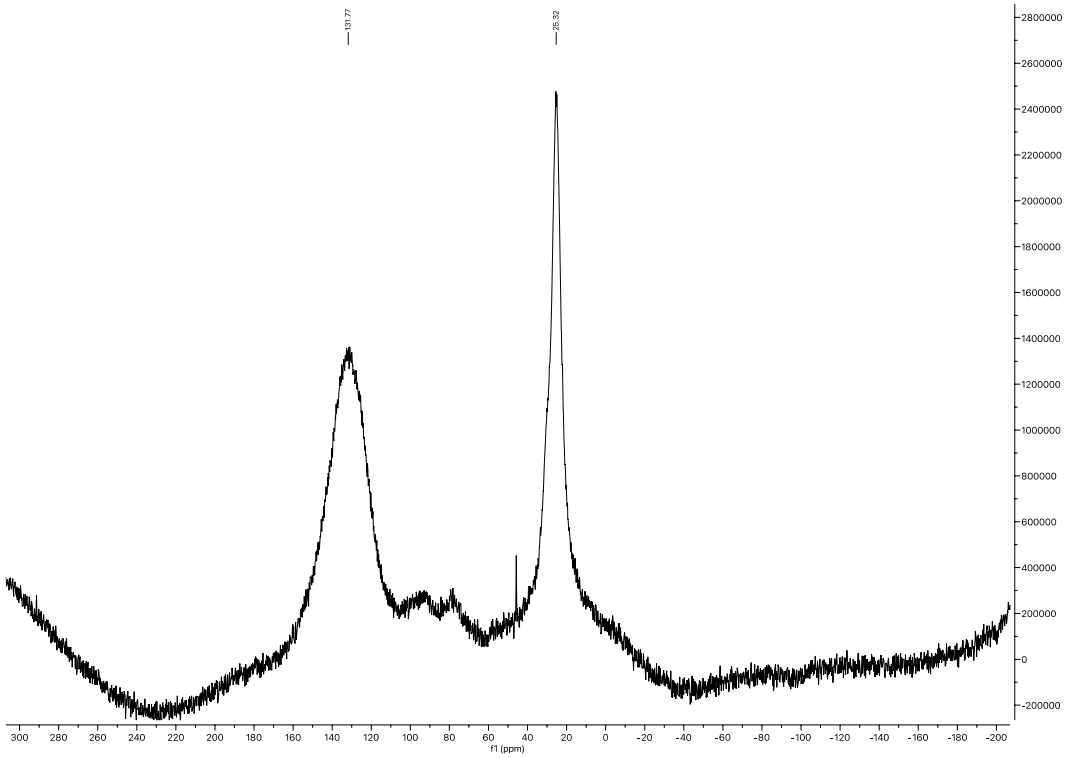


Figure S189 The ^{45}Sc NMR spectrum of [Sc(**L**^{102})] in D_2O.

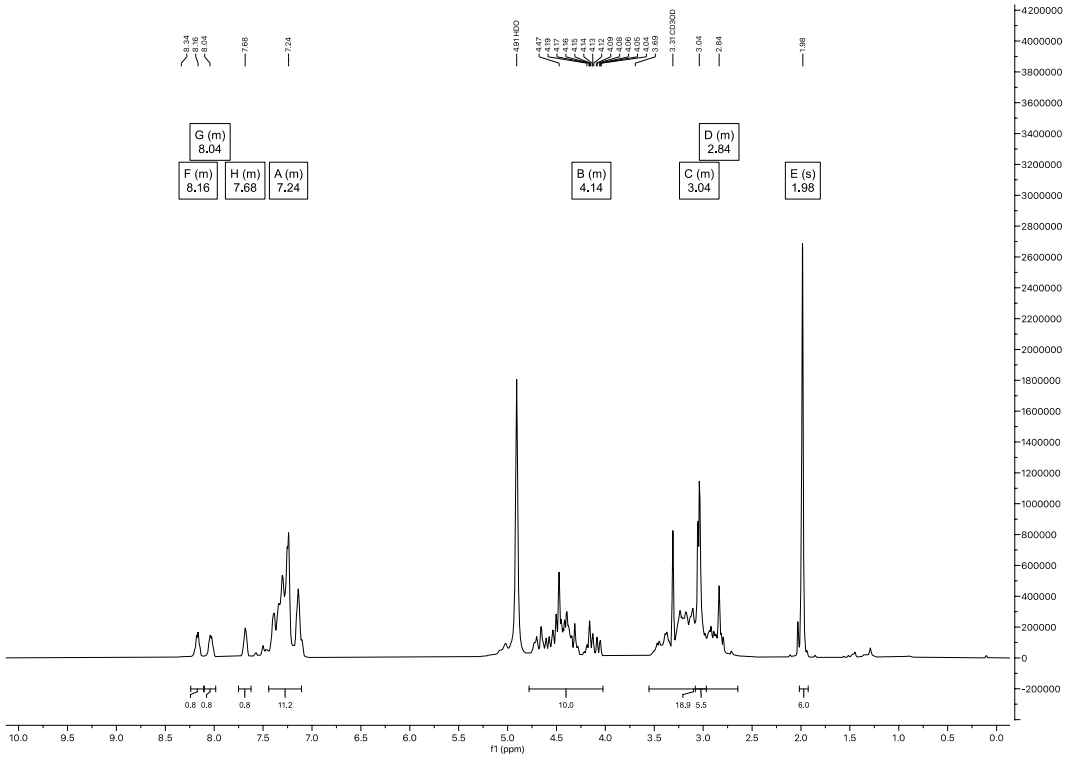


Figure S190 The ^{1}H NMR spectrum of [Sc(**L**^{021})]$^{2+}$ in MeOD.

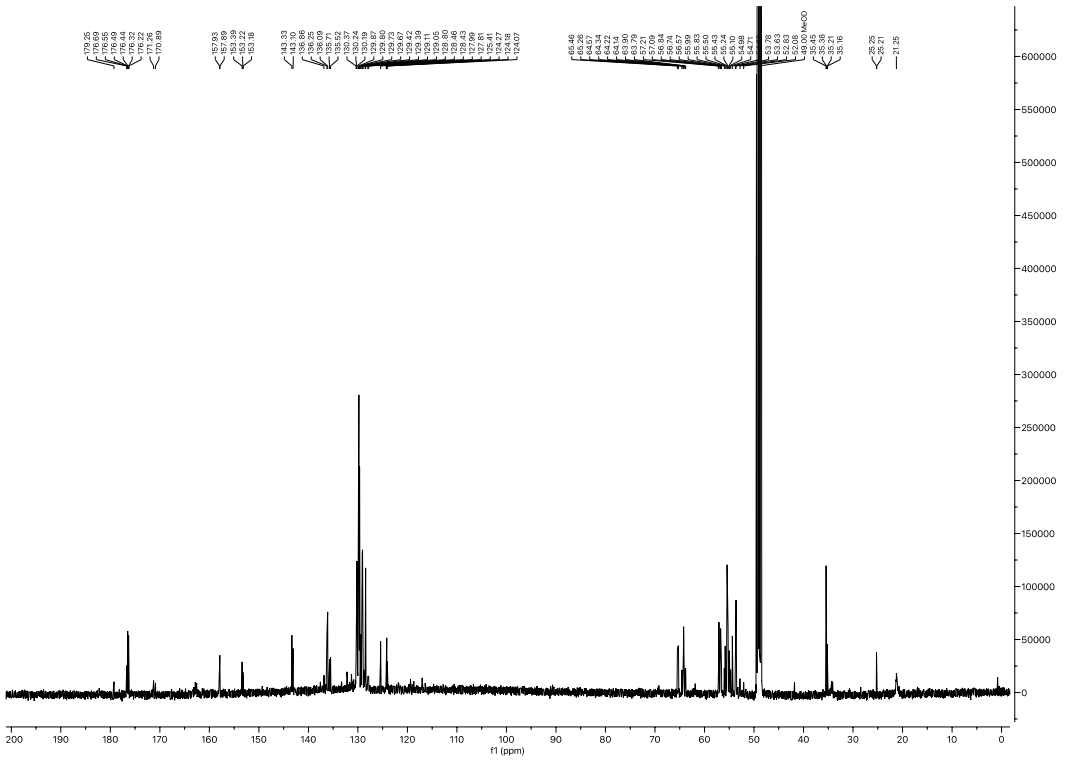


Figure S191 The $^{13}C\{^{1}H\}$ NMR spectrum of $[Sc(\mathbf{L^{021}})]^{2+}$ in MeOD.

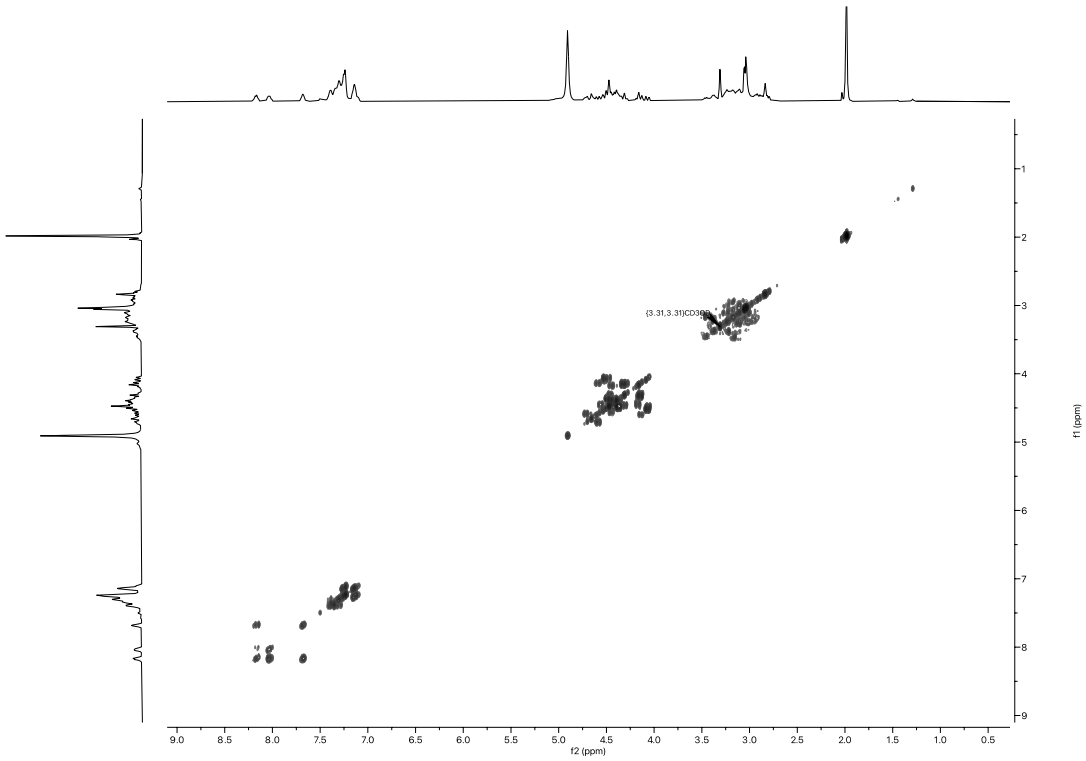


Figure S192 The ^{1}H-^{1}H COSY NMR spectrum of $[Sc(\mathbf{L^{021}})]^{2+}$ in MeOD.

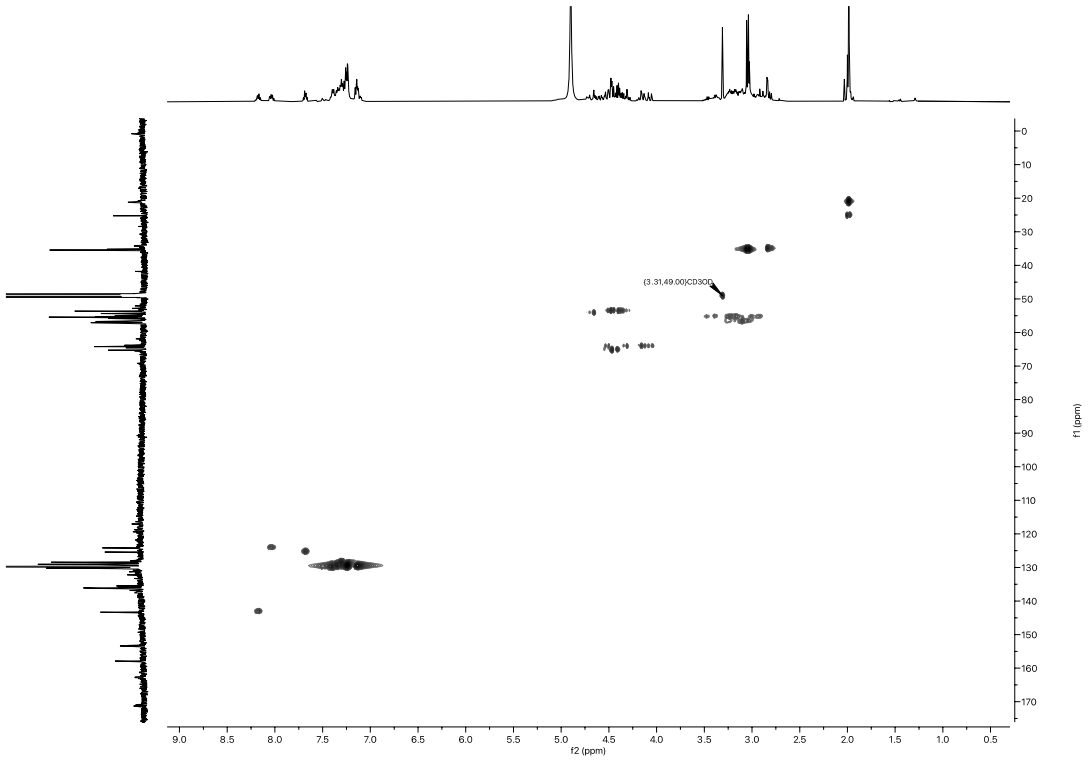


Figure S193 The ^{1}H-^{13}C HSQC NMR spectrum of $[Sc(\mathbf{L}^{\mathbf{021}})]^{2+}$ in MeOD.

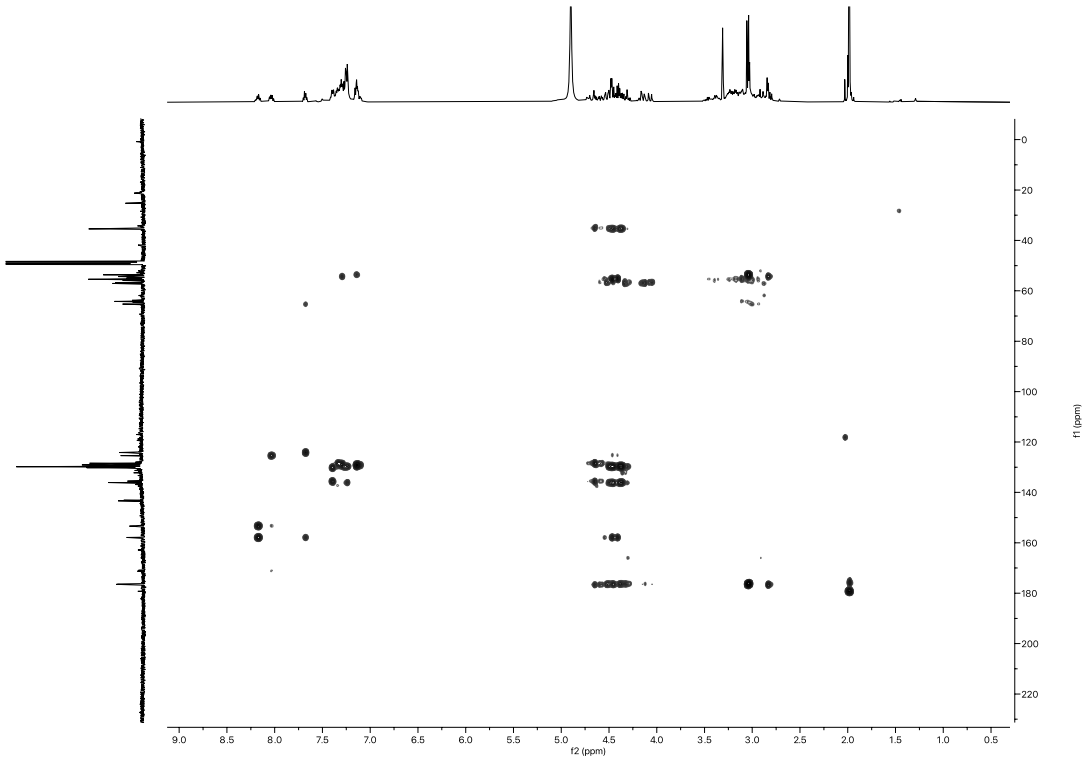


Figure S194 The ^{1}H-^{13}C HMBC NMR spectrum of $[Sc(\mathbf{L}^{\mathbf{021}})]^{2+}$ in MeOD.

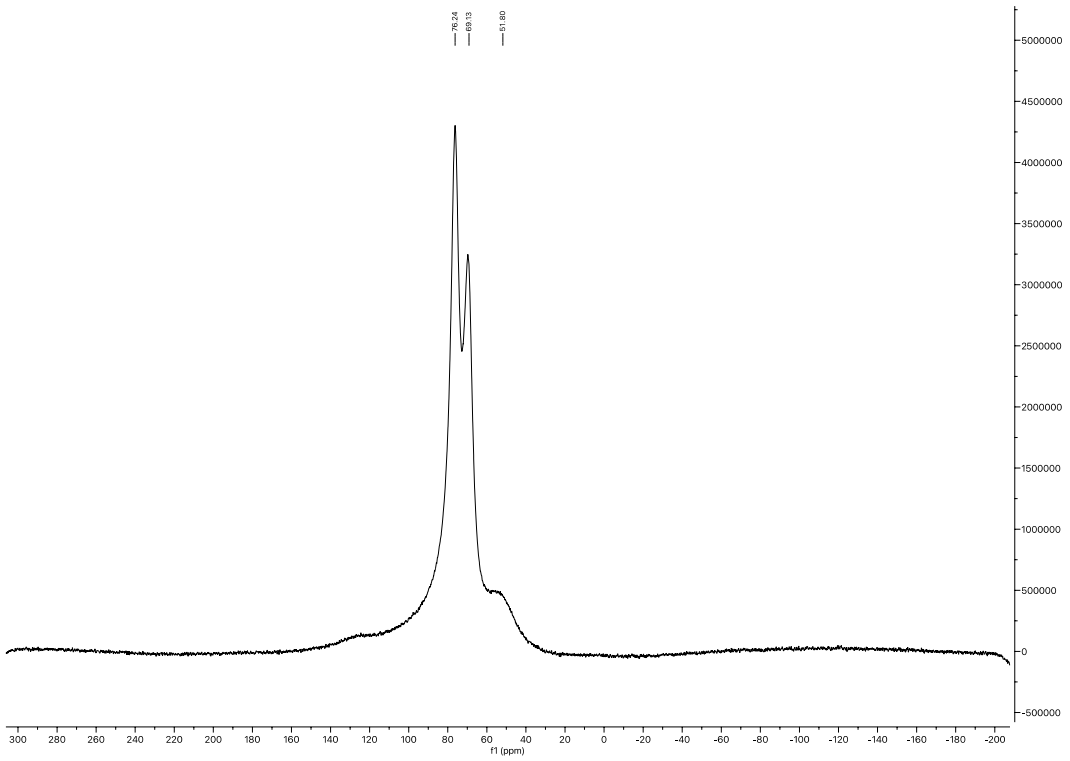


Figure S195 The ^{45}Sc NMR spectrum of [Sc(**L**$^{\mathbf{021}}$)]$^{2+}$ in MeOD.

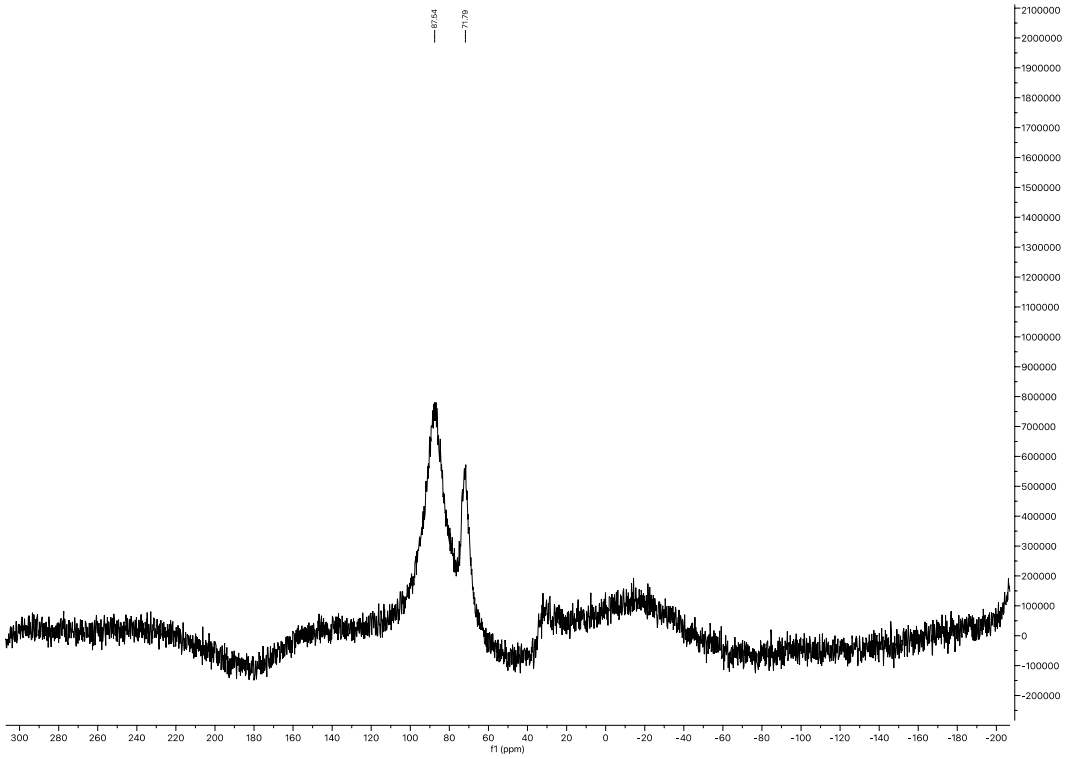


Figure S196 The ^{45}Sc NMR spectrum of [Sc(**L**$^{\mathbf{021}}$)]$^{2+}$ in D_2O.

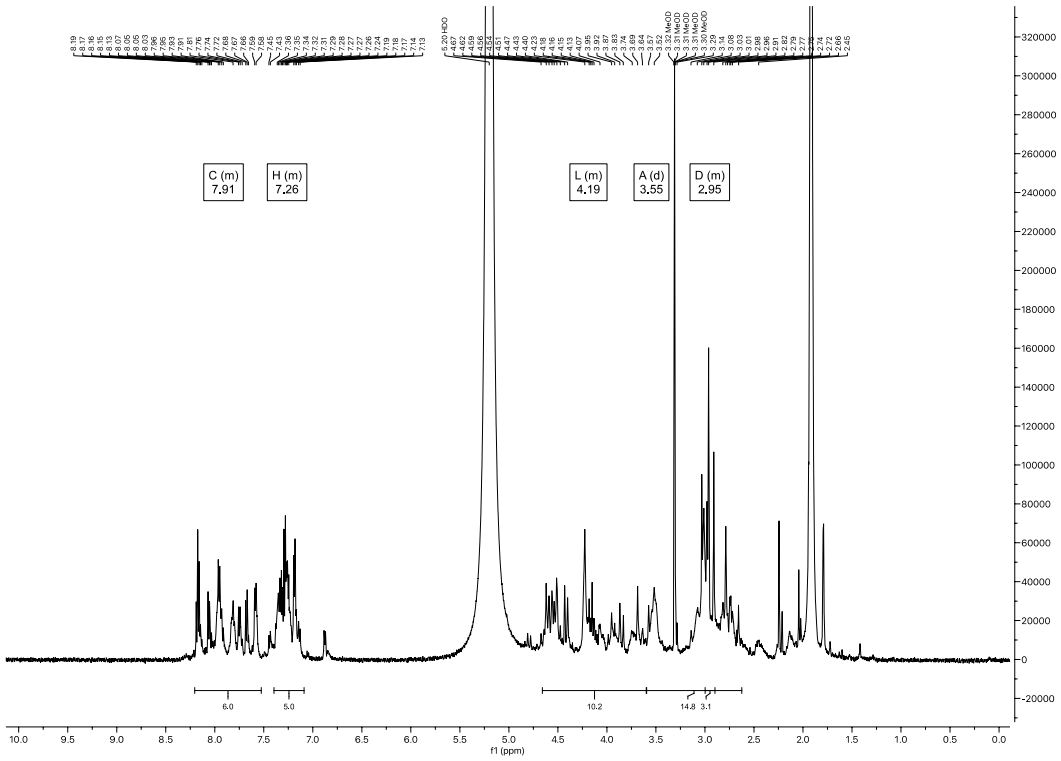


Figure S197 The ^{1}H NMR spectrum of [Sc(**L**$^{\mathbf{012}}$)]$^{+}$ in MeOD.

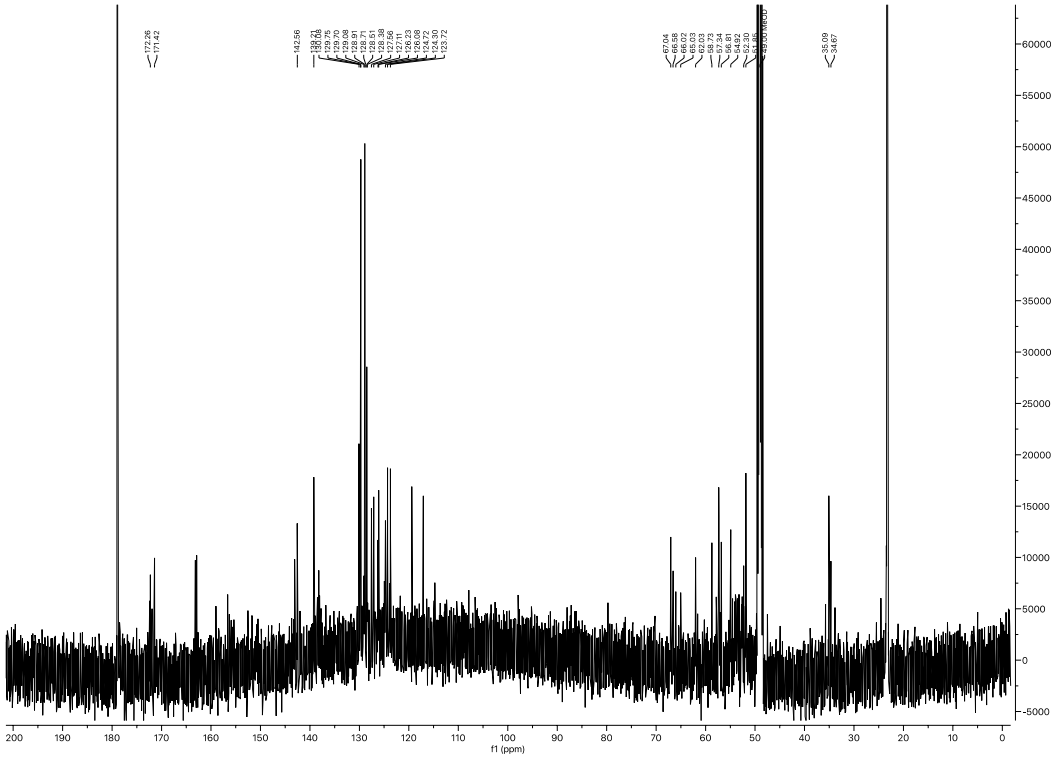


Figure S198 The ^{13}C{^{1}H} NMR spectrum of [Sc(**L**$^{\mathbf{012}}$)]$^{+}$ in MeOD.

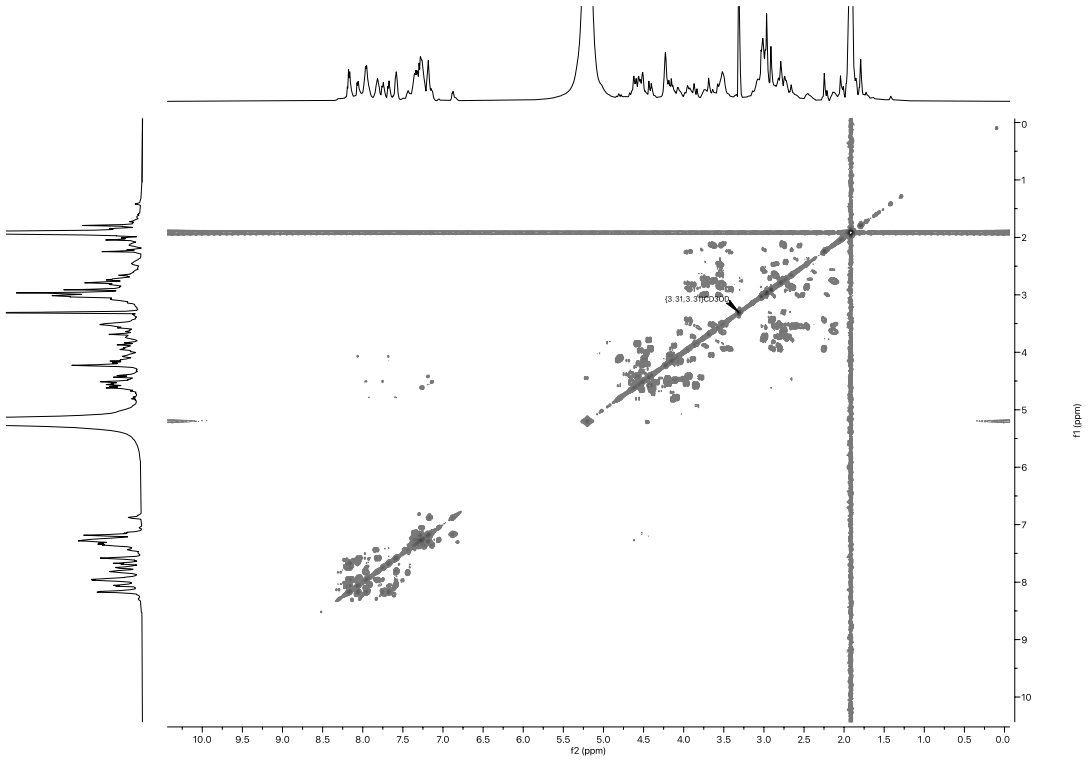


Figure S199 The ^{1}H-^{1}H COSY NMR spectrum of [Sc(**L**^{012})]$^{+}$ in MeOD.

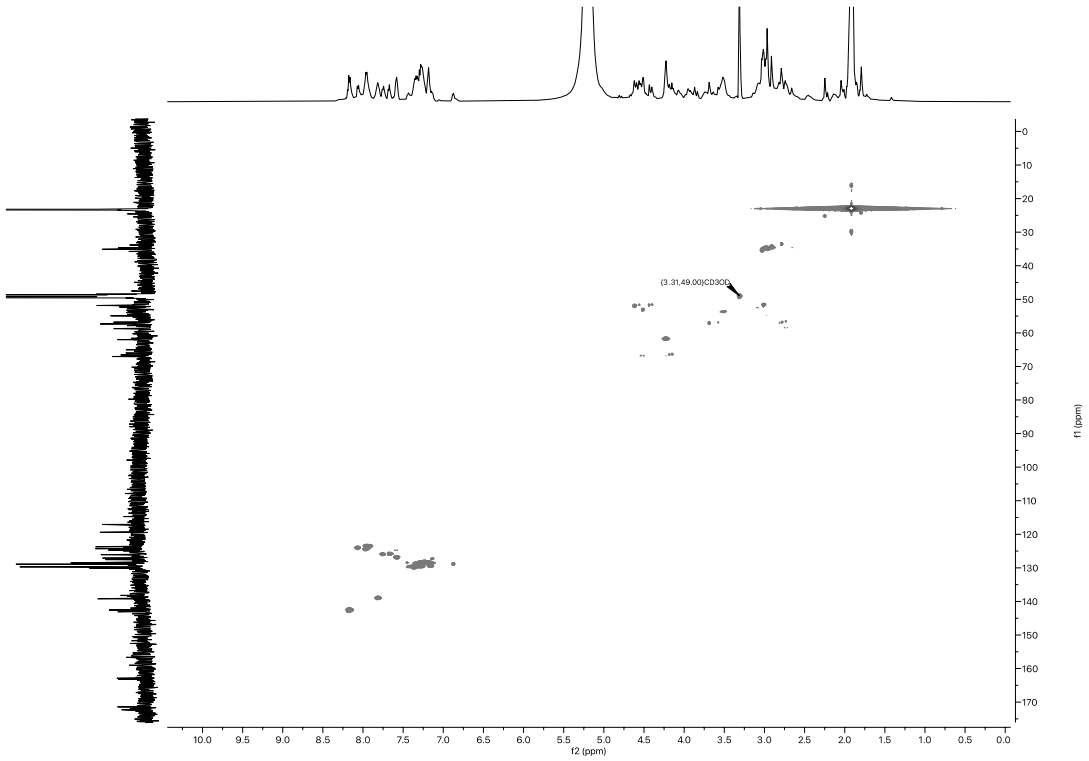


Figure S200 The ^{1}H-^{13}C HSQC NMR spectrum of [Sc(**L**^{012})]$^{+}$ in MeOD.

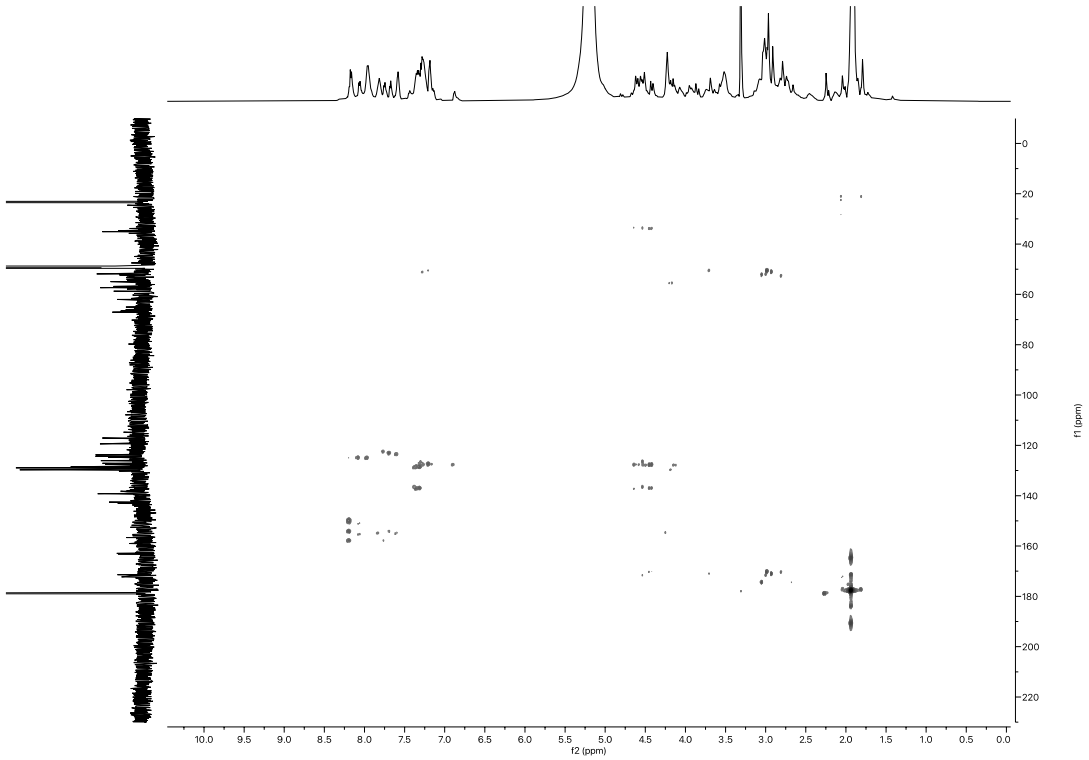


Figure S201 The ^{1}H-^{13}C HMBC NMR spectrum of [Sc(**L**^{012})]$^{+}$ in MeOD.

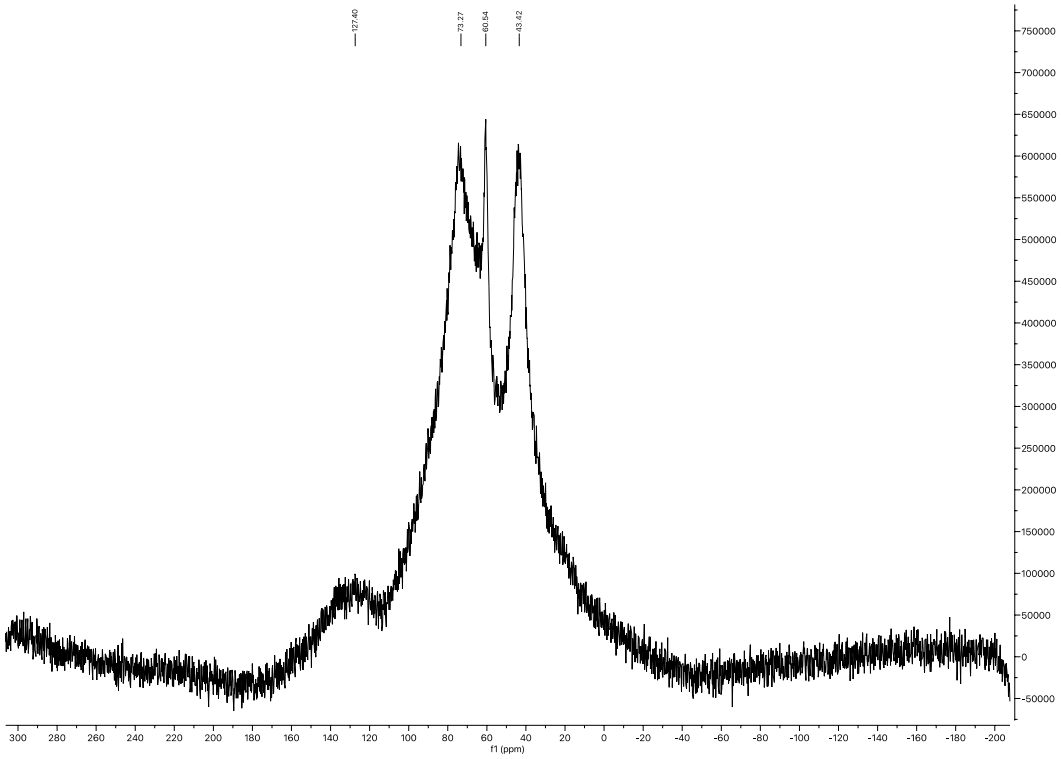


Figure S202 The ^{45}Sc NMR spectrum of [Sc(**L**^{012})]$^{+}$ in MeOD.

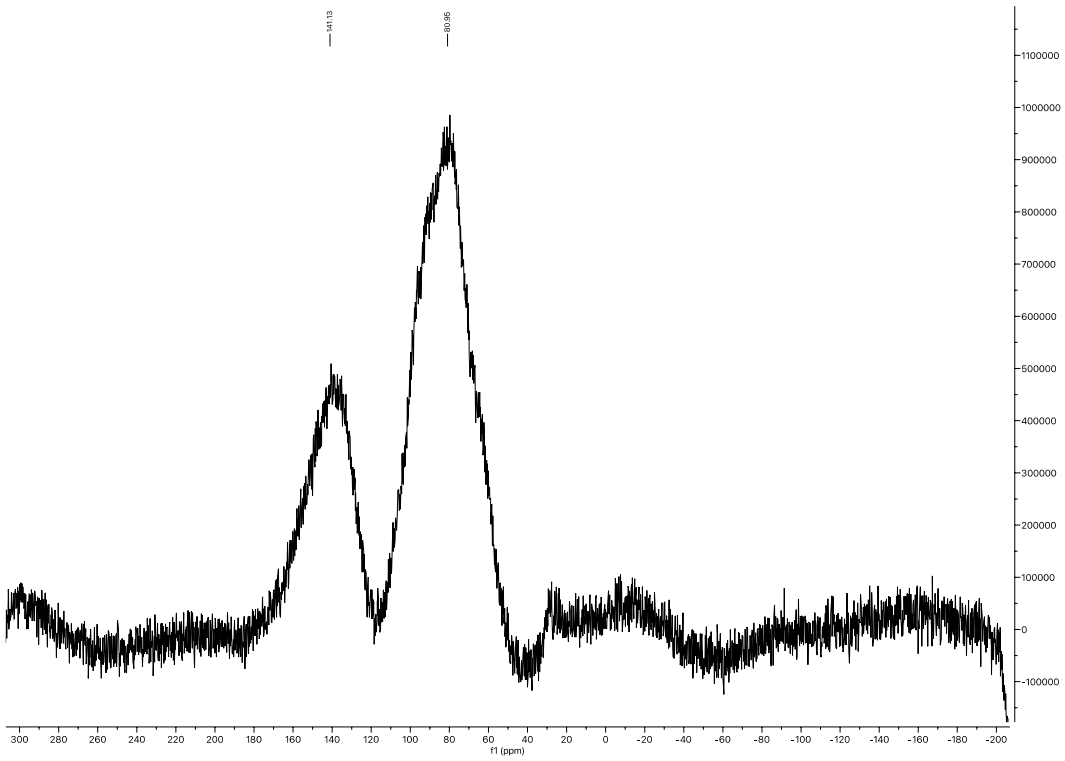


Figure S203 The ^{45}Sc NMR spectrum of [Sc(**L**^{012})]$^{+}$ in D_2O.

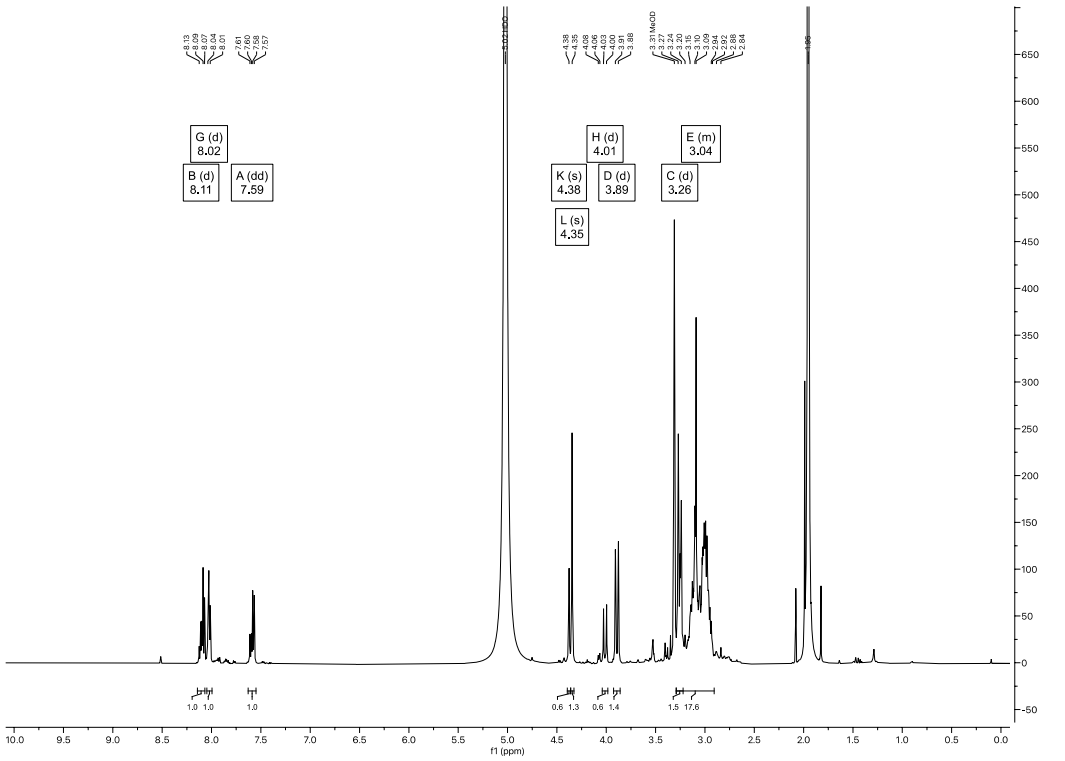


Figure S204 The ^{1}H NMR spectrum of [ScF(**L**^{201})]$^{-}$ in MeOD.

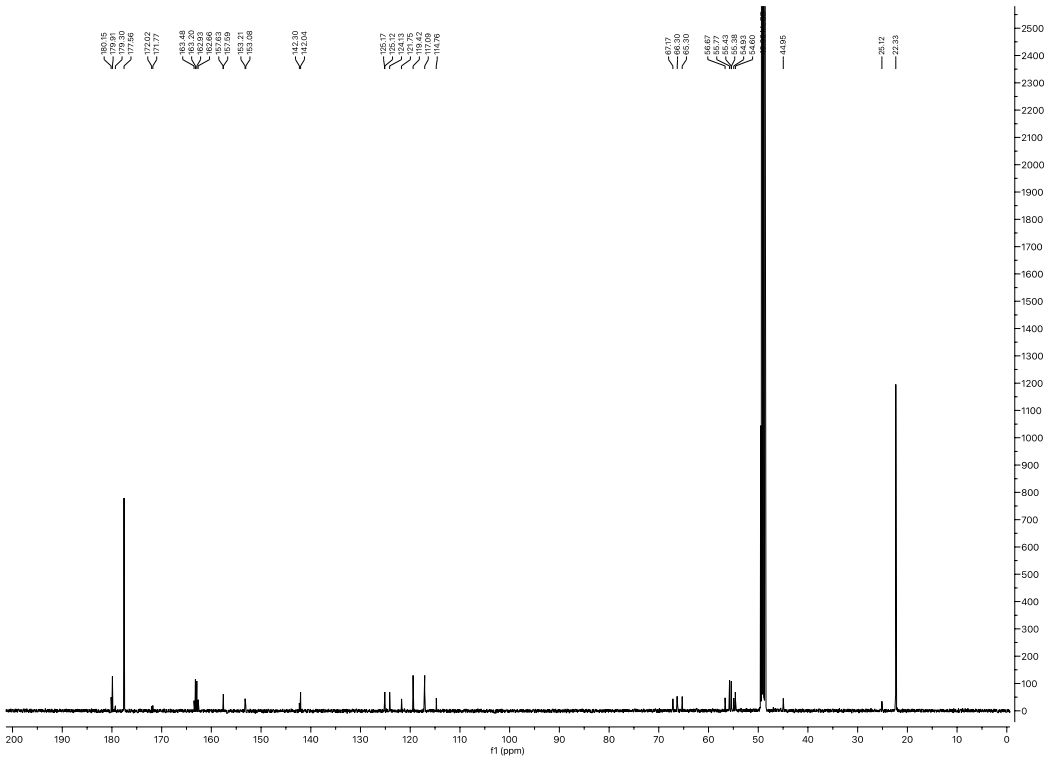


Figure S205 The $^{13}C\{^{1}H\}$ NMR spectrum of $[ScF(\mathbf{L^{201}})]^-$ in MeOD.

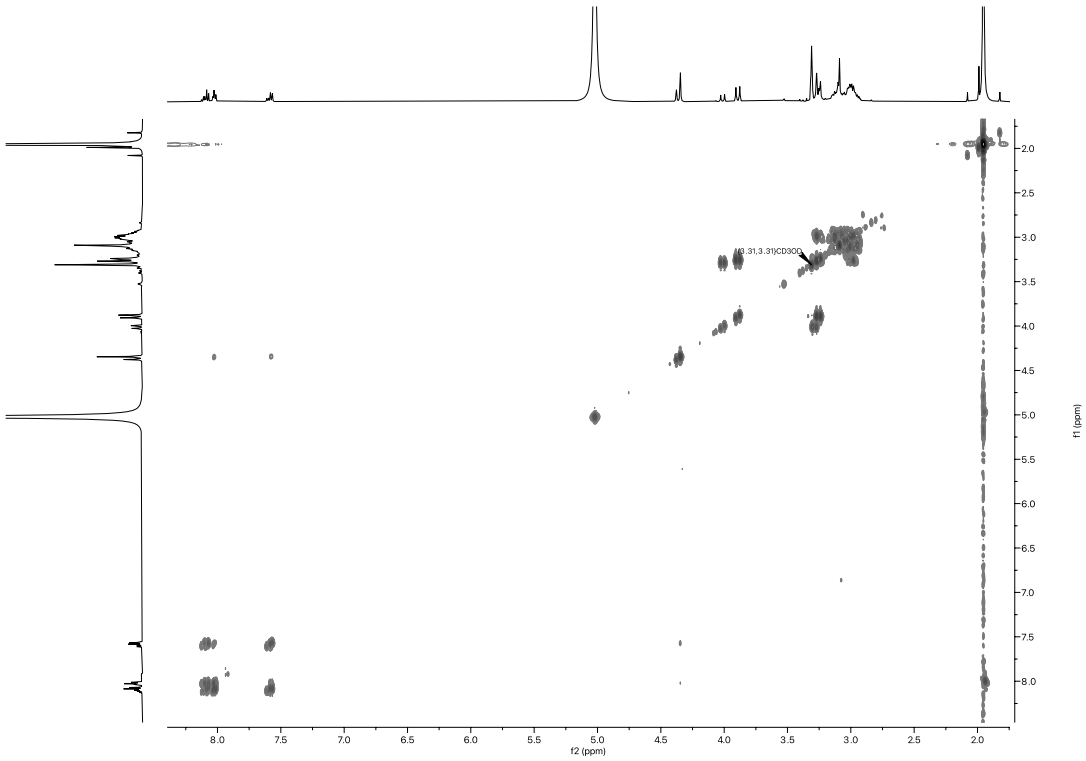


Figure S206 The ^{1}H-^{1}H COSY NMR spectrum of $[ScF(\mathbf{L^{201}})]^-$ in MeOD.

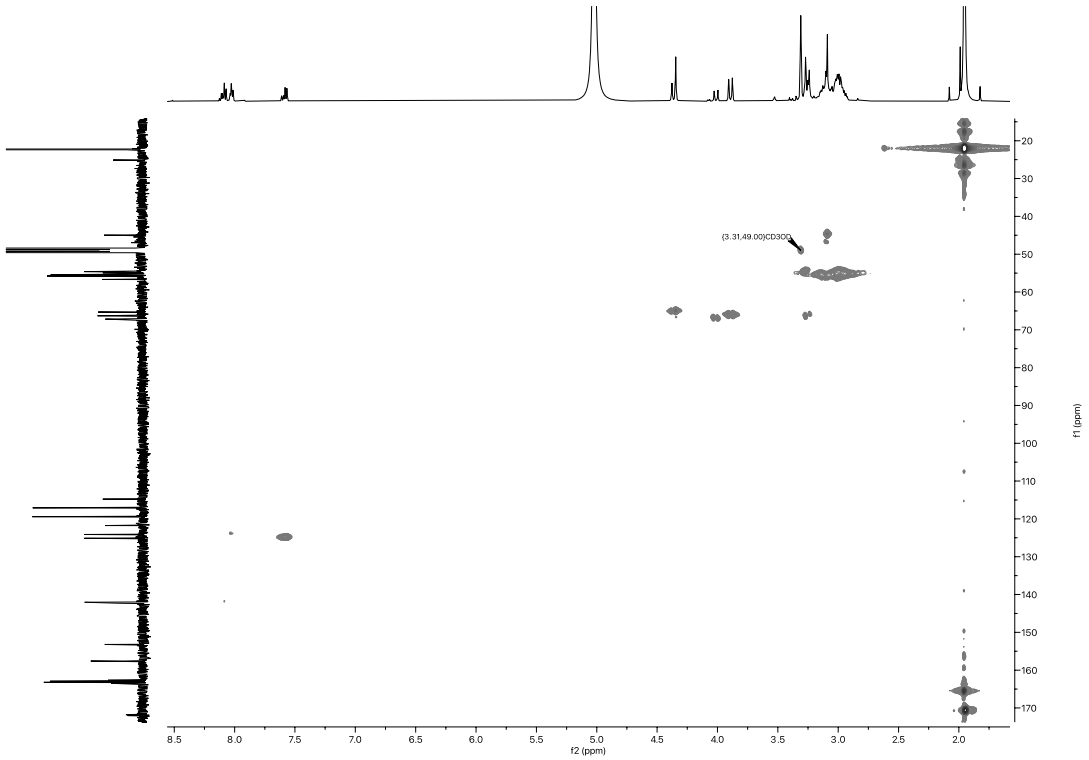


Figure S207 The ^{1}H-^{13}C HSQC NMR spectrum of [ScF(**L**^{201})]$^{-}$ in MeOD.

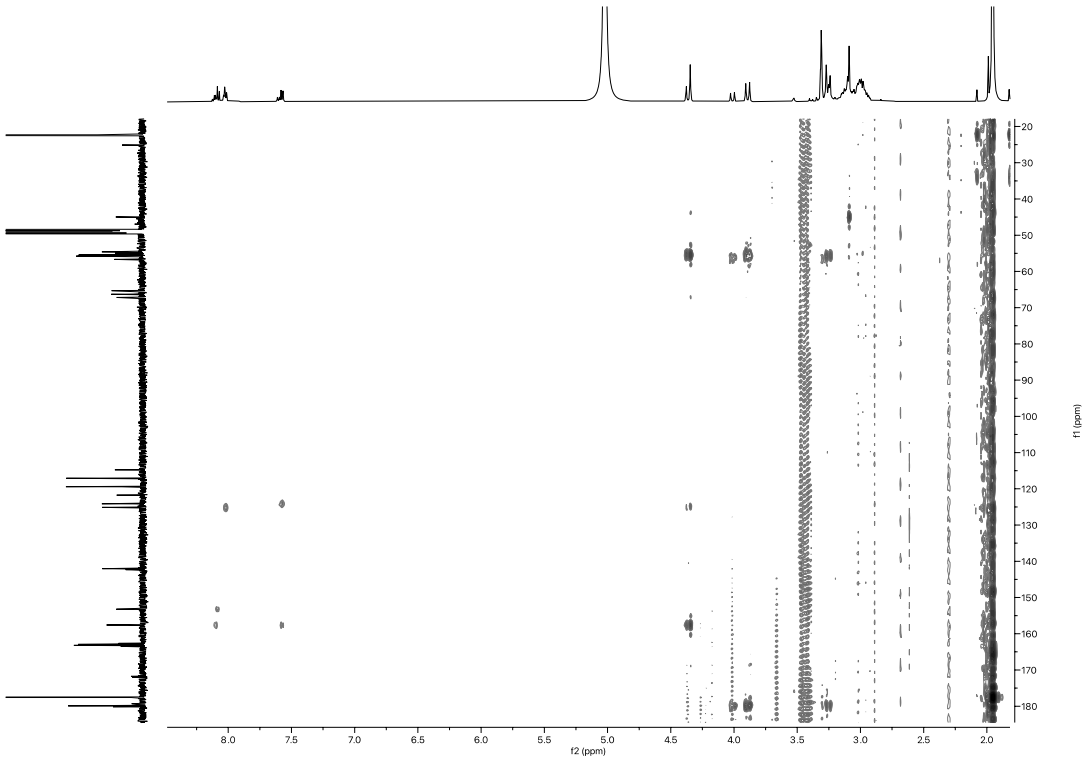


Figure S208 The ^{1}H-^{13}C HMBC NMR spectrum of [ScF(**L**^{201})]$^{-}$ in MeOD.

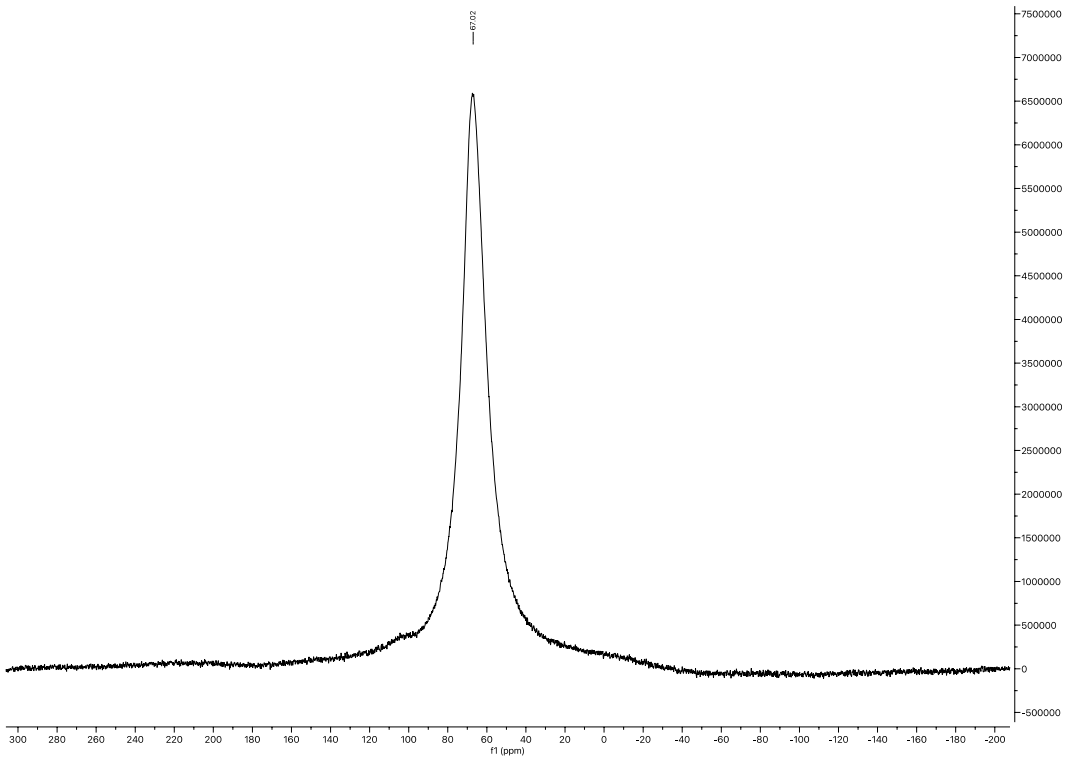


Figure S209 The ^{45}Sc NMR spectrum of [ScF(**L**^{201})]$^{-}$ in MeOD.

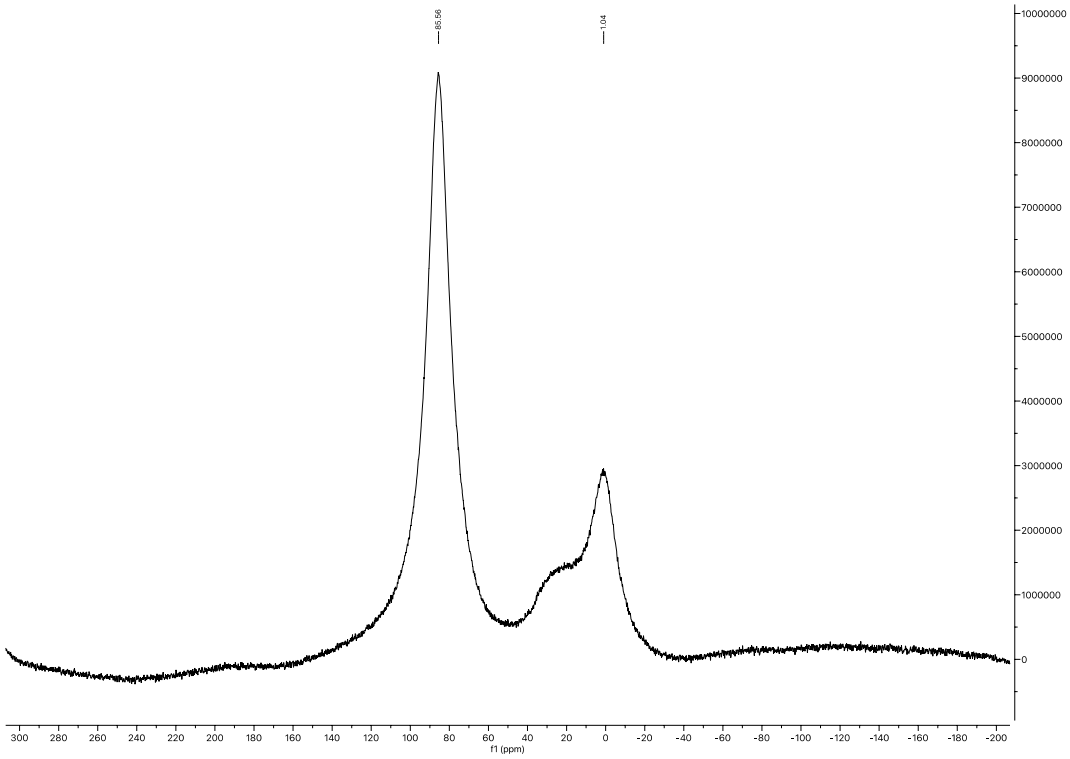


Figure S210 The ^{45}Sc NMR spectrum of [ScF(**L**^{201})]$^{-}$ in D_2O.

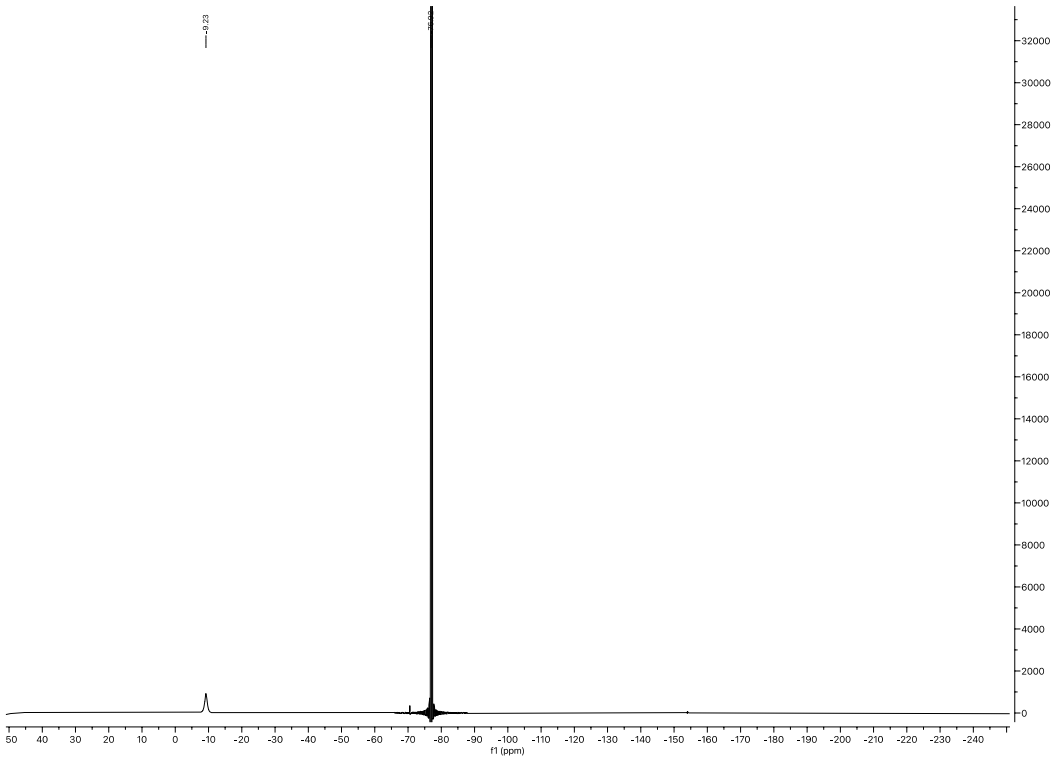


Figure S211 The ^{19}F NMR spectrum of $[ScF(\mathbf{L^{201}})]^-$ in MeOD.

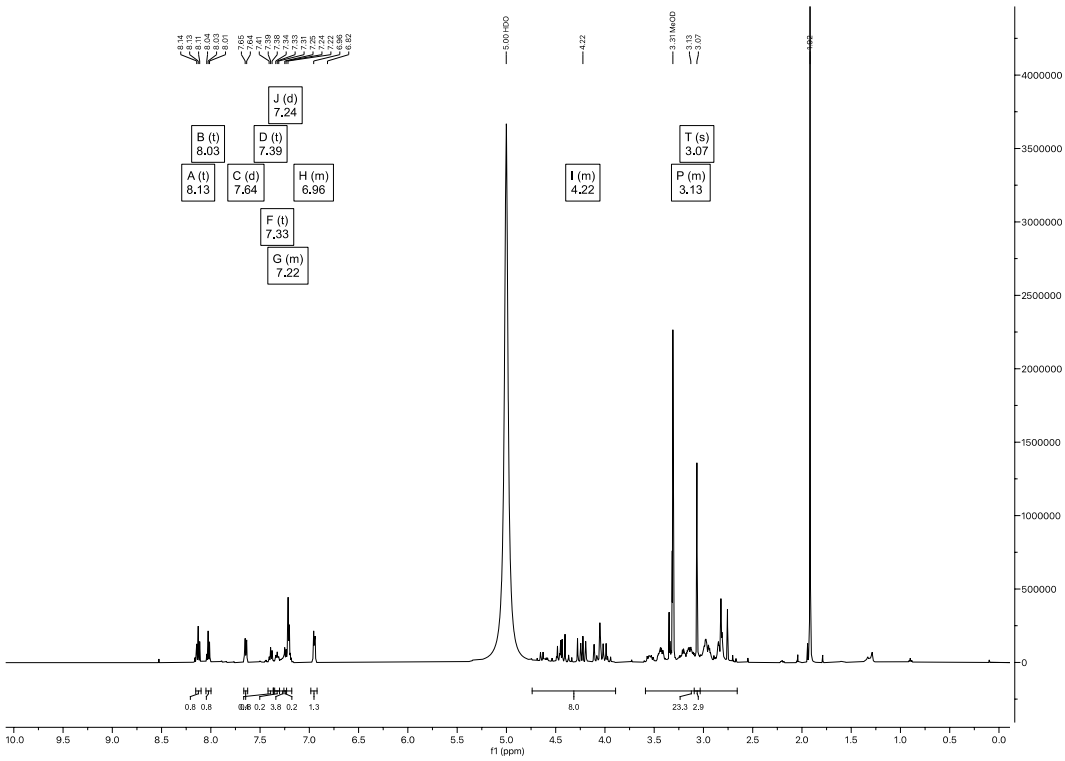


Figure S212 The ^{1}H NMR spectrum of $[ScF(\mathbf{L^{111}})]$ in MeOD.

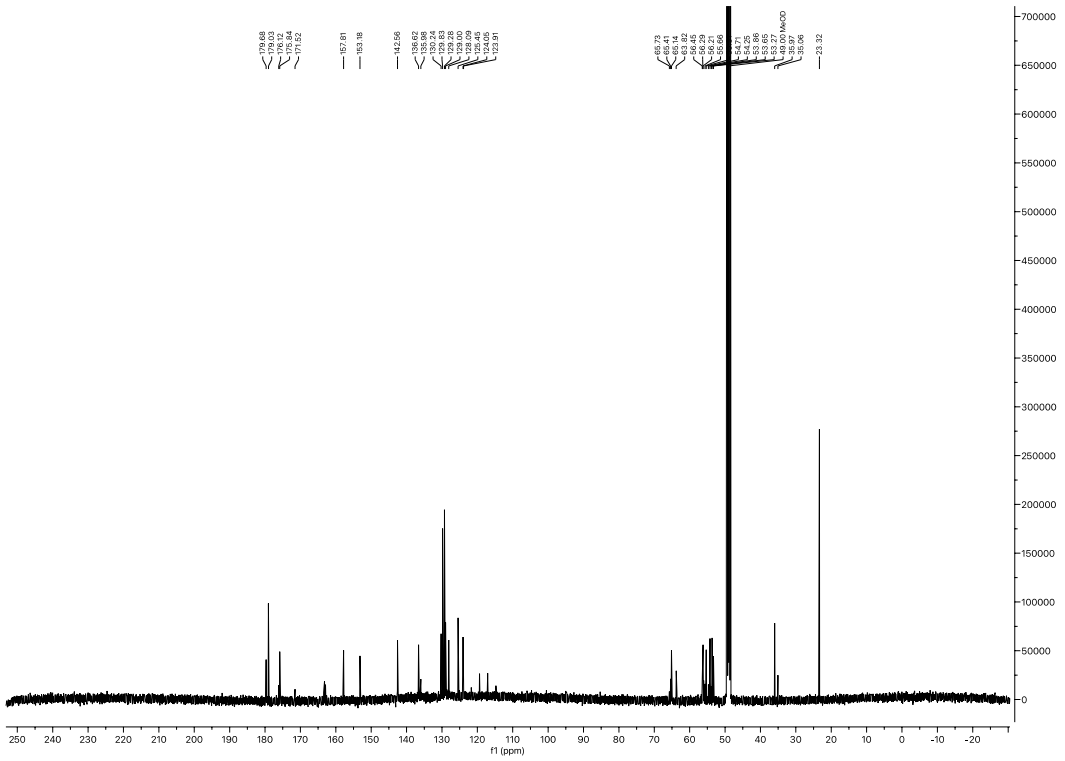


Figure S213 The $^{13}C\{^{1}H\}$ NMR spectrum of [ScF(**L**^{111})] in MeOD.

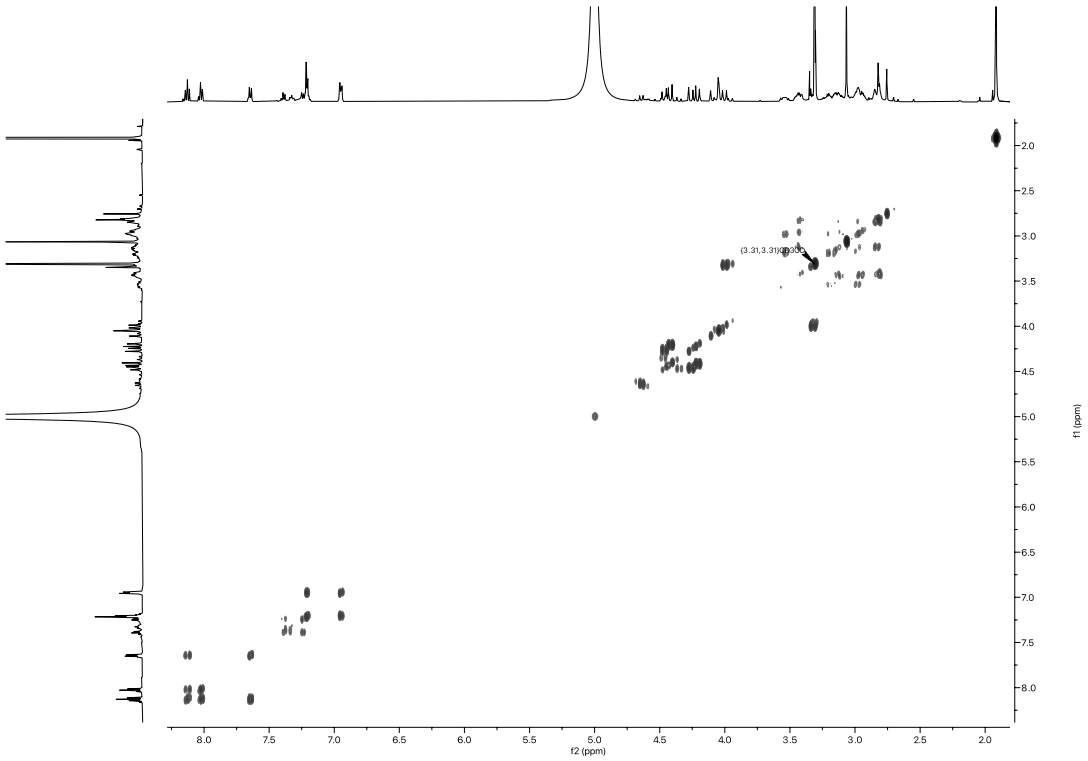


Figure S214 The ^{1}H-^{1}H COSY NMR spectrum of [ScF(**L**^{111})] in MeOD.

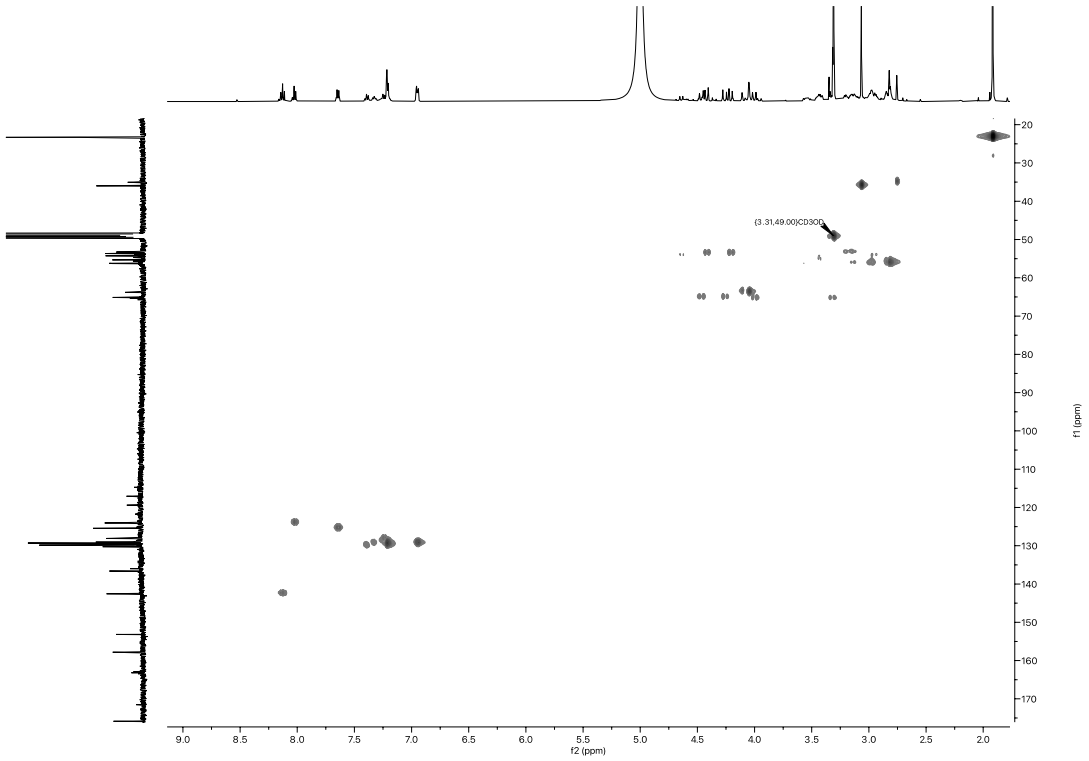


Figure S215 The ^{1}H-^{13}C HSQC NMR spectrum of [ScF(**L**^{111})] in MeOD.

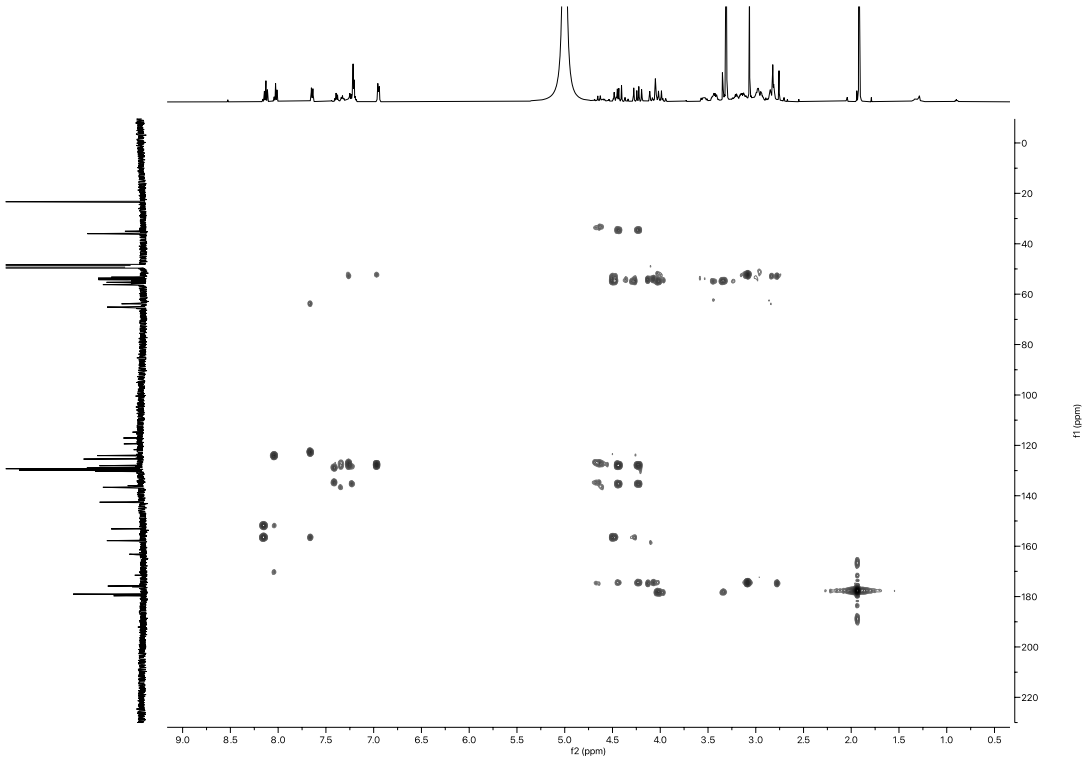


Figure S216 The ^{1}H-^{13}C HMBC NMR spectrum of [ScF(**L**^{111})] in MeOD.

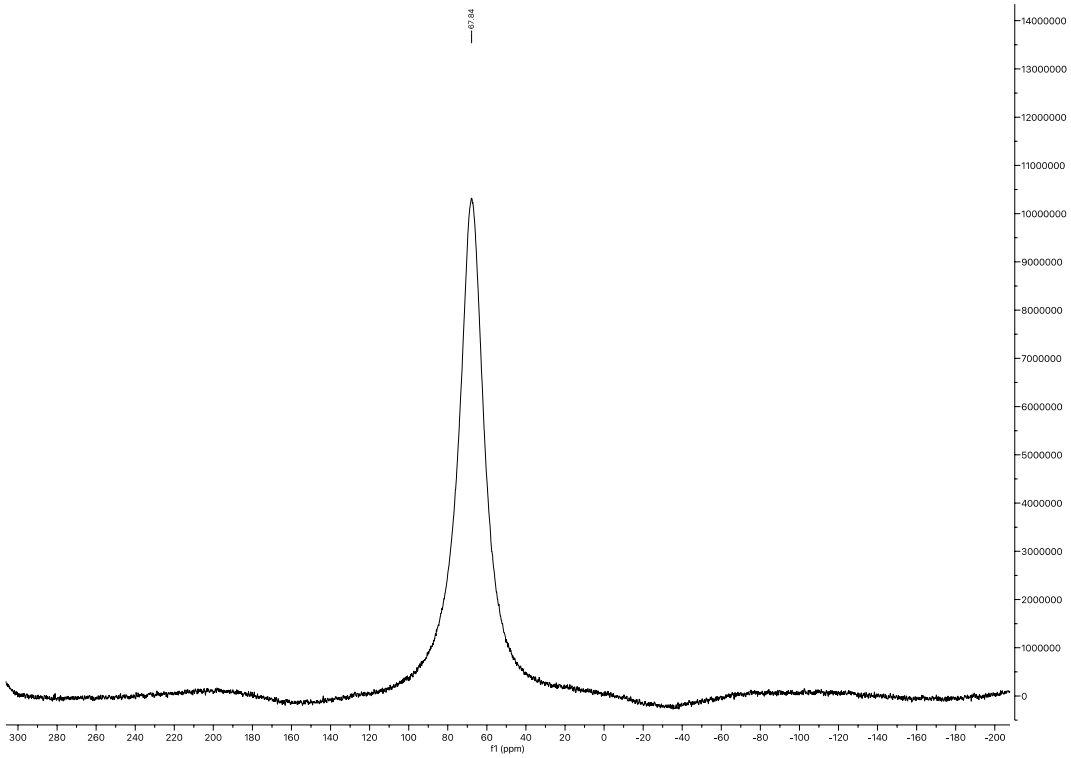


Figure S217 The ^{45}Sc NMR spectrum of [ScF(**L**^{111})] in MeOD.

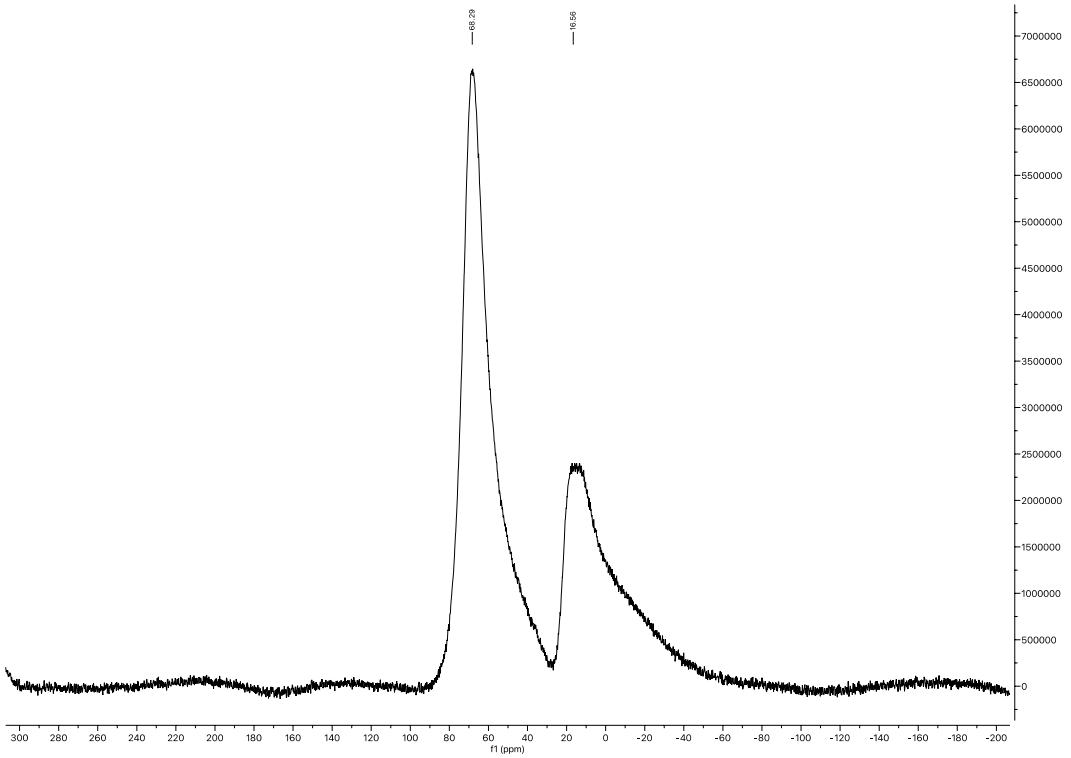


Figure S218 The ^{45}Sc NMR spectrum of [ScF(**L**^{111})] in D_2O.

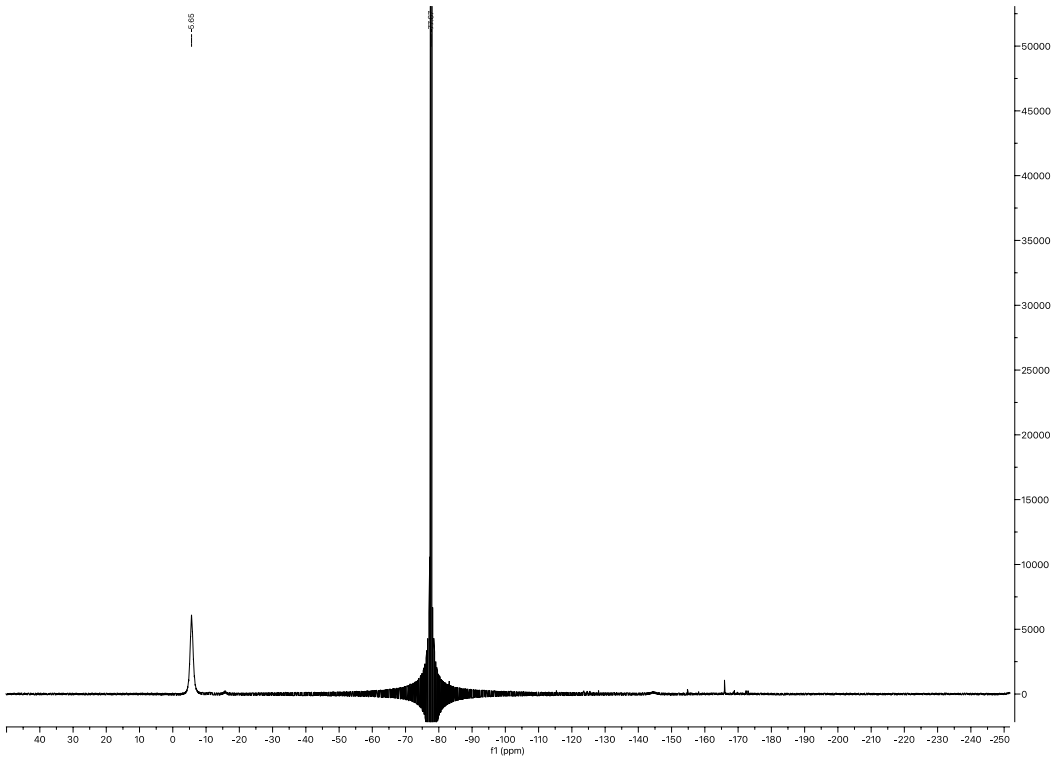


Figure S219 The ^{19}F NMR spectrum of [ScF(**L**^{111})] in MeOD.

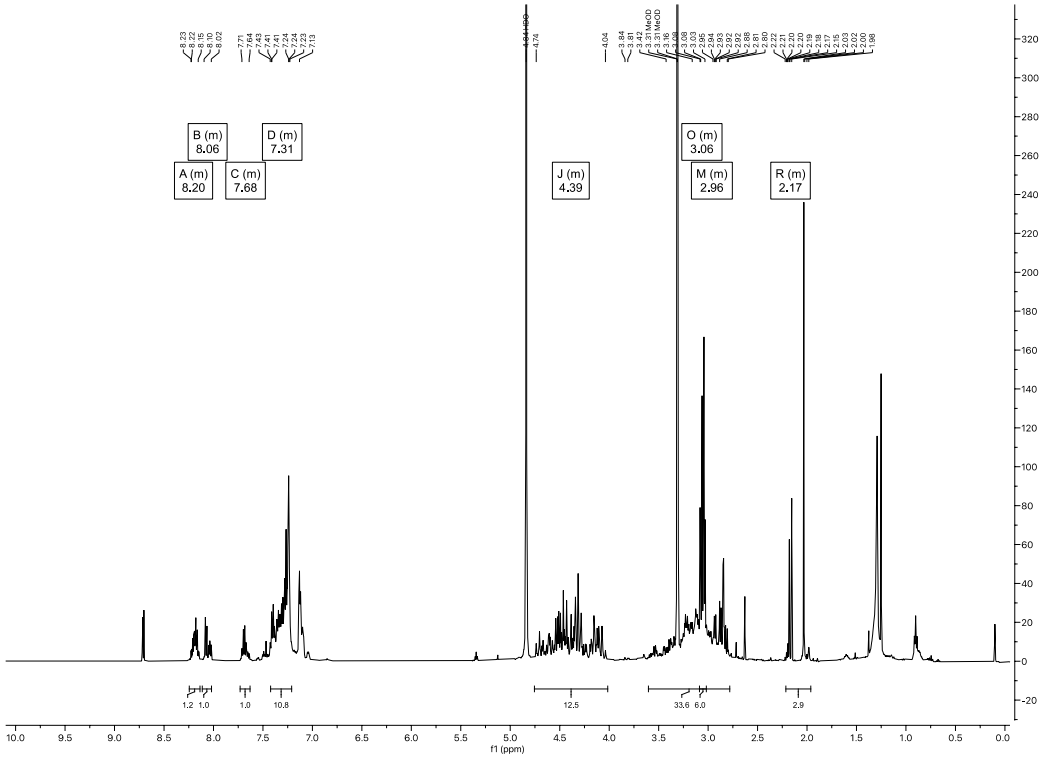


Figure S220 The ^{1}H NMR spectrum of [ScF(**L**^{021})]$^{+}$ in MeOD.

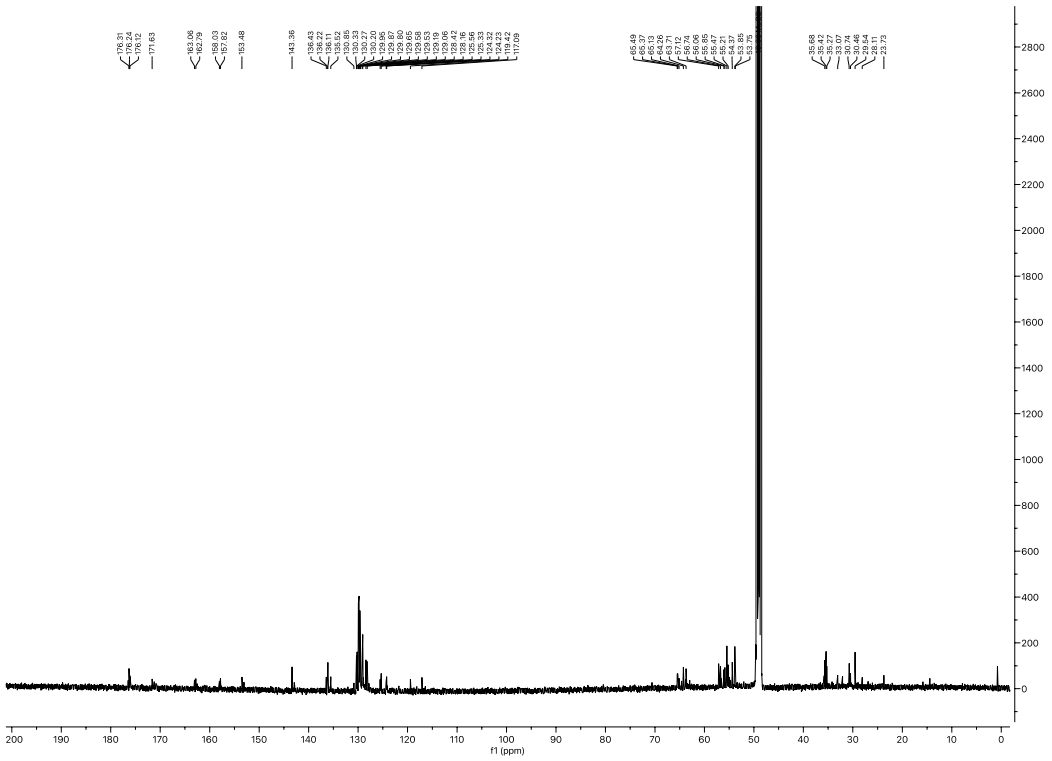


Figure S221 The $^{13}C\{^{1}H\}$ NMR spectrum of $[ScF(\mathbf{L^{021}})]^{+}$ in MeOD.

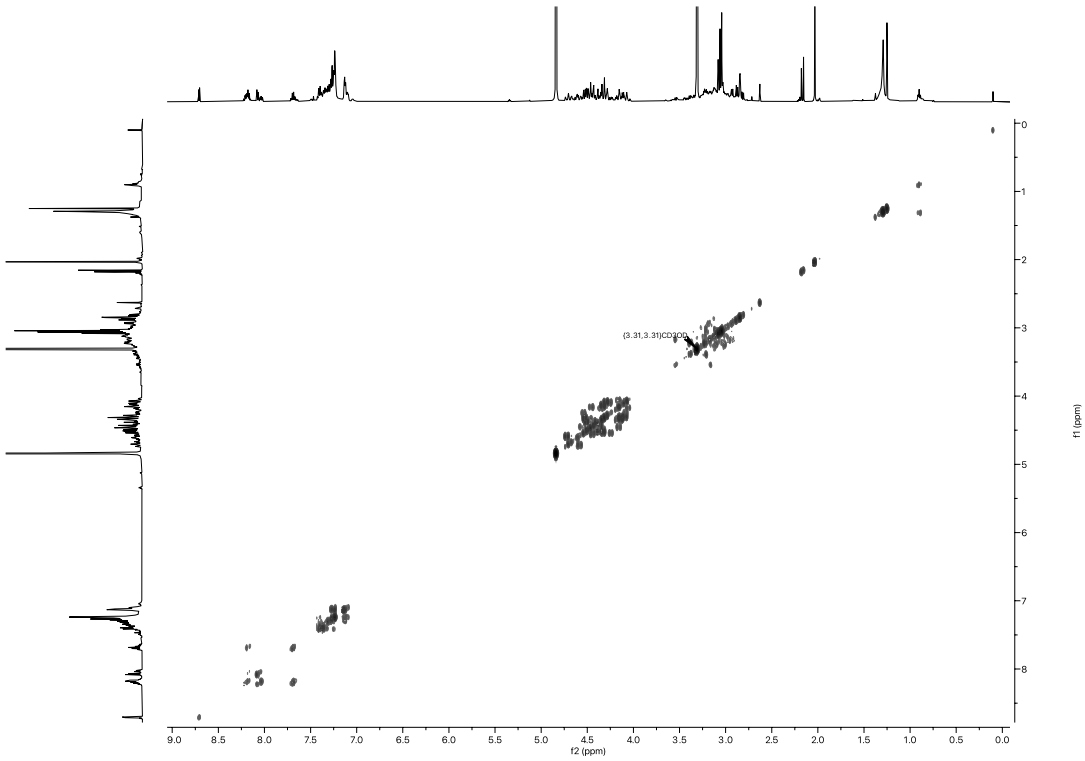


Figure S222 The ^{1}H-^{1}H COSY NMR spectrum of $[ScF(\mathbf{L^{021}})]^{+}$ in MeOD.

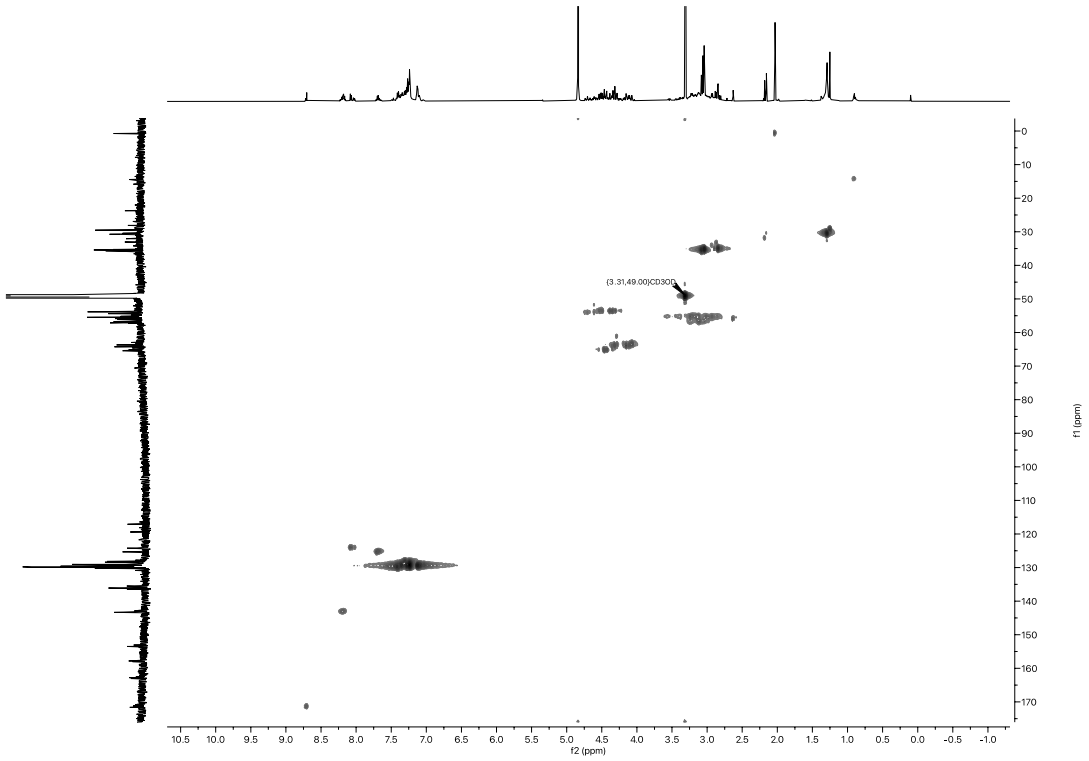


Figure S223 The ^{1}H-^{13}C HSQC NMR spectrum of [ScF(**L**^{021})]$^{+}$ in MeOD.

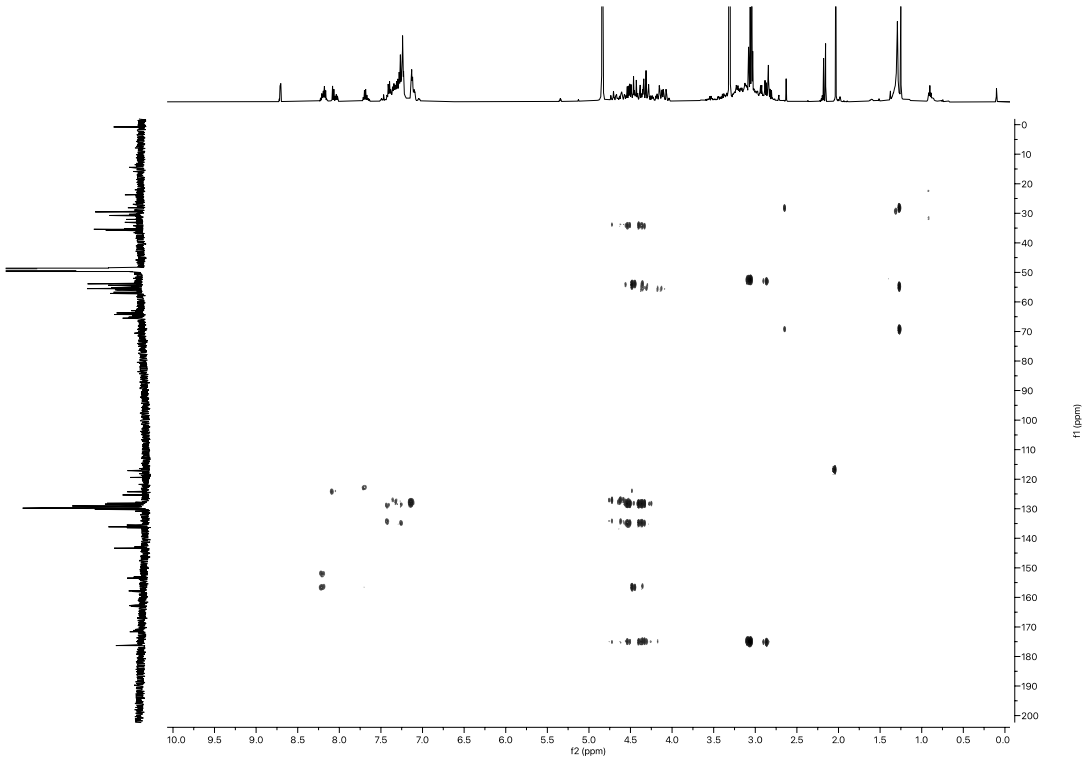


Figure S224 The ^{1}H-^{13}C HMBC NMR spectrum of [ScF(**L**^{021})]$^{+}$ in MeOD.

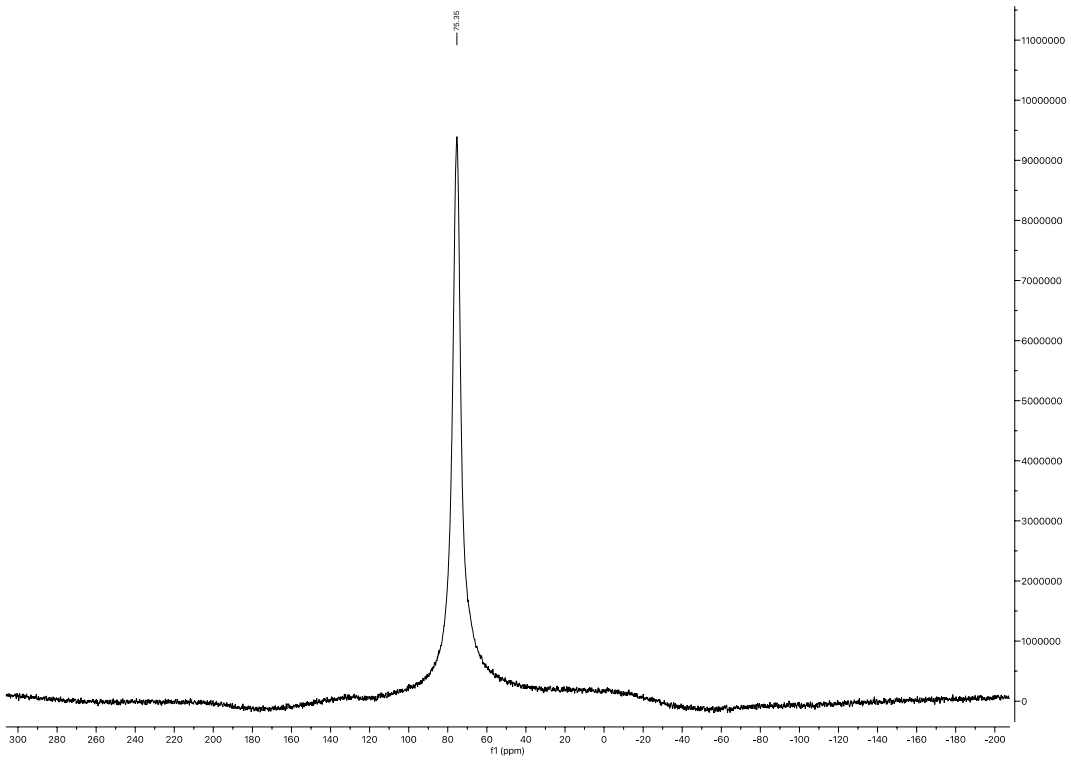


Figure S225 The ^{45}Sc NMR spectrum of [ScF(**L**$^{\mathbf{021}}$)]$^{+}$ in MeOD.

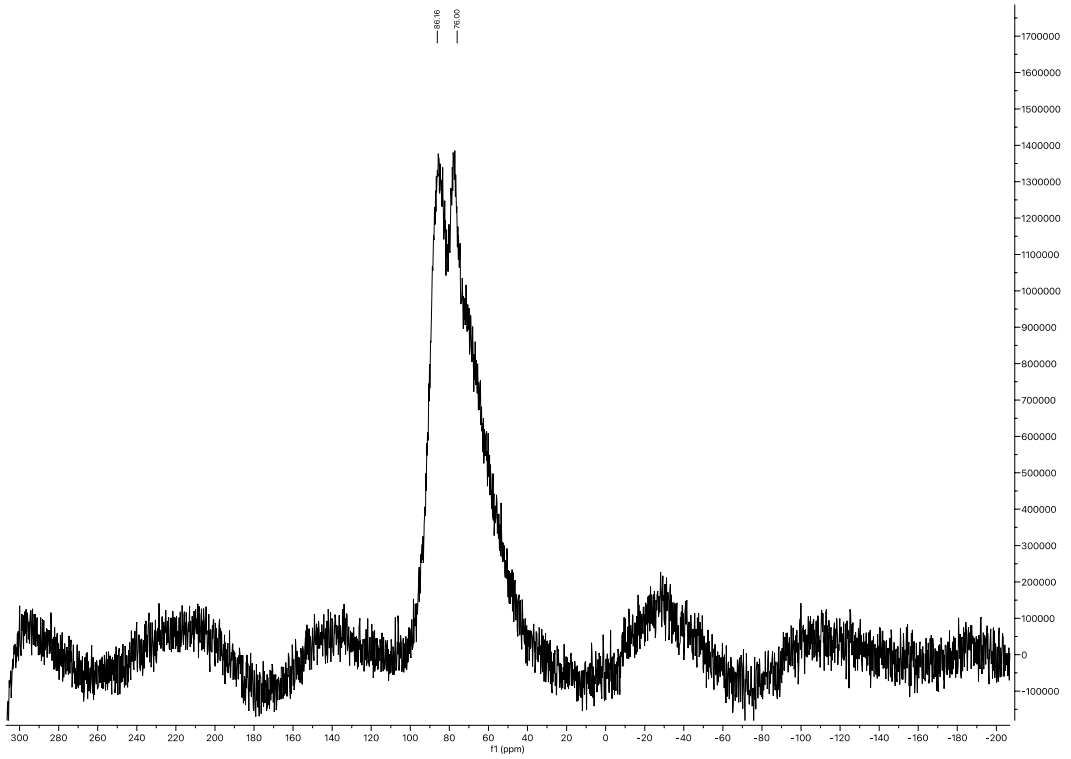


Figure S226 The ^{45}Sc NMR spectrum of [ScF(**L**$^{\mathbf{021}}$)]$^{+}$ in D_2O.

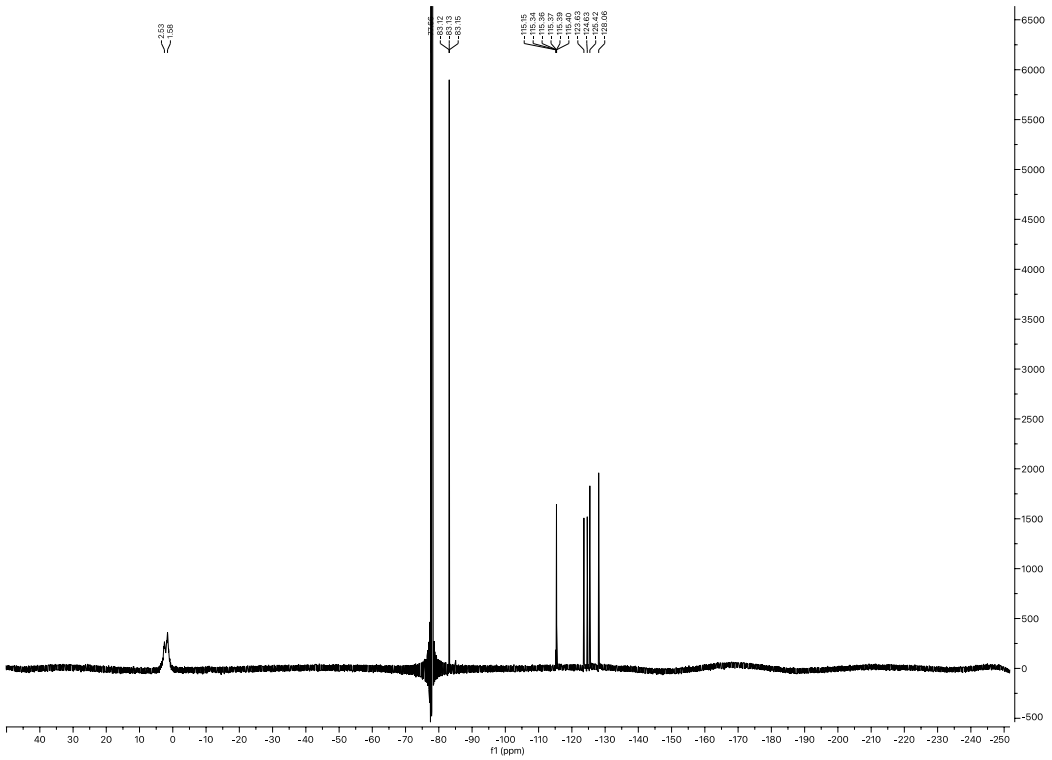


Figure S227 The ^{19}F NMR spectrum of $[ScF(\mathbf{L^{021}})]^+$ in MeOD.

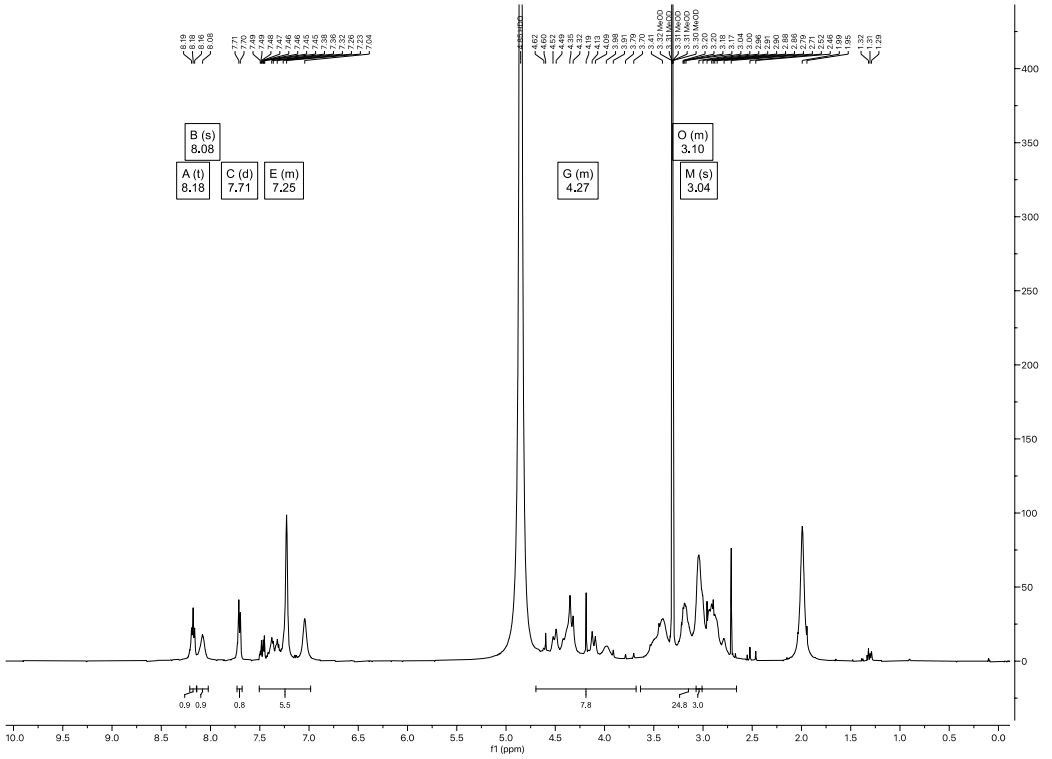


Figure S228 The ^{1}H NMR spectrum of $[Lu(\mathbf{L^{111}})]^+$ in MeOD.

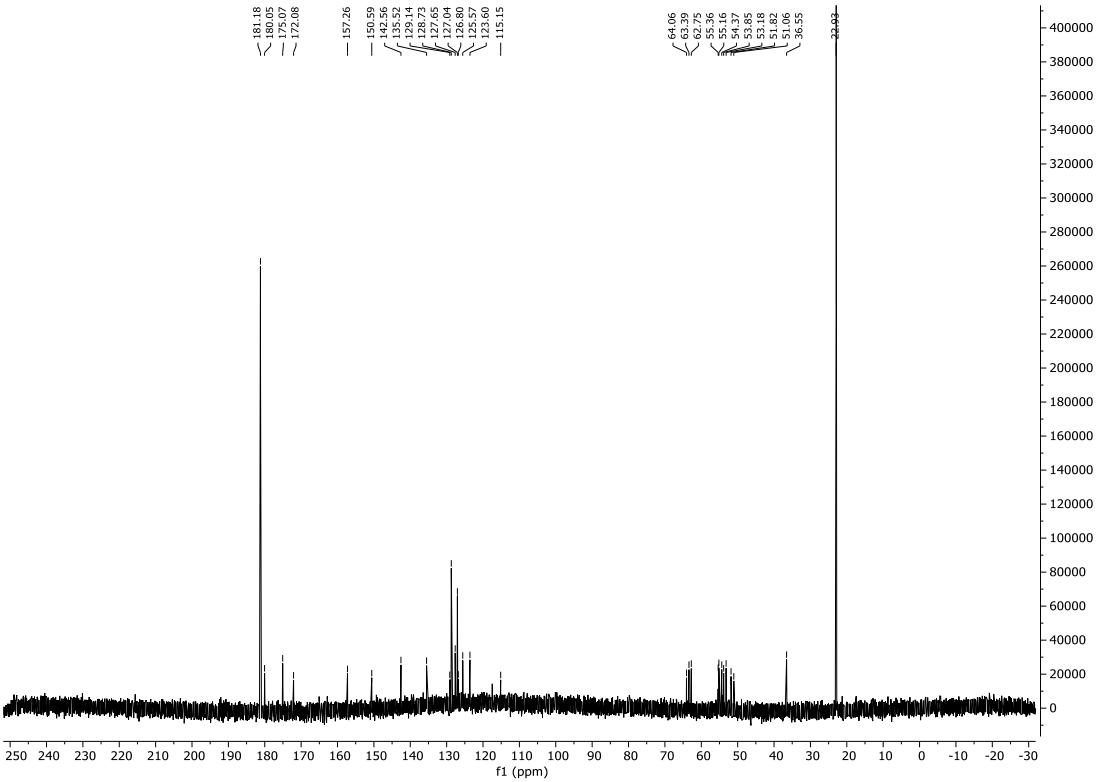


Figure S229 The $^{13}C\{^{1}H\}$ NMR spectrum of [Lu(**L**^{111})]$^{+}$ in MeOD.

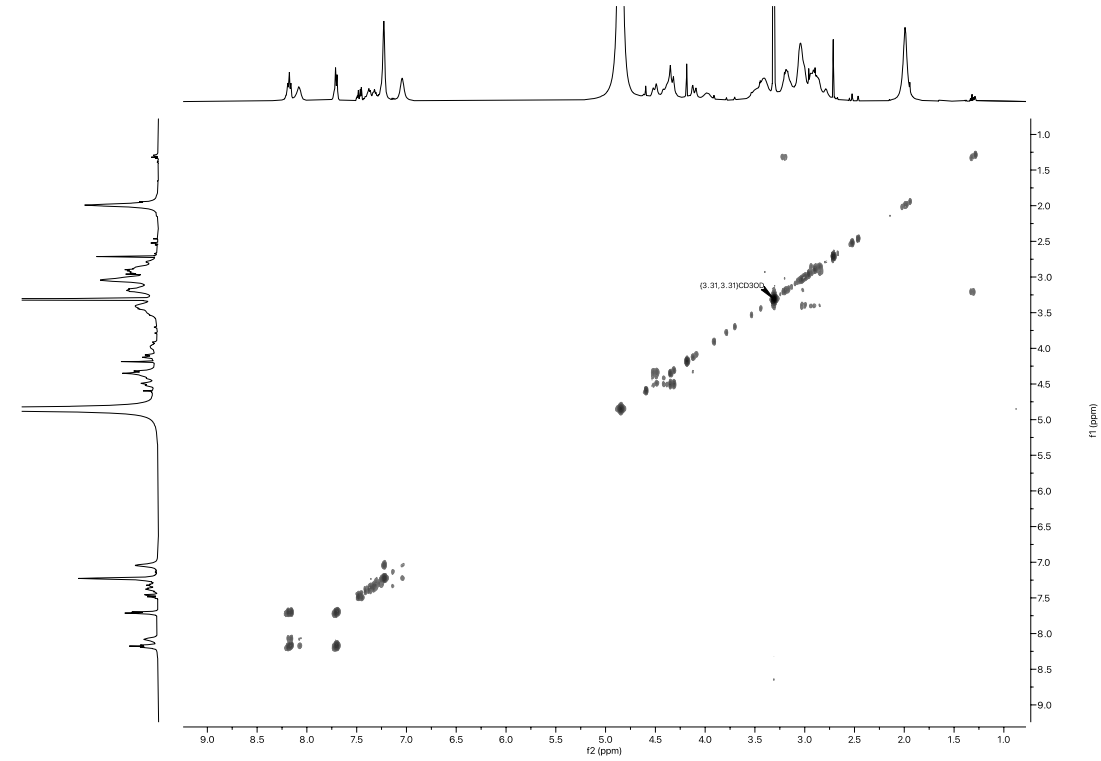


Figure S230 The ^{1}H-^{1}H COSY NMR spectrum of [Lu(**L**^{111})]$^{+}$ in MeOD.

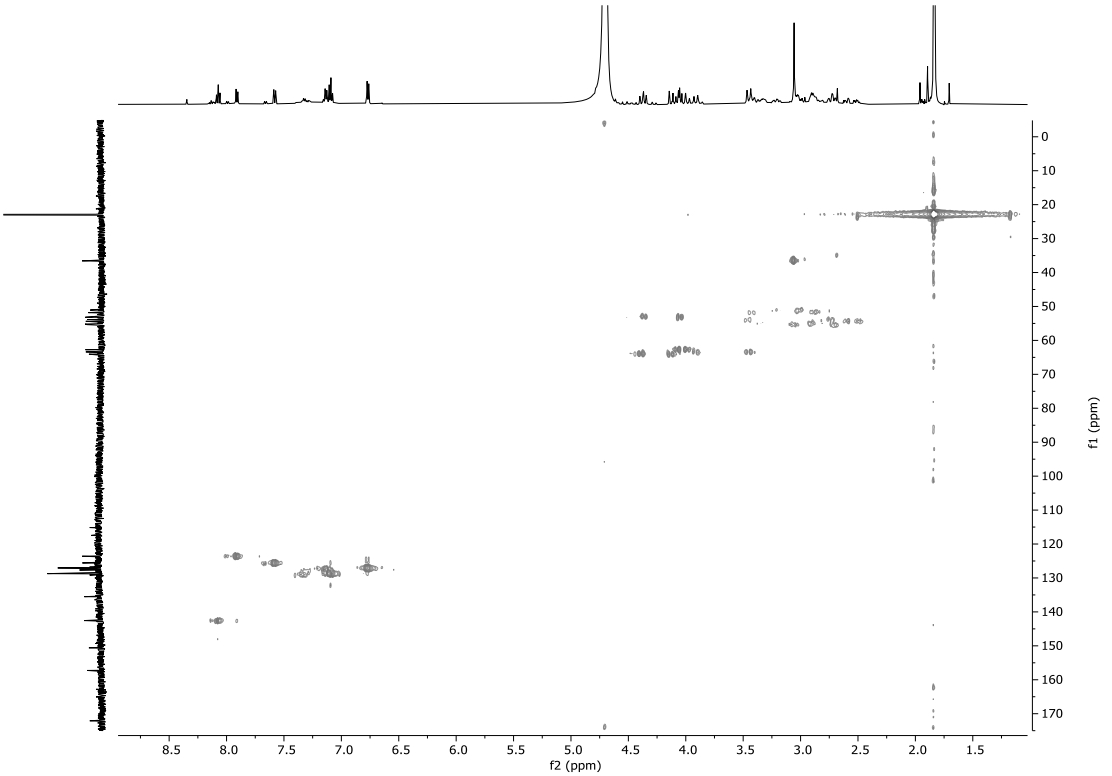


Figure S231 The ^{1}H-^{13}C HSQC NMR spectrum of [Lu(**L**^{111})]$^{+}$ in MeOD.

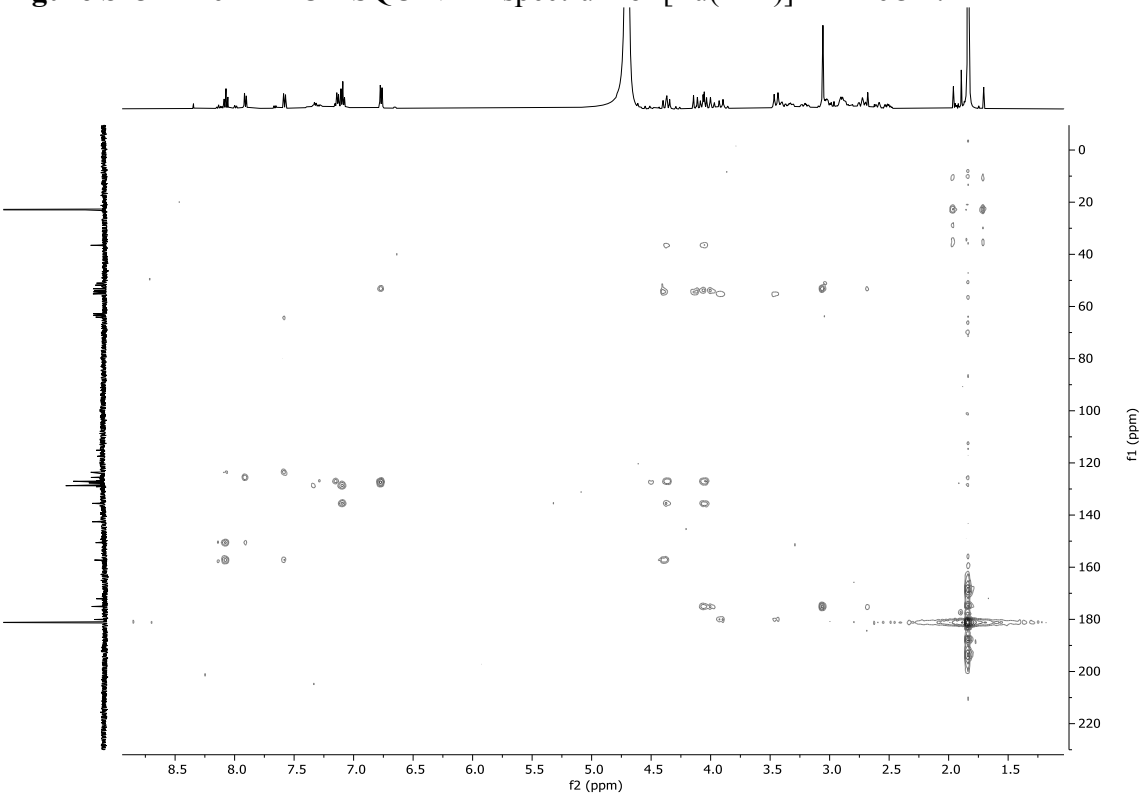


Figure S232 The ^{1}H-^{13}C HMBC NMR spectrum of [Lu(**L**^{111})]$^{+}$ in MeOD.

2.2 HRMS

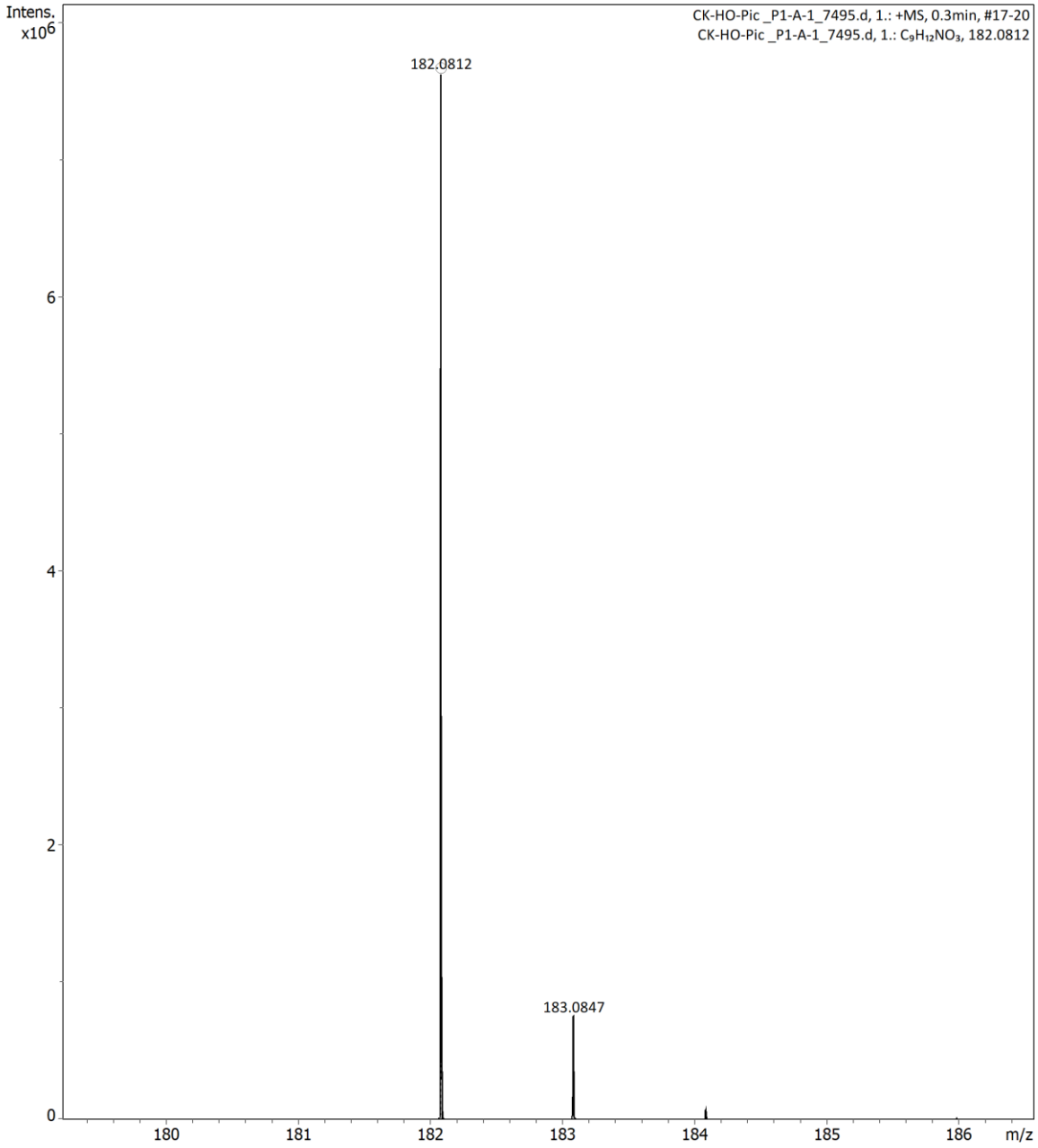


Figure S233 ESI-HRMS of ethyl 6-(hydroxymethyl)picolinate.

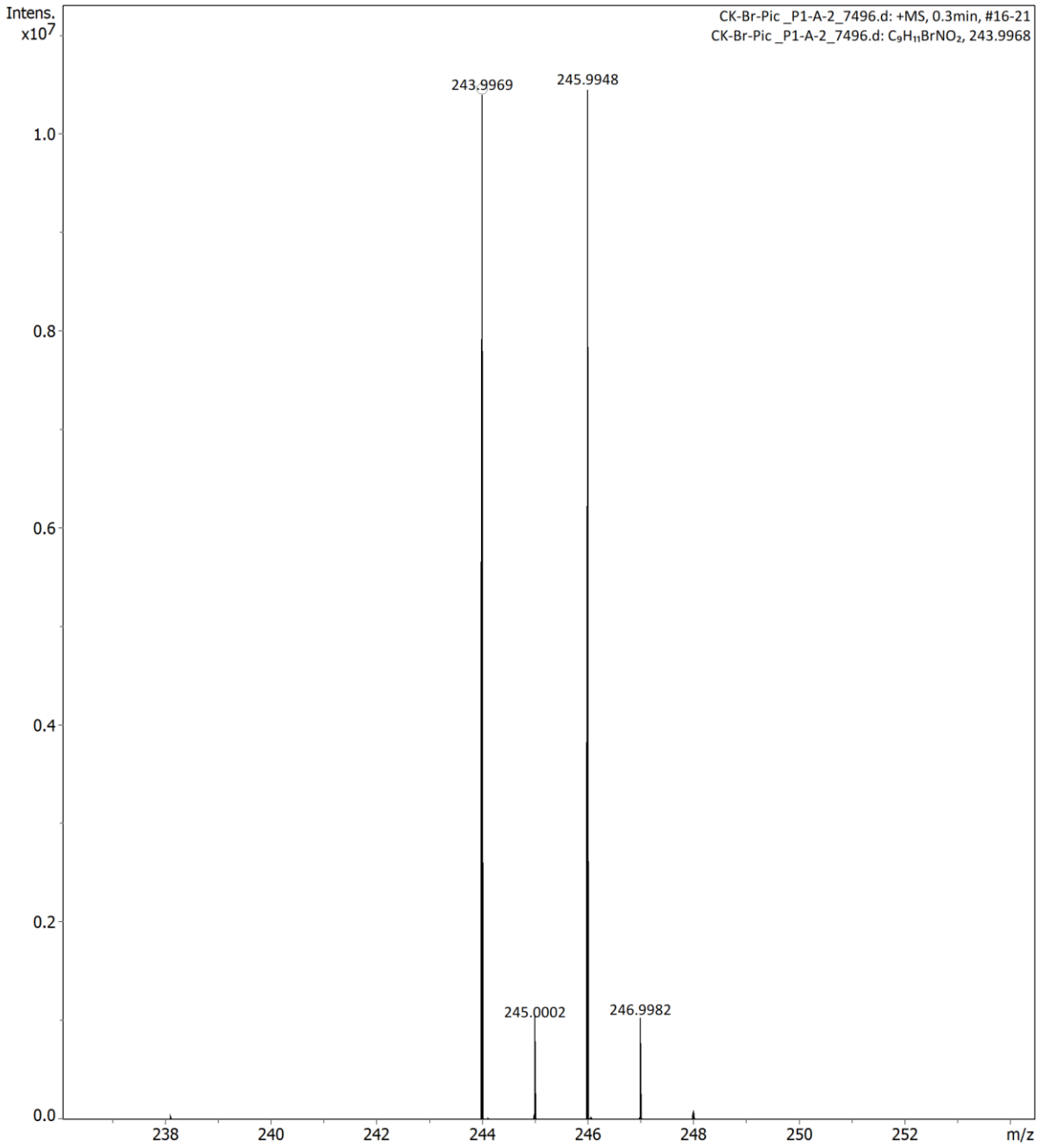


Figure S234 ESI-HRMS of ethyl 6-(bromomethyl)picolinate.

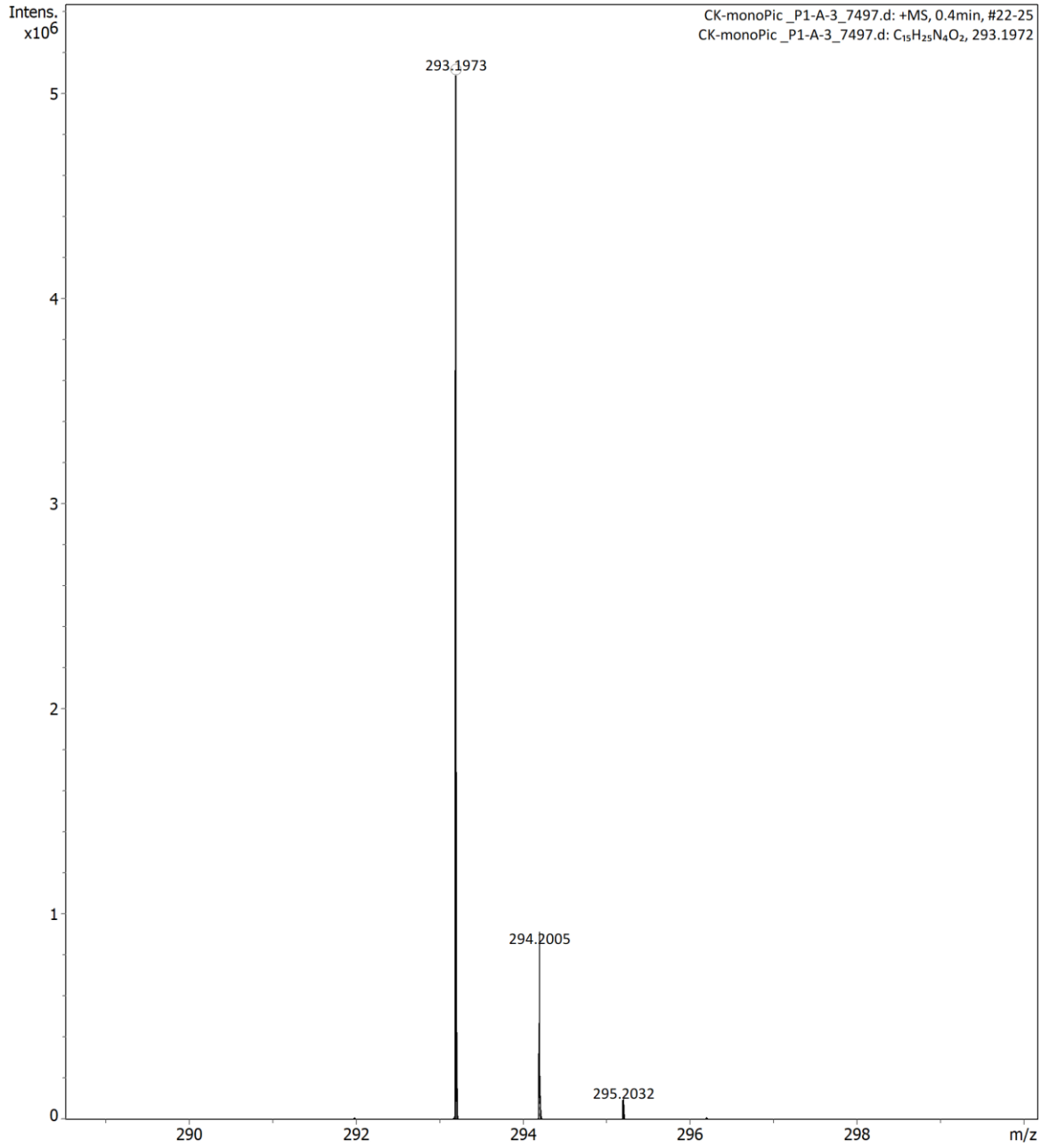


Figure S235 ESI-HRMS of monoPic.

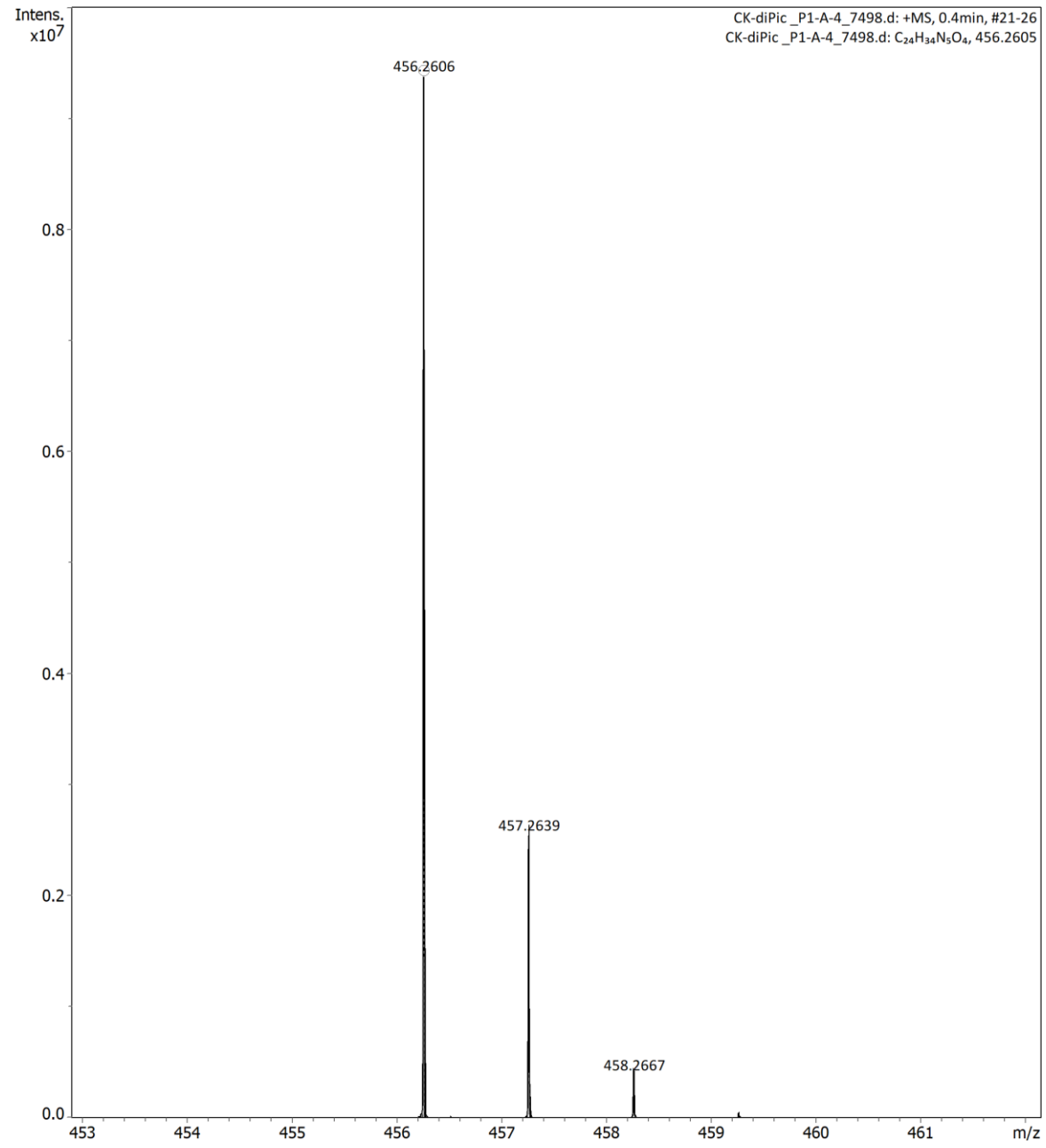


Figure S236 ESI-HRMS of diPic.

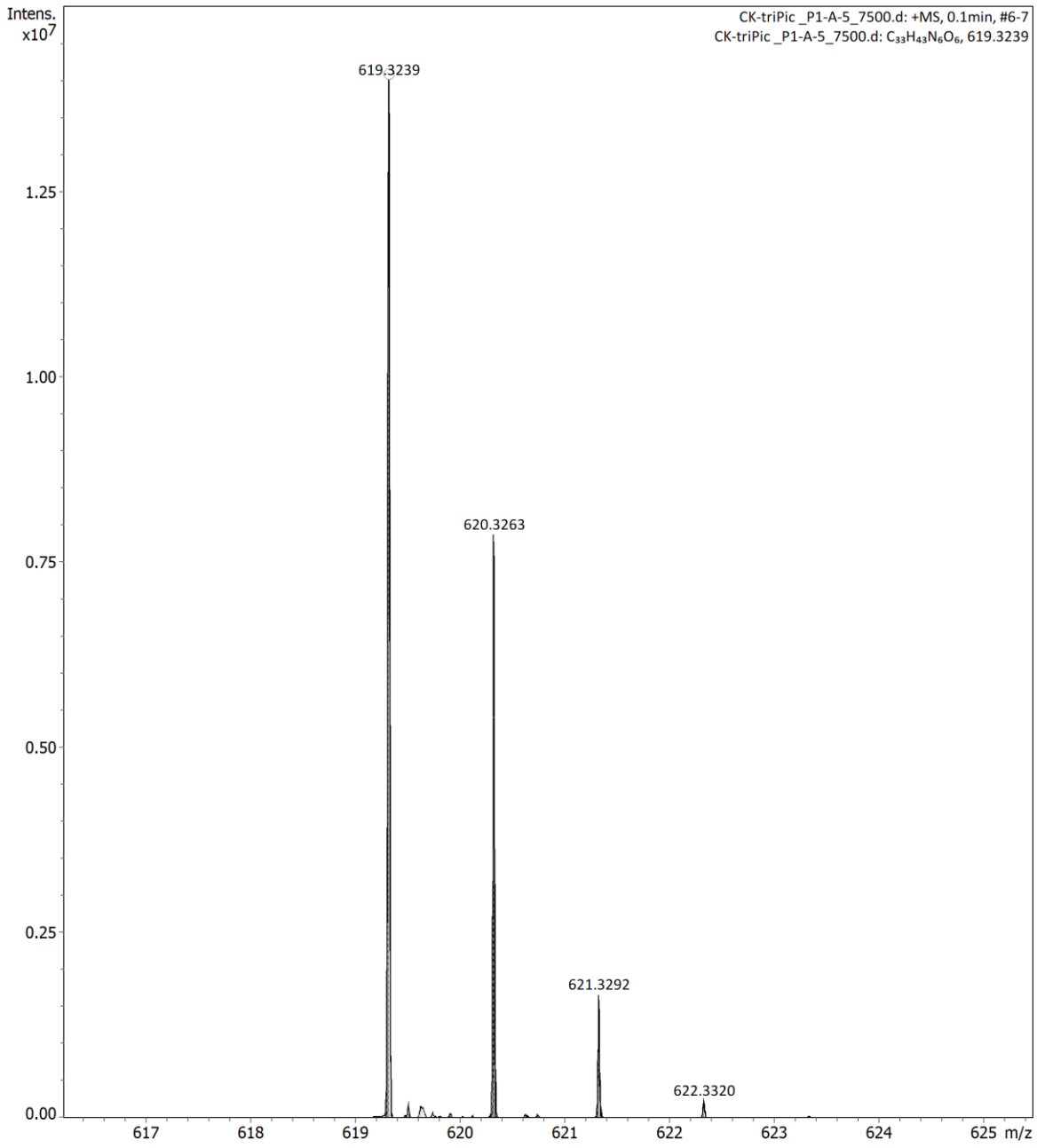


Figure S237 ESI-HRMS of triPic.

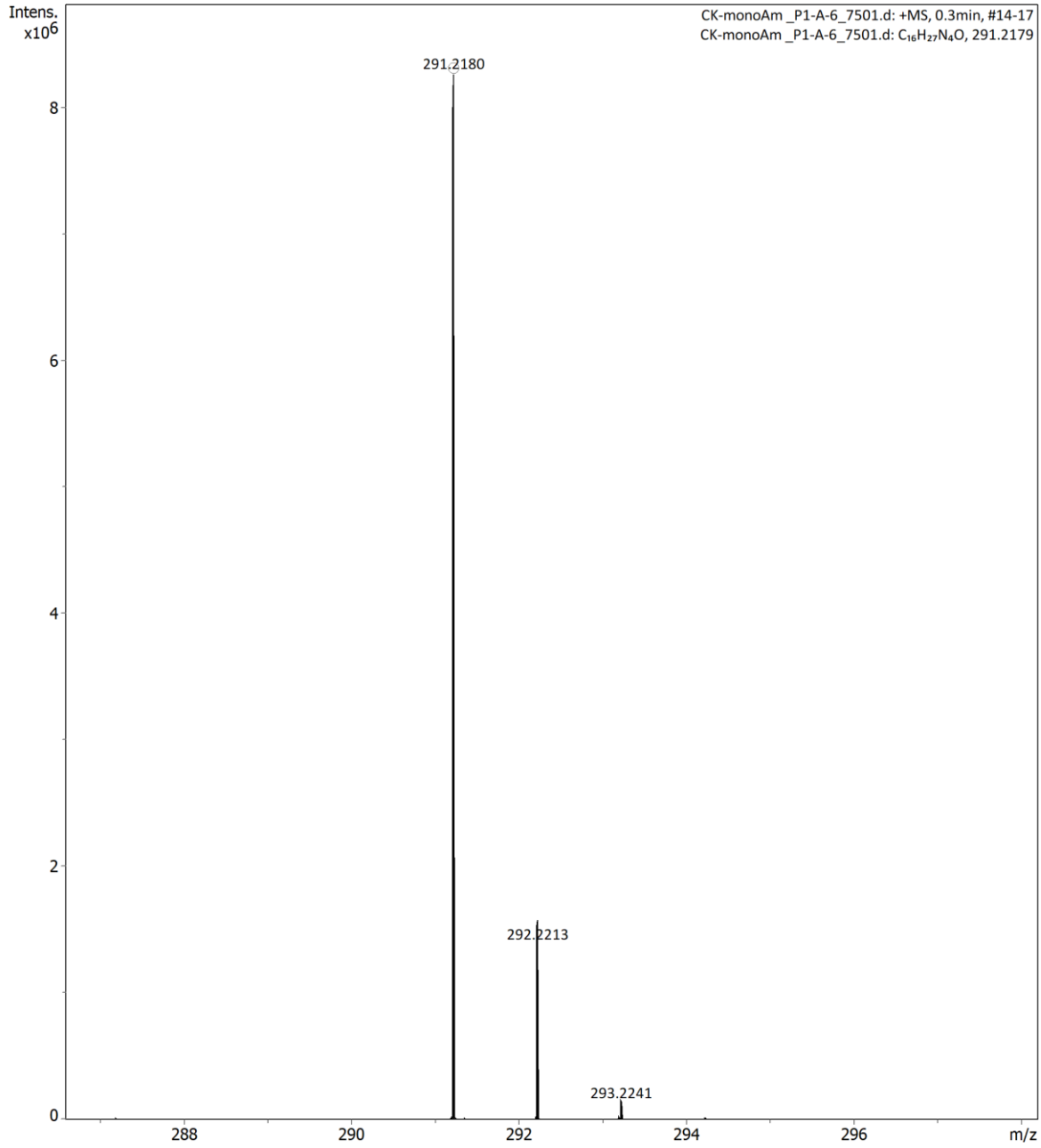


Figure S238 ESI-HRMS of **monoAm**.

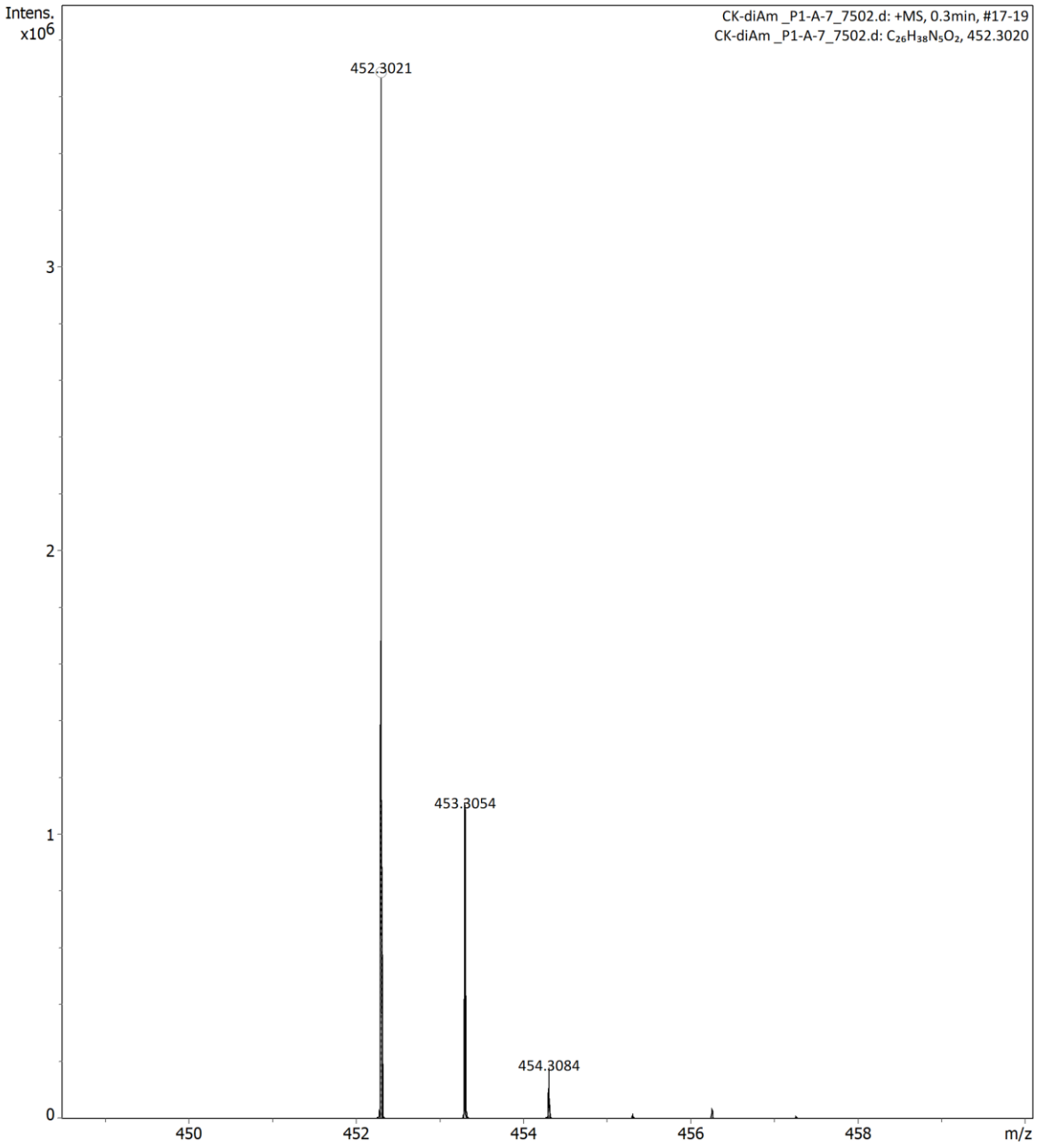


Figure S239 ESI-HRMS of **diAm**.

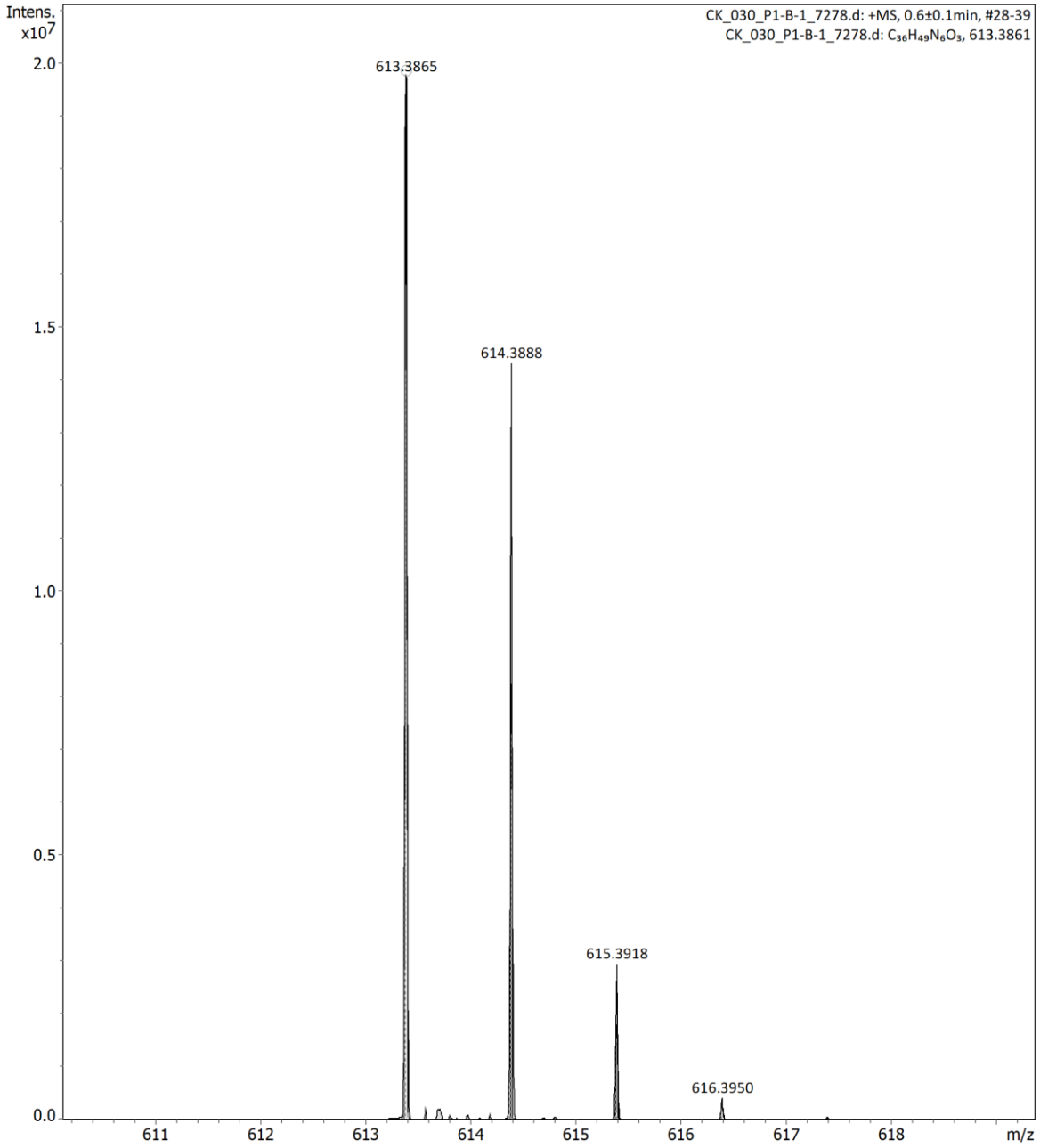


Figure S240 ESI-HRMS of $\mathbf{L}^{\mathbf{030}}$.

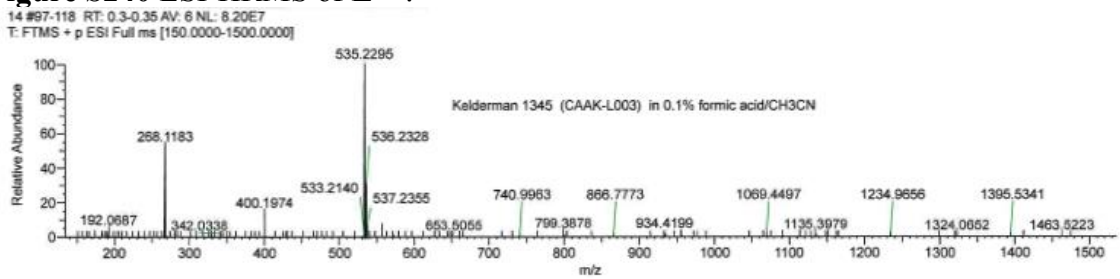


Figure S241 ESI-HRMS of $H_3\mathbf{L}^{\mathbf{003}}$.

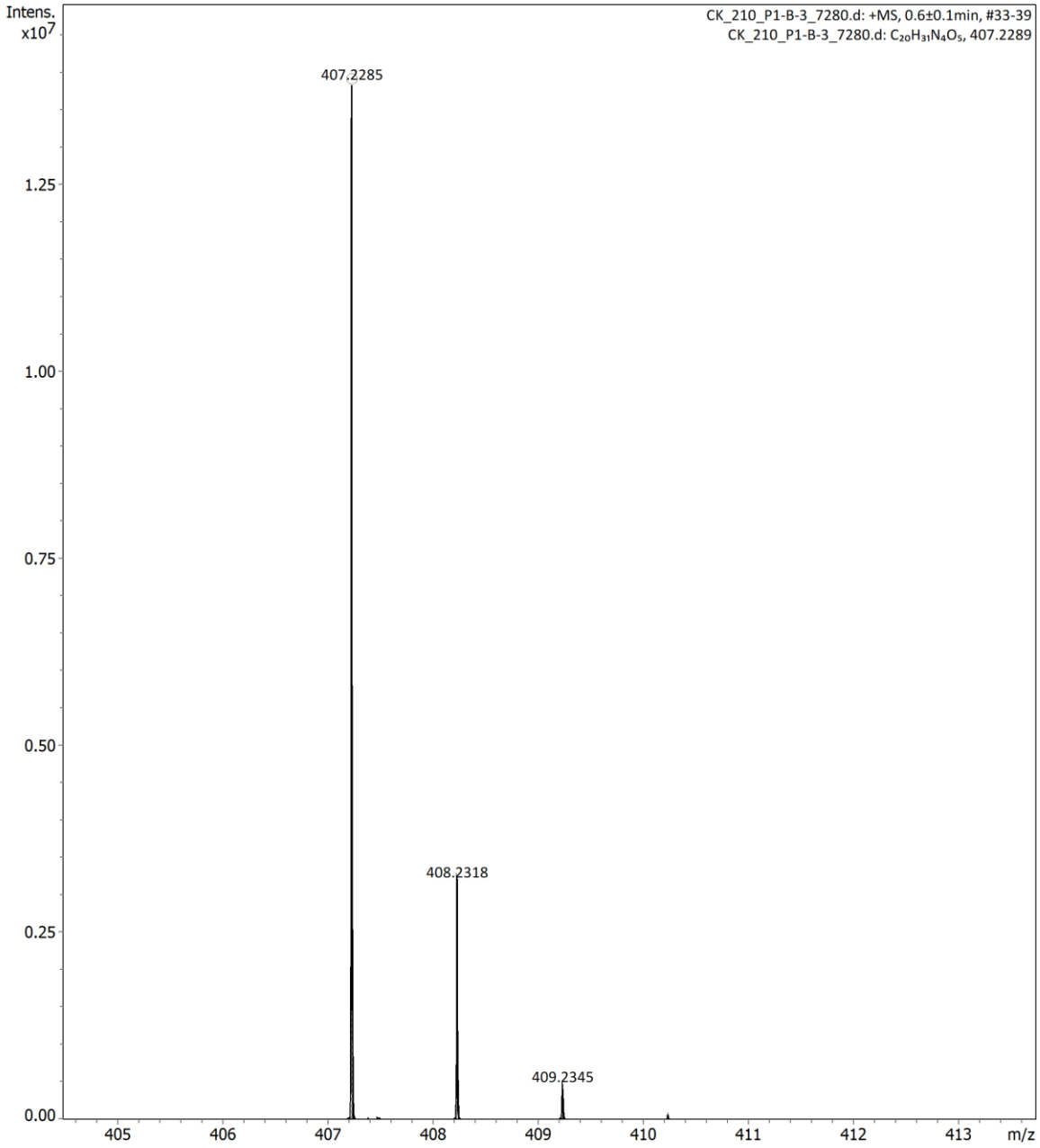


Figure S242 ESI-HRMS of H_2**L**^{210}.

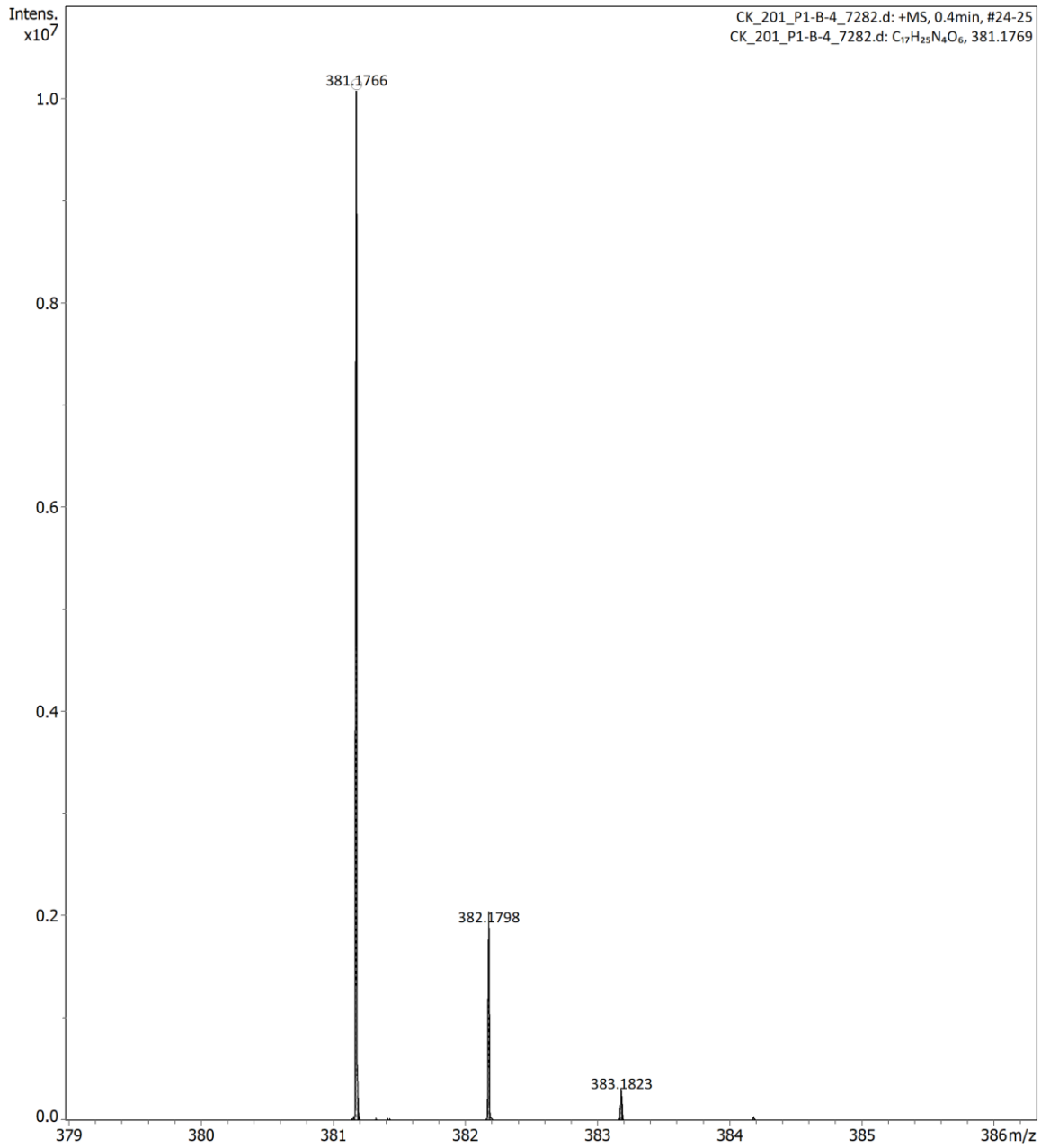


Figure S243 ESI-HRMS of $H_3\mathbf{L}^{\mathbf{201}}$ (H_3mptacn).

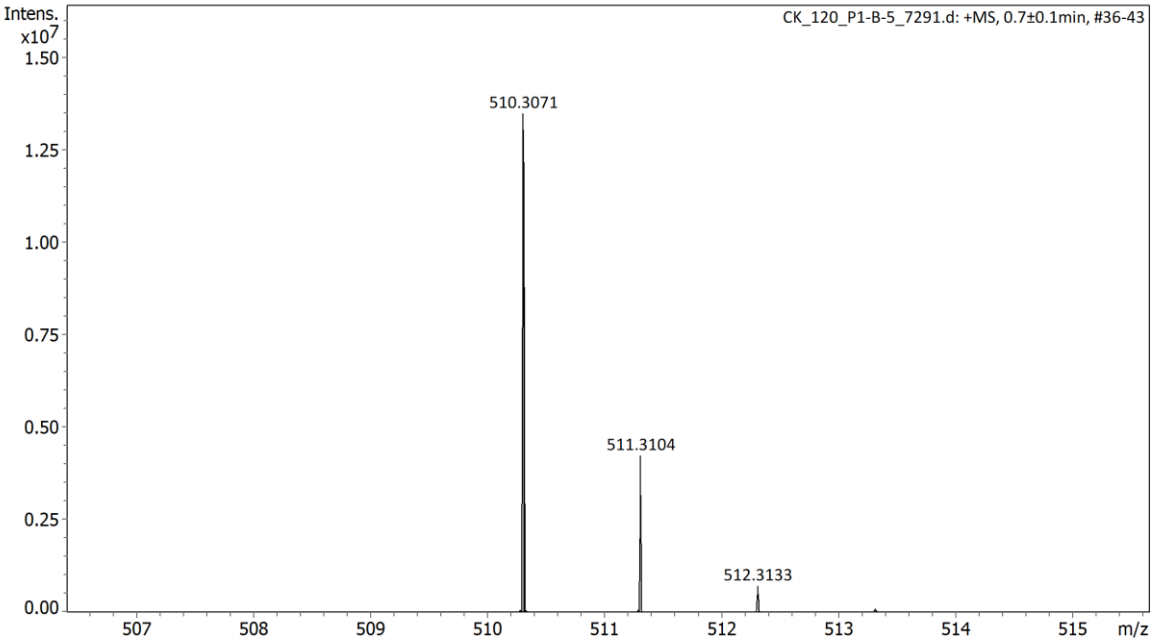


Figure S244 ESI-HRMS of H**L**[120].

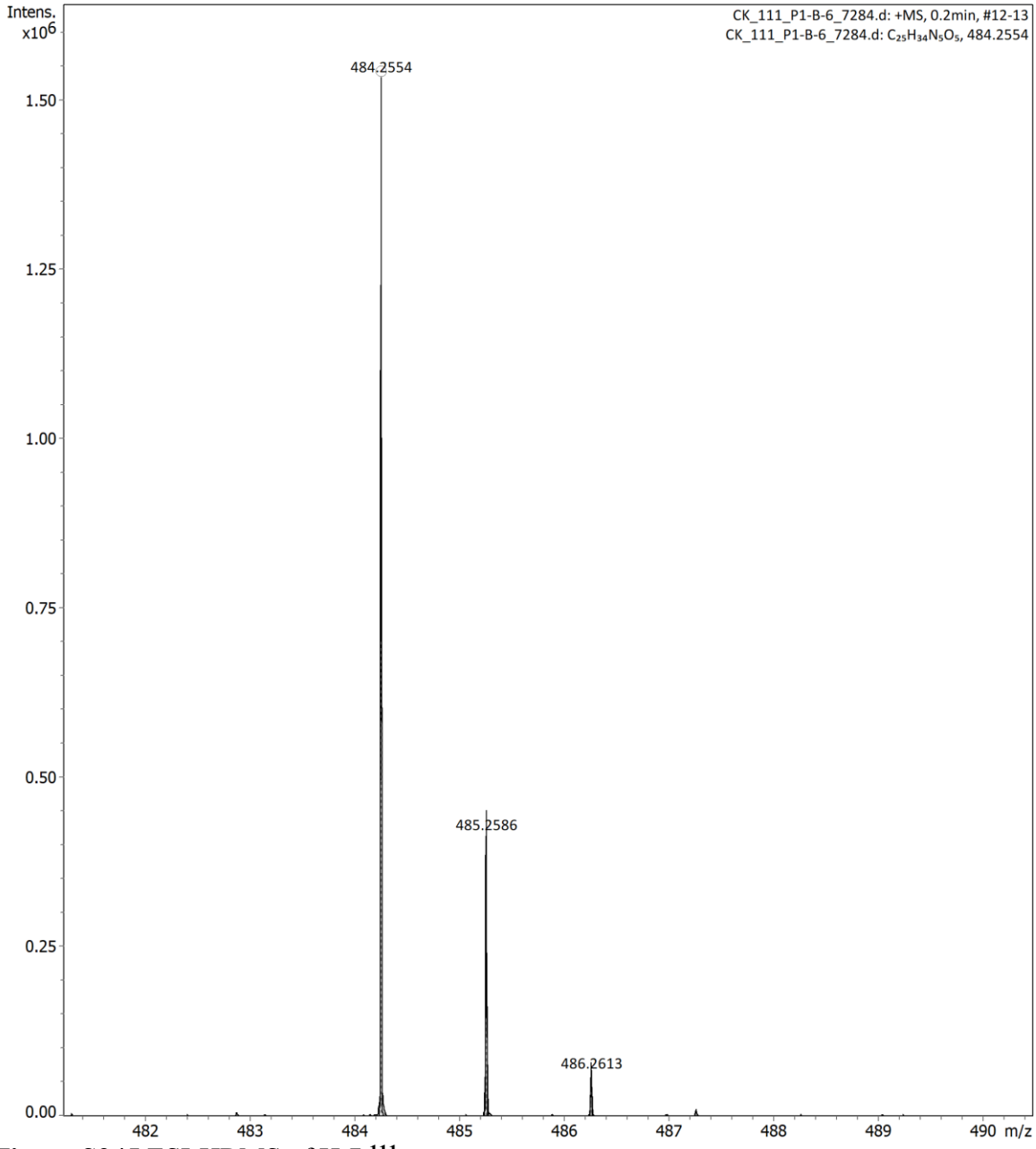


Figure S245 ESI-HRMS of H_2**L**^{111}.

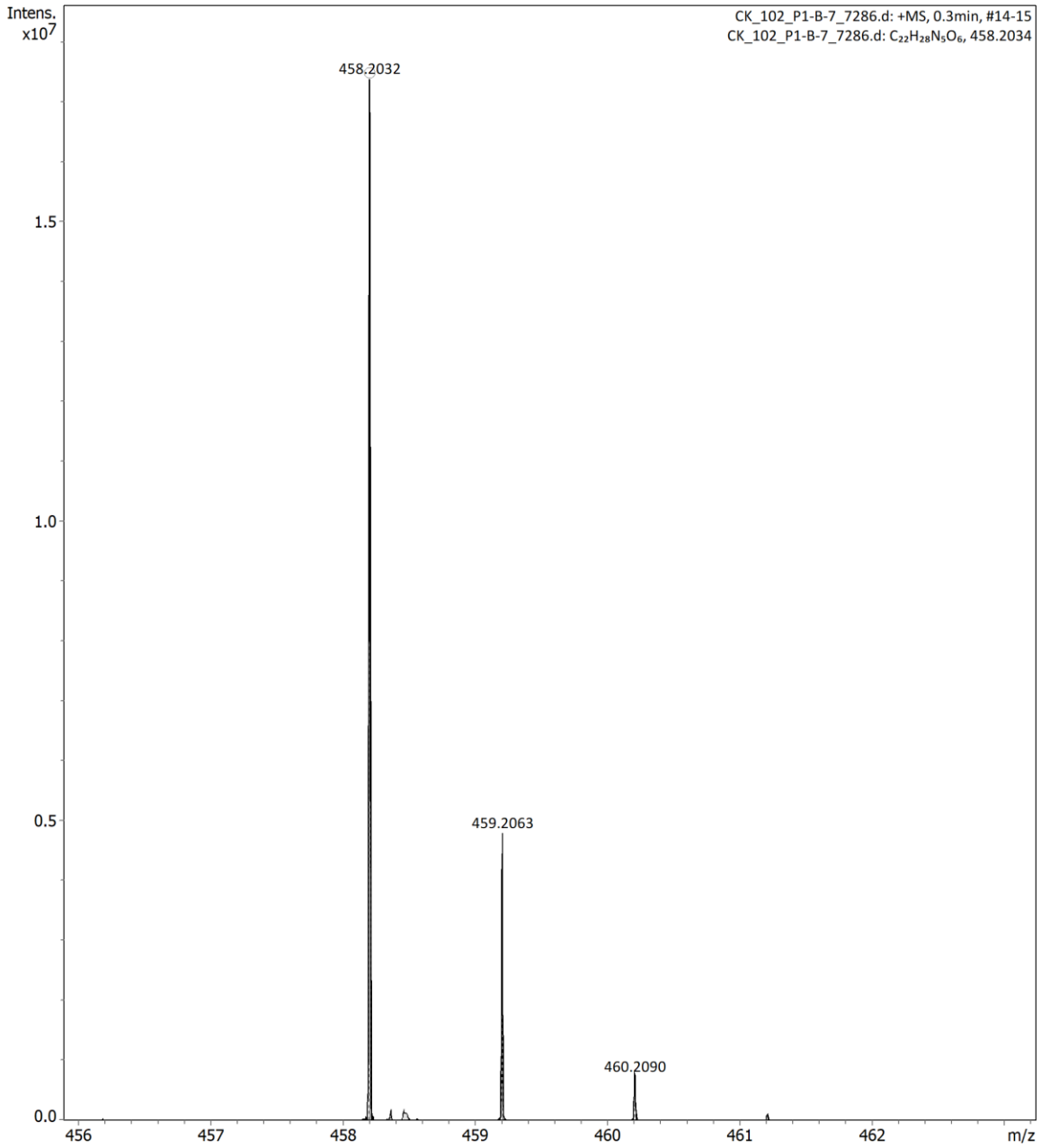


Figure S246 ESI-HRMS of $H_3\mathbf{L}^{\mathbf{102}}$.

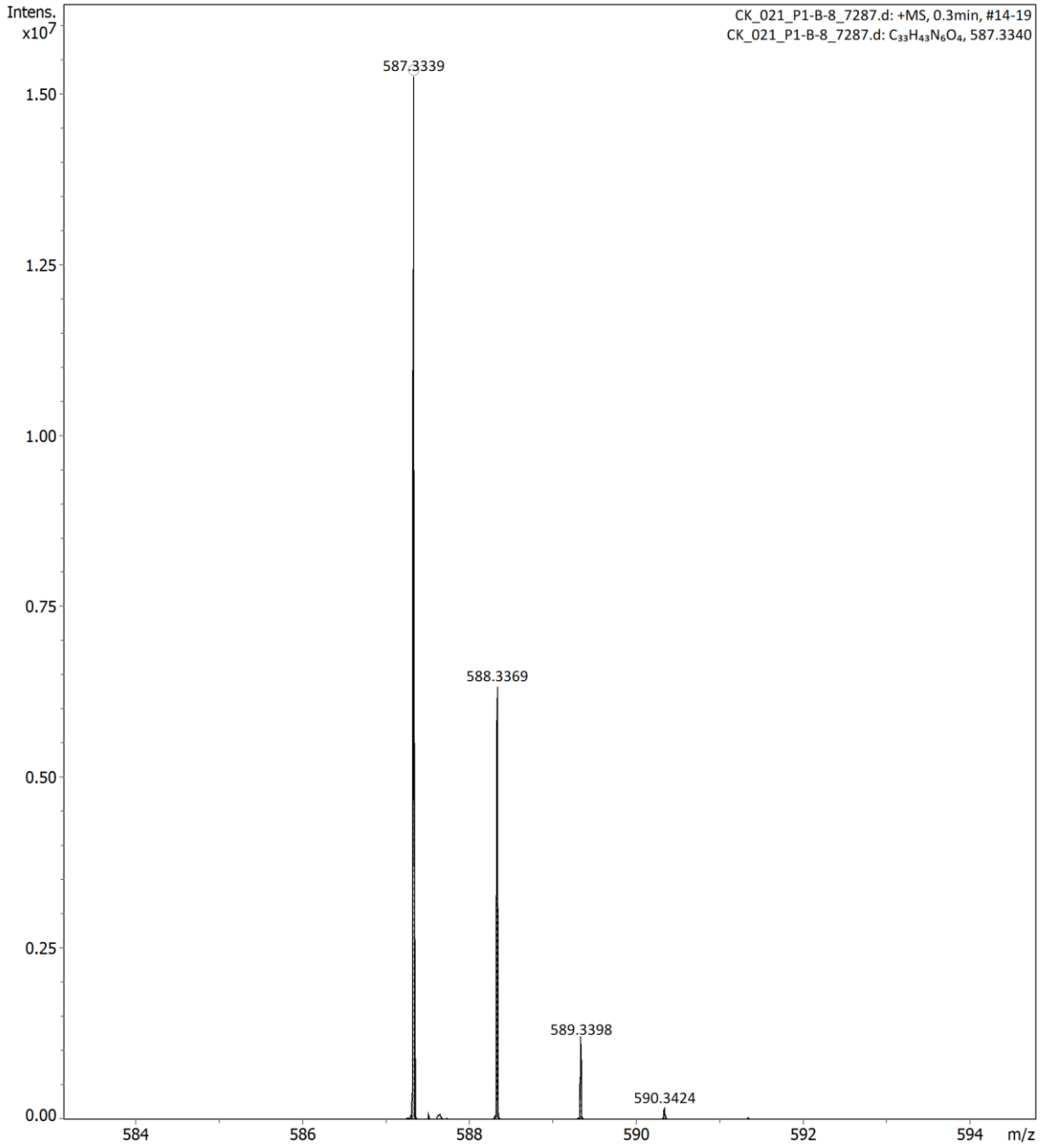


Figure S247 ESI-HRMS of H**L**^{021}.

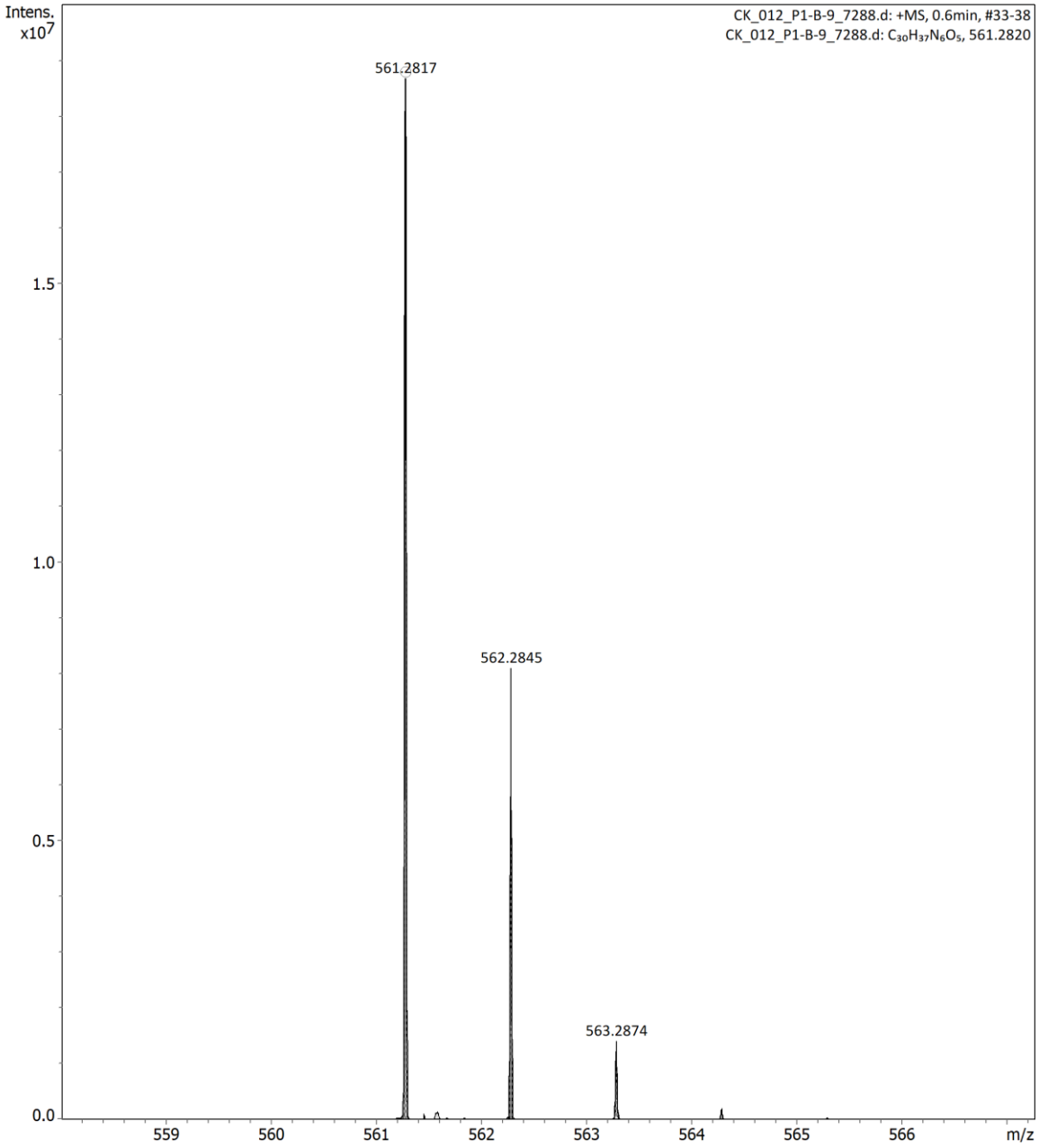


Figure S248 ESI-HRMS of $H_2\mathbf{L}^{012}$.

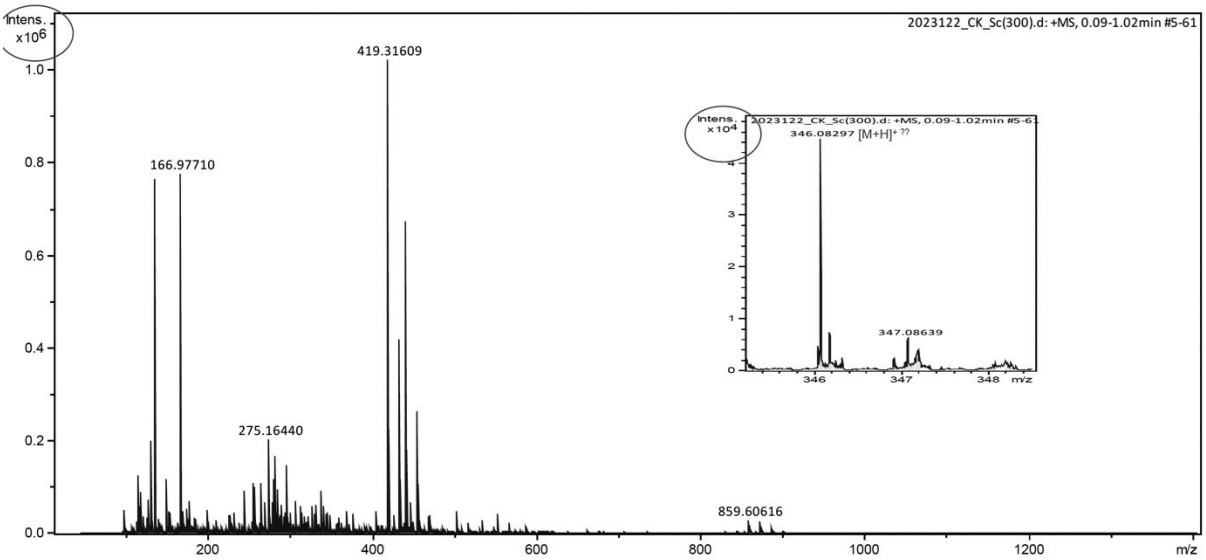


Figure S249 ESI-HRMS of [Sc(**L**^{300}) + H]$^{+}$.

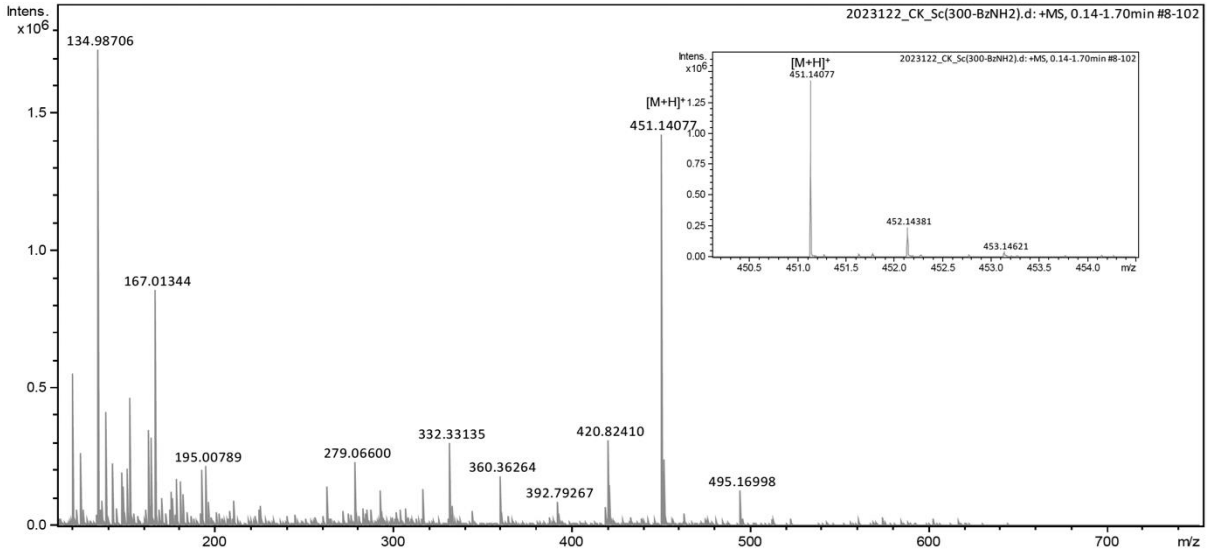


Figure S250 ESI-HRMS of [Sc(**L**$^{300\text{-}BzNH2}$) + H]$^{+}$.

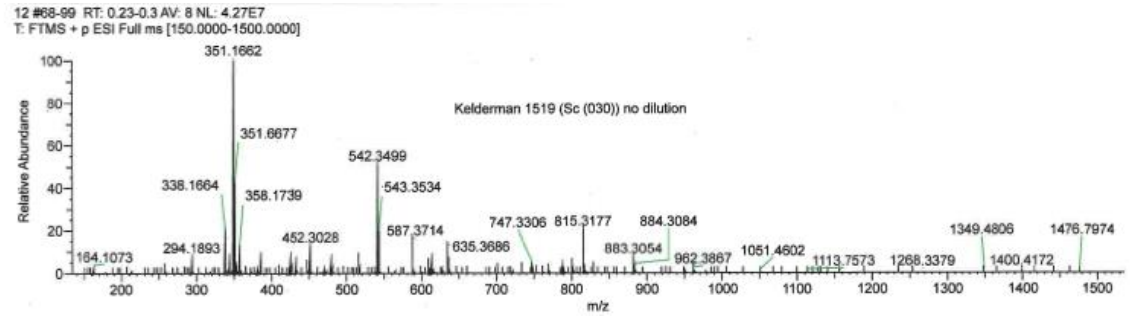


Figure S251 ESI-HRMS of $[Sc(\mathbf{L^{030}}) + HCOO]^{2+}$.

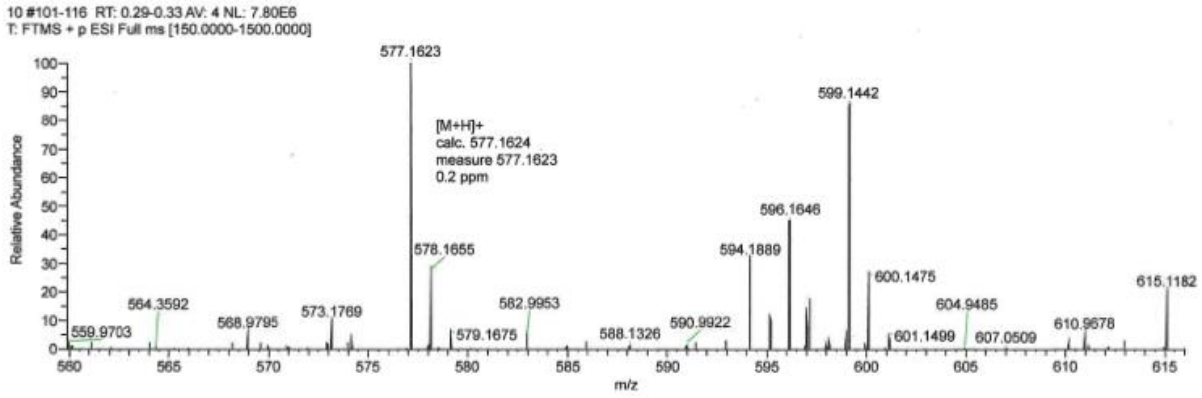


Figure S252 ESI-HRMS of $[Sc(\mathbf{L^{003}}) + H]^{+}$.

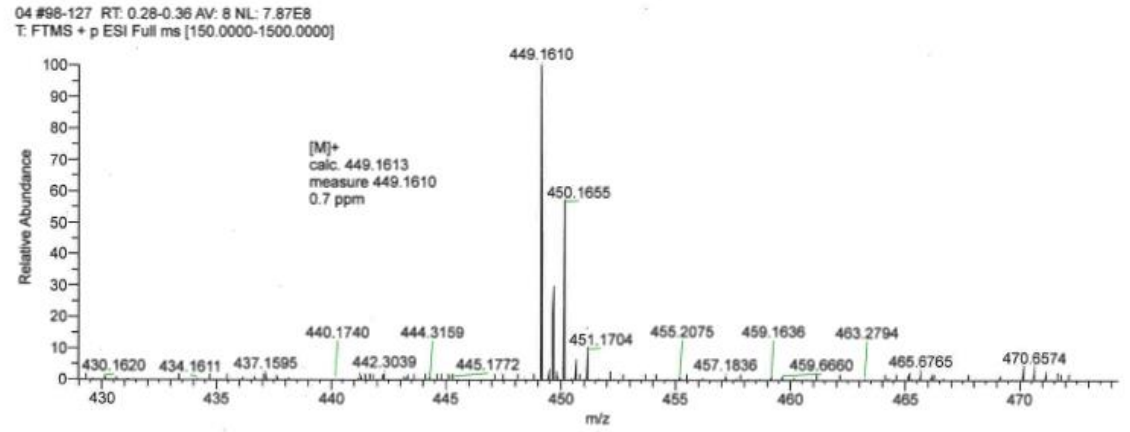


Figure S253 ESI-HRMS of $[Sc(\mathbf{L^{210}})]^{+}$.

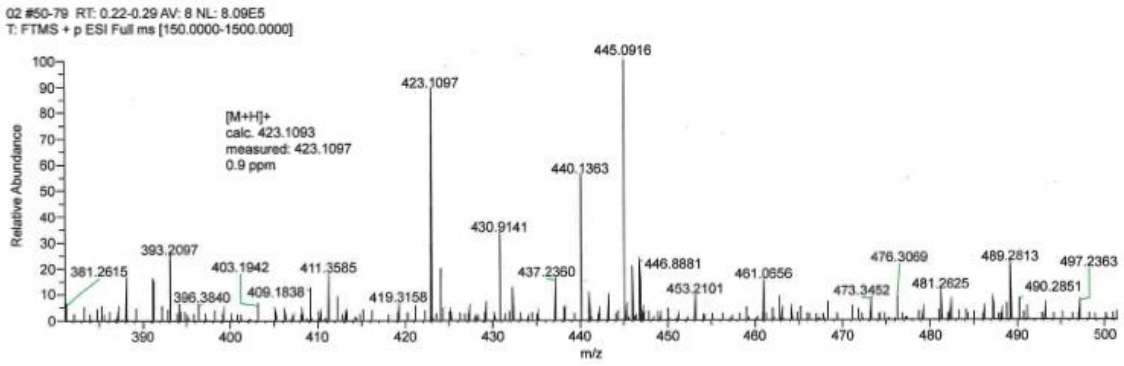


Figure S254 ESI-HRMS of [Sc(**L**^{201}) + H]$^{+}$.

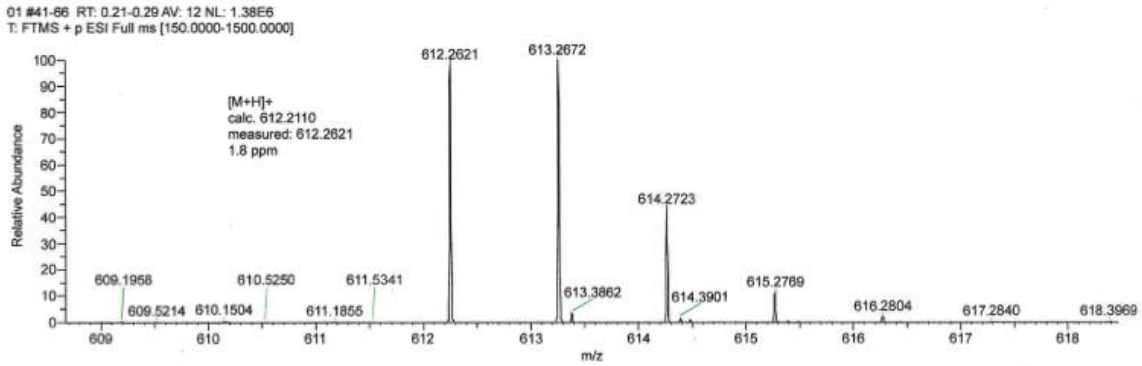


Figure S255 ESI-HRMS of [Sc(**L**^{120}) + OAc]$^{+}$.

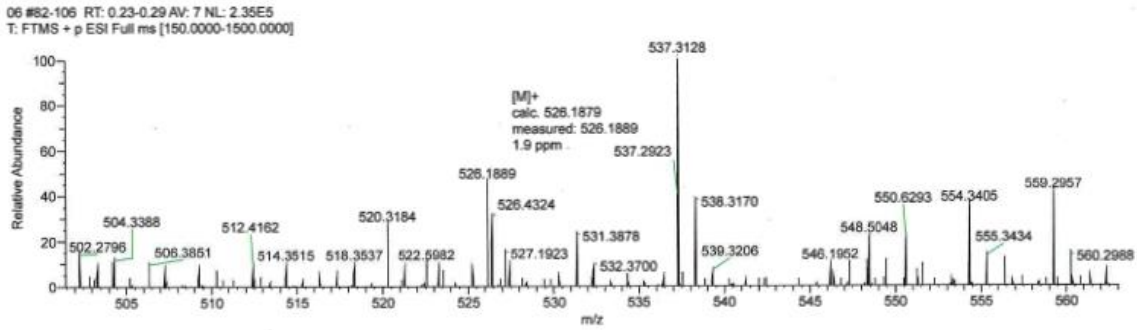


Figure S256 ESI-HRMS of [Sc(**L**^{111})]$^{+}$.

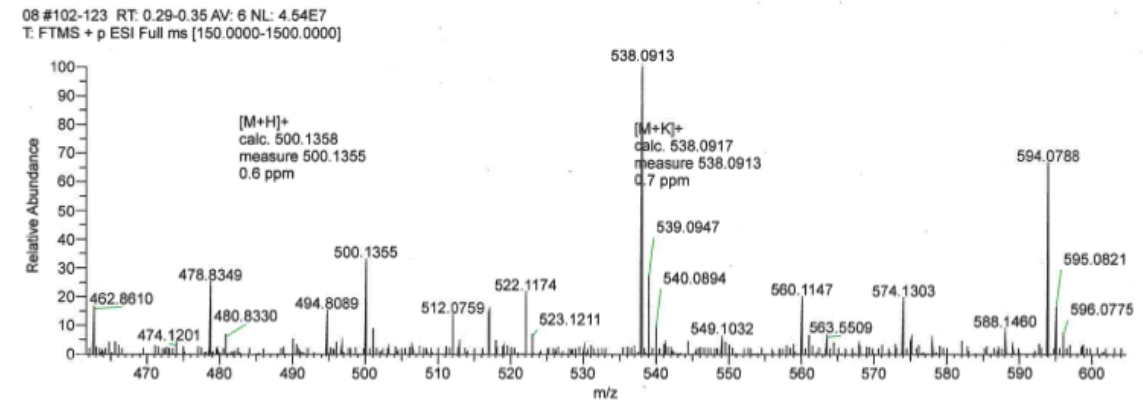


Figure S257 ESI-HRMS of [Sc(**L**^{102}) + H]$^{+}$.

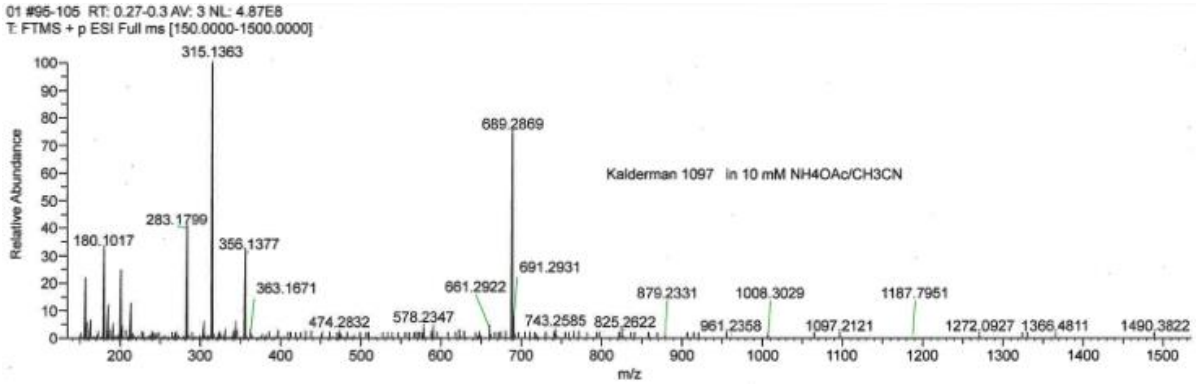


Figure S258 ESI-HRMS of [Sc(**L**^{021})]$^{2+}$.

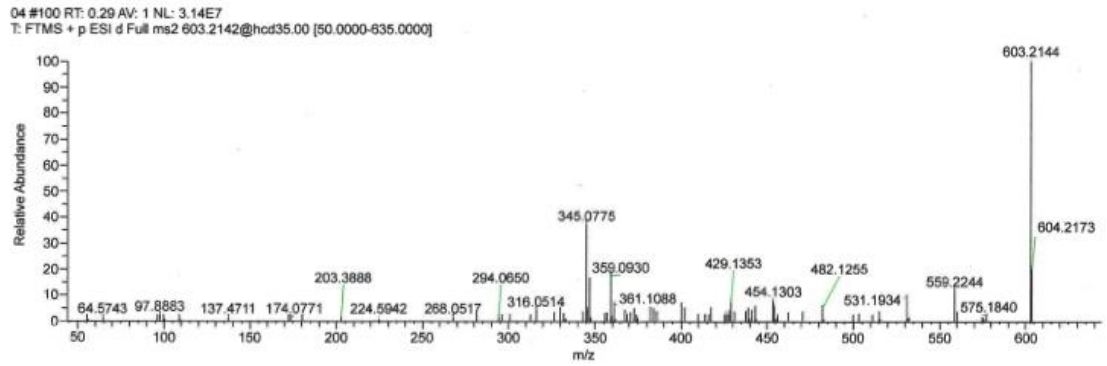


Figure S259 ESI-HRMS of [Sc(**L**^{012})]$^{+}$.

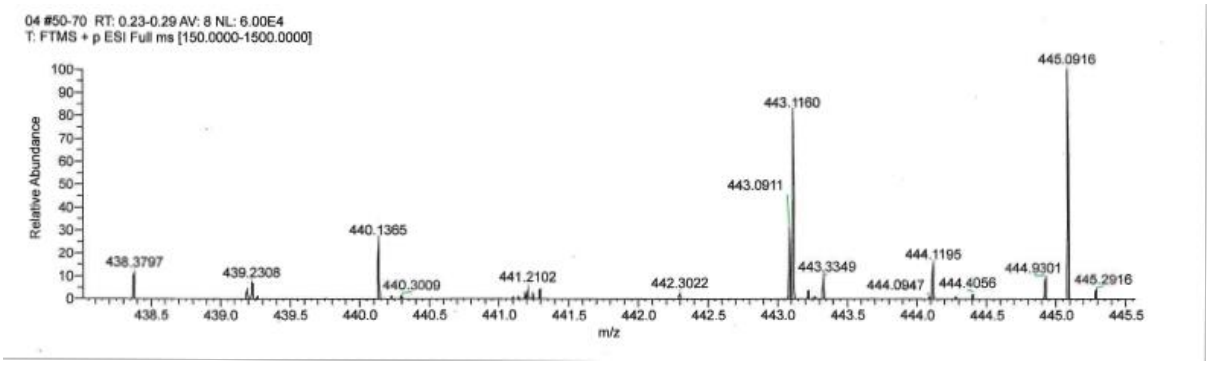


Figure S260 ESI-HRMS of [ScF($\mathbf{L^{201}}$)]$^-$.

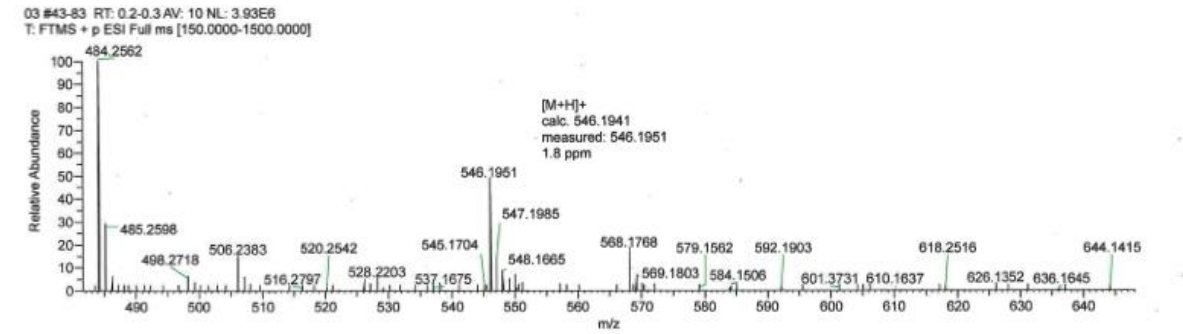


Figure S261 ESI-HRMS of [ScF($\mathbf{L^{111}}$) + H]$^+$.

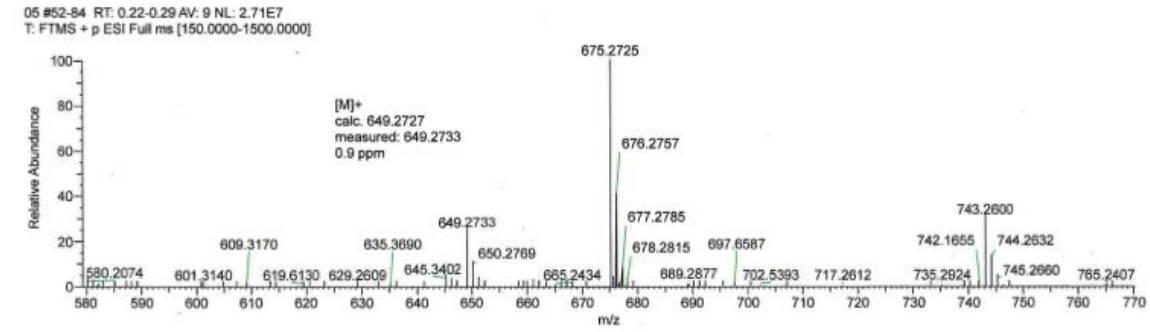


Figure S262 ESI-HRMS of [ScF($\mathbf{L^{021}}$)]$^+$.

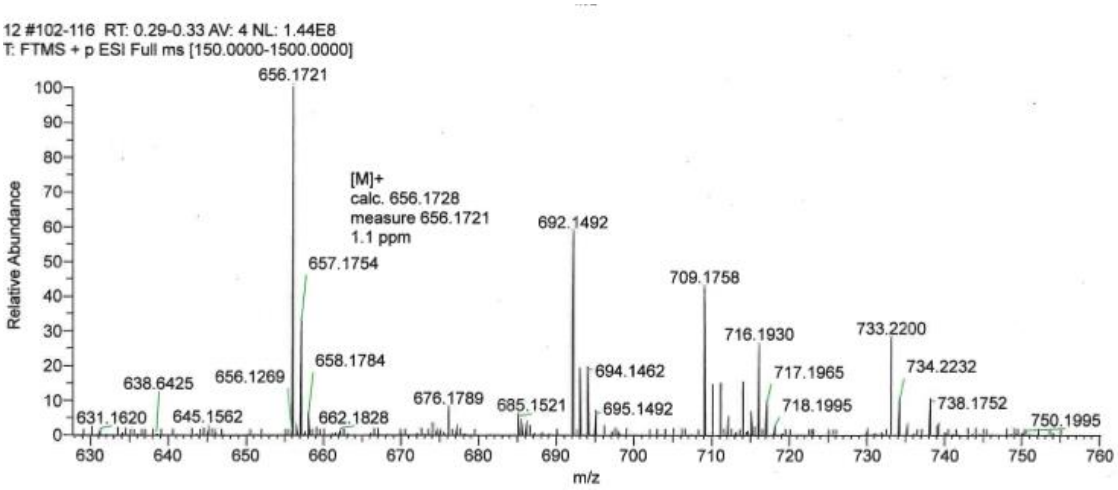


Figure S263 ESI-HRMS of [Lu(**L**^{111})]$^{+}$.

3 X-Ray Diffraction Analysis

3.1 Data collection

A colorless crystal with approximate dimensions 0.018 x 0.018 x 0.023 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera. The crystal evaluation and data collection were performed on a Bruker D8 VENTURE PhotonIII four-circle diffractometer with Cu Kα (λ = 1.54178 Å) radiation and the detector to crystal distance of 4.5 cm.[3] The initial cell constants were obtained from a 180° φ scan conducted at a 2θ = 50° angle with an exposure time of 1 second per frame. The reflections were successfully indexed by an automated indexing routine built into the APEX3 program. The final cell constants were calculated from a set of 9895 strong reflections from the actual data collection. The data were collected by using a full sphere data collection routine to survey reciprocal space to the extent of a full sphere to a resolution of 0.79 Å. A total of 34355 data were harvested by collecting 27 sets of frames with 0.8º scans in ω and φ with exposure times of 5-20 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements.[4]

3.2 Structure Solution and Refinement

The diffraction data were consistent with the space groups *Pn* and *P*2/*n*. The *E*-statistics strongly suggested the non-centrosymmetric space group *Pn* which yielded chemically reasonable and computationally stable results of refinement.[5-8] The atomic coordinates were taken from BILTEY, the metal atom changed from Yb to Sc, and the solvent water molecules were refined with a new disorder model. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. The absolute structure was unequivocally established by anomalous dispersion effects. There are 3 solvent water molecules per Sc complex in the lattice. Water molecule O3 is disordered over two positions with the major disorder component occupancy equal to 90.8(9)%. The water molecules O1, O2, and O3 were refined with H atoms and constrained water molecule geometries; it was not possible to reliably place H atoms on the oxygen atom in the minor disorder component. The final least-squares refinement of 401 parameters against 5395 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0441 and 0.1130, respectively. The final difference Fourier map was featureless.

3.3 Crystal Data Summary

Crystal Data for $C_{27}H_{32.82}N_6O_9Sc$ (M =630.37 g/mol): monoclinic, space group *Pn* (no. 7), a = 7.9195(6) Å, b = 11.7007(11) Å, c = 14.6519(15) Å, β = 98.998(8)°, V = 1341.0(2) $Å^3$, Z = 2, T = 100.00 K, μ(Cu Kα) = 2.942 mm^{-1}, *Dcalc* = 1.561 g/cm^3, 33522 reflections measured (7.556° ≤ 2Θ ≤ 154.962°), 5395 unique (R_{int} = 0.0653, R_{sigma} = 0.0412) which were used in all calculations. The final R_1 was 0.0441 (I > 2σ(I)) and wR_2 was 0.1130 (all data).

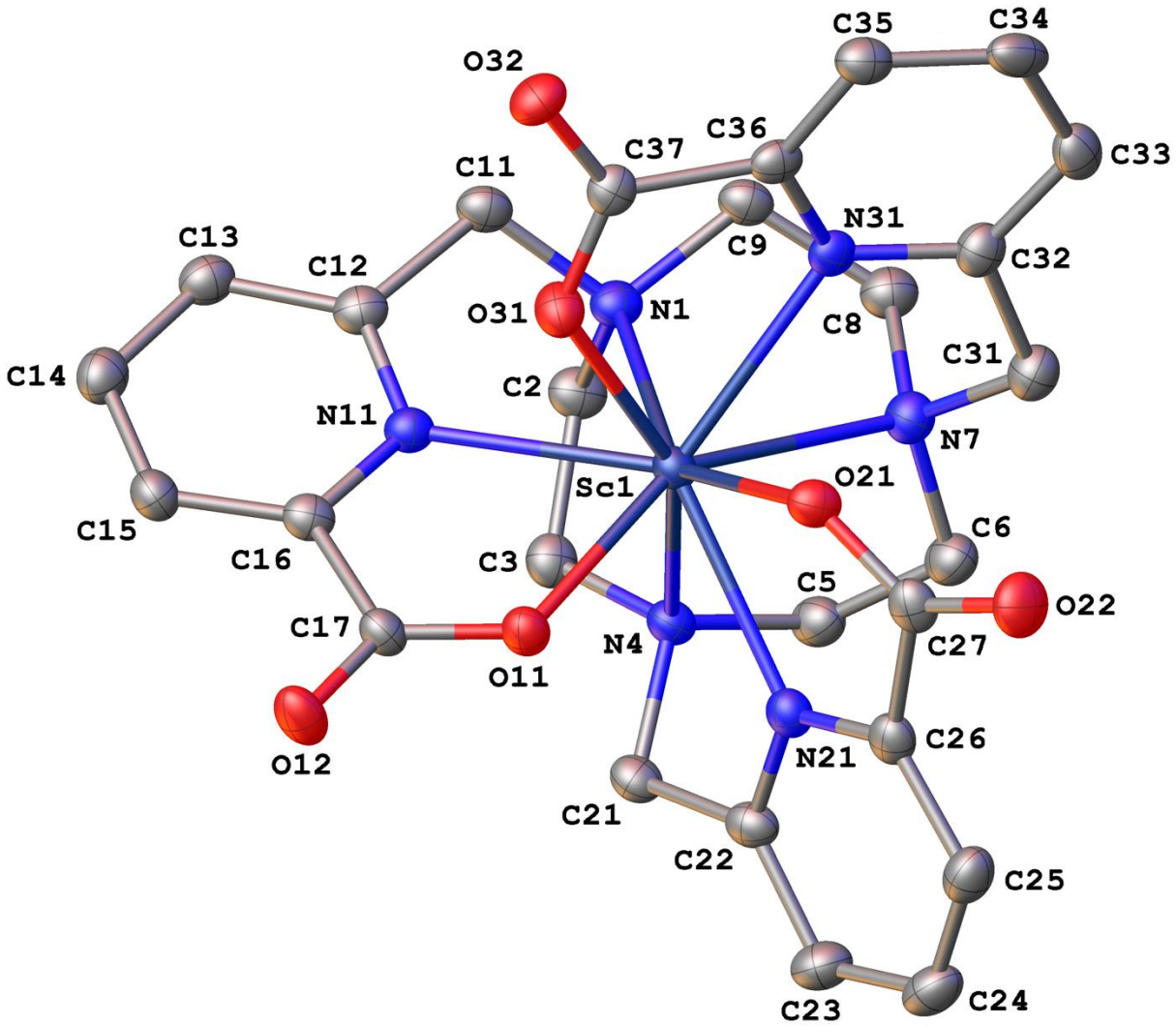


Figure S264 A molecular drawing of the entire complex [Sc(**L**^{003})] shown with 50% probability ellipsoids. All H atoms and solvent molecules are omitted.

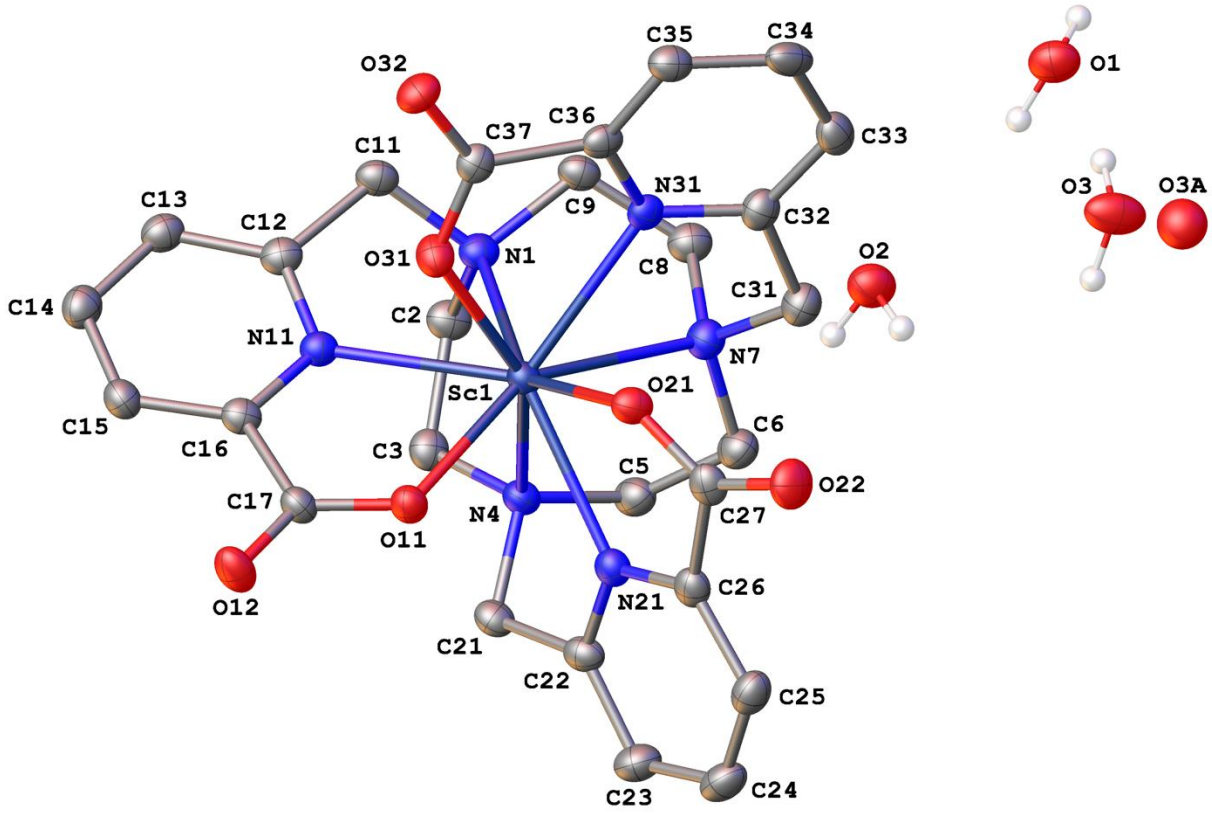


Figure S265 A molecular drawing of the entire complex in [Sc(**L**^{003})] shown with 50% probability ellipsoids. All H atoms on the Sc complex are omitted. All refined H atoms on the water molecules are shown.

Table S13 Crystal data and structure refinement for [Sc(L^{003})]

Identification code	2369298
Empirical formula	$C_{27}H_{27}N_6O_6Sc \bullet 3H_2O$
Formula weight	630.37
Temperature/K	100.00
Crystal system	monoclinic
Space group	*Pn*
a/Å	7.9195(6)
b/Å	11.7007(11)
c/Å	14.6519(15)
α/°	90
β/°	98.998(8)
γ/°	90
Volume/Å^3	1341.0(2)
Z	2
ρ_{calc}g/cm^3	1.561
μ/mm^{-1}	2.942
F(000)	660.0
Crystal size/mm^3	0.023 × 0.018 × 0.018
Radiation	Cu Kα (λ = 1.54178)
2Θ range for data collection/°	7.556 to 154.962
Index ranges	$-9 \le h \le 10$, $-14 \le k \le 14$, $-18 \le l \le 17$
Reflections collected	33522
Independent reflections	5395 [R_{int} = 0.0653, R_{sigma} = 0.0412]
Data/restraints/parameters	5395/2/401
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0441, wR_2 = 0.1105
Final R indexes [all data]	R_1 = 0.0473, wR_2 = 0.1130
Largest diff. peak/hole / e Å^{-3}	0.26/-0.46
Flack parameter	-0.009(9)

Table S14 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for [Sc(L^{003})]. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sc1	5474.8(7)	7229.6(5)	6013.0(5)	15.91(16)
O11	3892(4)	8777(2)	5779.3(19)	21.2(5)
O12	2806(4)	10414(3)	6228(2)	27.3(6)
O21	3140(4)	6413(2)	5225(2)	21.2(5)
O22	1844(4)	5619(3)	3906(2)	29.2(6)
O31	4023(4)	7000(2)	7150(2)	22.9(6)
O32	2845(4)	5991(3)	8175.3(19)	24.0(6)
N1	8313(4)	6977(3)	7095(2)	20.6(7)
N4	7939(4)	8204(3)	5385(2)	19.2(6)
N7	7464(4)	5771(3)	5394(2)	22.4(7)
N11	6139(4)	8632(3)	7244(2)	18.8(6)
N21	4968(4)	7738(3)	4405(2)	19.7(6)
N31	5089(4)	5223(3)	6385(2)	18.1(6)
C2	9734(5)	7752(3)	6878(3)	24.0(8)
C3	9119(5)	8686(3)	6179(3)	22.4(8)
C5	8941(6)	7428(4)	4849(3)	25.0(8)
C6	8104(6)	6282(4)	4591(3)	25.5(8)
C8	8975(5)	5391(4)	6105(3)	25.1(8)
C9	8828(5)	5762(3)	7080(3)	21.1(8)
C11	8018(5)	7248(3)	8043(3)	21.5(8)
C12	7183(5)	8402(4)	8028(3)	21.4(8)
C13	7404(5)	9161(4)	8774(3)	23.7(8)
C14	6451(6)	10166(4)	8703(3)	25.5(8)
C15	5274(5)	10363(3)	7905(3)	22.6(8)
C16	5154(5)	9569(3)	7198(3)	19.5(7)
C17	3851(5)	9606(3)	6329(3)	19.4(7)
C21	7164(5)	9122(3)	4767(3)	20.7(7)
C22	5842(5)	8576(3)	4058(3)	20.8(8)
C23	5537(6)	8847(4)	3120(3)	27.6(9)
C24	4325(6)	8229(4)	2534(3)	28.6(9)
C25	3395(6)	7378(4)	2901(3)	26.1(8)
C26	3754(5)	7174(3)	3845(3)	20.6(8)
C27	2822(5)	6320(3)	4353(3)	21.4(8)
C31	6433(6)	4751(4)	5086(3)	25.5(8)
C32	5438(6)	4372(4)	5834(3)	22.4(8)
C33	4800(6)	3273(4)	5895(3)	24.9(8)

Table S14 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for [Sc(L^{003})]. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C34	3725(6)	3059(4)	6540(3)	27.1(9)
C35	3335(5)	3947(4)	7100(3)	23.5(8)
C36	4041(5)	5011(3)	6996(3)	19.1(7)
C37	3600(5)	6070(3)	7490(3)	19.2(7)
O1	9899(4)	1566(3)	5388(2)	30.6(7)
O2	594(4)	3647(3)	4655(2)	32.3(7)
O3	6952(5)	1855(3)	4070(3)	35.6(11)
O3A	7730(60)	1480(40)	3690(30)	36

Table S15 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for [Sc(L^{003})]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sc1	14.5(3)	14.9(3)	18.0(3)	0.4(2)	1.8(2)	0.2(3)
O11	21.3(14)	19.8(13)	21.4(12)	-0.4(10)	-0.1(11)	2.6(10)
O12	24.5(14)	20.3(13)	34.2(15)	-2.1(11)	-4.9(12)	5.2(11)
O21	18.9(13)	21.5(13)	21.9(12)	2.2(10)	-0.5(10)	-2.5(11)
O22	25.1(15)	29.8(16)	30.7(14)	-6.7(12)	-1.4(12)	-7.3(12)
O31	22.3(14)	21.8(13)	25.9(14)	-2.3(11)	7.9(11)	-2.1(11)
O32	22.2(14)	30.9(14)	19.5(13)	1.2(11)	5.3(11)	-1.7(11)
N1	19.7(17)	20.9(16)	21.0(15)	2.0(12)	2.5(12)	-2.3(12)
N4	19.4(16)	17.1(15)	20.6(14)	1.6(12)	1.6(12)	-0.4(12)
N7	21.7(17)	23.7(16)	22.1(15)	-1.2(13)	4.0(13)	0.3(13)
N11	17.4(15)	19.5(15)	19.0(14)	1.7(12)	1.6(12)	-0.3(12)
N21	18.9(16)	18.2(15)	21.6(15)	-0.7(12)	1.6(13)	2.1(12)
N31	16.2(15)	20.6(15)	16.1(13)	-0.3(11)	-1.5(11)	-0.6(12)
C2	19.6(19)	25(2)	26.6(19)	2.5(15)	0.9(15)	-3.2(15)
C3	19.8(18)	22.6(19)	24.7(17)	-1.7(15)	3.5(15)	-3.4(14)
C5	27(2)	25.7(19)	23.2(18)	2.3(15)	5.5(16)	5.1(16)
C6	28(2)	27(2)	22.1(18)	0.4(15)	6.4(16)	3.1(17)
C8	23(2)	27(2)	24.8(18)	2.3(15)	2.9(16)	-0.6(15)
C9	18.3(19)	21.1(18)	23.1(18)	3.8(14)	0.2(14)	1.1(14)
C11	18.2(19)	22.4(19)	22.8(18)	3.9(14)	-0.2(15)	0.5(14)
C12	18.5(18)	24.2(19)	21.5(17)	2.3(14)	3.5(15)	-1.0(15)
C13	23(2)	27(2)	20.7(17)	1.7(15)	1.0(15)	-1.8(15)
C14	27(2)	25.4(19)	24.2(18)	-2.9(15)	3.1(16)	-3.7(16)

Table S15 Anisotropic Displacement Parameters ($Å^2×10^3$) for [Sc(L^{003})]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15	24.1(19)	18.2(17)	25.4(18)	-0.6(14)	3.8(15)	0.5(14)
C16	16.2(17)	19.9(17)	21.9(17)	2.1(14)	1.7(14)	-1.8(14)
C17	18.9(18)	15.5(17)	23.0(17)	0.4(14)	1.2(14)	0.7(14)
C21	19.7(18)	18.2(17)	24.7(18)	2.4(14)	4.8(15)	-1.3(14)
C22	19.4(19)	20.4(17)	23.1(18)	3.8(14)	5.0(15)	3.6(14)
C23	30(2)	31(2)	21.8(19)	5.5(16)	4.0(17)	1.3(17)
C24	29(2)	37(2)	18.5(17)	3.1(16)	1.8(16)	6.0(18)
C25	26(2)	30(2)	20.9(18)	-3.7(15)	0.1(16)	3.0(16)
C26	18.6(19)	19.9(18)	22.5(18)	-1.5(14)	0.4(15)	5.0(14)
C27	15.8(17)	21.0(19)	26.1(18)	-2.0(15)	-0.6(14)	3.5(14)
C31	26(2)	28(2)	23.0(18)	-2.4(15)	4.1(16)	0.5(16)
C32	20.0(17)	25.8(19)	20.7(18)	-2.5(14)	1.0(15)	-0.2(16)
C33	25.2(19)	22.0(19)	25.2(18)	-3.9(15)	-3.4(16)	-0.2(16)
C34	32(2)	22.5(19)	23.7(18)	6.4(15)	-6.9(16)	-5.5(16)
C35	22(2)	24.0(19)	23.0(17)	4.2(14)	0.2(15)	-3.0(15)
C36	16.3(17)	23.2(18)	16.3(16)	2.4(14)	-1.9(13)	-2.6(14)
C37	13.5(17)	23.0(17)	20.3(16)	-1.2(14)	0.7(14)	-0.8(14)
O1	26.5(16)	35.0(17)	28.7(14)	5.9(12)	-0.7(12)	4.2(13)
O2	31.0(17)	32.2(16)	31.5(16)	2.4(13)	-1.6(13)	-0.3(13)
O3	27(2)	36(2)	38(2)	12.5(16)	-9.6(16)	-6.7(16)

Table S16 Bond Lengths for [Sc(L^{003})].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sc1	O11	2.199(3)	N21	C22	1.346(5)
Sc1	O21	2.235(3)	N21	C26	1.336(5)
Sc1	O31	2.184(3)	N31	C32	1.338(5)
Sc1	N1	2.557(3)	N31	C36	1.336(5)
Sc1	N4	2.553(3)	C2	C3	1.524(6)
Sc1	N7	2.581(3)	C5	C6	1.517(6)
Sc1	N11	2.435(3)	C8	C9	1.515(6)
Sc1	N21	2.402(3)	C11	C12	1.502(6)
Sc1	N31	2.441(3)	C12	C13	1.398(6)
O11	C17	1.264(5)	C13	C14	1.392(6)
O12	C17	1.250(5)	C14	C15	1.395(6)
O21	C27	1.267(5)	C15	C16	1.384(5)
O22	C27	1.243(5)	C16	C17	1.508(5)

Table S16 Bond Lengths for [Sc(L^{003})].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O31	C37	1.262(5)	C21	C22	1.498(6)
O32	C37	1.250(5)	C22	C23	1.394(6)
N1	C2	1.517(5)	C23	C24	1.387(7)
N1	C9	1.480(5)	C24	C25	1.396(7)
N1	C11	1.478(5)	C25	C26	1.389(6)
N4	C3	1.485(5)	C26	C27	1.506(6)
N4	C5	1.506(5)	C31	C32	1.512(6)
N4	C21	1.475(5)	C32	C33	1.389(6)
N7	C6	1.478(5)	C33	C34	1.390(7)
N7	C8	1.525(5)	C34	C35	1.388(6)
N7	C31	1.476(5)	C35	C36	1.382(6)
N11	C12	1.333(5)	C36	C37	1.503(5)
N11	C16	1.341(5)			

Table S17 Bond Angles for [Sc(L^{003})].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O11	Sc1	O21	82.31(11)	C31	N7	C8	108.1(3)
O11	Sc1	N1	128.05(11)	C12	N11	Sc1	122.3(3)
O11	Sc1	N4	91.46(11)	C12	N11	C16	119.1(3)
O11	Sc1	N7	148.68(11)	C16	N11	Sc1	117.2(3)
O11	Sc1	N11	67.18(11)	C22	N21	Sc1	122.3(3)
O11	Sc1	N21	68.88(11)	C26	N21	Sc1	118.3(3)
O11	Sc1	N31	137.64(11)	C26	N21	C22	119.4(4)
O21	Sc1	N1	147.86(11)	C32	N31	Sc1	122.4(3)
O21	Sc1	N4	128.45(11)	C36	N31	Sc1	116.1(3)
O21	Sc1	N7	92.10(11)	C36	N31	C32	118.4(3)
O21	Sc1	N11	137.41(12)	N1	C2	C3	113.6(3)
O21	Sc1	N21	66.49(11)	N4	C3	C2	110.5(3)
O21	Sc1	N31	65.28(10)	N4	C5	C6	114.7(3)
O31	Sc1	O11	82.23(11)	N7	C6	C5	110.6(3)
O31	Sc1	O21	81.36(11)	C9	C8	N7	113.1(3)
O31	Sc1	N1	91.68(11)	N1	C9	C8	110.6(3)
O31	Sc1	N4	148.59(11)	N1	C11	C12	108.3(3)
O31	Sc1	N7	127.56(11)	N11	C12	C11	114.0(3)
O31	Sc1	N11	66.19(11)	N11	C12	C13	122.0(4)
O31	Sc1	N21	138.73(12)	C13	C12	C11	124.0(4)
O31	Sc1	N31	67.16(11)	C14	C13	C12	118.6(4)

Table S17 Bond Angles for [Sc(L^{003})].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Sc1	N7	67.42(11)	C13	C14	C15	119.0(4)
N4	Sc1	N1	68.15(11)	C16	C15	C14	118.4(4)
N4	Sc1	N7	68.03(11)	N11	C16	C15	122.6(4)
N11	Sc1	N1	63.34(11)	N11	C16	C17	112.5(3)
N11	Sc1	N4	82.96(11)	C15	C16	C17	124.8(4)
N11	Sc1	N7	129.28(12)	O11	C17	C16	115.7(3)
N11	Sc1	N31	120.20(11)	O12	C17	O11	125.9(4)
N21	Sc1	N1	129.25(12)	O12	C17	C16	118.3(3)
N21	Sc1	N4	63.63(11)	N4	C21	C22	107.1(3)
N21	Sc1	N7	80.59(11)	N21	C22	C21	113.2(3)
N21	Sc1	N11	122.94(11)	N21	C22	C23	121.2(4)
N21	Sc1	N31	116.71(11)	C23	C22	C21	125.5(4)
N31	Sc1	N1	83.05(11)	C24	C23	C22	119.2(4)
N31	Sc1	N4	129.77(11)	C23	C24	C25	119.3(4)
N31	Sc1	N7	63.06(11)	C26	C25	C24	117.9(4)
C17	O11	Sc1	127.1(2)	N21	C26	C25	122.9(4)
C27	O21	Sc1	125.1(3)	N21	C26	C27	112.6(4)
C37	O31	Sc1	127.6(3)	C25	C26	C27	124.5(4)
C2	N1	Sc1	114.2(2)	O21	C27	C26	113.9(3)
C9	N1	Sc1	108.6(2)	O22	C27	O21	126.7(4)
C9	N1	C2	110.9(3)	O22	C27	C26	119.4(4)
C11	N1	Sc1	107.7(2)	N7	C31	C32	110.0(3)
C11	N1	C2	107.5(3)	N31	C32	C31	113.5(3)
C11	N1	C9	107.7(3)	N31	C32	C33	122.5(4)
C3	N4	Sc1	108.1(2)	C33	C32	C31	123.7(4)
C3	N4	C5	108.6(3)	C32	C33	C34	118.6(4)
C5	N4	Sc1	114.4(2)	C35	C34	C33	118.9(4)
C21	N4	Sc1	106.2(2)	C36	C35	C34	118.5(4)
C21	N4	C3	110.8(3)	N31	C36	C35	123.0(4)
C21	N4	C5	108.7(3)	N31	C36	C37	112.6(3)
C6	N7	Sc1	108.4(2)	C35	C36	C37	124.1(4)
C6	N7	C8	109.3(3)	O31	C37	C36	115.1(3)
C8	N7	Sc1	114.2(2)	O32	C37	O31	124.8(4)
C31	N7	Sc1	107.7(2)	O32	C37	C36	120.1(4)
C31	N7	C6	109.1(3)				

Table S18 Hydrogen Bonds for [Sc(L^{003})].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1	H1A	O2[1]	0.87	1.90	2.751(5)	167.2
O1	H1B	O12[2]	0.87	1.93	2.784(4)	166.7
O2	H2C	O22	0.87	1.97	2.801(5)	158.9
O2	H2D	O32[3]	0.87	2.01	2.854(4)	163.8
O3	H3C	O1	0.87	1.94	2.807(5)	170.7
O3	H3D	O32[4]	0.87	2.11	2.977(5)	177.1

[1]1+X,+Y,+Z; [2]1+X,-1+Y,+Z; [3]-1/2+X,1-Y,-1/2+Z; [4]1/2+X,1-Y,-1/2+Z

Table S19 Torsion Angles for [Sc(L^{003})].

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Sc1	O11	C17	O12	-171.2(3)	C3	N4	C21	C22	-173.1(3)
Sc1	O11	C17	C16	6.3(5)	C5	N4	C3	C2	-68.0(4)
Sc1	O21	C27	O22	157.9(3)	C5	N4	C21	C22	67.6(4)
Sc1	O21	C27	C26	-22.4(4)	C6	N7	C8	C9	132.9(3)
Sc1	O31	C37	O32	176.0(3)	C6	N7	C31	C32	-167.1(3)
Sc1	O31	C37	C36	-5.2(5)	C8	N7	C6	C5	-70.6(4)
Sc1	N1	C2	C3	11.0(4)	C8	N7	C31	C32	74.2(4)
Sc1	N1	C9	C8	57.7(3)	C9	N1	C2	C3	134.1(3)
Sc1	N1	C11	C12	-52.5(3)	C9	N1	C11	C12	-169.5(3)
Sc1	N4	C3	C2	56.7(4)	C11	N1	C2	C3	-108.4(4)
Sc1	N4	C5	C6	12.8(4)	C11	N1	C9	C8	174.1(3)
Sc1	N4	C21	C22	-56.0(3)	C11	C12	C13	C14	-174.8(4)
Sc1	N7	C6	C5	54.5(4)	C12	N11	C16	C15	5.4(6)
Sc1	N7	C8	C9	11.2(4)	C12	N11	C16	C17	-170.6(3)
Sc1	N7	C31	C32	-49.6(4)	C12	C13	C14	C15	2.0(6)
Sc1	N11	C12	C11	5.1(5)	C13	C14	C15	C16	-2.7(6)
Sc1	N11	C12	C13	-172.4(3)	C14	C15	C16	N11	-1.0(6)
Sc1	N11	C16	C15	172.4(3)	C14	C15	C16	C17	174.6(4)
Sc1	N11	C16	C17	-3.7(4)	C15	C16	C17	O11	-177.0(4)
Sc1	N21	C22	C21	1.4(4)	C15	C16	C17	O12	0.8(6)
Sc1	N21	C22	C23	179.3(3)	C16	N11	C12	C11	171.3(3)
Sc1	N21	C26	C25	-178.1(3)	C16	N11	C12	C13	-6.2(6)
Sc1	N21	C26	C27	2.9(4)	C21	N4	C3	C2	172.6(3)
Sc1	N31	C32	C31	12.5(5)	C21	N4	C5	C6	-105.8(4)
Sc1	N31	C32	C33	-161.7(3)	C21	C22	C23	C24	176.8(4)
Sc1	N31	C36	C35	162.4(3)	C22	N21	C26	C25	3.0(6)

Table S19 Torsion Angles for [Sc(L^{003})].

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Sc1	N31	C36	C37	-12.5(4)	C22	N21	C26	C27	-176.1(3)
N1	C2	C3	N4	-45.7(5)	C22	C23	C24	C25	2.2(7)
N1	C11	C12	N11	33.3(5)	C23	C24	C25	C26	-1.1(7)
N1	C11	C12	C13	-149.2(4)	C24	C25	C26	N21	-1.5(6)
N4	C5	C6	N7	-45.9(5)	C24	C25	C26	C27	177.5(4)
N4	C21	C22	N21	38.3(4)	C25	C26	C27	O21	-168.0(4)
N4	C21	C22	C23	-139.4(4)	C25	C26	C27	O22	11.7(6)
N7	C8	C9	N1	-46.1(4)	C26	N21	C22	C21	-179.6(3)
N7	C31	C32	N31	27.2(5)	C26	N21	C22	C23	-1.8(6)
N7	C31	C32	C33	-158.6(4)	C31	N7	C6	C5	171.5(3)
N11	C12	C13	C14	2.4(6)	C31	N7	C8	C9	-108.5(4)
N11	C16	C17	O11	-1.0(5)	C31	C32	C33	C34	-172.1(4)
N11	C16	C17	O12	176.7(4)	C32	N31	C36	C35	1.6(6)
N21	C22	C23	C24	-0.8(6)	C32	N31	C36	C37	-173.3(3)
N21	C26	C27	O21	11.0(5)	C32	C33	C34	C35	-0.2(6)
N21	C26	C27	O22	-169.3(4)	C33	C34	C35	C36	-0.4(6)
N31	C32	C33	C34	1.5(6)	C34	C35	C36	N31	-0.3(6)
N31	C36	C37	O31	11.7(5)	C34	C35	C36	C37	174.0(4)
N31	C36	C37	O32	-169.3(3)	C35	C36	C37	O31	-163.1(4)
C2	N1	C9	C8	-68.5(4)	C35	C36	C37	O32	15.9(6)
C2	N1	C11	C12	71.0(4)	C36	N31	C32	C31	172.0(3)
C3	N4	C5	C6	133.6(4)	C36	N31	C32	C33	-2.2(6)

Table S20 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for [Sc(L^{003})].

Atom	*x*	*y*	*z*	U(eq)
H2A	10602.31	7282.21	6634.54	29
H2B	10293.19	8114.59	7457.9	29
H3A	8523.16	9288.43	6480.61	27
H3B	10113.89	9038.89	5954.88	27
H5A	10078.78	7292.09	5219.89	30
H5B	9122.05	7824.63	4274.78	30
H6A	7142.87	6386.1	4078.66	31
H6B	8945.24	5760.73	4377.17	31
H8A	9063.25	4547.33	6088.27	30
H8B	10039.48	5711	5933.2	30
H9A	7971.06	5281.11	7322.85	25

Table S20 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for [Sc(L^{003})].

Atom	*x*	*y*	*z*	U(eq)
H9B	9942.16	5655.18	7483.34	25
H11A	9117.91	7255.66	8469.68	26
H11B	7269.63	6662.16	8258.93	26
H13	8187.16	8994.89	9317.61	28
H14	6600.62	10710.22	9189.98	31
H15	4572.54	11025.31	7849.1	27
H21A	8046.88	9502.53	4464.49	25
H21B	6629.22	9702	5122.76	25
H23	6153.07	9447.23	2885.24	33
H24	4129.72	8384.54	1889.75	34
H25	2542.4	6951.3	2516.39	31
H31A	7193.26	4124.91	4945.92	31
H31B	5632.02	4930.75	4515.73	31
H33	5091.52	2680.98	5504.64	30
H34	3265.78	2317.59	6597.26	33
H35	2597.97	3826.94	7544.11	28
H1A	10250.34	2229.18	5225.25	46
H1B	10831.55	1178.77	5560.72	46
H2C	1085.25	4295.04	4569.87	48
H2D	-271.03	3612.41	4210.2	48
H3C	7835.39	1684.31	4478.57	53
H3D	7248.39	2474.5	3808.07	53

Table S21 Atomic Occupancy for [Sc(L^{003})].

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O3	0.909(9)	H3C	0.909(9)	H3D	0.909(9)
O3A	0.091(9)				

4 DFT Atomic Coordinates

Table S22 Atomic coordinates (x,y,z) of [Sc($\mathbf{L}^{300}$)] isomers.

[Sc($\mathbf{L}^{300}$)] Δ				[Sc($\mathbf{L}^{300}$)] Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.01303300	-0.00278700	2.37235300	N	-0.02086300	-0.00585000	2.36819900
C	1.39751000	-0.00498300	2.93407000	C	1.35407000	-0.04558200	2.95133800
C	2.45182200	0.34426600	1.89034300	C	2.41452900	-0.41871200	1.92171400
N	2.25340400	-0.43677300	0.64311600	N	2.25468100	0.37432500	0.67589600
C	2.50436500	-1.89539700	0.84202400	C	2.54944800	1.82197400	0.88822600
C	1.40985000	-2.76241100	0.23191200	C	1.49135200	2.72465600	0.26653100
N	0.06079700	-2.28686100	0.63067700	N	0.12308100	2.28341800	0.63846200
C	-0.19240800	-2.46913700	2.09240400	C	-0.15050900	2.46729800	2.09636900
C	-0.75432600	-1.21552500	2.75395200	C	-0.75877400	1.22765100	2.74272700
H	-0.76679100	-1.35298700	3.84975200	H	-0.78570400	1.36059900	3.83878500
H	-1.78934200	-1.05422900	2.42422800	H	-1.79242300	1.09753500	2.39520900
H	0.74222000	-2.77630800	2.57536300	H	0.78419400	2.74715700	2.59588600
H	-0.90381500	-3.29403500	2.24854700	H	-0.84137600	3.31114600	2.24333900
C	-1.00129900	-2.91216100	-0.18273900	C	-0.90447300	2.94309400	-0.19153800
C	-2.20586300	-1.98593900	-0.33710100	C	-2.13620700	2.05785000	-0.36906100
O	-3.33885900	-2.44033700	-0.49895500	O	-3.24925100	2.55123000	-0.55458500
O	-1.91549900	-0.70941000	-0.34005200	O	-1.89036500	0.77210100	-0.36500300
H	-0.61308000	-3.07153100	-1.20134600	H	-0.49313200	3.09106400	-1.20278900
H	-1.31283800	-3.88801800	0.22010700	H	-1.19075200	3.92835300	0.20733800
H	1.56626200	-3.81524600	0.52696400	H	1.67144500	3.77042100	0.57294400
H	1.45667200	-2.70915400	-0.86426400	H	1.55575100	2.67883100	-0.82904000
H	2.59711900	-2.09347900	1.91601300	H	2.63096700	2.00948000	1.96504500
H	3.46891600	-2.17517700	0.39194300	H	3.52961000	2.07335500	0.45551200
C	3.05848300	0.10113200	-0.47255500	C	3.05521900	-0.18162100	-0.43415000
C	2.36433800	-0.10168700	-1.81712400	C	2.38541900	0.05731600	-1.78550700
O	3.01074300	-0.23920400	-2.85576300	O	3.04965900	0.19093900	-2.81320900
O	1.05611700	-0.05468300	-1.76528700	O	1.07532700	0.04568500	-1.75224400
H	4.07335500	-0.32405100	-0.49404000	H	4.08418200	0.20883000	-0.43902100
H	3.14812600	1.19163700	-0.34496400	H	3.10541500	-1.27562400	-0.31525300
H	3.45830700	0.17672700	2.31332100	H	3.41877900	-0.28037900	2.36005000
H	2.37257000	1.40534200	1.61806300	H	2.31034800	-1.47586700	1.64301100
H	1.59929500	-0.99044200	3.36959700	H	1.57518000	0.93110100	3.39695300
H	1.46801800	0.71804200	3.76078400	H	1.39070500	-0.77530600	3.77424500
C	-0.71524300	1.23097800	2.73196900	C	-0.78962600	-1.21905200	2.71289600
C	-0.39805900	2.37471700	1.77111800	C	-0.49080400	-2.36853500	1.75348400
O	-0.43363100	3.54789100	2.14365600	O	-0.59090700	-3.54157100	2.11438600
O	-0.15580300	1.99833600	0.54091800	O	-0.19208100	-1.99451100	0.53541800
H	-0.52702200	1.53647600	3.77252400	H	-0.62680400	-1.53285600	3.75522400
H	-1.79499800	1.04252300	2.62253400	H	-1.86196600	-0.99996400	2.58781300

Table S23 Atomic coordinates (x,y,z) of [ScF($\mathbf{L}^{300}$)]$^{-}$ isomers.

[ScF($\mathbf{L^{300}}$)]$^-$ Δ				[ScF($\mathbf{L^{300}}$)]$^-$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.01038900	0.01706600	2.48025900	N	0.02581500	-0.00491300	2.48438200
C	1.37596500	0.01119100	3.08005600	C	1.39480600	0.00000700	3.07562800
C	2.48139700	0.29544400	2.06784300	C	2.49281600	-0.29189000	2.05754700
N	2.27742300	-0.50155000	0.84334500	N	2.28367000	0.50025900	0.83079600
C	2.50436700	-1.95483500	1.09406000	C	2.51630000	1.95405200	1.07312100
C	1.41109900	-2.85054400	0.51703600	C	1.42190600	2.85017200	0.49873900
N	0.07318400	-2.31454900	0.83679800	N	0.08464500	2.31900500	0.82878300
C	-0.23658200	-2.43629500	2.29300800	C	-0.21544100	2.44795900	2.28631400
C	-0.77948600	-1.15085500	2.91526700	C	-0.75857000	1.16715200	2.91759600
H	-0.77434700	-1.25671300	4.01637600	H	-0.74761300	1.27868100	4.01814200
H	-1.81547600	-0.98085900	2.60220900	H	-1.79665400	0.99845000	2.61065100
H	0.67337400	-2.75066700	2.81772400	H	0.69901000	2.76133000	2.80371600
H	-0.97095300	-3.24214600	2.45212900	H	-0.94592700	3.25708500	2.44679000
C	-0.98638500	-2.93830500	0.03338600	C	-0.97851700	2.94190500	0.02948500
C	-2.23415400	-2.05525600	0.05848500	C	-2.22789600	2.06142400	0.06483800
O	-3.36077600	-2.55085500	-0.08099100	O	-3.35433300	2.55890500	-0.06885100
O	-1.99395700	-0.78882300	0.19722900	O	-1.98968700	0.79462800	0.20478600
H	-0.65135100	-2.99028300	-1.01558800	H	-0.64970500	2.98947100	-1.02166900
H	-1.22986100	-3.96103800	0.36755700	H	-1.21809600	3.96629100	0.36141600
H	1.54093200	-3.87536600	0.91249300	H	1.55683000	3.87630400	0.88912100
H	1.49187000	-2.90242900	-0.57467900	H	1.49636900	2.89725200	-0.59363000
H	2.58007500	-2.11276200	2.17635500	H	2.59975300	2.11709100	2.15409900
H	3.47514000	-2.26240200	0.67290900	H	3.48520100	2.25664800	0.64410600
C	3.10788800	-0.03297900	-0.27235800	C	3.10677800	0.02440600	-0.28727300
C	2.53125800	-0.53736800	-1.59365000	C	2.52480300	0.52523100	-1.60756400
O	3.26586700	-0.72877200	-2.57214600	O	3.25489400	0.71078200	-2.59060500
O	1.24496500	-0.69927400	-1.59408600	O	1.23909500	0.69120700	-1.60201400
H	4.16488900	-0.33338100	-0.17335400	H	4.16529300	0.32164400	-0.19510200
H	3.06611100	1.06801100	-0.30582900	H	3.06110200	-1.07658800	-0.31609800
H	3.46069000	0.07878100	2.53461500	H	3.47585100	-0.07650100	2.51700700
H	2.47774200	1.35198600	1.77741700	H	2.48385300	-1.34969200	1.77168500
H	1.54608100	-0.96413600	3.55101400	H	1.57050500	0.97693100	3.54125800
H	1.43406300	0.75506200	3.89103500	H	1.45620200	-0.74050300	3.88948700
C	-0.66674600	1.28966400	2.75809800	C	-0.65332800	-1.27421800	2.77177500
C	-0.08256900	2.38899100	1.87077400	C	-0.07798700	-2.37914200	1.88556300
O	-0.08974000	3.57054200	2.24063300	O	-0.08403600	-3.55869300	2.26163200
O	0.36199000	1.97664100	0.72402300	O	0.35846100	-1.97356700	0.73312100
H	-0.61213800	1.58101800	3.82058400	H	-0.59312900	-1.56143900	3.83510800
H	-1.72962400	1.19195200	2.48259200	H	-1.71753700	-1.17450300	2.50223400
F	-0.85696900	0.98718600	-1.46991100	F	-0.86281700	-0.99047800	-1.46413400

Table S24 Atomic coordinates (x,y,z) of [Sc(OH_2)($\mathbf{L^{300}}$)] isomers.							
[Sc(OH_2)($\mathbf{L^{300}}$)] Δ				[Sc(OH_2)($\mathbf{L^{300}}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000

N	-1.03026300	1.35285600	1.69220100
C	-0.05372600	1.84927300	2.70958500
C	1.39763900	1.66495100	2.28018700
N	1.61303400	0.30427200	1.73607700
C	1.51733600	-0.74084000	2.80216800
C	0.63968300	-1.92402100	2.40296100
N	-0.62361500	-1.45139400	1.79201600
C	-1.51434800	-0.79965000	2.80048900
C	-2.08912700	0.52734200	2.31521200
H	-2.56001500	1.05326500	3.16510800
H	-2.86157200	0.35895900	1.55620500
H	-0.94116500	-0.64949100	3.72261200
H	-2.34321000	-1.47601000	3.06046400
C	-1.33978300	-2.52420200	1.08148400
C	-2.29367400	-1.92439200	0.04936500
O	-3.30975700	-2.52725600	-0.30609500
O	-1.90754800	-0.77752000	-0.43548300
H	-0.60678400	-3.12370100	0.51753600
H	-1.88079100	-3.19638900	1.76667700
H	0.44545500	-2.54919800	3.29293300
H	1.14894100	-2.54806100	1.65939600
H	1.12793400	-0.27189000	3.71324100
H	2.52295300	-1.11192600	3.05334400
C	2.89164100	0.19785100	1.01342400
C	2.84551000	-0.96569300	0.02586500
O	3.87874600	-1.53397500	-0.33795600
O	1.65239100	-1.25200900	-0.41247800
H	3.75304700	0.09755900	1.69308500
H	3.03436100	1.11069700	0.41294700
H	2.06015900	1.86086500	3.14233700
H	1.65782800	2.37742300	1.48868500
H	-0.23742300	1.32123300	3.65250300
H	-0.23395300	2.91617100	2.91342800
C	-1.58394600	2.46995200	0.90899700
C	-0.56748100	2.93855500	-0.12919400
O	-0.57372700	4.09741700	-0.55241500
O	0.24541100	2.00671300	-0.54253100
H	-1.90793600	3.31076300	1.54331600
H	-2.45925100	2.10708200	0.34641400
O	0.00319300	-0.20970200	-2.33936600
H	0.69251400	-0.87843300	-2.50296500
H	-0.83064500	-0.67911100	-2.52195300

N	-1.61386900	0.30810900	1.73521900
C	-1.52133300	-0.73680900	2.80174900
C	-0.64637400	-1.92224600	2.40334700
N	0.61834500	-1.45280600	1.79282700
C	1.51003100	-0.80295100	2.80165900
C	2.08813400	0.52261300	2.31644300
N	1.03144400	1.35052300	1.69285300
C	0.05551100	1.84921900	2.70971500
C	-1.39594400	1.66841800	2.27919900
H	-2.05876700	1.86598300	3.14072900
H	-1.65381700	2.38137700	1.48735500
H	0.23737600	1.32061100	3.65267900
H	0.23824600	2.91564000	2.91379600
C	1.58820600	2.46641200	0.91007900
C	0.57343300	2.93729400	-0.12873000
O	0.58224300	4.09610000	-0.55193000
O	-0.24077400	2.00692800	-0.54290800
H	2.46303400	2.10159600	0.34798500
H	1.91379200	3.30640700	1.54465400
H	2.55987900	1.04760500	3.16643400
H	2.86048600	0.35231600	1.55776200
H	0.93669000	-0.65128600	3.72343900
H	2.33721100	-1.48115500	3.06220000
C	1.33216900	-2.52759500	1.08295800
C	2.28797900	-1.93088500	0.05081200
O	3.30324100	-2.53602800	-0.30314700
O	1.90525900	-0.78297900	-0.43439300
H	1.87108200	-3.20091100	1.76869700
H	0.59787500	-3.12542100	0.51893100
H	-0.45393700	-2.54757500	3.29359400
H	-1.15679500	-2.54539100	1.65982000
H	-1.13130100	-0.26852300	3.71288700
H	-2.52800000	-1.10532600	3.05254700
C	-2.89198800	0.20399500	1.01143500
C	-2.84728200	-0.96065400	0.02503700
O	-3.88108700	-1.52845800	-0.33797200
O	-1.65459000	-1.24800800	-0.41374400
H	-3.75430900	0.10632400	1.69030100
H	-3.03197300	1.11656900	0.40988100
O	-0.00165800	-0.20961800	-2.34017900
H	0.83073300	-0.68250900	-2.52030100
H	-0.69311200	-0.87580200	-2.50492200

Table S25 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{300})]$^{-}$ isomers.

[Sc(OH)(**L**^{300})]$^{-}$ Δ				[Sc(OH)(**L**^{300})]$^{-}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-1.24923100	1.09524700	1.84831000	N	-1.57680300	0.45904700	1.83722900
C	-0.35841700	1.72627100	2.86524300	C	-1.61588600	-0.62800200	2.86130900
C	1.10076600	1.81601900	2.42643000	C	-0.89324500	-1.90402500	2.43052500
N	1.55524700	0.54145900	1.83651200	N	0.42271900	-1.58618700	1.84349300
C	1.65132200	-0.54103300	2.86091800	C	1.37465800	-1.07987400	2.87533400
C	0.99875000	-1.85364700	2.42963300	C	2.12056700	0.18349700	2.45165600
N	-0.33283300	-1.60667200	1.84402400	N	1.19370200	1.16002500	1.84757700
C	-1.30993000	-1.15151000	2.87643500	C	0.27183900	1.74134500	2.86722200
C	-2.12135900	0.07143500	2.45469600	C	-1.18974100	1.75512800	2.42878300
H	-2.65650200	0.46786200	3.33813300	H	-1.82305800	2.00698200	3.30020700
H	-2.87249900	-0.20484700	1.70699500	H	-1.35407300	2.52441600	1.66530100
H	-0.76244300	-0.93357100	3.80109000	H	0.37634400	1.16981800	3.79692600
H	-2.00549300	-1.97069800	3.12077700	H	0.57802200	2.77225700	3.10789400
C	-0.85903100	-2.76909200	1.11579400	C	1.89851800	2.22319700	1.11992800
C	-1.96617700	-2.31623400	0.16276500	C	0.94586000	2.89624000	0.13401000
O	-2.87519100	-3.09443500	-0.16122100	O	1.10463300	4.08227600	-0.18701500
O	-1.83895600	-1.10497800	-0.27644300	O	0.02279200	2.12015000	-0.34167600
H	-0.05343500	-3.19194400	0.49326300	H	2.70457400	1.76792100	0.52158300
H	-1.22847400	-3.56278100	1.78712800	H	2.35047000	2.97272400	1.79161700
H	0.93842900	-2.52715300	3.30519400	H	2.63630400	0.60752300	3.33377200
H	1.60578700	-2.35279900	1.66591200	H	2.88331300	-0.05331100	1.70204700
H	1.18878300	-0.18392800	3.78869800	H	0.81658000	-0.88927200	3.79937000
H	2.70855900	-0.73522300	3.10336700	H	2.11161300	-1.86173700	3.12068600
C	2.82816300	0.68655300	1.11914200	C	1.01090300	-2.71782400	1.11418900
C	3.00687400	-0.47410300	0.14281500	C	2.09207100	-2.20632500	0.16048300
O	4.13925400	-0.85401500	-0.18698800	O	3.04139000	-2.93504300	-0.16386700
O	1.90014200	-0.96832700	-0.31303600	O	1.89860400	-1.00439800	-0.28105000
H	3.69454800	0.75670300	1.79870800	H	1.42240900	-3.49085600	1.78517700
H	2.79142000	1.60786400	0.51524100	H	0.22857800	-3.18296500	0.49201800
H	1.72019700	2.10237600	3.29727400	H	-0.79588400	-2.57266600	3.30657000
H	1.22402300	2.59177600	1.66185000	H	-1.47305100	-2.43593900	1.66795100
H	-0.43233500	1.15233700	3.79657400	H	-1.17436000	-0.24600200	3.78941700
H	-0.71843100	2.74021200	3.10381800	H	-2.66142300	-0.87840300	3.10272200
C	-2.01219300	2.11843200	1.12183400	C	-2.85576200	0.53990700	1.12012300
C	-1.09935500	2.84181100	0.13382300	C	-2.97525400	-0.62969800	0.14511300
O	-1.32143900	4.01751600	-0.18688900	O	-4.08634100	-1.06838700	-0.18383200
O	-0.13709500	2.11554600	-0.34253200	O	-1.84494300	-1.06664600	-0.31094500
H	-2.50202400	2.84315100	1.79429300	H	-3.72449500	0.56758400	1.79967900
H	-2.79380600	1.62023600	0.52554400	H	-2.86466900	1.46138500	0.51536800
O	0.05191600	-0.10581700	-2.03936000	O	-0.04803000	-0.10622400	-2.03965200
H	-0.79290000	0.21544700	-2.39531800	H	0.78195300	0.25199900	-2.39509400

.

Table S26 Atomic coordinates (x,y,z) of [Sc(**L**^{210})]$^{+}$ isomers

$[Sc(\mathbf{L^{210}})]^+$ Δ				$[Sc(\mathbf{L^{210}})]^+$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.38392300	1.54651300	1.76499500	N	-0.38437100	1.54663400	1.76488100
C	1.61767100	1.21948700	2.54172400	C	-1.61806800	1.21943600	2.54158200
C	2.50328400	0.20623700	1.82758200	C	-2.50350600	0.20607300	1.82737300
N	1.70854000	-0.94960900	1.33216000	N	-1.70850200	-0.94958700	1.33191100
C	1.16586900	-1.77887300	2.45154200	C	-1.16586000	-1.77883700	2.45133700
C	-0.31055700	-2.10907100	2.27623700	C	0.31063700	-2.10887700	2.27623100
N	-1.09728600	-0.89589000	1.92822800	N	1.09724700	-0.89560900	1.92823600
C	-1.14872900	0.08331600	3.05831800	C	1.14842200	0.08367200	3.05829400
C	-0.83746900	1.50427700	2.60936400	C	0.83699500	1.50458900	2.60928900
H	-0.73212600	2.15413800	3.49590400	H	0.73153700	2.15443400	3.49583400
H	-1.66237000	1.89723800	2.00111500	H	1.66188200	1.89763100	2.00107600
H	-0.44284500	-0.23956100	3.83177200	H	0.44247900	-0.23929600	3.83165700
H	-2.14612900	0.06885100	3.52243500	H	2.14577100	0.06939000	3.52252900
C	-2.45413800	-1.26834800	1.47740800	C	2.45419200	-1.26793500	1.47756300
C	-2.95810600	-0.24521900	0.47891100	C	2.95814700	-0.24482000	0.47905900
O	-2.08458100	0.40285100	-0.18909700	N	4.25127600	-0.05289200	0.27904900
N	-4.25125200	-0.05341100	0.27890500	C	4.70928200	0.94966000	-0.68597200
C	-4.70958900	0.94934300	-0.68572000	H	3.95991600	1.74056300	-0.79131700
H	-5.64743500	1.38063600	-0.31215000	H	5.64871100	1.37899000	-0.31418500
H	-3.95901400	1.73878400	-0.79324000	H	4.89293700	0.48242400	-1.66623400
H	-4.89628600	0.48172900	-1.66522100	C	5.30574400	-0.84876700	0.91168400
C	-5.30561300	-0.84918500	0.91189100	H	4.91010300	-1.77581200	1.33586100
H	-6.04445200	-1.11082000	0.14183300	H	6.04343800	-1.11204000	0.14106900
H	-4.91026000	-1.77714600	1.33434100	H	5.80746100	-0.26355200	1.69702000
H	-5.80588700	-0.26456500	1.69859400	O	2.08461700	0.40316700	-0.18903000
H	-2.40290300	-2.22725000	0.93802400	H	2.40308200	-2.22684800	0.93819300
H	-3.13326200	-1.39637800	2.33059500	H	3.13325200	-1.39584700	2.33082100
H	-0.69355400	-2.58235700	3.19711000	H	0.69355900	-2.58203900	3.19720000
H	-0.43937800	-2.82219700	1.45130500	H	0.43965200	-2.82205700	1.45137800
H	1.33181300	-1.24689600	3.39506700	H	-1.33194500	-1.24687200	3.39484600
H	1.72848200	-2.72140700	2.52512300	H	-1.72839800	-2.72142300	2.52484200
C	2.48695400	-1.77153700	0.38061100	C	-2.48675400	-1.77156400	0.38025200
C	1.58367200	-2.43652800	-0.65324700	C	-1.58327900	-2.43671800	-0.65331300
O	1.90589700	-3.48956800	-1.20085900	O	-1.90535300	-3.48985300	-1.20082400
O	0.49475900	-1.76241200	-0.93499800	O	-0.49433300	-1.76259100	-0.93499700
H	3.10816800	-2.52209900	0.89241400	H	-3.10815800	-2.52199700	0.89201400
H	3.15584400	-1.10706200	-0.18900400	H	-3.15542300	-1.10707200	-0.18960000
H	3.30693300	-0.12645700	2.50759800	H	-3.30710200	-0.12684200	2.50734100
H	2.97332500	0.66974800	0.95045500	H	-2.97361400	0.66956100	0.95027400
H	1.32173700	0.84584900	3.52869700	H	-1.32210800	0.84578000	3.52853900
H	2.20126900	2.13516900	2.71938300	H	-2.20180800	2.13502500	2.71926900
C	0.50989600	2.84534600	1.07232700	C	-0.51054100	2.84536500	1.07206700
C	1.23919900	2.70021800	-0.25886700	C	-1.23964400	2.70000000	-0.25921100
O	1.86450800	3.63799400	-0.75116500	O	-1.86503400	3.63760600	-0.75171700

O	1.08635100	1.53288200	-0.83660800	O	-1.08657700	1.53259100	-0.83680900
H	0.99871100	3.60532100	1.70090200	H	-0.99960200	3.60530000	1.70050300
H	-0.49978700	3.20857600	0.82247400	H	0.49909600	3.20877100	0.82229800

Table S27 Atomic coordinates (x,y,z) of [ScF($\mathbf{L}^{210}$)] isomers.

[ScF($\mathbf{L}^{210}$)] Δ				[ScF($\mathbf{L}^{210}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.33496400	1.50031400	1.89504200	N	-0.33505800	1.50026200	1.89500700
C	1.56620300	1.18863300	2.68342800	C	-1.56631400	1.18859900	2.68337400
C	2.49295800	0.18487200	2.00133300	C	-2.49305900	0.18482600	2.00128000
N	1.72111800	-0.95354900	1.46420300	N	-1.72118500	-0.95356300	1.46411400
C	1.16790300	-1.80792900	2.55547200	C	-1.16799400	-1.80797100	2.55536700
C	-0.30059400	-2.16807000	2.35717300	C	0.30050000	-2.16812700	2.35707700
N	-1.08659300	-0.97225400	1.98107000	N	1.08653300	-0.97229900	1.98107200
C	-1.19132400	-0.00945300	3.12271300	C	1.19118800	-0.00950800	3.12272700
C	-0.87596500	1.43415700	2.73858400	C	0.87583100	1.43411500	2.73861600
H	-0.75628700	2.03086200	3.66158300	H	0.75607800	2.03078600	3.66162400
H	-1.70187700	1.86972200	2.16601300	H	1.70176600	1.86971100	2.16610700
H	-0.51134200	-0.34099700	3.91579500	H	0.51117200	-0.34107000	3.91577200
H	-2.20430700	-0.04868200	3.55296200	H	2.20414700	-0.04872800	3.55303600
C	-2.42379900	-1.35046000	1.49952300	C	2.42376700	-1.35048300	1.49958300
C	-2.97952300	-0.18840600	0.69788100	C	2.97949800	-0.18841600	0.69796300
O	-2.14544100	0.60731600	0.17578900	N	4.28916700	-0.02247200	0.53809800
N	-4.28920300	-0.02246000	0.53810900	C	4.78784700	1.11252000	-0.23964000
C	-4.78808400	1.11254800	-0.23945300	H	4.11441200	1.96933500	-0.12930000
H	-5.78327500	1.37988800	0.13894500	H	5.78367700	1.37902300	0.13763900
H	-4.11393300	1.96894300	-0.13030200	H	4.86911600	0.84917200	-1.30663400
H	-4.87088300	0.84879400	-1.30623000	C	5.29786900	-0.99134400	0.96449000
C	-5.29787200	-0.99123800	0.96479400	H	4.83917200	-1.91919400	1.31753000
H	-5.94055600	-1.23111500	0.10473400	H	5.93993600	-1.23175600	0.10411500
H	-4.83919900	-1.91937400	1.31711900	H	5.92491800	-0.56508500	1.76239200
H	-5.92430900	-0.56515700	1.76327800	O	2.14542400	0.60737600	0.17596400
H	-2.33314500	-2.20837700	0.81428100	H	2.33317100	-2.20842200	0.81436400
H	-3.08368600	-1.64282400	2.32976500	H	3.08363500	-1.64281300	2.32985500
H	-0.68779800	-2.62600600	3.28573500	H	0.68767400	-2.62613400	3.28561500
H	-0.41228900	-2.90201200	1.55151800	H	0.41219600	-2.90200600	1.55136200
H	1.29916800	-1.28471100	3.50943300	H	-1.29925600	-1.28477300	3.50933900
H	1.75127900	-2.73905600	2.63626300	H	-1.75137900	-2.73909500	2.63613500
C	2.49639700	-1.76727300	0.51797400	C	-2.49646500	-1.76725600	0.51784700
C	1.54478600	-2.57961200	-0.35995100	C	-1.54488600	-2.57951100	-0.36019900
O	1.89439700	-3.66500700	-0.83923700	O	-1.89459300	-3.66480800	-0.83963300
O	0.39560000	-2.01281300	-0.57431600	O	-0.39566000	-2.01277500	-0.57448700
H	3.22071600	-2.43032300	1.01982700	H	-3.22072200	-2.43038400	1.01968400
H	3.05351500	-1.09428400	-0.15387600	H	-3.05364800	-1.09424000	-0.15391700
H	3.25561900	-0.15079600	2.72828300	H	-3.25569200	-0.15089200	2.72823300
H	3.01615700	0.65242100	1.15974000	H	-3.01628000	0.65237700	1.15970600
H	1.25984600	0.80628500	3.66415500	H	-1.25997100	0.80625500	3.66410700
H	2.12828700	2.11549900	2.87924500	H	-2.12839200	2.11547100	2.87917800
C	0.47154300	2.79788800	1.21602600	C	-0.47161500	2.79781900	1.21594400

C 1.42367700 2.65837300 0.02947700	C -1.42372000 2.65828800 0.02935300
O 2.07731600 3.62673900 -0.37641800	O -2.07714100 3.62674000 -0.37668500
O 1.43991100 1.47696600 -0.50971300	O -1.44014600 1.47682700 -0.50969900
H 0.81142400 3.59836400 1.89400100	H -0.81154500 3.59830800 1.89387800
H -0.50930600 3.08707000 0.80441400	H 0.50925400 3.08700000 0.80438200
F -0.51098700 0.18196000 -1.87999900	F 0.51110600 0.18214800 -1.87989900

Table S28 Atomic coordinates (x,y,z) of $[Sc(OH_2)(\mathbf{L^{210}})]^+$ isomers.

$[Sc(OH_2)(\mathbf{L^{210}})]^+$ Δ				$[Sc(OH_2)(\mathbf{L^{210}})]^+$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.30858900	1.37482700	1.91158800	N	-0.30858600	1.37483300	1.91158400
C	1.53885800	1.03070500	2.69205600	C	-1.53885300	1.03071200	2.69205400
C	2.47258600	0.08193400	1.94769900	C	-2.47258200	0.08194100	1.94769900
N	1.70977700	-1.02755600	1.32930400	N	-1.70977300	-1.02755000	1.32930600
C	1.16190800	-1.96388200	2.35848800	C	-1.16190500	-1.96387500	2.35849200
C	-0.29926800	-2.32201500	2.12032000	C	0.29927100	-2.32200900	2.12032600
N	-1.10310500	-1.10612800	1.84628500	N	1.10310700	-1.10612400	1.84628500
C	-1.20734800	-0.21915300	3.04919700	C	1.20735300	-0.21914500	3.04919400
C	-0.91480100	1.24554900	2.73731700	C	0.91480600	1.24555600	2.73731000
H	-0.81752600	1.80520100	3.68439000	H	0.81753400	1.80521100	3.68438200
H	-1.74157300	1.68967500	2.17047800	H	1.74157700	1.68967900	2.17046800
H	-0.51887900	-0.59040200	3.81647800	H	0.51888500	-0.59039100	3.81647600
H	-2.21705200	-0.29374000	3.48008300	H	2.21705700	-0.29373200	3.48007800
C	-2.44478900	-1.46196200	1.35063600	C	2.44479100	-1.46195800	1.35063300
C	-2.98490500	-0.28790100	0.55943200	C	2.98490500	-0.28789900	0.55942500
O	-2.13196100	0.48195400	0.01437200	N	4.28529300	-0.08181700	0.41760300
N	-4.28529500	-0.08182500	0.41760700	C	4.76678000	1.06924100	-0.34939100
C	-4.76678500	1.06923400	-0.34938400	H	4.03385500	1.88150100	-0.30713400
H	-5.71415900	1.40543100	0.09157900	H	5.71415800	1.40543600	0.09156400
H	-4.03385900	1.88149200	-0.30713400	H	4.94173100	0.78647400	-1.39951300
H	-4.94174600	0.78646500	-1.39950400	C	5.31821000	-0.99552000	0.90823600
C	-5.31820800	-0.99553400	0.90823400	H	4.89527100	-1.96252800	1.19424700
H	-6.04379400	-1.16353000	0.09986500	H	6.04379800	-1.16351700	0.09986800
H	-4.89526600	-1.96254200	1.19424100	H	5.84344700	-0.55166700	1.76746200
H	-5.84344800	-0.55168700	1.76746200	O	2.13195900	0.48194900	0.01435700
H	-2.35902900	-2.30734800	0.64942700	H	2.35903000	-2.30734600	0.64942700
H	-3.10728600	-1.76343200	2.17356800	H	3.10728900	-1.76342600	2.17356500
H	-0.68707600	-2.86719700	2.99915300	H	0.68707900	-2.86718600	2.99916200
H	-0.39659300	-2.97962500	1.24773600	H	0.39659600	-2.97962400	1.24774600
H	1.28380900	-1.50769900	3.34735200	H	-1.28380700	-1.50768900	3.34735500
H	1.75472200	-2.89112800	2.37384800	H	-1.75472000	-2.89112000	2.37385400
C	2.51095700	-1.75750700	0.33091500	C	-2.51095100	-1.75750300	0.33091700
C	1.60215100	-2.43044300	-0.69284900	C	-1.60214200	-2.43045000	-0.69283600
O	1.95786900	-3.44050200	-1.30164600	O	-1.95786300	-3.44051000	-1.30163000
O	0.46682000	-1.81390300	-0.88955400	O	-0.46680500	-1.81391900	-0.88953500
H	3.19060300	-2.49174000	0.79104900	H	-3.19060400	-2.49172800	0.79105300
H	3.11993000	-1.03016300	-0.22939200	H	-3.11991700	-1.03015900	-0.22939800
H	3.23671300	-0.30018800	2.64773600	H	-3.23671000	-0.30017900	2.64773500
H	2.99164800	0.60905900	1.13905600	H	-2.99164400	0.60906500	1.13905500
H	1.23169800	0.58939700	3.64695400	H	-1.23169200	0.58940500	3.64695200
H	2.08973700	1.95014900	2.94154700	H	-2.08973200	1.95015700	2.94154600
C	0.43444800	2.71565300	1.30977100	C	-0.43444500	2.71565900	1.30976600

C	1.36182900	2.65860000	0.09775200	C	-1.36182600	2.65860500	0.09774700
O	2.00427200	3.64582200	-0.26530500	O	-2.00427100	3.64582600	-0.26531000
O	1.36051800	1.50899800	-0.51968900	O	-1.36051200	1.50900300	-0.51969600
H	0.78278400	3.46890600	2.03391700	H	-0.78278100	3.46891200	2.03391100
H	-0.55308900	3.02896400	0.93333200	H	0.55309200	3.02897000	0.93332600
O	-0.61777100	0.57795400	-2.17477200	O	0.61773500	0.57792700	-2.17478200
H	-0.02050400	1.30932200	-2.41320800	H	0.02045100	1.30928900	-2.41319400
H	-1.49237000	0.99739200	-2.08688600	H	1.49233200	0.99737400	-2.08692900

Table S29 Atomic coordinates (x,y,z) of Sc(OH)(**L**^{210}) isomers.

Sc(OH)(**L**^{210}) Δ				Sc(OH)(**L**^{210}) Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.32735000	1.48427100	1.90852000	N	-0.33234400	1.48215000	1.90903800
C	1.54741200	1.16743100	2.71118300	C	-1.55224200	1.16244300	2.71076700
C	2.48165400	0.16408100	2.03841400	C	-2.48409400	0.15787300	2.03659700
N	1.71529900	-0.96735700	1.48065700	N	-1.71500300	-0.97181000	1.47905900
C	1.14973100	-1.83086600	2.55741200	C	-1.14931300	-1.83497800	2.55588400
C	-0.31708100	-2.18762900	2.34230300	C	0.31822100	-2.18924100	2.34179500
N	-1.10200500	-0.98982200	1.97115500	N	1.10164200	-0.99014200	1.97165900
C	-1.21230700	-0.02973200	3.11428700	C	1.20928700	-0.02995700	3.11499800
C	-0.89366400	1.41586600	2.73649000	C	0.88826900	1.41534600	2.73773800
H	-0.78657100	2.01031800	3.66266300	H	0.77945700	2.00891500	3.66428400
H	-1.71313900	1.85183200	2.15483800	H	1.70736300	1.85313000	2.15694600
H	-0.53740900	-0.36383500	3.91069600	H	0.53450500	-0.36558000	3.91088400
H	-2.22794000	-0.06888600	3.53845600	H	2.22470500	-0.06721500	3.53987400
C	-2.43643100	-1.36701300	1.48323500	C	2.43695200	-1.36555600	1.48502800
C	-2.98885700	-0.20261500	0.68348000	C	2.98901400	-0.20025200	0.68643900
O	-2.15385900	0.59272100	0.16344100	N	4.29856400	-0.02955500	0.53007200
N	-4.29862500	-0.03338500	0.52723000	C	4.79496200	1.11519300	-0.23492900
C	-4.79871200	1.11040900	-0.23653800	H	4.12842300	1.97438500	-0.10173900
H	-5.79085000	1.37685300	0.15049900	H	5.79650600	1.36934500	0.13537300
H	-4.12169300	1.96393000	-0.12229900	H	4.86181300	0.87038700	-1.30720300
H	-4.88835900	0.85789900	-1.30535500	C	5.30907000	-0.99580000	0.95854800
C	-5.30763500	-0.99906500	0.96082600	H	4.85282000	-1.93337800	1.28854300
H	-5.97679700	-1.21051900	0.11390600	H	5.96724600	-1.21704100	0.10541100
H	-4.85118100	-1.94133200	1.27704700	H	5.91912800	-0.57741100	1.77370500
H	-5.90628300	-0.58523300	1.78675600	O	2.15395900	0.59545200	0.16708500
H	-2.34287800	-2.22294200	0.79587900	H	2.34524400	-2.22155500	0.79755400
H	-3.10001700	-1.66214300	2.30963500	H	3.10009400	-1.65995300	2.31210100
H	-0.71186100	-2.65648600	3.26242800	H	0.71309800	-2.65789600	3.26198700
H	-0.42104200	-2.91279300	1.52743800	H	0.42394800	-2.91396800	1.52675400
H	1.27177700	-1.31677100	3.51771500	H	-1.27304500	-1.32161800	3.51635800
H	1.73055400	-2.76400100	2.63573200	H	-1.72876600	-2.76906500	2.63315100
C	2.50304700	-1.76953900	0.53571600	C	-2.49985900	-1.77472200	0.53239700
C	1.56811500	-2.57940700	-0.36159000	C	-1.56188400	-2.58235500	-0.36385800
O	1.93156900	-3.66109000	-0.84098000	O	-1.92172700	-3.66531300	-0.84302300
O	0.42132100	-2.01705000	-0.59322100	O	-0.41640800	-2.01684800	-0.59479800
H	3.22538700	-2.43383300	1.03930200	H	-3.22173700	-2.44075500	1.03433800
H	3.06439300	-1.08775900	-0.12361000	H	-3.06134200	-1.09351500	-0.12739600
H	3.23024200	-0.17950500	2.77643800	H	-3.23284000	-0.18748700	2.77363000
H	3.02126400	0.63528100	1.20977200	H	-3.02368900	0.62854400	1.20765400
H	1.22768500	0.78169400	3.68627000	H	-1.23229100	0.77654400	3.68570800
H	2.10842400	2.09268400	2.91816200	H	-2.11506800	2.08648700	2.91819600
C	0.47752000	2.78000900	1.22971800	C	-0.48488600	2.77789200	1.23081300
C	1.45521400	2.63831600	0.06303700	C	-1.46158100	2.63463400	0.06338500

O	2.10995200	3.61105400	-0.33365500	O	-2.11851200	3.60601900	-0.33288200
O	1.49246500	1.45546800	-0.46830700	O	-1.49567000	1.45202700	-0.46890800
H	0.80372300	3.58252400	1.91231200	H	-0.81332500	3.57932700	1.91359600
H	-0.49501800	3.06837300	0.79779800	H	0.48730500	3.06862200	0.79967200
O	-0.55502600	0.25916900	-1.93756900	O	0.55721200	0.26403100	-1.93584500
H	0.21765300	0.14868500	-2.51592200	H	-0.21575300	0.16164000	-2.51528200

Table S30 Atomic coordinates (x,y,z) of $[Sc(\mathbf{L^{120}})]^{2+}$ isomers.

$[Sc(\mathbf{L^{120}})]^{2+}$ Δ				$[Sc(\mathbf{L^{120}})]^{2+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.37101800	N	0.63149400	2.02495700	1.09954700
C	1.38603000	0.00000000	2.93240900	C	-0.44604300	2.54397900	1.99141900
C	2.43524100	0.35587700	1.88969200	C	-1.79077200	1.89473100	1.70449800
N	2.24096900	-0.42195900	0.63415000	N	-1.67575600	0.41010700	1.64890900
C	2.50955200	-1.88183400	0.83848600	C	-1.30214200	-0.17096400	2.97673000
C	1.41708300	-2.76919900	0.26054900	C	-0.16708400	-1.17948500	2.87756600
N	0.06363500	-2.30640900	0.66970700	N	0.97601700	-0.64849500	2.08491000
C	-0.17296200	-2.46686400	2.13851700	C	1.65914900	0.49376100	2.77032700
C	-0.76233100	-1.21235600	2.76862400	C	1.87014300	1.68625100	1.84654200
H	-0.78427200	-1.32666900	3.86645700	H	2.23066400	2.54816600	2.43483300
H	-1.79524600	-1.06991700	2.42252400	H	2.63578700	1.44242800	1.09771000
H	0.77507300	-2.73707700	2.61757200	H	1.06900400	0.77731400	3.64955900
H	-0.85928800	-3.30668300	2.32018000	H	2.63882300	0.16907000	3.14986800
C	-0.97745600	-3.00245700	-0.11896500	C	1.92845000	-1.73666400	1.77036900
C	-2.14824000	-2.07192200	-0.35520900	C	2.56139000	-1.49834700	0.41511900
O	-1.89755000	-0.81920400	-0.38549800	N	3.71923300	-2.04100900	0.08088400
N	-3.37258200	-2.52369600	-0.56140700	C	4.28353800	-1.80316500	-1.25092100
C	-4.47605500	-1.58489900	-0.78283900	H	3.98322500	-0.81565000	-1.61614300
H	-5.39198200	-2.03157800	-0.37510200	H	5.37701000	-1.85058600	-1.17272700
H	-4.27087300	-0.63737400	-0.27454300	H	3.94037900	-2.57643500	-1.95610100
H	-4.61480500	-1.40375200	-1.86018000	C	4.45739200	-2.98711000	0.91996800
C	-3.71777500	-3.94216200	-0.68035200	H	3.85743900	-3.32549400	1.76888300
H	-4.35152900	-4.06738900	-1.56956700	H	4.71396500	-3.86316800	0.30734300
H	-2.82709000	-4.56381700	-0.80335800	H	5.38715600	-2.52449800	1.28286600
H	-4.28170800	-4.27026100	0.20555800	O	1.90922100	-0.78464000	-0.41937800
H	-0.57325700	-3.24359600	-1.11458100	H	1.37536100	-2.68526700	1.68632600
H	-1.27081500	-3.94414600	0.36190400	H	2.67246800	-1.85219500	2.56926800
H	1.59226700	-3.81396200	0.57052100	H	0.15486300	-1.47044800	3.89254200
H	1.44809900	-2.72956500	-0.83647700	H	-0.52101300	-2.08186300	2.36100000
H	2.63322300	-2.06533800	1.91165500	H	-1.03792800	0.64838100	3.65442400
H	3.46460900	-2.15500000	0.36713000	H	-2.17282600	-0.67188500	3.42380800
C	3.08690000	0.13638500	-0.44304500	C	-2.93094900	-0.17934100	1.13390600
C	2.40297500	-0.03399900	-1.78326700	C	-2.63337800	-1.39348100	0.27755400
O	1.13379700	-0.17604900	-1.78171700	O	-1.45761500	-1.50458500	-0.20913500
N	3.07667300	0.01344400	-2.91974100	N	-3.57152900	-2.28454700	0.00825200
C	2.35992300	-0.08361500	-4.19487200	C	-4.96588400	-2.15113100	0.43659200
H	1.50978400	-0.76736400	-4.09921800	H	-5.19126700	-1.13034100	0.75731400
H	1.99848100	0.90874700	-4.50769900	H	-5.61182700	-2.39303600	-0.41869800
H	3.05664600	-0.46565400	-4.95099800	H	-5.18247800	-2.85461800	1.25448900
C	4.49967900	0.33999300	-3.01942800	C	-3.27633300	-3.44558200	-0.83504800
H	5.03593300	-0.48772600	-3.50549700	H	-3.55910700	-3.23935200	-1.87923600
H	4.61061500	1.24389900	-3.63681800	H	-2.21012700	-3.68710100	-0.78383800
H	4.93876000	0.53242100	-2.03723400	H	-3.86493000	-4.29627500	-0.46757000

H	4.09147100	-0.30609900	-0.42369100	H	-3.62087700	-0.41379500	1.95532500
H	3.19419500	1.22130900	-0.28705300	H	-3.42800600	0.55169600	0.47735900
H	3.44309000	0.18741700	2.30660400	H	-2.52213800	2.20555700	2.47058400
H	2.35278100	1.41724300	1.62170200	H	-2.16457500	2.22203700	0.72517900
H	1.59149500	-0.98427100	3.36782700	H	-0.14995400	2.38129700	3.03379600
H	1.45610400	0.72211500	3.75910600	H	-0.54781400	3.63228500	1.86640200
C	-0.72464400	1.23757400	2.73474600	C	0.91079700	2.96179900	-0.01069700
C	-0.42033800	2.37093300	1.75982600	C	-0.01611500	2.72502400	-1.19864000
O	-0.49542700	3.54874400	2.10324100	O	-0.31690700	3.63448500	-1.96816500
O	-0.13874400	1.97745200	0.53917100	O	-0.39694800	1.47669900	-1.35202800
H	-0.51788500	1.54919000	3.76953100	H	0.86359400	4.01235200	0.31200100
H	-1.80640600	1.04931000	2.64559700	H	1.92811500	2.76694500	-0.38527900

Table S31 Atomic coordinates (x,y,z) of [ScF(**L**^{120})]$^{+}$ isomers.

[ScF(**L**^{120})]$^{+}$ Δ			[ScF(**L**^{120})]$^{+}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.83324400	1.88357200	1.35742500	N	0.83326200	1.88354700	1.35756300
C	0.20916900	2.45516300	2.26150000	C	-0.20893000	2.45505800	2.26192600
C	1.61989300	1.97798400	1.94160600	C	-1.61971300	1.97801200	1.94221400
N	1.65485100	0.51111800	1.74194900	N	-1.65479000	0.51119400	1.74237300
C	1.37813300	-0.23275400	3.01193800	C	-1.37784200	-0.23288500	3.01216600
C	0.33505700	-1.33845000	2.86628100	C	-0.33477200	-1.33855600	2.86622200
N	-0.85168600	-0.85350600	2.12690700	N	0.85191500	-0.85355600	2.12686500
C	-1.62763600	0.14903800	2.92283500	C	1.62790000	0.14899600	2.92274800
C	-1.99546800	1.40047400	2.13018800	C	1.99563500	1.40045700	2.13008600
H	-2.36223700	2.17260900	2.83112000	H	2.36248400	2.17256200	2.83101000
H	-2.80099800	1.18745000	1.41950100	H	2.80108000	1.18751500	1.41927300
H	-1.03324900	0.42258900	3.80207900	H	1.03355800	0.42252200	3.80203400
H	-2.54927600	-0.31297100	3.30986600	H	2.54958100	-0.31299400	3.30970800
C	-1.72400900	-1.96480400	1.71431000	C	1.72426900	-1.96477100	1.71414500
C	-2.59994200	-1.46521100	0.57829400	C	2.60029000	-1.46480600	0.57834600
O	-2.14226900	-0.51598000	-0.12544500	N	3.78712400	-2.00154100	0.32021700
N	-3.78617500	-2.00299700	0.31967600	C	4.59409100	-1.47465000	-0.78233200
C	-4.59360100	-1.47635200	-0.78265900	H	4.41733100	-0.39982100	-0.89744700
H	-5.65178900	-1.65104800	-0.54994600	H	5.65240100	-1.64884700	-0.54979900
H	-4.41734800	-0.40143100	-0.89768100	H	4.34607200	-1.98730300	-1.72563000
H	-4.34553400	-1.98878500	-1.72606300	C	4.31231000	-3.19714800	0.97897600
C	-4.31091200	-3.19851700	0.97897000	H	3.54928700	-3.68417900	1.59256100
H	-4.63635300	-3.90872500	0.20479300	H	4.63566000	-3.90802000	0.20450900
H	-3.54692100	-3.68650000	1.59060700	H	5.18047900	-2.93963000	1.60450100
H	-5.17760200	-2.94076700	1.60646800	O	2.14206600	-0.51605800	-0.12566600
H	-1.10384500	-2.78329800	1.31472500	H	1.10416900	-2.78311800	1.31415400
H	-2.30675100	-2.35662900	2.56065100	H	2.30682700	-2.35684100	2.56049200
H	0.05971500	-1.70233200	3.87280300	H	-0.05939300	-1.70260200	3.87268100
H	0.74606500	-2.18518400	2.30460000	H	-0.74584000	-2.18520300	2.30443900
H	1.05518400	0.48897600	3.77087900	H	-1.05480200	0.48871300	3.77120600
H	2.30867400	-0.68091400	3.39338600	H	-2.30830300	-0.68117300	3.39366500
C	2.94644000	0.09733100	1.17109000	C	-2.94650200	0.09762400	1.17169600
C	2.74972400	-1.23247600	0.47217600	C	-2.75004800	-1.23200300	0.47239600
O	1.57101500	-1.52756400	0.11129400	O	-1.57140900	-1.52700700	0.11124000
N	3.76952300	-2.04559600	0.22405000	N	-3.76996900	-2.04493400	0.22417400
C	3.53897900	-3.31061200	-0.47594300	C	-5.17021500	-1.70382000	0.47168000
H	2.53884600	-3.69197800	-0.24466300	H	-5.28051900	-0.66151400	0.78301600
H	3.63376100	-3.17269200	-1.56510800	H	-5.73687700	-1.84790300	-0.46024800
H	4.29435600	-4.03367400	-0.14191200	H	-5.59129400	-2.36450100	1.24455900
C	5.16991600	-1.70434500	0.47056100	C	-3.53983300	-3.30983800	-0.47613800
H	5.59172600	-2.36538200	1.24272800	H	-3.63645200	-3.17196600	-1.56514600
H	5.73584900	-1.84780200	-0.46191500	H	-2.53912400	-3.69063000	-0.24645000
H	5.28027500	-0.66220300	0.78241500	H	-4.29427800	-4.03333800	-0.14091700

H 3.73361000 0.05853800 1.93856000	H -3.73353000 0.05874000 1.93931000
H 3.25349200 0.82652600 0.40474200	H -3.25365300 0.82697100 0.40553000
H 2.29743400 2.28663800 2.75847500	H -2.29707300 2.28660800 2.75926500
H 1.98152500 2.43942800 1.01517400	H -1.98153200 2.43960800 1.01593000
H -0.04636900 2.19689900 3.29589500	H 0.04677200 2.19656200 3.29622200
H 0.19019800 3.55528700 2.20905700	H -0.18987300 3.55519200 2.20968700
C -1.21370400 2.85630700 0.32259600	C 1.21339500 2.85633400 0.32268100
C -0.13389500 2.92118800 -0.75464400	C 0.13322000 2.92126700 -0.75417400
O 0.05060900 3.95114700 -1.41054700	O -0.05176400 3.95135400 -1.40976000
O 0.51743800 1.80792400 -0.93375600	O -0.51797500 1.80791000 -0.93336100
H -1.40965800 3.85999600 0.73423000	H 1.40951100 3.86000100 0.73429600
H -2.13199600 2.50231500 -0.17318300	H 2.13149800 2.50235000 -0.17345900
F -0.08060500 -0.71640200 -1.81397200	F 0.08057400 -0.71645200 -1.81404300

Table S32 Atomic coordinates (x,y,z) of $[Sc(OH_2)(\mathbf{L^{120}})]^{2+}$ isomers.

$[Sc(OH_2)(\mathbf{L^{120}})]^{2+}$ Δ				$[Sc(OH_2)(\mathbf{L^{120}})]^{2+}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.80381200	1.88947600	1.26345800	N	0.80184300	1.88691400	1.26735900
C	0.24388600	2.47664400	2.15351000	C	-0.25276100	2.47742000	2.14726200
C	1.64588800	1.98103500	1.82424000	C	-1.65281700	1.98465100	1.80574500
N	1.65575600	0.50696600	1.65213300	N	-1.66425500	0.51030700	1.63420000
C	1.40330800	-0.20280200	2.94847200	C	-1.42523000	-0.19948800	2.93335400
C	0.35844800	-1.30804700	2.83828100	C	-0.38096800	-1.30653400	2.83367900
N	-0.82971400	-0.83450200	2.08605400	N	0.81423500	-0.83543300	2.09105400
C	-1.60483300	0.18616200	2.86394700	C	1.58482700	0.18327600	2.87580100
C	-1.97323300	1.41167200	2.03611900	C	1.96312900	1.40799600	2.05164400
H	-2.35898700	2.19950100	2.70718600	H	2.34277200	2.19572400	2.72627400
H	-2.76433600	1.16893500	1.31702600	H	2.76094400	1.16403900	1.34063000
H	-1.00670300	0.48126500	3.73345100	H	0.97970800	0.47966000	3.74004600
H	-2.52504400	-0.26727400	3.26198900	H	2.50040400	-0.27242600	3.28184600
C	-1.69809800	-1.96187100	1.69999500	C	1.68338900	-1.96375100	1.70971100
C	-2.53032000	-1.53382900	0.50658800	C	2.52167800	-1.53936600	0.51881100
O	-2.03438600	-0.63331900	-0.24727500	N	3.68072600	-2.11312800	0.24252700
N	-3.70030000	-2.08738100	0.23632900	C	4.45662700	-1.68031500	-0.92232700
C	-4.47359500	-1.64308900	-0.92602100	H	4.25005500	-0.62784800	-1.14155100
H	-5.54034600	-1.74503000	-0.68866500	H	5.52234400	-1.80623800	-0.69200300
H	-4.24568100	-0.59622200	-1.15096100	H	4.20461600	-2.29549000	-1.80054200
H	-4.24024500	-2.26725800	-1.80299600	C	4.22114900	-3.25985500	0.97537000
C	-4.26228900	-3.21615400	0.98117000	H	3.46111400	-3.72488000	1.60928100
H	-4.64288200	-3.94911500	0.25631200	H	4.56170200	-4.00562400	0.24346100
H	-3.50357500	-3.70713500	1.59691400	H	5.07980800	-2.95005300	1.58981700
H	-5.09650600	-2.87921900	1.61475000	O	2.04137500	-0.62494300	-0.22805000
H	-1.06956100	-2.80301800	1.36678900	H	1.05553500	-2.80512100	1.37577600
H	-2.30850000	-2.30438600	2.54692700	H	2.29066200	-2.30549700	2.55932000
H	0.07912900	-1.64226900	3.85276400	H	-0.11097500	-1.63953200	3.85106900
H	0.76305500	-2.17211800	2.29907000	H	-0.78227500	-2.17089900	2.29247400
H	1.08969100	0.54033700	3.68972200	H	-1.11773900	0.54361300	3.67712000
H	2.34063200	-0.63833400	3.32613800	H	-2.36696300	-0.63329800	3.30183500
C	2.92693600	0.06109700	1.05049100	C	-2.93141100	0.06739100	1.02198300
C	2.69212200	-1.27989000	0.38786200	C	-2.69640700	-1.27889000	0.37094600
O	1.49774200	-1.54859500	0.03820400	O	-1.50118800	-1.54972300	0.02491800
N	3.68542600	-2.12332600	0.15985500	N	-3.68957800	-2.12424000	0.15087100
C	3.42699000	-3.42045600	-0.46888100	C	-5.09389800	-1.81737700	0.43227300
H	2.38865900	-3.72024500	-0.29577200	H	-5.25697600	-0.73986000	0.52596700
H	3.62038800	-3.36605500	-1.55175100	H	-5.69931700	-2.18277000	-0.40863900
H	4.10396900	-4.16142200	-0.02333300	H	-5.42182400	-2.32597900	1.35159600
C	5.09066500	-1.81787200	0.43680500	C	-3.43223100	-3.42931100	-0.46152300
H	5.42968300	-2.35304700	1.33677200	H	-3.64085700	-3.39227000	-1.54223100
H	5.69019700	-2.15370400	-0.42071800	H	-2.39000300	-3.72053500	-0.29797800
H	5.24915400	-0.74308000	0.56320100	H	-4.09884400	-4.16724400	0.00441900

H	3.73347900	0.03161500	1.79650800	H	-3.74581600	0.04788900	1.75960500
H	3.21794600	0.76896400	0.25827300	H	-3.20960600	0.77139200	0.22170700
H	2.34045600	2.29124500	2.62438300	H	-2.35388900	2.29626800	2.59957000
H	1.99867500	2.41984200	0.88356800	H	-1.99657800	2.42370000	0.86186400
H	-0.00829700	2.24115700	3.19388600	H	-0.01107400	2.24235200	3.19020100
H	0.22916100	3.57439200	2.07516600	H	-0.23493900	3.57504100	2.06798400
C	-1.19008100	2.84482200	0.20882800	C	1.20099600	2.84088300	0.21637300
C	-0.14868200	2.84898600	-0.90628500	C	0.17058500	2.84856100	-0.90851100
O	0.01429300	3.83081700	-1.63102100	O	0.01951700	3.83006900	-1.63623800
O	0.49790000	1.72015600	-1.04236300	O	-0.47962100	1.72249900	-1.04969000
H	-1.34815700	3.86215300	0.59925500	H	1.35888200	3.85770200	0.60824700
H	-2.13182700	2.50175800	-0.24884500	H	2.14581300	2.49468300	-0.23246200
O	0.04569400	-0.72704000	-2.20469500	O	-0.03488000	-0.75812700	-2.19607300
H	0.49431900	-1.59027200	-2.24073400	H	-0.71470600	-1.45168300	-2.26616100
H	0.64535000	-0.12613200	-2.68127200	H	-0.38690900	-0.02328300	-2.72940500

Table S33 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{120})]$^{+}$ isomers.

[Sc(OH)(**L**^{120})]$^{+}$ Δ				[Sc(OH)(**L**^{120})]$^{+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.83332300	1.87632800	1.36677300	N	0.83336100	1.87629400	1.36681900
C	0.21565700	2.44288400	2.26644000	C	-0.21562100	2.44285800	2.26648200
C	1.62562900	1.95904300	1.94424000	C	-1.62560400	1.95908100	1.94425000
N	1.65407800	0.49190900	1.74984200	N	-1.65409000	0.49195400	1.74980800
C	1.38074600	-0.24284000	3.02459600	C	-1.38078700	-0.24283100	3.02455300
C	0.33583300	-1.34751300	2.88881600	C	-0.33588800	-1.34752300	2.88880600
N	-0.84732600	-0.86685400	2.14228600	N	0.84729400	-0.86690100	2.14230500
C	-1.62448300	0.13775800	2.93352600	C	1.62445500	0.13769400	2.93355800
C	-1.99337200	1.38674400	2.13822000	C	1.99338200	1.38668900	2.13828900
H	-2.36727100	2.15747500	2.83730600	H	2.36725300	2.15739700	2.83741500
H	-2.79567100	1.16865600	1.42486300	H	2.79571000	1.16862000	1.42495900
H	-1.03104800	0.41518300	3.81234600	H	1.03101300	0.41511400	3.81237600
H	-2.54648500	-0.32290000	3.32174700	H	2.54644400	-0.32298700	3.32178700
C	-1.71482900	-1.98276900	1.73535500	C	1.71479100	-1.98280700	1.73537000
C	-2.58715800	-1.50087000	0.58990100	C	2.58712100	-1.50088800	0.58991800
O	-2.13316000	-0.55738800	-0.12329200	N	3.76714700	-2.05287700	0.33050200
N	-3.76721100	-2.05282600	0.33052400	C	4.57395800	-1.54902700	-0.78260100
C	-4.57401400	-1.54901500	-0.78259800	H	4.39136800	-0.47862500	-0.92501600
H	-5.63293900	-1.71143800	-0.54369000	H	5.63287300	-1.71161300	-0.54376700
H	-4.39129400	-0.47865700	-0.92516000	H	4.33114800	-2.08669500	-1.71328000
H	-4.33132200	-2.08683700	-1.71322000	C	4.28559400	-3.24354500	1.00341600
C	-4.28568800	-3.24348200	1.00343300	H	3.51721000	-3.72464300	1.61504800
H	-4.61316500	-3.96135500	0.23726700	H	4.61326700	-3.96132700	0.23725100
H	-3.51739000	-3.72447000	1.61525700	H	5.14980700	-2.98302300	1.63331200
H	-5.15004200	-2.98296700	1.63313800	O	2.13314500	-0.55736000	-0.12322200
H	-1.09034800	-2.80332500	1.34685600	H	1.09031500	-2.80336200	1.34685900
H	-2.30105500	-2.36923000	2.58200500	H	2.30102600	-2.36928000	2.58200900
H	0.05731000	-1.69959200	3.89885600	H	-0.05740500	-1.69958200	3.89886600
H	0.74582200	-2.20122800	2.33788800	H	-0.74587400	-2.20124700	2.33788700
H	1.05961900	0.48433000	3.77905100	H	-1.05966900	0.48432300	3.77902900
H	2.31208500	-0.68835100	3.40780100	H	-2.31214400	-0.68833400	3.40772700
C	2.93430000	0.06068200	1.16855700	C	-2.93433500	0.06079000	1.16852800
C	2.71785100	-1.27906800	0.49107600	C	-2.71793600	-1.27900000	0.49110600
O	1.53391800	-1.57563900	0.15164500	O	-1.53402300	-1.57561200	0.15167400
N	3.73182100	-2.10001000	0.24021300	N	-3.73194900	-2.09990700	0.24028300
C	3.48436700	-3.37429900	-0.43664100	C	-5.13712000	-1.76005300	0.45961100
H	2.49299800	-3.75585100	-0.16981100	H	-5.25630600	-0.71185900	0.74703600
H	3.54460900	-3.25060400	-1.52995100	H	-5.68915600	-1.92552300	-0.47758400
H	4.25167200	-4.09101600	-0.11665700	H	-5.56801500	-2.40582800	1.23973900
C	5.13701400	-1.76025500	0.45957600	C	-3.48456400	-3.37423600	-0.43652300
H	5.56786600	-2.40614000	1.23963700	H	-3.54483700	-3.25059000	-1.52983700
H	5.68903800	-1.92566300	-0.47763800	H	-2.49320100	-3.75581500	-0.16970700

H	5.25626100	-0.71210000	0.74711200	H	-4.25188500	-4.09091000	-0.11648100
H	3.73185200	0.02475500	1.92564100	H	-3.73189900	0.02494900	1.92560300
H	3.23694300	0.77717500	0.38838800	H	-3.23691000	0.77726300	0.38831500
H	2.30515200	2.26855900	2.75933900	H	-2.30511500	2.26858500	2.75936200
H	1.98658800	2.41640600	1.01570900	H	-1.98655300	2.41648200	1.01573300
H	-0.03842500	2.18803300	3.30217300	H	0.03841800	2.18795700	3.30221300
H	0.20239500	3.54309100	2.21244000	H	-0.20231500	3.54306700	2.21252300
C	-1.22045100	2.85379900	0.33968100	C	1.22052800	2.85377000	0.33975000
C	-0.14181900	2.93197900	-0.73787600	C	0.14188800	2.93201000	-0.73779900
O	0.02869200	3.96662600	-1.39225300	O	-0.02859000	3.96666600	-1.39216500
O	0.52240800	1.82892500	-0.91744100	O	-0.52235500	1.82897100	-0.91739700
H	-1.42196300	3.85356600	0.75873100	H	1.42207400	3.85352100	0.75882200
H	-2.13773300	2.49848900	-0.15714300	H	2.13779200	2.49843100	-0.15708500
O	-0.00657800	-0.62388400	-1.92130100	O	0.00641700	-0.62393000	-1.92127400
H	-0.15134300	-1.58320900	-1.97036000	H	0.15078500	-1.58332200	-1.97024300

Table S34 Atomic coordinates (x,y,z) of $[Sc(\mathbf{L}^{030})]^{3+}$ isomers.

$[Sc(\mathbf{L}^{030})]^{3+}$ Δ				$[Sc(\mathbf{L}^{030})]^{3+}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.91628900	-1.42532300	1.65767200	N	-1.61538400	-0.08059800	1.74638700
C	-1.69982200	-0.66927100	2.68676200	C	-1.29468000	-1.13731300	2.75983500
C	-2.04044200	0.74149800	2.23195200	C	-0.24704000	-2.12430100	2.26420100
N	-0.83875400	1.43384100	1.68978700	N	0.91857100	-1.41850400	1.66630100
C	0.18220000	1.69750000	2.75675900	C	1.69701000	-0.65592500	2.69436500
C	1.58891700	1.28729200	2.34464500	C	2.03333100	0.75407700	2.23478100
N	1.61309800	-0.07771400	1.75074100	N	0.82973900	1.43908400	1.68752700
C	1.29346700	-1.14040400	2.75810600	C	-0.19538700	1.70312900	2.75072500
C	0.25148100	-2.12892900	2.25398100	C	-1.59980100	1.28646200	2.33559000
H	-0.06385000	-2.78775300	3.08103400	H	-2.27295000	1.34929000	3.20769800
H	0.68182900	-2.75789400	1.46341800	H	-1.98161600	1.96881100	1.56467600
H	0.96189500	-0.65666300	3.68377000	H	0.11115900	1.18486200	3.66591200
H	2.20552100	-1.69845500	3.01378800	H	-0.21054200	2.77524500	2.99435300
C	2.92031500	-0.33219400	1.10235000	C	1.22091000	2.69292700	1.00471900
C	2.72499100	-1.21810900	-0.11000700	C	0.24331900	2.97976800	-0.11421800
O	1.58183400	-1.17177600	-0.68201200	N	-0.02232000	4.20720900	-0.52061900
N	3.69217400	-1.97537700	-0.59207400	C	0.65033600	5.40658900	-0.01538000
C	3.45756900	-2.80997000	-1.77457800	H	0.99107500	5.99882700	-0.87633200
H	2.39898800	-3.08035000	-1.84130900	H	-0.05441800	6.01135300	0.57429900
H	3.75962700	-2.27173300	-2.68648900	H	1.52059300	5.15136900	0.59448400
H	4.06526000	-3.71867000	-1.67829800	C	-0.97590200	4.43298200	-1.61110500
C	5.06189500	-1.98850700	-0.07328800	H	-1.48081400	5.39079500	-1.43155700
H	5.24559300	-1.14785000	0.60079100	H	-0.44727500	4.48202200	-2.57575400
H	5.25750200	-2.93634600	0.44990300	H	-1.71529500	3.62621800	-1.63715100
H	5.75128200	-1.90594300	-0.92520200	O	-0.29802700	1.96770900	-0.68073200
H	3.32426200	0.61982200	0.72442100	H	2.20233100	2.54818700	0.52651700
H	3.64090100	-0.74440800	1.81968300	H	1.30825500	3.51642400	1.72386400
H	2.25918000	1.35066200	3.21892200	H	2.46472100	1.32448900	3.07493900
H	1.96965400	1.97380300	1.57688800	H	2.77786100	0.72326500	1.42816000
H	-0.12541600	1.17502700	3.66926900	H	1.11789500	-0.63184500	3.62321100
H	0.19333900	2.76870800	3.00464800	H	2.63209400	-1.18637900	2.92584300
C	-1.23352100	2.68775900	1.00990100	C	1.78826000	-2.37640900	0.94702900
C	-0.26307800	2.97682800	-0.11495700	C	2.48108500	-1.66167300	-0.19378400
O	0.28732000	1.96757000	-0.67770600	O	1.82464300	-0.72285900	-0.76422800
N	-0.01206900	4.20536500	-0.52731600	N	3.68744900	-1.99840700	-0.61024200
C	0.93373600	4.43922500	-1.62283500	C	4.32705400	-1.25850600	-1.70228300
H	1.67113800	3.63130100	-1.66234400	H	4.15927700	-1.77298700	-2.66110000
H	0.39737900	4.49849200	-2.58262900	H	3.92527600	-0.24177700	-1.75422200
H	1.44210500	5.39442800	-1.43858600	H	5.40566600	-1.21948500	-1.50210600
C	-0.69015900	5.39929400	-0.01638500	C	4.45548900	-3.12894800	-0.08074900
H	-1.03106500	5.99474900	-0.87487400	H	3.81406400	-3.83354400	0.45508400
H	-1.56113400	5.13707600	0.58978700	H	4.91323400	-3.65592900	-0.92883200
H	0.01056300	6.00352000	0.57874300	H	5.25351200	-2.76674500	0.58457800

H	-1.31710800	3.51182900	1.72900500	H	2.48415600	-2.86718300	1.63815900
H	-2.21789100	2.54390000	0.53737900	H	1.15818000	-3.15211300	0.48466400
H	-2.47653500	1.30664500	3.07327900	H	0.06955300	-2.77554400	3.09673900
H	-2.78314400	0.71034400	1.42358800	H	-0.67232600	-2.76117500	1.47732600
H	-1.12349900	-0.64706000	3.61722400	H	-0.96754200	-0.64793400	3.68399500
H	-2.63380000	-1.20378200	2.91351100	H	-2.20555700	-1.69737500	3.01525700
C	-1.78159700	-2.38421000	0.93414100	C	-2.91869700	-0.34626500	1.09417100
C	-2.47651000	-1.66667800	-0.20412500	C	-2.71289100	-1.24935800	-0.10385900
O	-1.81869800	-0.72819600	-0.77422600	O	-1.56943100	-1.19830900	-0.67507900
N	-3.68395800	-1.99769800	-0.62227000	N	-3.67037100	-2.02561500	-0.57480300
C	-4.45739300	-3.13067800	-0.10812200	C	-5.04055800	-2.04679100	-0.05756300
H	-3.83617900	-3.80296400	0.48859800	H	-5.23640900	-1.19510700	0.59927100
H	-5.30141500	-2.76610300	0.49607600	H	-5.72935100	-1.98988600	-0.91203000
H	-4.85228800	-3.69296400	-0.96569500	H	-5.22478300	-2.98671800	0.48370600
C	-4.31096000	-1.25774800	-1.72201200	C	-3.42402600	-2.87563000	-1.74383500
H	-4.10283500	-1.75342300	-2.68288100	H	-3.73049200	-2.35504700	-2.66448300
H	-5.39511200	-1.24897500	-1.55228400	H	-2.36227500	-3.13468500	-1.80445600
H	-3.93412400	-0.23040500	-1.74856000	H	-4.02132500	-3.78971300	-1.63441300
H	-2.47372400	-2.88112400	1.62439700	H	-3.64298500	-0.74948400	1.81290000
H	-1.14747400	-3.15439900	0.46828000	H	-3.32130000	0.59949400	0.69935200

Table S35 Atomic coordinates (x,y,z) of $[ScF(\mathbf{L}^{030})]^{2+}$ isomers.

$[ScF(\mathbf{L}^{030})]^{2+}$ Δ				$[ScF(\mathbf{L}^{030})]^{2+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.02344000	0.01565200	2.45519000	N	0.02088600	0.01248500	2.45713700
C	1.40311900	0.01524600	3.03623400	C	1.39898000	0.03146900	3.04086900
C	2.48785200	0.32426300	2.01366800	C	2.48791700	-0.28041000	2.02346800
N	2.28032300	-0.46234000	0.77710200	N	2.27361100	0.48802500	0.77659500
C	2.52249600	-1.92174300	1.00949000	C	2.50671300	1.95206100	0.99147000
C	1.42836500	-2.81982100	0.44310900	C	1.40641400	2.83808800	0.41794700
N	0.08488200	-2.30607000	0.79621100	N	0.06589900	2.32069700	0.77588300
C	-0.19251900	-2.44134700	2.26165700	C	-0.21319600	2.46513900	2.23971000
C	-0.74555600	-1.16971900	2.89649500	C	-0.76049800	1.19532800	2.88270400
H	-0.71894400	-1.27706300	3.99569300	H	-0.74210700	1.31320400	3.98102900
H	-1.78890900	-1.01239200	2.60157600	H	-1.80069400	1.02696200	2.58212100
H	0.73377300	-2.74403100	2.76257600	H	0.71101400	2.77557200	2.73964600
H	-0.90933100	-3.25934300	2.43139200	H	-0.93419500	3.28076100	2.40314700
C	-0.96247600	-2.98243600	0.01192600	C	-0.98515700	2.98407800	-0.01363600
C	-2.19516100	-2.09878200	0.02091000	C	-2.21061000	2.09065400	-0.00348300
O	-2.01034400	-0.85368900	0.19062200	N	-3.43059000	2.57570800	-0.18983800
N	-3.41177000	-2.59237600	-0.16465000	C	-3.71691600	3.96247700	-0.55782500
C	-4.56614500	-1.69066900	-0.16071600	H	-4.34980900	3.96196500	-1.45736200
H	-4.41204800	-0.88379800	0.56413300	H	-4.25988700	4.46770800	0.25497600
H	-4.72266300	-1.25631800	-1.16104200	H	-2.80049800	4.51414400	-0.78452800
H	-5.45442800	-2.27023000	0.12015000	C	-4.57955600	1.66728800	-0.18305600
C	-3.68880600	-3.98110000	-0.53183400	H	-5.46995500	2.24080200	0.10364800
H	-2.76791000	-4.52930700	-0.74854800	H	-4.73837300	1.23511400	-1.18396400
H	-4.23676200	-4.48640400	0.27752300	H	-4.41727300	0.85929500	0.53868800
H	-4.31367200	-3.98588800	-1.43700000	O	-2.01706800	0.84699300	0.16746000
H	-0.63166600	-3.06799100	-1.03559700	H	-0.65311900	3.06704000	-1.06099200
H	-1.15909600	-3.99445100	0.39378400	H	-1.19078800	3.99638700	0.36257600
H	1.57564800	-3.84661100	0.82323600	H	1.54868100	3.86918800	0.78839200
H	1.48673000	-2.85731500	-0.65079200	H	1.46398400	2.86557400	-0.67628900
H	2.62500500	-2.08686300	2.08799300	H	2.61132800	2.13022000	2.06771900
H	3.48497100	-2.21685500	0.56391100	H	3.46610100	2.24805000	0.53977100
C	3.14271100	0.03977300	-0.30473000	C	3.13983900	-0.02180100	-0.29864600
C	2.55166300	-0.40966100	-1.62483600	C	2.54846100	0.41021600	-1.62450300
O	1.30098700	-0.62285900	-1.65144500	O	1.29714500	0.62007800	-1.65426500
N	3.29824000	-0.55543600	-2.71180700	N	3.29471800	0.54377900	-2.71320400
C	2.68023200	-0.98530300	-3.96777900	C	2.67413400	0.95321800	-3.97485200
H	1.82107600	-1.63222500	-3.76202300	H	2.33683600	0.07193800	-4.54362500
H	2.34925500	-0.11313500	-4.55404900	H	1.81872500	1.60796700	-3.77820600
H	3.42834400	-1.54091500	-4.54798100	H	3.42266000	1.49444100	-4.56779300
C	4.70796200	-0.17451300	-2.80059500	C	4.70506500	0.16407200	-2.79778500
H	4.83270300	0.50875000	-3.65371400	H	5.04403400	-0.33125700	-1.88385800
H	5.04344100	0.34021000	-1.89613400	H	4.82951800	-0.53607300	-3.63721300
H	5.33095000	-1.06565600	-2.96936700	H	5.32541700	1.05309300	-2.98604800

H	4.18430800	-0.28458700	-0.17026400	H	4.17983200	0.30878300	-0.16652700
H	3.12247200	1.14131900	-0.29831800	H	3.12474800	-1.12331000	-0.28014800
H	3.47523300	0.11185100	2.46156600	H	3.47277300	-0.05217600	2.46903000
H	2.47031000	1.38359800	1.73367000	H	2.48114600	-1.34338800	1.75757900
H	1.58636600	-0.96346300	3.49340400	H	1.57297800	1.01712500	3.48673600
H	1.46679400	0.74997400	3.85374200	H	1.46728900	-0.69310400	3.86706200
C	-0.67900000	1.26122100	2.80830400	C	-0.67066700	-1.23602100	2.82039500
C	-0.14739200	2.36324500	1.91378100	C	-0.12492200	-2.34142500	1.93823000
O	0.29165400	2.01362900	0.77294300	O	0.32163500	-1.99736700	0.79866600
N	-0.15438900	3.63785700	2.27718700	N	-0.12830000	-3.61339500	2.31105000
C	-0.79204100	4.14994300	3.49004000	C	-0.77636100	-4.11958300	3.52080900
H	-1.26361100	3.34794600	4.06379700	H	-1.24986800	-3.31438800	4.08843300
H	-0.04554700	4.65815200	4.11784900	H	-1.55048500	-4.84616700	3.23140800
H	-1.56648300	4.87729700	3.20368900	H	-0.03569900	-4.62735500	4.15577600
C	0.34906500	4.64956100	1.34381000	C	0.38526300	-4.63010600	1.38880400
H	-0.41982900	4.90697800	0.59820000	H	-0.38005400	-4.90085100	0.64417200
H	0.60722600	5.54764900	1.91757600	H	1.27531900	-4.25504000	0.87095900
H	1.24095500	4.27644400	0.82756900	H	0.64901100	-5.52059900	1.97187700
H	-0.58093600	1.48843200	3.87885000	H	-0.57345300	-1.45231100	3.89334300
H	-1.75009200	1.14822700	2.57663300	H	-1.74216700	-1.13568600	2.58493800
F	-0.86649700	0.96325100	-1.44547000	F	-0.84991100	-0.99532400	-1.43256700

Table S36 Atomic coordinates (x,y,z) of $[Sc(OH_2)(\mathbf{L^{030}})]^{3+}$ isomers.

$[Sc(OH_2)(\mathbf{L^{030}})]^{3+}$ Δ				$[Sc(OH_2)(\mathbf{L^{030}})]^{3+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.39568200	N	-1.65745800	-0.00591800	1.70877700
C	1.38091800	0.00000000	2.98181400	C	-1.39652600	-1.07482900	2.73392900
C	2.45765500	0.33496100	1.96149500	C	-0.36628900	-2.10629300	2.28540800
N	2.24628200	-0.43352400	0.70933100	N	0.82633400	-1.43352200	1.70573600
C	2.50149900	-1.89843400	0.91328000	C	1.60183800	-0.68244900	2.75274900
C	1.40704500	-2.78621300	0.33450200	C	1.98725400	0.72976000	2.32396100
N	0.06300900	-2.28002500	0.71014000	N	0.81652500	1.42573600	1.72968100
C	-0.21080600	-2.45376800	2.17398300	C	-0.23083700	1.71422700	2.76813900
C	-0.76579100	-1.19522600	2.82946500	C	-1.64106900	1.34928800	2.32012300
H	-0.73056100	-1.31085500	3.92645000	H	-2.32318200	1.40573300	3.18517200
H	-1.81088100	-1.03750100	2.54126600	H	-2.00560800	2.05286200	1.56292300
H	0.71700700	-2.76534900	2.66586900	H	0.03122900	1.16468300	3.67825900
H	-0.92600800	-3.27607100	2.32334200	H	-0.20601600	2.77882100	3.04233700
C	-0.98965400	-2.93283000	-0.09326800	C	1.21990800	2.67278000	1.04390300
C	-2.20399700	-2.02664100	-0.10333600	C	0.15990900	2.99037400	0.00247500
N	-3.41741100	-2.47981000	-0.36761800	N	-0.03852000	4.20657000	-0.46393200
C	-3.70620400	-3.85081100	-0.79058500	C	0.75386000	5.37557200	-0.07578000
H	-4.24663300	-3.81403000	-1.74788000	H	1.10275400	5.87540800	-0.99010600
H	-4.34276400	-4.34792900	-0.04413900	H	0.12648500	6.07386100	0.49719800
H	-2.78874600	-4.42797200	-0.93311900	H	1.62602000	5.09062700	0.51785600
C	-4.54980700	-1.55002800	-0.40703100	C	-1.07122800	4.45668300	-1.47550900
H	-5.46176200	-2.10864900	-0.16236600	H	-1.63845200	5.34944900	-1.17883900
H	-4.65428200	-1.11543500	-1.41382000	H	-0.59402200	4.64054300	-2.44987300
H	-4.40350500	-0.74734500	0.32341400	H	-1.73754500	3.59267700	-1.54387000
O	-1.99710300	-0.78795000	0.11966300	O	-0.51731800	1.99450100	-0.42272200
H	-0.64535300	-3.02049700	-1.13624700	H	2.16590700	2.49825600	0.50738200
H	-1.21118700	-3.94200800	0.28018600	H	1.38361600	3.48892800	1.75997000
H	1.55475500	-3.82100400	0.68883300	H	2.38055400	1.27842400	3.19617500
H	1.45722000	-2.79539900	-0.76065800	H	2.77494700	0.70778700	1.56226300
H	2.61236300	-2.08241000	1.98761300	H	1.00060300	-0.65194400	3.66739600
H	3.46147600	-2.17645500	0.45354700	H	2.51390400	-1.23862200	3.01234300
C	3.10002000	0.10145700	-0.36766600	C	1.71040700	-2.39944900	1.01716300
C	2.47626900	-0.25925900	-1.69821000	C	2.52589700	-1.62491700	-0.00483300
O	1.22480400	-0.50039400	-1.69901200	O	1.99968900	-0.54143700	-0.42873400
N	3.17582000	-0.28045800	-2.82035600	N	3.69023700	-2.04720700	-0.45523600
C	2.49905800	-0.55664500	-4.09087400	C	4.42937200	-1.26709700	-1.45387500
H	2.06543200	0.36834600	-4.50302200	H	4.35929700	-1.76394000	-2.43333500
H	1.70462700	-1.29582600	-3.94261300	H	4.01290100	-0.25829500	-1.51657000
H	3.24082500	-0.94995400	-4.79650600	H	5.48340600	-1.22275900	-1.14780200
C	4.57237400	0.14381400	-2.92557400	C	4.31666000	-3.31164100	-0.06241100
H	4.97670900	0.44005800	-1.95418000	H	3.63698400	-3.93148900	0.52732800
H	4.63096800	1.00440900	-3.60896200	H	4.58754100	-3.86163000	-0.97434800
H	5.17740500	-0.67649400	-3.33761800	H	5.22892300	-3.10648000	0.51641400

H	4.13472300	-0.25363700	-0.26950700	H	2.32695300	-2.95647300	1.73449200
H	3.10842900	1.20127100	-0.30555400	H	1.09506900	-3.12721500	0.46476400
H	3.44948100	0.11948500	2.39535200	H	-0.09075700	-2.74049400	3.14456900
H	2.43114900	1.39883400	1.69928700	H	-0.78080900	-2.76014900	1.50917500
H	1.56988500	-0.98554100	3.42066800	H	-1.06966900	-0.58760500	3.65868800
H	1.43594700	0.72174800	3.81046000	H	-2.33374300	-1.59262500	2.98379500
C	-0.71566600	1.23792000	2.75547000	C	-2.93925200	-0.25841100	1.01511100
C	-0.23059500	2.34704800	1.84503200	C	-2.69258700	-1.32532900	-0.03606300
O	0.21228700	1.99897900	0.69880800	O	-1.49794500	-1.40197000	-0.48138200
N	-0.28727500	3.61436300	2.21188000	N	-3.64817000	-2.11143100	-0.48869800
C	-0.88321700	4.06178900	3.47451900	C	-5.04923200	-2.02747100	-0.06824600
H	-1.60506800	3.33314600	3.85551500	H	-5.25073400	-1.10158200	0.47663600
H	-1.41622800	5.00231800	3.28269900	H	-5.67929700	-2.04386400	-0.96796900
H	-0.10142500	4.24340200	4.22745800	H	-5.30092900	-2.89369200	0.56117700
C	0.21923000	4.67230000	1.33509700	C	-3.35682500	-3.13163200	-1.50168000
H	-0.61531200	5.16274200	0.81064700	H	-3.78503400	-2.82267200	-2.46704800
H	0.91794700	4.25131900	0.60581100	H	-2.27521200	-3.25892800	-1.59645500
H	0.73604800	5.41669500	1.95583600	H	-3.82318700	-4.07532700	-1.18715400
H	-0.59522900	1.47478900	3.82120600	H	-3.73202900	-0.52331700	1.72685600
H	-1.78981300	1.10257000	2.55175700	H	-3.24904200	0.65767200	0.48794400
O	-0.97841000	1.06897600	-1.76610300	O	0.12084800	-0.08167400	-2.24214000
H	-0.96713500	0.49167000	-2.54987600	H	0.93686700	0.24360800	-2.65778400
H	-1.92294700	1.24141000	-1.60562000	H	-0.60853800	0.25069200	-2.79114400

Table S37 Atomic coordinates (x,y,z) of $[Sc(OH)(\mathbf{L}^{\mathbf{030}})]^{2+}$ isomers.

$[Sc(OH)(\mathbf{L}^{\mathbf{030}})]^{2+}$ Δ				$[Sc(OH)(\mathbf{L}^{\mathbf{030}})]^{2+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	1.42631500	0.85217400	1.80043300	N	1.43140600	-0.83786300	1.79700000
C	1.74909600	-0.18951000	2.82640900	C	1.75423300	0.20855000	2.81845800
C	1.38189400	-1.60863200	2.39888100	C	1.38276200	1.62523900	2.38737700
N	0.02213000	-1.64827100	1.81776800	N	0.02278100	1.65922100	1.80567100
C	-1.02270100	-1.40604300	2.86055300	C	-1.02210200	1.41618400	2.84912500
C	-2.07596800	-0.38629300	2.44379800	C	-2.07188800	0.39246300	2.43330600
N	-1.44411500	0.79937300	1.82300900	N	-1.43610400	-0.79425400	1.81710500
C	-0.69303500	1.60281900	2.83935500	C	-0.68622400	-1.59668400	2.83643200
C	0.70627400	2.00306300	2.38908400	C	0.71790200	-1.98965700	2.39301300
H	1.25447000	2.41878300	3.25397100	H	1.26677600	-2.39496700	3.26222100
H	0.65540600	2.78193900	1.61899200	H	0.67427700	-2.77488900	1.62922900
H	-0.63968700	1.02039100	3.76629700	H	-0.64109100	-1.01740500	3.76564500
H	-1.25657600	2.51616300	3.08556800	H	-1.24713600	-2.51323300	3.07656400
C	-2.45302800	1.63114600	1.14774900	C	-2.44252100	-1.62997000	1.14220000
C	-1.74733200	2.49287300	0.12005500	C	-1.72889000	-2.50280800	0.12948800
O	-0.65157800	2.05414100	-0.34945400	N	-2.23721700	-3.65934000	-0.27390500
N	-2.26144400	3.64496600	-0.28759300	C	-3.56474700	-4.14801500	0.09836600
C	-1.54695800	4.46407900	-1.26824600	H	-4.11420400	-4.40116200	-0.82022200
H	-0.47056600	4.27493900	-1.20267400	H	-3.47664400	-5.05369000	0.71712700
H	-1.89753900	4.23881500	-2.28804400	H	-4.13386100	-3.38810500	0.64055000
H	-1.74907700	5.52053000	-1.04810300	C	-1.51762000	-4.46888300	-1.25921400
C	-3.58241300	4.13538000	0.10736900	H	-1.76590400	-5.52375000	-1.08542100
H	-4.17948800	3.34615300	0.57257400	H	-1.82130600	-4.19403700	-2.28198500
H	-3.48624700	4.98472200	0.80081800	H	-0.43776300	-4.32354800	-1.14954600
H	-4.10889400	4.47576300	-0.79559700	O	-0.62905800	-2.06880600	-0.33482700
H	-3.14903100	0.97680400	0.59906800	H	-3.13262000	-0.97930700	0.58175000
H	-3.03572600	2.22253000	1.86898300	H	-3.03147100	-2.21263800	1.86508800
H	-2.66938000	-0.10178400	3.33141900	H	-2.66748900	0.10974700	3.31990700
H	-2.76238800	-0.81676600	1.70726700	H	-2.75700700	0.81885900	1.69302300
H	-0.52280600	-1.07944200	3.77934700	H	-0.52289300	1.09191200	3.76882400
H	-1.52767300	-2.35200500	3.10986000	H	-1.52999500	2.36117900	3.09656100
C	-0.23284500	-2.92044900	1.12214700	C	-0.23588700	2.92933500	1.10839600
C	-1.38619400	-2.70234600	0.15892000	C	-1.38738100	2.70533200	0.14442100
O	-1.57933500	-1.51875700	-0.25315400	O	-1.57487000	1.52094900	-0.26814800
N	-2.14974300	-3.70601600	-0.25580100	N	-2.15236700	3.70814900	-0.26972300
C	-3.23234200	-3.44438200	-1.20675000	C	-3.24066500	3.44877600	-1.21422300
H	-3.67251000	-2.45965300	-1.01533900	H	-2.87922900	3.52490300	-2.25228300
H	-2.85667200	-3.47969600	-2.24197800	H	-3.65373300	2.44820100	-1.04711700
H	-3.99846200	-4.21949100	-1.07919000	H	-4.02416000	4.20046100	-1.05420900
C	-1.89478300	-5.11445600	0.04260600	C	-1.90837700	5.11486300	0.04739000
H	-1.80714300	-5.66638700	-0.90519100	H	-0.94891100	5.25108900	0.55364800
H	-0.96522000	-5.24402600	0.60334800	H	-1.88703700	5.68736500	-0.89150400
H	-2.73223600	-5.53545100	0.61866900	H	-2.71764000	5.50827100	0.68095200

H	-0.42164300	-3.73898800	1.83178000	H	-0.42907800	3.74788300	1.81678600
H	0.65024500	-3.18604500	0.51930500	H	0.64691000	3.19759300	0.50620500
H	1.46248100	-2.27755000	3.27469100	H	1.46139300	2.29611700	3.26194900
H	2.07716900	-1.97374500	1.63474000	H	2.07650100	1.99127700	1.62247200
H	1.23524200	0.07308400	3.75828900	H	1.24217400	-0.05060800	3.75192800
H	2.82545200	-0.16271100	3.05635600	H	2.83078700	0.18405700	3.04752200
C	2.65201400	1.29461300	1.11798600	C	2.65632800	-1.27798400	1.11169900
C	3.04459400	0.21684500	0.12636300	C	3.04442700	-0.19931900	0.11931000
O	2.11399500	-0.52529200	-0.31301900	O	2.11322400	0.54420700	-0.31525500
N	4.29744800	0.06788900	-0.28427200	N	4.29721100	-0.05160700	-0.29249700
C	5.38832100	0.98108700	0.05542200	C	5.38666900	-0.96582300	0.05002100
H	5.02938600	1.83622100	0.63446300	H	5.01443900	-1.85906100	0.55917900
H	6.16135200	0.44850400	0.62926500	H	5.88393900	-1.28165500	-0.87872900
H	5.83739700	1.35719700	-0.87593600	H	6.12425800	-0.45764600	0.68940400
C	4.62216600	-0.97094500	-1.26423100	C	4.62916500	1.00022900	-1.25551700
H	4.48104200	-0.59409700	-2.28985500	H	4.51457300	0.63173200	-2.28744800
H	5.67374100	-1.25396100	-1.12975800	H	3.97789500	1.86799300	-1.10562000
H	3.98458800	-1.84810500	-1.10939900	H	5.67427300	1.29493500	-1.09629400
H	3.45261300	1.52353800	1.83527900	H	3.45877500	-1.50472100	1.82804500
H	2.43557600	2.20823700	0.54150000	H	2.44022600	-2.19222300	0.53613800
O	0.06882500	-0.13126800	-2.00166600	O	0.07232000	0.10398000	-2.00198000
H	-0.81649200	-0.04386900	-2.39198600	H	-0.79904600	-0.06907400	-2.39528700

Table S38 Atomic coordinates (x,y,z) of [Sc($\mathbf{L}^{201}$)] isomers.

[Sc($\mathbf{L}^{201}$)] Δ				[Sc($\mathbf{L}^{201}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.44231500	0.47283900	-2.30601600	N	0.44670300	0.47693000	-2.30343600
C	-1.88196000	0.36824900	-2.69772600	C	1.88673600	0.37011300	-2.69280300
C	-2.82415200	0.24001700	-1.50262000	C	2.82675300	0.23792500	-1.49635000
N	-2.28364900	-0.71910400	-0.51344200	N	2.28234900	-0.72167300	-0.50983600
C	-2.36445700	-2.11394800	-1.03911300	C	2.36212700	-2.11580800	-1.03769200
C	-1.08389300	-2.90752100	-0.85129400	C	1.08001700	-2.90800300	-0.85358900
N	0.11560300	-2.15727700	-1.29768900	N	-0.11761200	-2.15460700	-1.29977700
C	0.11697300	-1.89285700	-2.76877300	C	-0.11722300	-1.88734600	-2.77047300
C	0.41433600	-0.43571400	-3.09938400	C	-0.41077400	-0.42883500	-3.09899800
H	0.28089100	-0.26948500	-4.18364700	H	-0.27566900	-0.26158700	-4.18291100
H	1.45891600	-0.19648000	-2.85452400	H	-1.45512300	-0.18761100	-2.85510400
H	-0.85163800	-2.19348000	-3.18553000	H	0.85073600	-2.18981400	-3.18741500
H	0.87119400	-2.52321000	-3.26279900	H	-0.87291600	-2.51478200	-3.26595000
C	1.32811000	-2.91233100	-0.91658000	C	-1.33179400	-2.90841300	-0.92101900
C	2.49670500	-1.98546600	-0.76196000	C	-2.49957800	-1.98075300	-0.76546400
C	3.81280300	-2.30013000	-1.10609600	C	-3.81624900	-2.29507500	-1.10768500
C	4.82003600	-1.37340600	-0.83032100	C	-4.82302400	-1.36847800	-0.82981800
C	4.49357000	-0.16954800	-0.19950500	C	-4.49546300	-0.16486900	-0.19921800
C	3.15858800	0.06702900	0.11088700	C	-3.15996600	0.07139000	0.10913600
N	2.18778900	-0.81435600	-0.18543300	C	-2.66478900	1.29617600	0.83842900
C	2.66446800	1.29243800	0.84007800	O	-3.45506000	2.19444400	1.15866900
O	3.45586500	2.18979500	1.16015900	O	-1.39474000	1.28065100	1.08157100
O	1.39463200	1.27758100	1.08503600	N	-2.18966400	-0.80997500	-0.18877200
H	5.24701700	0.57524800	0.05306800	H	-5.24842500	0.57985500	0.05504400
H	5.85477100	-1.59136600	-1.09962000	H	-5.85821300	-1.58640200	-1.09738300
H	4.03564800	-3.25450500	-1.58361400	H	-4.04005100	-3.24935200	-1.58494700
H	1.14868900	-3.37533700	0.06655800	H	-1.15380500	-3.37318900	0.06154800
H	1.54545800	-3.72278300	-1.62981200	H	-1.54955000	-3.71748400	-1.63567800
H	-1.17582300	-3.86736600	-1.39229200	H	1.17103800	-3.86666300	-1.39677800
H	-0.93455800	-3.13850900	0.21168900	H	0.92869700	-3.14129900	0.20859500
H	-2.62955000	-2.07132900	-2.10191700	H	2.62909800	-2.07174900	-2.09993900
H	-3.18422000	-2.65475100	-0.54099500	H	3.18034800	-2.65855800	-0.53913600
C	-2.95733700	-0.60594100	0.79180400	C	2.95249800	-0.61141900	0.79753600
C	-2.04611400	-1.07862300	1.92031400	C	2.03768500	-1.08500000	1.92296200
O	-2.50282100	-1.58650700	2.94528200	O	2.49147200	-1.59247600	2.94932800
O	-0.77426200	-0.84071100	1.72422300	O	0.76597700	-0.84730300	1.72344900
H	-3.91559300	-1.14859600	0.81894900	H	3.91006300	-1.15519000	0.82655900
H	-3.15927600	0.45859300	0.99128200	H	3.15494500	0.45259300	0.99923400
H	-3.82013100	-0.07743000	-1.86093200	H	3.82250900	-0.08126300	-1.85368600
H	-2.93952300	1.20410900	-0.99859400	H	2.94369100	1.20093300	-0.99062500
H	-1.99680100	-0.49220800	-3.36627200	H	2.00105800	-0.48940000	-3.36265600
H	-2.17221400	1.25260900	-3.28567100	H	2.17971500	1.25490300	-3.27878900

C	0.00953100	1.87301300	-2.38593100	C	-0.00258200	1.87811000	-2.38092700
C	-0.58730200	2.66396900	-1.22292600	C	0.59510000	2.66589900	-1.21610400
O	-0.75314900	3.88646900	-1.30578900	O	0.76533400	3.88799000	-1.29739000
O	-0.85330100	1.94705900	-0.17450900	O	0.85714900	1.94688900	-0.16824100
H	-0.23824500	2.34328400	-3.35115500	H	0.24674700	2.34958500	-3.34518700
H	1.10500400	1.89844800	-2.25904400	H	-1.09808100	1.90523700	-2.25464600

.

Table S39 Atomic coordinates (x,y,z) of ScF($\mathbf{L}^{201}$)]$^-$ isomers.

[ScF($\mathbf{L}^{201}$)]$^-$ Δ				ScF($\mathbf{L}^{201}$)]$^-$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.55952200	0.93090000	2.27008800	N	-0.55950000	0.93092600	2.27007800
C	1.94412500	0.77885100	2.78564100	C	-1.94410200	0.77888600	2.78563900
C	2.93714800	0.48152200	1.67130000	C	-2.93713000	0.48156800	1.67130300
N	2.42506100	-0.63555900	0.86923100	N	-2.42504900	-0.63551100	0.86922600
C	2.45319600	-1.88977700	1.66074700	C	-2.45319900	-1.88973800	1.66073900
C	1.17401300	-2.70327000	1.56499900	C	-1.17402200	-2.70323900	1.56499700
N	-0.06113600	-1.88709500	1.66090700	N	0.06113300	-1.88707200	1.66089600
C	-0.25112100	-1.30723800	3.03443400	C	0.25112800	-1.30721500	3.03442600
C	-0.43623700	0.21823600	3.09184800	C	0.43625800	0.21825900	3.09184000
H	-0.39329000	0.52386100	4.15522600	H	0.39331300	0.52388800	4.15521600
H	-1.42736600	0.49478300	2.70807400	H	1.42738500	0.49480000	2.70806100
H	0.60692400	-1.60192200	3.65293000	H	-0.60692000	-1.60189300	3.65292000
H	-1.13530800	-1.76256000	3.50595000	H	1.13531100	-1.76254700	3.50593900
C	-1.18110000	-2.78505200	1.30531500	C	1.18109200	-2.78503700	1.30530600
C	-2.42778400	-2.00632400	1.02265900	C	2.42778000	-2.00631600	1.02264800
C	-3.71645700	-2.51978800	1.20011900	C	3.71645200	-2.51978300	1.20009900
C	-4.80810300	-1.71844200	0.86997500	H	3.84934800	-3.52816100	1.59332700
C	-4.58335800	-0.41734200	0.41116600	C	4.80809800	-1.71843400	0.86995900
C	-3.26984700	0.02673300	0.29379600	C	4.58335500	-0.41733300	0.41115700
N	-2.21810300	-0.76799900	0.56088300	C	3.26984200	0.02674400	0.29379000
C	-2.90895000	1.44999400	-0.05885400	C	2.90894100	1.44999500	-0.05887500
O	-3.80209100	2.21585900	-0.48246200	O	3.80208700	2.21586400	-0.48247700
O	-1.68845400	1.74789900	0.14901400	O	1.68844400	1.74790000	0.14898600
H	-5.40091300	0.26067200	0.17006600	N	2.21810100	-0.76798600	0.56088000
H	-5.82531000	-2.09509700	0.99047500	H	5.40091300	0.26067800	0.17005700
H	-3.84935100	-3.52816200	1.59335800	H	5.82530400	-2.09509400	0.99045400
H	-0.89925900	-3.32615600	0.38858600	H	0.89924700	-3.32614400	0.38857900
H	-1.36031800	-3.54062900	2.08987800	H	1.36030900	-3.54061300	2.08987000
H	1.18486800	-3.47689700	2.35573000	H	-1.18488200	-3.47686000	2.35573400
H	1.13246300	-3.22184300	0.60159000	H	-1.13248000	-3.22182000	0.60159300
H	2.65757900	-1.64356200	2.70862800	H	-2.65759200	-1.64352800	2.70861900
H	3.29088500	-2.52920600	1.33334300	H	-3.29088800	-2.52916000	1.33332200
C	3.11631000	-0.80178000	-0.40762200	C	-3.11631400	-0.80172800	-0.40762100
C	2.26383100	-1.65929300	-1.34124500	C	-2.26386100	-1.65928700	-1.34122300
O	2.80168900	-2.36865500	-2.20786200	O	-2.80174200	-2.36866000	-2.20782000
O	0.98942000	-1.55393500	-1.16602700	O	-0.98944600	-1.55392500	-1.16604000
H	4.12209300	-1.24620900	-0.29937300	H	-4.12211300	-1.24611200	-0.29935700
H	3.22675900	0.18654000	-0.88259900	H	-3.22672600	0.18659000	-0.88261300
H	3.92680400	0.25388500	2.11314100	H	-3.92678500	0.25393000	2.11314600
H	3.05900100	1.34900900	1.01316600	H	-3.05898500	1.34905700	1.01317300
H	1.96040200	-0.02457200	3.53021600	H	-1.96038200	-0.02453900	3.53021100
H	2.25087700	1.69282500	3.31903700	H	-2.25084100	1.69286100	3.31904100

C 0.29053000 2.35757900 2.05237800	C -0.29050800 2.35760000 2.05235200
C 0.85672900 2.80012200 0.69743600	C -0.85670700 2.80012800 0.69740800
O 1.11108900 3.99697800 0.49779400	O -1.11105500 3.99698300 0.49774700
O 1.01180400 1.86396600 -0.18908300	O -1.01180300 1.86395700 -0.18909500
H 0.71202600 2.99023300 2.85100500	H -0.71199700 2.99026400 2.85097700
H -0.79125600 2.52759400 2.00877200	H 0.79127800 2.52761900 2.00874500
F -0.76589800 0.21803500 -1.78890100	F 0.76592100 0.21800400 -1.78890000

Table S40 Atomic coordinates (x,y,z) of [Sc(OH_2)($\mathbf{L}^{201}$)] isomers.

[Sc(OH_2)($\mathbf{L}^{201}$)] Δ				[Sc(OH_2)($\mathbf{L}^{201}$)] Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.38761600	0.80714300	-2.25036900	N	0.38761200	0.80714300	-2.25037600
C	-1.76491100	0.70929600	-2.81452900	C	1.76490500	0.70930300	-2.81453800
C	-2.81581600	0.49202200	-1.73599300	C	2.81581200	0.49203100	-1.73600300
N	-2.36504000	-0.59074000	-0.84861400	N	2.36504100	-0.59073100	-0.84862400
C	-2.41366900	-1.89281400	-1.56303400	C	2.41367100	-1.89280700	-1.56304200
C	-1.16852100	-2.73683100	-1.36262100	C	1.16852500	-2.73682600	-1.36262400
N	0.08842800	-1.95731600	-1.49062700	N	-0.08842400	-1.95731300	-1.49063000
C	0.33006600	-1.48667900	-2.89877700	C	-0.33006300	-1.48668000	-2.89878200
C	0.58828900	0.02059500	-3.03366300	C	-0.58829000	0.02059200	-3.03367000
H	0.55879600	0.28486700	-4.10683100	H	-0.55879700	0.28486300	-4.10683900
H	1.58823300	0.27432400	-2.65860600	H	-1.58823500	0.27432000	-2.65861600
H	-0.52985800	-1.77940200	-3.51378900	H	0.52986400	-1.77940000	-3.51379100
H	1.19856200	-2.01426700	-3.32010700	H	-1.19855600	-2.01427300	-3.32011200
C	1.18734600	-2.84382100	-1.04291000	C	-1.18734100	-2.84381900	-1.04290900
C	2.43895300	-2.05017100	-0.83859200	C	-2.43894800	-2.05016800	-0.83859500
C	3.72811400	-2.54941300	-1.04001000	C	-3.72810900	-2.54941100	-1.04001500
C	4.81721300	-1.71257400	-0.79715200	H	-3.86481800	-3.57401600	-1.38663600
C	4.58805600	-0.39763800	-0.38398300	C	-4.81720800	-1.71257100	-0.79716000
C	3.27254200	0.02329200	-0.21825300	C	-4.58805200	-0.39763500	-0.38399100
N	2.22576200	-0.79479400	-0.42319600	C	-3.27253900	0.02329500	-0.21825900
C	2.89668400	1.42955000	0.17153200	C	-2.89668300	1.42955200	0.17153100
O	3.79035700	2.26548200	0.40012700	O	-3.79035700	2.26548500	0.40011800
O	1.63420800	1.64160300	0.22359200	O	-1.63420800	1.64160400	0.22360500
H	5.40156100	0.30302800	-0.20139900	N	-2.22575900	-0.79479000	-0.42320100
H	5.83530300	-2.07674700	-0.94408000	H	-5.40155900	0.30303000	-0.20140900
H	3.86482300	-3.57401800	-1.38663200	H	-5.83529800	-2.07674400	-0.94409000
H	0.89286100	-3.28510800	-0.07799900	H	-0.89285600	-3.28510000	-0.07799600
H	1.35159000	-3.67204100	-1.75220100	H	-1.35158300	-3.67204200	-1.75219700
H	-1.17850100	-3.57105100	-2.08767400	H	1.17850400	-3.57104700	-2.08767700
H	-1.16508900	-3.17402500	-0.35784800	H	1.16509500	-3.17401900	-0.35785100
H	-2.56482100	-1.70334800	-2.63169300	H	2.56481900	-1.70334200	-2.63170200
H	-3.28786700	-2.47718300	-1.23139800	H	3.28787100	-2.47717400	-1.23140700
C	-3.10730700	-0.64804500	0.41204500	C	3.10731000	-0.64803300	0.41203500
C	-2.29729300	-1.41368500	1.45261900	C	2.29730000	-1.41367100	1.45261300
O	-2.85493600	-2.02072500	2.37463600	O	2.85494800	-2.02070300	2.37463300
O	-1.00908300	-1.33869800	1.30144200	O	1.00909100	-1.33869500	1.30143400
H	-4.10823900	-1.09925700	0.30101700	H	4.10824200	-1.09924400	0.30100600
H	-3.23239800	0.37692000	0.79587500	H	3.23240100	0.37693300	0.79586200
H	-3.78477700	0.25285200	-2.21310000	H	3.78477400	0.25286300	-2.21311200
H	-2.95502100	1.39476400	-1.13274800	H	2.95501600	1.39477400	-1.13276000
H	-1.79083900	-0.11448700	-3.53582900	H	1.79083600	-0.11447900	-3.53584000
H	-2.00009100	1.62190600	-3.38364800	H	2.00008100	1.62191500	-3.38365500

C	-0.03941000	2.22777700	-2.07846000	C	0.03940300	2.22777600	-2.07846700
C	-0.68757900	2.76501400	-0.79572400	C	0.68757400	2.76501300	-0.79573200
O	-0.88306700	3.97805400	-0.65645000	O	0.88306000	3.97805300	-0.65645700
O	-0.97473000	1.86694000	0.10182700	O	0.97472700	1.86693900	0.10181900
H	-0.34544000	2.84014800	-2.94175000	H	0.34543000	2.84014800	-2.94175800
H	1.04635200	2.32599900	-1.95019400	H	-1.04635800	2.32599500	-1.95019900
O	0.86540400	0.12504300	2.18529100	O	-0.86540600	0.12502700	2.18528700
H	1.08180900	1.05931100	2.34560300	H	-1.08182700	1.05929200	2.34560100
H	0.11883800	-0.08382600	2.77171800	H	-0.11884400	-0.08383300	2.77172200

Table S41 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{201})]$^{-}$ isomers.

[Sc(OH)(**L**^{201})]$^{-}$ Δ				[Sc(OH)(**L**^{201})]$^{-}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.04717500	-1.89760800	-1.64816800	N	-0.04813700	-1.89696700	-1.64826900
C	-1.23784500	-2.63245200	-1.59617700	C	1.23656900	-2.63241200	-1.59701600
C	-2.44158000	-1.72407000	-1.78143300	C	2.44069600	-1.72445300	-1.78185600
N	-2.35833000	-0.46365100	-1.00134700	N	2.35812600	-0.46421700	-1.00134000
C	-2.73674400	0.68373900	-1.83782400	C	2.73725100	0.68311900	-1.83761300
C	-1.67054700	0.90411500	-2.90438700	C	1.67121500	0.90415700	-2.90430700
N	-0.29565400	0.92576500	-2.33992900	N	0.29644700	0.92656300	-2.33991600
C	0.65555900	0.11167500	-3.11676700	C	-0.65555900	0.11308800	-3.11639400
C	0.33902600	-1.38755300	-3.02881000	C	-0.34015300	-1.38642300	-3.02875600
H	-0.51858400	-1.62537400	-3.67108000	H	0.51704700	-1.62474600	-3.67139500
H	1.19493700	-1.93465100	-3.45355000	H	-1.19666900	-1.93275400	-3.45326000
H	0.66644700	0.39632300	-4.18693000	H	-0.66675100	0.39771600	-4.18656700
H	1.65599600	0.31264200	-2.71274000	H	-1.65569900	0.31469900	-2.71194600
C	0.12333500	2.31755800	-2.13510300	C	-0.12166100	2.31835100	-2.13398400
C	-0.49833000	2.86458900	-0.84628000	C	0.50064700	2.86437300	-0.84498900
O	-0.65700900	4.08645600	-0.70415100	O	0.66040300	4.08610500	-0.70251200
O	-0.80012100	1.98070100	0.05361500	O	0.80178000	1.97998000	0.05449100
H	-0.14245900	2.96868700	-2.98491600	H	0.14425000	2.96992700	-2.98343800
H	1.21057900	2.35212300	-1.99076400	H	-1.20885000	2.35340100	-1.98935300
H	-1.73150900	0.11657000	-3.66408600	H	1.73174300	0.11658400	-3.66400700
H	-1.87606200	1.84983800	-3.43151700	H	1.87734900	1.84979700	-3.43138000
H	-3.71629300	0.52713800	-2.32973100	H	3.71672600	0.52599900	-2.32947900
H	-2.82738000	1.56145700	-1.18859500	H	2.82833500	1.56076400	-1.18834900
C	-3.13542600	-0.55923300	0.23435100	C	3.13500900	-0.56046100	0.23446000
C	-2.40979400	-1.46472500	1.22868400	C	2.40919700	-1.46573500	1.22895000
O	-3.04814700	-2.10985700	2.07519800	O	3.04754800	-2.10975400	2.07631400
O	-1.12134000	-1.46619800	1.12284700	O	1.12074500	-1.46838100	1.12230500
H	-4.16412900	-0.92592500	0.06918200	H	4.16356600	-0.92760400	0.06925700
H	-3.19681300	0.44144800	0.69224700	H	3.19701000	0.44012000	0.69251000
H	-2.55397500	-1.47538200	-2.84259700	H	2.55320900	-1.47551200	-2.84295900
H	-3.34978200	-2.28539500	-1.50377000	H	3.34857300	-2.28636500	-1.50435300
H	-1.26291800	-3.42232000	-2.37034300	H	1.26108200	-3.42171400	-2.37177400
H	-1.28229900	-3.12845800	-0.62108400	H	1.28096800	-3.12912200	-0.62228300
C	1.09820200	-2.82657700	-1.18956000	C	-1.09923600	-2.82573500	-1.18934900
C	2.38888200	-2.10112600	-0.96199700	C	-2.38969600	-2.10002800	-0.96155100
C	3.63301800	-2.69542400	-1.18992400	C	-3.63411700	-2.69382000	-1.18935600
C	4.78691500	-1.95524500	-0.94203100	H	-3.68345900	-3.71700900	-1.56304500
C	4.65776100	-0.63636900	-0.50542700	C	-4.78763200	-1.95315000	-0.94119700
C	3.38083700	-0.10887200	-0.32119600	C	-4.65784900	-0.63426900	-0.50478100
N	2.26571500	-0.83997400	-0.51807400	C	-3.38070300	-0.10733500	-0.32083900
C	3.18419000	1.34350300	0.06268800	C	-3.18298700	1.34485400	0.06284500
O	4.19973700	2.02519200	0.33194100	O	-4.19804200	2.02762600	0.33115800

O	1.97917400	1.75110500	0.06048900	O	-1.97752500	1.75104500	0.06160000
H	5.52259100	-0.00081600	-0.32328400	N	-2.26593900	-0.83901000	-0.51761100
H	5.77292700	-2.39284500	-1.10748800	H	-5.52242300	0.00161100	-0.32247600
H	3.68188800	-3.71861400	-1.56367700	H	-5.77389000	-2.39029700	-1.10636600
H	0.76674200	-3.26213400	-0.23365800	H	-0.76757400	-3.26110800	-0.23344400
H	1.24308300	-3.65913400	-1.90001800	H	-1.24438600	-3.65837300	-1.89964300
O	0.66107500	0.25093900	1.89693000	O	-0.66050600	0.25067100	1.89730600
H	1.30477800	0.97529900	1.82435200	H	-1.30291200	0.97613500	1.82446200

Table S42 Atomic coordinates (x,y,z) of [Sc($\mathbf{L^{111}}$)]$^+$ isomers.

[Sc($\mathbf{L^{111}}$)]$^+$ ΔM				[Sc($\mathbf{L^{111}}$)]$^+$ ΛM			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.54482300	1.93611200	1.23026100	N	0.74262100	0.39588700	-2.23132100
C	0.63048100	2.66442300	1.80457700	C	1.70648500	-0.62469400	-2.75860900
C	1.96900800	2.18129800	1.25328400	C	2.25191700	-1.55996400	-1.68058200
N	2.00477600	0.69863400	1.18883700	N	1.16140700	-1.99777500	-0.78168100
C	2.10834100	0.12065200	2.56708800	C	0.26684700	-2.96616700	-1.48290600
C	1.12720500	-1.00784000	2.83050200	C	-1.20857500	-2.66994000	-1.28342700
N	-0.25076800	-0.67346000	2.39569800	N	-1.51744600	-1.23450400	-1.49781500
C	-0.85833700	0.44842200	3.17845200	C	-1.30831200	-0.81253200	-2.92116900
C	-1.49196400	1.51078300	2.28626300	C	-0.48891400	0.46677500	-3.05237400
H	-1.81092400	2.36759900	2.90597100	H	-0.25007900	0.63679500	-4.11713400
H	-2.38555800	1.11403400	1.78511200	H	-1.06580400	1.33288200	-2.70109000
H	-0.08730100	0.89548600	3.81662600	H	-0.82830800	-1.63402900	-3.46510100
H	-1.62962100	0.05734800	3.85820500	H	-2.28051800	-0.65008800	-3.40949600
C	-1.09854200	-1.88012100	2.50448600	C	-2.92131100	-0.98025200	-1.10013000
C	-2.26941100	-1.77183200	1.57531600	C	-3.11184200	0.48331400	-0.83697100
C	-3.54923000	-2.26063400	1.84218800	C	-4.25965000	1.21845900	-1.13677900
C	-4.52798100	-2.15774400	0.85165600	C	-4.30220800	2.56923200	-0.78371200
C	-4.20030300	-1.59243000	-0.38399700	C	-3.21110900	3.14780200	-0.12806700
C	-2.90019000	-1.13550600	-0.57185900	C	-2.10924300	2.34373000	0.14221700
N	-1.97049000	-1.20653400	0.39622800	C	-0.88304800	2.79739600	0.89511200
C	-2.38040400	-0.57381700	-1.87233400	O	-0.75205100	3.98134500	1.22862200
O	-3.14567200	-0.40775200	-2.83145100	O	-0.04359400	1.84167600	1.14429600
O	-1.11097800	-0.32437400	-1.86234700	N	-2.06455300	1.05188100	-0.22300900
H	-4.92438300	-1.50907900	-1.19334600	H	-3.20665200	4.19339300	0.17687500
H	-5.53875100	-2.52336500	1.03957500	H	-5.18464400	3.16754200	-1.01595000
H	-3.76750800	-2.71089600	2.81072300	H	-5.09792500	0.73699800	-1.64037700
H	-0.50230500	-2.74832100	2.18315100	H	-3.11198500	-1.51930400	-0.15902000
H	-1.41742300	-2.06126600	3.54286800	H	-3.63083800	-1.35635100	-1.85358400
H	1.15524000	-1.26076800	3.90603000	H	-1.80076800	-3.30658600	-1.96520700
H	1.42388400	-1.90474700	2.26989700	H	-1.51305400	-2.91006000	-0.25671100
H	1.96350600	0.92747800	3.29441900	H	0.51397200	-2.95968200	-2.55027900
H	3.12695900	-0.26055500	2.73568700	H	0.47064100	-3.98888700	-1.12962700
C	3.12051600	0.23745200	0.34085700	C	1.66383400	-2.56780800	0.48006600
C	2.78199300	-1.11999700	-0.24334100	C	0.60805300	-2.45778100	1.57768300
O	1.54796200	-1.37978400	-0.44352700	O	0.55873100	-3.26396800	2.50499600
N	3.72290700	-1.99027800	-0.56946700	O	-0.18611300	-1.41823900	1.46590800
C	3.36379500	-3.29974900	-1.11972000	H	1.99761500	-3.61188800	0.37062200
H	2.34768800	-3.56950000	-0.81589000	H	2.52175100	-1.96545300	0.81938800
H	3.42838200	-3.28264100	-2.21890100	H	2.73729700	-2.42414700	-2.16816700
H	4.07377600	-4.04267100	-0.73268500	H	3.00508200	-1.05328300	-1.07056500
C	5.15961500	-1.71629100	-0.47543200	H	1.19854600	-1.20128400	-3.53960900
H	5.64464000	-2.14339000	-1.36350800	H	2.54882100	-0.11740300	-3.25269600

H	5.36373400	-0.64190900	-0.46025300	C	1.39589600	1.71549700	-2.12996100
H	5.58375900	-2.19111200	0.42224600	C	2.33578200	1.66808100	-0.93768500
H	4.06821300	0.23504200	0.89530400	O	2.07929900	0.80671000	-0.04384400
H	3.22713300	0.92208000	-0.51520400	N	3.36063200	2.50363500	-0.82782800
H	2.78287900	2.56683500	1.89222000	C	3.62857200	3.60094900	-1.75719400
H	2.12772600	2.56069300	0.24011700	H	2.79992300	3.74542400	-2.45620200
H	0.60566400	2.55417600	2.89392400	H	3.75544700	4.52669700	-1.17724400
H	0.53238500	3.74192000	1.60274500	H	4.55492300	3.40727600	-2.31905800
C	-1.18798300	2.74892600	0.17834800	C	4.23501900	2.43544100	0.34456300
C	-0.28830100	2.75352400	-1.05902800	H	3.87428700	3.11259900	1.13515700
O	-0.32882700	3.67651300	-1.87784400	H	4.26736100	1.41117800	0.73027900
O	0.46513100	1.69799300	-1.16691800	H	5.24389100	2.74545600	0.04262500
H	-1.40809600	3.77453900	0.51407300	H	1.90430600	1.98241100	-3.06738700
H	-2.13614700	2.26495000	-0.11118200	H	0.63151100	2.48117800	-1.91890000

Table S43 Atomic coordinates (x,y,z) of [ScF($\mathbf{L}^{111}$)] isomers.

[ScF($\mathbf{L}^{111}$)] ΔM				[ScF($\mathbf{L}^{111}$)] ΛM			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.35178800	1.73733300	1.75131700	N	-0.85863200	0.03353100	2.32283200
C	0.82110900	2.24946000	2.50790500	C	-0.91002900	-1.34745200	2.91572300
C	2.13503400	1.96969200	1.79521700	C	-0.58219600	-2.47488500	1.92922600
N	2.18590800	0.54740200	1.42785400	N	0.61087200	-2.11502900	1.14414000
C	2.30496700	-0.29320900	2.64738000	C	1.81998400	-2.17164700	2.01307700
C	1.34478600	-1.47017000	2.68000800	C	2.75778400	-0.98961100	1.84110500
N	-0.03015400	-1.13585500	2.23367000	N	2.00548000	0.27389500	1.80677300
C	-0.74452200	-0.24521300	3.21311100	C	1.44693900	0.60293800	3.14437200
C	-1.32350500	1.04999900	2.62221200	C	-0.03415500	0.96590700	3.12900000
H	-1.65186200	1.69056200	3.46302600	H	-0.39715100	1.00589900	4.17294700
H	-2.20790600	0.82947900	2.01055900	H	-0.17532800	1.96427700	2.69628700
H	-0.05043100	-0.00600400	4.02915500	H	1.61481500	-0.24894900	3.81498400
H	-1.57601400	-0.79808100	3.67588800	H	1.99420500	1.44904100	3.59208900
C	-0.74140500	-2.42538800	2.08123800	C	2.87089800	1.34560500	1.29967400
C	-2.02750300	-2.23543700	1.34027800	C	2.04759900	2.54541400	0.93842300
C	-3.15636500	-3.04031800	1.51894100	C	2.46463200	3.85803500	1.17502800
C	-4.29227000	-2.78081200	0.75305500	C	1.62468200	4.91202100	0.81711700
C	-4.28043400	-1.70711000	-0.14176900	C	0.38252400	4.62335400	0.25011700
C	-3.12294200	-0.94160700	-0.24102700	C	0.04196600	3.28881100	0.04831100
N	-2.01440400	-1.22284700	0.46514400	C	-1.28685200	2.86802200	-0.52399600
C	-3.01752600	0.30211500	-1.08705000	O	-2.13641900	3.73016500	-0.81007800
O	-3.95270400	0.59970800	-1.85817100	O	-1.42846200	1.60018700	-0.65929300
O	-1.94465900	0.96932200	-0.90420900	N	0.86176100	2.27248000	0.37025100
H	-5.15073900	-1.44368800	-0.74121000	H	-0.32366400	5.40397300	-0.02867700
H	-5.18639800	-3.39585500	0.86792400	H	1.92808200	5.94526800	0.99356400
H	-3.13626800	-3.84812500	2.25116000	H	3.43199300	4.03910300	1.64437300
H	-0.09763800	-3.09697400	1.49195300	H	3.36676500	0.97682500	0.38859600
H	-0.91716500	-2.90885600	3.05749200	H	3.65994000	1.62320400	2.02173600
H	1.32515900	-1.88284500	3.70578200	H	3.49365600	-0.99680200	2.66848700
H	1.70457400	-2.26330500	2.01641000	H	3.31617300	-1.07033900	0.90429200
H	2.14778600	0.33908600	3.52821400	H	1.48924900	-2.23120900	3.05583100
H	3.33086500	-0.68713300	2.74089600	H	2.37363800	-3.10435500	1.81635600
C	3.26373400	0.26121300	0.48183000	C	0.82820900	-2.91140000	-0.07138300
C	2.95723800	-1.06947000	-0.17898500	C	1.77494800	-2.15076700	-1.01477500
O	1.74960300	-1.42487500	-0.24309400	O	2.43324100	-2.77495900	-1.86131000
N	3.93280200	-1.83140100	-0.67437300	O	1.80055000	-0.86718200	-0.85708300
C	3.61331200	-3.12567600	-1.27513600	H	1.23645200	-3.91376600	0.14370300
H	2.71030700	-3.54077200	-0.81481800	H	-0.13068800	-3.03705400	-0.59693300
H	3.45331800	-3.02530300	-2.36112900	H	-0.42596100	-3.40839100	2.50171800
H	4.45722300	-3.80727700	-1.10359000	H	-1.41106900	-2.63689400	1.23456500
C	5.33047300	-1.41411700	-0.76884400	H	-0.21621800	-1.38132900	3.76408900
H	5.69476700	-1.64131600	-1.78131200	H	-1.91062700	-1.53095200	3.33610200

H	5.43950400	-0.33837100	-0.60354000	C	-2.22322100	0.57739300	2.22242200
H	5.95086000	-1.96255200	-0.04267800	C	-2.93522300	-0.15016000	1.10117100
H	4.25127800	0.26576800	0.96987800	O	-2.22832200	-0.78578300	0.27920700
H	3.26734500	1.03114100	-0.30629700	N	-4.26591600	-0.09694800	1.00517200
H	2.97619600	2.25243700	2.45675300	C	-5.11396700	0.71742300	1.87152200
H	2.21983400	2.56316800	0.87861200	H	-4.52440500	1.42396700	2.46302000
H	0.82808100	1.79533700	3.50450600	H	-5.80836400	1.29564400	1.24400800
H	0.71880600	3.33410000	2.67051400	H	-5.70438300	0.07966000	2.54846100
C	-0.90060800	2.83143900	0.93909400	C	-4.95543500	-0.80276000	-0.07224500
C	-0.08201700	2.98014600	-0.34974000	H	-5.17584800	-0.11808100	-0.90752700
O	-0.07150800	4.06186200	-0.95357700	H	-4.33587800	-1.62850000	-0.43663000
O	0.55005300	1.91557700	-0.74479500	H	-5.90292700	-1.20078500	0.31706900
H	-0.91345700	3.79029800	1.48299000	H	-2.75916200	0.48517400	3.18006000
H	-1.92584800	2.58864000	0.63628400	H	-2.17179300	1.64571200	1.96443000
F	-0.12902200	-0.72849300	-1.80552600	F	-0.57179200	-0.68182100	-1.73952300

Table S44 Atomic coordinates (x,y,z) of $[Sc(OH_2)(\mathbf{L^{111}})]^+$ isomers.

$Sc(OH_2)(\mathbf{L^{111}})]^+$ ΔM				$[Sc(OH_2)(\mathbf{L^{111}})]^+$ ΛM			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.45110300	1.74778300	1.60267400	N	-0.79300600	-0.36779600	-2.23754000
C	0.69647600	2.32541700	2.36145700	C	-1.67785000	0.70012000	-2.80775600
C	2.03912100	2.01502200	1.71674300	C	-2.21999600	1.64840300	-1.74425000
N	2.09710500	0.57708400	1.40138400	N	-1.10775900	2.05741100	-0.86767300
C	2.19598000	-0.21812400	2.65581900	C	-0.20263900	2.97933200	-1.61202000
C	1.24288800	-1.39864600	2.70000600	C	1.26651100	2.66385500	-1.41463800
N	-0.12220100	-1.06715900	2.21980600	N	1.54070900	1.20810300	-1.50045700
C	-0.85268000	-0.14725600	3.16105900	C	1.36597300	0.69184800	-2.90049900
C	-1.43706400	1.10681200	2.49828900	C	0.45707500	-0.53494900	-3.01670000
H	-1.77558100	1.79706500	3.29247100	H	0.24325600	-0.71343800	-4.08577600
H	-2.31348200	0.84920200	1.88952400	H	0.96380500	-1.42688500	-2.62620500
H	-0.16588600	0.13755500	3.96733800	H	0.97773300	1.50814400	-3.52190900
H	-1.67898600	-0.69053700	3.64298500	H	2.34585700	0.42531200	-3.32389300
C	-0.84966600	-2.35018900	2.07982100	C	2.92892600	1.00017200	-1.02897000
C	-2.11408900	-2.14325600	1.30762700	C	3.17072700	-0.44995900	-0.75452600
C	-3.29293100	-2.85924600	1.52731000	C	4.40678200	-1.08127400	-0.91252900
C	-4.40583400	-2.58044000	0.73419400	C	4.51082000	-2.43946100	-0.61386200
C	-4.31740700	-1.58033900	-0.23753000	C	3.37326200	-3.13477400	-0.19507100
C	-3.11011300	-0.90508000	-0.38279800	C	2.17803700	-2.43407900	-0.07525900
N	-2.02902200	-1.19788000	0.36089700	C	0.87025100	-3.08344300	0.29218900
C	-2.90801300	0.23598300	-1.34473700	O	0.83165700	-4.29758900	0.55434400
O	-3.83002100	0.57346000	-2.10705000	O	-0.13381200	-2.28357300	0.28115900
O	-1.74951500	0.78445700	-1.27213200	N	2.08936600	-1.11563900	-0.32531800
H	-5.16333700	-1.30722200	-0.86667700	H	3.39303500	-4.20157000	0.02302300
H	-5.33951900	-3.12452100	0.88534600	H	5.46523400	-2.95619300	-0.72619000
H	-3.33001600	-3.61236000	2.31484400	H	5.26379800	-0.51063300	-1.27101900
H	-0.20583700	-3.04407200	1.51732800	H	3.05164800	1.55797100	-0.08790100
H	-1.05362000	-2.80597400	3.06273100	H	3.66305500	1.39651800	-1.74963300
H	1.20247600	-1.78873200	3.73303000	H	1.85985700	3.21344400	-2.16735900
H	1.61333900	-2.20581900	2.05846300	H	1.60021600	2.99398600	-0.42563400
H	2.01205100	0.44649400	3.50704900	H	-0.45364300	2.92889900	-2.67676600
H	3.22252800	-0.59744600	2.78502100	H	-0.38903700	4.02054100	-1.30342200
C	3.19418100	0.25838500	0.48302200	C	-1.54632400	2.66907700	0.39298200
C	2.86998300	-1.05557600	-0.19944300	C	-0.38977500	2.65362800	1.39242400
O	1.64941700	-1.39659700	-0.26014200	O	-0.30753200	3.50427100	2.28491100
N	3.81721500	-1.81714800	-0.73013500	O	0.44619500	1.66917000	1.23367500
C	3.45798200	-3.07708200	-1.38439300	H	-1.92746400	3.69511400	0.25959900
H	2.57591200	-3.51280000	-0.90326100	H	-2.35242500	2.05192800	0.82238800
H	3.24659300	-2.91225800	-2.45314600	H	-2.68516000	2.52014500	-2.23924100
H	4.30493600	-3.76889700	-1.29152800	H	-2.98415700	1.16397900	-1.13001000
C	5.22612200	-1.43199000	-0.81261700	H	-1.10532300	1.26094000	-3.55461400
H	5.57449200	-1.60979700	-1.84002000	H	-2.51596400	0.23749900	-3.34991100

H	5.36496000	-0.37179300	-0.58306700	C	-1.56195800	-1.61994800	-2.12912600
H	5.83158200	-2.04173000	-0.12476100	C	-2.42638900	-1.51976400	-0.88158600
H	4.16651800	0.23086500	0.99774800	O	-2.12263300	-0.64094400	-0.01779700
H	3.24326100	1.02991500	-0.30160900	N	-3.46155000	-2.33087600	-0.70473100
H	2.85091100	2.31201900	2.40597900	C	-3.78734500	-3.44632800	-1.59253100
H	2.16981500	2.57534000	0.78597000	H	-3.04074200	-3.56101800	-2.38322700
H	0.66925900	1.93732200	3.38517300	H	-3.81130100	-4.37400200	-1.00155400
H	0.57457600	3.41620900	2.44504500	H	-4.77781300	-3.29210200	-2.04634500
C	-1.00629000	2.78080900	0.71115400	C	-4.24804800	-2.24337700	0.52691700
C	-0.11836800	2.90557400	-0.53337700	H	-3.78610000	-2.84832200	1.32371600
O	-0.12000800	3.94442600	-1.20242300	H	-4.31549400	-1.20128000	0.85795600
O	0.58926700	1.84941300	-0.81596600	H	-5.25484600	-2.62875900	0.32280500
H	-1.09908800	3.75815800	1.21097500	H	-2.16239300	-1.79511300	-3.03317000
H	-2.00105900	2.47012500	0.36590300	H	-0.87727500	-2.46767700	-1.99845800
O	-0.03505100	-0.95101700	-2.10608400	O	-0.06777100	-0.64350300	2.24521400
H	0.85645700	-1.11543400	-2.45621800	H	-0.59181800	-0.02018900	2.77581500
H	-0.45558000	-0.31574100	-2.71069000	H	-0.55964700	-1.48331400	2.25057400

Table S45 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{111})] isomers.

[Sc(OH)(**L**^{111})] ΔM				[Sc(OH)(**L**^{111})] ΛM			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.49964200	1.71742900	1.76837800	N	0.85352200	-0.44215300	2.33242300
C	0.63329000	2.24822900	2.57002500	C	1.75976800	0.58424800	2.92122000
C	1.98638200	1.97247500	1.93070900	C	2.35008200	1.51381000	1.86908200
N	2.07284200	0.55196600	1.55376200	N	1.26390600	2.01763600	1.01512200
C	2.14470400	-0.29640500	2.77460800	C	0.41419100	2.95837900	1.79332200
C	1.18685900	-1.47746700	2.77099300	C	-1.07636600	2.72358300	1.62241300
N	-0.16056600	-1.13746100	2.25936100	N	-1.44147600	1.28867500	1.64467400
C	-0.91636000	-0.25951300	3.21618500	C	-1.27683800	0.68979300	3.00997200
C	-1.49399700	1.02485200	2.60549800	C	-0.41335600	-0.57803400	3.08001700
H	-1.85589700	1.66435100	3.43381900	H	-0.23583500	-0.80607200	4.14845200
H	-2.35680400	0.79382500	1.96803600	H	-0.95239100	-1.42969600	2.64553100
H	-0.24841700	-0.00642700	4.04919900	H	-0.86358900	1.45822400	3.67574000
H	-1.74995200	-0.82523400	3.66020500	H	-2.26431000	0.43383400	3.42419800
C	-0.87953000	-2.41197200	2.04928000	C	-2.84395100	1.19579000	1.18581600
C	-2.14430500	-2.16960200	1.28551000	C	-3.19978300	-0.22387100	0.87076600
C	-3.31613500	-2.91068200	1.45910100	C	-4.48214700	-0.76009600	1.02044700
C	-4.43106200	-2.59530700	0.68272000	C	-4.69078500	-2.10067900	0.69823500
C	-4.35010200	-1.53761300	-0.22650300	C	-3.60770000	-2.87694600	0.27647600
C	-3.14789300	-0.84394200	-0.32976900	C	-2.36021900	-2.26942100	0.17404100
N	-2.06674400	-1.16859800	0.39896500	C	-1.09234300	-3.02160300	-0.14286800
C	-2.95495400	0.34624700	-1.23564500	O	-1.15461000	-4.22611000	-0.46054400
O	-3.88923300	0.70709300	-1.97837800	O	-0.02615600	-2.32776500	-0.01876700
O	-1.80634900	0.90100800	-1.14336900	N	-2.17504000	-0.96309700	0.42926400
H	-5.19691800	-1.23616400	-0.84139000	H	-3.70852800	-3.93793500	0.05213900
H	-5.35937700	-3.15731300	0.79780500	H	-5.68255000	-2.54409400	0.80178600
H	-3.34616600	-3.71208500	2.19798800	H	-5.29224300	-0.13284800	1.39367100
H	-0.23061600	-3.07209400	1.45231100	H	-2.93548500	1.79215200	0.26477400
H	-1.08830500	-2.92514900	3.00388500	H	-3.54443100	1.61961000	1.92620900
H	1.11920400	-1.88149400	3.79852700	H	-1.61788200	3.27405000	2.41454200
H	1.57650200	-2.27308800	2.12881700	H	-1.41120900	3.12000900	0.65900700
H	1.95301100	0.33395400	3.65055700	H	0.68263100	2.87879100	2.85285100
H	3.16823800	-0.68560100	2.90479600	H	0.63843900	3.99870500	1.50378100
C	3.21693600	0.30531300	0.67528800	C	1.74661500	2.64987100	-0.21408700
C	3.01623900	-1.03003500	-0.01437700	C	0.59139000	2.79722600	-1.20393600
O	1.84981000	-1.50452900	-0.04849300	O	0.60761900	3.70112700	-2.05592900
N	4.03966900	-1.66854400	-0.58891700	O	-0.33740800	1.90782200	-1.09049200
C	3.77596100	-2.90116300	-1.33183900	H	2.22132300	3.63064000	-0.03406600
H	3.03211700	-3.50926000	-0.80473200	H	2.49365700	1.98787000	-0.68231400
H	3.40321700	-2.67719600	-2.34521300	H	2.88734900	2.33925200	2.37396000
H	4.71416200	-3.46389500	-1.41504900	H	3.07043400	0.98642700	1.23578100
C	5.36338200	-1.08260500	-0.78304300	H	1.19870000	1.16389000	3.66257000
H	5.51977300	-0.86694200	-1.85233600	H	2.57616300	0.09457600	3.47498900

H	5.47527000	-0.15240300	-0.21925100	C	1.58886800	-1.70474300	2.19492100
H	6.13501200	-1.79371700	-0.45370800	C	2.40897400	-1.63552500	0.91315500
H	4.17248200	0.34590300	1.22367600	O	2.10750300	-0.76688400	0.04376900
H	3.24485600	1.08049200	-0.10731900	N	3.42139700	-2.47568800	0.70775000
H	2.78664800	2.25267000	2.64212000	C	3.73667800	-3.60924900	1.57397100
H	2.12201600	2.57337600	1.02592000	H	3.11260100	-3.61253800	2.47155400
H	0.59539100	1.80682900	3.57193500	H	3.56437100	-4.54796700	1.02458800
H	0.51673500	3.33472000	2.71355100	H	4.79430900	-3.56691100	1.87335600
C	-1.03570400	2.78852100	0.92201800	C	4.13518800	-2.42338500	-0.56984000
C	-0.13175000	2.98357800	-0.30313400	H	3.53950100	-2.89222400	-1.36961800
O	-0.12165700	4.07324500	-0.89426800	H	4.34421800	-1.38300400	-0.84635400
O	0.56955100	1.95117000	-0.65974800	H	5.08123100	-2.96688400	-0.46030000
H	-1.13809800	3.74401900	1.46414700	H	2.22612400	-1.89294300	3.07209100
H	-2.02397100	2.49686300	0.54392000	H	0.88729200	-2.54114900	2.09278100
O	0.07386800	-0.86987400	-1.81512300	O	-0.12467600	-0.52842800	-1.95011600
H	0.82003700	-1.49011700	-1.79178800	H	-0.22965500	0.30944100	-2.42841700

Table S46 Atomic coordinates (x,y,z) of $[Sc(\mathbf{L^{111}})]^+$ isomers.

$[Sc(\mathbf{L^{111}})]^+$ ΔP				$[Sc(\mathbf{L^{111}})]^+$ ΛP			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.74195000	0.39613300	-2.23134800	N	0.52585000	1.99078900	1.15503100
C	-1.70505800	-0.62497400	-2.75909900	C	-0.65703500	2.72261500	1.70868700
C	-2.25030200	-1.56082800	-1.68146900	C	-1.99148900	2.20314000	1.18095600
N	-1.15985400	-1.99805700	-0.78219600	N	-2.00803100	0.71837200	1.16924000
C	-0.26452100	-2.96591900	-1.48326700	C	-2.09279200	0.19036600	2.56794200
C	1.21073700	-2.66882400	-1.28371200	C	-1.09625400	-0.91646000	2.85896500
N	1.51875600	-1.23318700	-1.49782600	N	0.27602900	-0.57800100	2.40935600
C	1.30968400	-0.81103100	-2.92113600	C	0.87188400	0.57736500	3.15118600
C	0.48968400	0.46791300	-3.05216300	C	1.48470400	1.61726600	2.21932400
H	0.25093400	0.63809200	-4.11691900	H	1.79532600	2.49952200	2.80677400
H	1.06605300	1.33423800	-2.70057000	H	2.38059600	1.21486800	1.72652400
H	0.83009600	-1.63263900	-3.46526500	H	0.09845400	1.03375500	3.77985300
H	2.28189700	-0.64806800	-3.40927700	H	1.65299000	0.21964000	3.83787000
C	2.92230300	-0.97798800	-1.09963100	C	1.13784900	-1.77067500	2.56140500
C	3.11169700	0.48567600	-0.83623900	C	2.29823100	-1.69333000	1.61660600
C	4.25906400	1.22166700	-1.13561900	C	3.58205100	-2.16977300	1.88723500
C	4.30049100	2.57249200	-0.78257300	C	4.54824900	-2.10604900	0.88135700
C	3.20867800	3.15029800	-0.12746700	C	4.20433900	-1.59086400	-0.37171000
C	2.10732700	2.34538100	0.14247100	C	2.90193400	-1.14130600	-0.56078100
N	2.06378000	1.05346900	-0.22260200	C	2.36655900	-0.62999300	-1.87525700
C	0.88042000	2.79827100	0.89464300	O	3.11717200	-0.51342500	-2.85291700
O	0.74793500	3.98240200	1.22699800	O	1.10045400	-0.36535200	-1.85509300
O	0.04197600	1.84183700	1.14443600	N	1.98408300	-1.17458000	0.42059900
H	3.20326900	4.19592600	0.17733100	H	4.91766200	-1.54014800	-1.19325800
H	5.18259300	3.17142700	-1.01446600	H	5.56166100	-2.46344000	1.07085500
H	5.09788900	0.74084300	-1.63891200	H	3.81254600	-2.58091400	2.87022400
H	3.11302700	-1.51705100	-0.15853800	H	0.54779500	-2.65816300	2.28448600
H	3.63236100	-1.35345600	-1.85289900	H	1.46804200	-1.90346800	3.60350900
H	1.80327300	-3.30503200	-1.96559800	H	-1.11686600	-1.13999500	3.94118400
H	1.51534700	-2.90893200	-0.25702900	H	-1.38454600	-1.83185700	2.32415300
H	-0.51151700	-2.95962300	-2.55066900	H	-1.94896200	1.02506800	3.26324800
H	-0.46773100	-3.98873600	-1.12993800	H	-3.10496900	-0.19618600	2.76081600
C	-1.66233600	-2.56850500	0.47932800	C	-3.12324600	0.21313900	0.34594800
C	-0.60664400	-2.45846200	1.57706200	C	-2.76527100	-1.14990900	-0.21271900
O	-0.55634200	-3.26542100	2.50361800	O	-1.52821900	-1.39687900	-0.41258900
O	0.18639900	-1.41791100	1.46616300	N	-3.69578200	-2.03749900	-0.52034500
H	-1.99593400	-3.61260800	0.36954200	C	-3.32356600	-3.35314400	-1.04665100
H	-2.52037000	-1.96634300	0.81870500	H	-3.40317200	-3.36087100	-2.14491900
H	-2.73482400	-2.42526400	-2.16945400	H	-2.29954100	-3.60055800	-0.75066300
H	-3.00411700	-1.05485600	-1.07168000	H	-4.01683500	-4.09819100	-0.63409800
H	-1.19646200	-1.20114100	-3.53998000	C	-5.13519900	-1.77712300	-0.42411500
H	-2.54750200	-0.11810700	-3.25343400	H	-5.35276300	-0.70558700	-0.45763800

C	-1.39604700	1.71530900	-2.12978400	H	-5.62249400	-2.25067100	-1.28677600
C	-2.33634200	1.66694700	-0.93784700	H	-5.54578300	-2.21466500	0.49852800
O	-2.07981300	0.80523600	-0.04434600	H	-4.06445400	0.20248800	0.91147100
N	-3.36177700	2.50182600	-0.82807700	H	-3.25569800	0.87562500	-0.52376400
C	-3.62936000	3.60014300	-1.75631300	H	-2.80730300	2.59967800	1.81052100
H	-2.80181300	3.74341300	-2.45685900	H	-2.16036500	2.54401100	0.15589200
H	-4.55710800	3.40838400	-2.31650100	H	-0.62667800	2.65035800	2.80108900
H	-3.75351600	4.52587300	-1.17569900	H	-0.57392000	3.79384800	1.46988500
C	-4.23652300	2.43276900	0.34397300	C	1.15079400	2.77136700	0.06891000
H	-3.87696900	3.11056400	1.13455900	C	0.24291500	2.71938100	-1.16181200
H	-5.24567700	2.74146800	0.04159100	O	0.26762400	3.61345900	-2.01297700
H	-4.26771000	1.40854700	0.72987300	O	-0.49783400	1.65224900	-1.22467500
H	-1.90436100	1.98214600	-3.06729600	H	1.35912200	3.81186000	0.36430500
H	-0.63220900	2.48141100	-1.91830900	H	2.10365700	2.28991200	-0.20897900

Table S47 Atomic coordinates (x,y,z) of [ScF(**L**^{111})] isomers.

[ScF(**L**^{111})] ΔP				[ScF(**L**^{111})] ΛP		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.86327700	0.03106700	2.31901300	N	0.35179500	1.73783700	1.75073300
C	0.90366700	-1.35004900	2.91263700	C	-0.82119600	2.25014300	2.50708200
C	0.56411100	-2.47452500	1.92685000	C	-2.13512100	1.97007500	1.79446300
N	-0.62727200	-2.10392100	1.14365600	N	-2.18586700	0.54765900	1.42758000
C	-1.83512000	-2.15028900	2.01557400	C	-2.30494200	-0.29252700	2.64741100
C	-2.76384300	-0.96141600	1.84387900	C	-1.34463900	-1.46937600	2.68065400
N	-2.00186200	0.29612200	1.80774300	N	0.03029500	-1.13515800	2.23426600
C	-1.43726700	0.62148400	3.14370900	C	0.74457700	-0.24408000	3.21334700
C	0.04684300	0.97118900	3.12503400	C	1.32350000	1.05094500	2.62195400
H	0.41192600	1.00956500	4.16830800	H	1.65175900	1.69186200	3.46253700
H	0.19566800	1.96776500	2.69086100	H	2.20795400	0.83023000	2.01043700
H	-1.61171500	-0.22791400	3.81575900	H	0.05045500	-0.00457800	4.02928200
H	-1.97550700	1.47320000	3.59170200	H	1.57610800	-0.79669800	3.67635600
C	-2.85940900	1.37444000	1.30141400	C	0.74165500	-2.42466200	2.08233600
C	-2.02561600	2.56577500	0.93593100	C	2.02756200	-2.23500600	1.34098000
C	-2.42870100	3.88281500	1.17233500	C	3.15638900	-3.03995500	1.51963600
C	-1.57834200	4.92768900	0.81258100	C	4.29210800	-2.78088500	0.75334700
C	-0.34003000	4.62569000	0.24397000	C	4.28014800	-1.70751800	-0.14189200
C	-0.01354900	3.28753300	0.04258000	C	3.12273900	-0.94191200	-0.24109200
N	-0.84380200	2.28002300	0.36596100	C	3.01716500	0.30153900	-1.08751700
C	1.31117300	2.85243200	-0.52785600	O	3.95195800	0.59870600	-1.85923200
O	2.16754700	3.70573800	-0.81991700	O	1.94450000	0.96899200	-0.90430400
O	1.44138100	1.58268800	-0.65900300	N	2.01433900	-1.22273500	0.46548700
H	0.37395100	5.39892800	-0.03543500	H	5.15031700	-1.44443600	-0.74168400
H	-1.87041400	5.96416200	0.98924100	H	5.18619100	-3.39599700	0.86820000
H	-3.39311800	4.07408800	1.64371400	H	3.13638900	-3.84747300	2.25217800
H	-3.36149700	1.00852300	0.39262300	H	0.09785300	-3.09666100	1.49355700
H	-3.64356900	1.66038800	2.02554500	H	0.91770000	-2.90760900	3.05880000
H	-3.49919000	-0.96263100	2.67182700	H	-1.32507300	-1.88154400	3.70663700
H	-3.32362200	-1.03845800	0.90753200	H	-1.70430700	-2.26287400	2.01742900
H	-1.50235800	-2.21128600	3.05754200	H	-2.14795900	0.34010700	3.52803600
H	-2.39603200	-3.07903800	1.82100300	H	-3.33080400	-0.68654000	2.74094000
C	-0.85470700	-2.90068300	-0.07027700	C	-3.26366200	0.26101700	0.48162900
C	-1.79561900	-2.13231000	-1.01290200	C	-2.95706700	-1.07001800	-0.17843900
O	-2.46239200	-2.75091300	-1.85683800	O	-1.74934600	-1.42520800	-0.24242300
O	-1.80710400	-0.84821000	-0.85732300	N	-3.93212800	-1.83293500	-0.67326800
H	-1.27206400	-3.89855300	0.14779300	C	-3.61052200	-3.12662300	-1.27432500
H	0.10184900	-3.03659800	-0.59750000	H	-3.44108600	-3.02433300	-2.35871500
H	0.40041900	-3.40675600	2.49921300	H	-2.71232000	-3.54494300	-0.80745300
H	1.39035200	-2.64331100	1.23066900	H	-4.45736800	-3.80656600	-1.11128500
H	0.21138700	-1.37752200	3.76250800	C	-5.32971900	-1.41621200	-0.77068600
H	1.90345300	-1.54240600	3.33092600	H	-5.44051000	-0.34187500	-0.59776700

C	2.23200000	0.56470900	2.21938500	H	-5.68990000	-1.63635700	-1.78623900
C	2.94101000	-0.17025300	1.10114800	H	-5.95232000	-1.97053200	-0.05095600
O	2.23185400	-0.80576500	0.28169600	H	-4.25120300	0.26590000	0.96967800
N	4.27218500	-0.12165400	1.00498400	H	-3.26717500	1.03051400	-0.30691400
C	5.12337900	0.69576300	1.86507300	H	-2.97627000	2.25295500	2.45595500
H	4.53555500	1.40097700	2.45986900	H	-2.22000300	2.56325300	0.87767600
H	5.71975900	0.05972700	2.53843000	H	-0.82821100	1.79631300	3.50381100
H	5.81247200	1.27563300	1.23304800	H	-0.71895200	3.33483600	2.66937900
C	4.95968300	-0.83517300	-0.06847600	C	0.90058300	2.83177500	0.93824000
H	5.18977900	-0.15375000	-0.90387400	C	0.08186600	2.98012500	-0.35057500
H	5.90225900	-1.24087300	0.32493800	O	0.07116700	4.06170300	-0.95465700
H	4.33425600	-1.65596100	-0.43391900	O	-0.55012400	1.91539700	-0.74529900
H	2.76485000	0.46993500	3.17858000	H	0.91341400	3.79075700	1.48191100
H	2.18891400	1.63301000	1.96016500	H	1.92579500	2.58888300	0.63542400
F	0.57098000	-0.70038000	-1.73203200	F	0.12901700	-0.72896300	-1.80538300

Table S48 Atomic coordinates (x,y,z) of $[Sc(OH_2)(\mathbf{L^{111}})]^+$ isomers.

$Sc(OH_2)(\mathbf{L^{111}})]^+$ ΔP				$[Sc(OH_2)(\mathbf{L^{111}})]^+$ ΛP			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.79535400	-0.36680300	-2.23616700	N	0.45266300	1.74567500	1.60468300
C	1.67810900	0.70330800	-2.80587700	C	-0.69495000	2.32480400	2.36239200
C	2.21640800	1.65386800	-1.74236600	C	-2.03751100	2.01641400	1.71648100
N	1.10197000	2.06026500	-0.86738800	N	-2.09725100	0.57868800	1.40060200
C	0.19494700	2.97893700	-1.61346600	C	-2.19841700	-0.21686900	2.65461700
C	-1.27356000	2.65929600	-1.41760400	C	-1.24719100	-1.39889500	2.69888900
N	-1.54341900	1.20272200	-1.50260400	N	0.11865500	-1.06901000	2.21988000
C	-1.36620600	0.68613200	-2.90209700	C	0.84948100	-0.15088900	3.16247100
C	-0.45348000	-0.53787200	-3.01664400	C	1.43653500	1.10266200	2.50112600
H	-0.23790800	-0.71629700	-4.08537800	H	1.77512400	1.79195000	3.29612200
H	-0.95799400	-1.43111900	-2.62628800	H	2.31329600	0.84405400	1.89327400
H	-0.97989900	1.50318800	-3.52370600	H	0.16223600	0.13452600	3.96815000
H	-2.34493700	0.41635700	-3.32613700	H	1.67441300	-0.69571700	3.64502000
C	-2.93113300	0.99073600	-1.03164900	C	0.84446700	-2.35287100	2.07938800
C	-3.16855500	-0.46008000	-0.75676700	C	2.10990300	-2.14701800	1.30857200
C	-4.40252700	-1.09538200	-0.91516600	C	3.28768500	-2.86442500	1.52924100
C	-4.50253200	-2.45368100	-0.61557500	C	4.40181200	-2.58650800	0.73752200
C	-3.36315700	-3.14514100	-0.19532200	C	4.31562100	-1.58589300	-0.23386400
C	-2.17020600	-2.44063900	-0.07516800	C	3.10921700	-0.90922100	-0.38022400
N	-2.08544100	-1.12216300	-0.32640400	C	2.90950900	0.23243900	-1.34198500
C	-0.86073800	-3.08540300	0.29439500	O	3.83281100	0.56917100	-2.10307900
O	-0.81845700	-4.29921300	0.55772600	O	1.75154700	0.78224700	-1.27058900
O	0.14070000	-2.28233400	0.28340400	N	2.02699800	-1.20112800	0.36210600
H	-3.37986100	-4.21179600	0.02371100	H	5.16260400	-1.31343700	-0.86187300
H	-5.45526100	-2.97345500	-0.72816800	H	5.33470600	-3.13170300	0.88955600
H	-5.26110100	-0.52764800	-1.27454400	H	3.32302400	-3.61791000	2.31650800
H	-3.05593700	1.54846900	-0.09081700	H	0.20019500	-3.04532200	1.51563000
H	-3.66618200	1.38459200	-1.75274100	H	1.04690200	-2.80986600	3.06205600
H	-1.86759300	3.20656100	-2.17148600	H	-1.20810600	-1.78957400	3.73173800
H	-1.60943500	2.98927500	-0.42930900	H	-1.61834600	-2.20524000	2.05671100
H	0.44737400	2.92839600	-2.67787700	H	-2.01411500	0.44705000	3.50630300
H	0.37786300	4.02094000	-1.30543700	H	-3.22567300	-0.59461000	2.78285300
C	1.53680000	2.67387400	0.39367700	C	-3.19405000	0.26163700	0.48125100
C	0.37819500	2.65584900	1.39096300	C	-2.87160000	-1.05378300	-0.19914600
O	0.29200200	3.50687300	2.28274600	O	-1.65120700	-1.39512600	-0.26141300
O	-0.45452700	1.66869900	1.23169900	N	-3.81859000	-1.81804700	-0.72650000
H	1.91546000	3.70083600	0.26033900	C	-3.45441600	-3.07650600	-1.38136700
H	2.34375700	2.05910300	0.82490600	H	-3.21223200	-2.90598800	-2.44268100
H	2.67961100	2.52660800	-2.23744300	H	-2.58986400	-3.52541600	-0.88051200
H	2.98122700	1.17203700	-1.12692500	H	-4.31039600	-3.76004000	-1.31649100
H	1.10509300	1.26231400	-3.55375500	C	-5.22751100	-1.43482400	-0.81428900
H	2.51817200	0.24270400	-3.34673300	H	-5.37247900	-0.38167800	-0.55828600

C	1.56721600	-1.61697800	-2.12673600	H	-5.56583100	-1.58737900	-1.84927900
C	2.43087200	-1.51411800	-0.87889900	H	-5.83712900	-2.06401000	-0.14811400
O	2.12535400	-0.63514500	-0.01590100	H	-4.16693800	0.23739300	0.99504600
N	3.46730000	-2.32364900	-0.70278600	H	-3.24012100	1.03222200	-0.30450400
C	3.79524200	-3.43588200	-1.59404400	H	-2.84942600	2.31430200	2.40520700
H	3.02883800	-3.57380100	-2.36188400	H	-2.16675300	2.57719800	0.78580200
H	4.76882300	-3.26227100	-2.07681500	H	-0.66921300	1.93654900	3.38608700
H	3.85690300	-4.35858600	-0.99840700	H	-0.57162100	3.41540600	2.44623800
C	4.26122200	-2.23105400	0.52354000	C	1.01090100	2.77832400	0.71465400
H	3.81484700	-2.84792900	1.32009800	C	0.12452200	2.90594800	-0.53056100
H	5.27247700	-2.59957100	0.30990500	O	0.12906100	3.94518400	-1.19898900
H	4.31490300	-1.18996300	0.85992200	O	-0.58523900	1.85149300	-0.81446700
H	2.16891700	-1.79109500	-3.03017600	H	1.10526400	3.75506100	1.21539600
H	0.88439700	-2.46628900	-1.99641100	H	2.00536300	2.46585800	0.37011700
O	0.06824300	-0.64128400	2.24589200	O	0.03437500	-0.94919200	-2.10642500
H	0.58988400	-0.01525700	2.77574400	H	-0.85733200	-1.11083000	-2.45736100
H	0.56398200	-1.47882500	2.25099100	H	0.45687700	-0.31435200	-2.71014100

Table S49 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{111})] isomers.

[Sc(OH)(**L**^{111})] ΔP			[Sc(OH)(**L**^{111})] ΛP		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.85344800	-0.44227100	2.33262600	N	0.49966600	1.71735900	1.76856500
C	-1.75966100	0.58404000	2.92154900	C	-0.63322700	2.24816700	2.57025500
C	-2.35015400	1.51357600	1.86948600	C	-1.98633500	1.97253400	1.93097300
N	-1.26409500	2.01749900	1.01543200	N	-2.07286200	0.55204600	1.55391500
C	-0.41439900	2.95831300	1.79355800	C	-2.14475800	-0.29641100	2.77471900
C	1.07617800	2.72366200	1.62253600	C	-1.18699300	-1.47752000	2.77093600
N	1.44143200	1.28879500	1.64462700	N	0.16043500	-1.13753100	2.25940200
C	1.27697700	0.68977300	3.00989700	C	0.91626900	-0.25968400	3.21627700
C	0.41356000	-0.57810200	3.07998900	C	1.49397600	1.02469100	2.60566700
H	0.23625500	-0.80619700	4.14845100	H	1.85589800	1.66412700	3.43402900
H	0.95257500	-1.42971300	2.64538300	H	2.35678800	0.79365200	1.96821100
H	0.86378700	1.45813700	3.67578200	H	0.24833900	-0.00661800	4.04930800
H	2.26451400	0.43381800	3.42396900	H	1.74982000	-0.82548600	3.66027100
C	2.84388100	1.19610800	1.18563700	C	0.87938200	-2.41203000	2.04919700
C	3.19984600	-0.22350300	0.87049200	C	2.14419300	-2.16957900	1.28551500
C	4.48229800	-0.75958500	1.01995800	C	3.31606500	-2.91056100	1.45922900
C	4.69101000	-2.10016800	0.69780400	C	4.43104900	-2.59509800	0.68296700
C	3.60790800	-2.87659100	0.27636600	C	4.35010100	-1.53740100	-0.22624800
C	2.36036000	-2.26919100	0.17408100	C	3.14785100	-0.84382100	-0.32963700
N	2.17511100	-0.96284600	0.42918400	C	2.95495500	0.34639900	-1.23545900
C	1.09246800	-3.02151400	-0.14245300	O	3.88932500	0.70738600	-1.97800400
O	1.15468700	-4.22623300	-0.45929100	O	1.80628800	0.90105900	-1.14333100
O	0.02630600	-2.32752200	-0.01893300	N	2.06663900	-1.16857800	0.39896000
H	3.70877500	-3.93760300	0.05215500	H	5.19696000	-1.23587000	-0.84103700
H	5.68284300	-2.54347300	0.80117700	H	5.35939900	-3.15702700	0.79814400
H	5.29239500	-0.13222600	1.39299100	H	3.34608300	-3.71194800	2.19813400
H	2.93526000	1.79253700	0.26462200	H	0.23047600	-3.07208400	1.45214300
H	3.54437500	1.61996900	1.92599400	H	1.08813500	-2.92531900	3.00375000
H	1.61768100	3.27410100	2.41469300	H	-1.11942100	-1.88175500	3.79839900
H	1.41091900	3.12022500	0.65915300	H	-1.57668400	-2.27299100	2.12860000
H	-0.68272300	2.87869900	2.85311300	H	-1.95300600	0.33387800	3.65070600
H	-0.63875400	3.99862400	1.50404100	H	-3.16830700	-0.68556200	2.90490900
C	-1.74698900	2.64970000	-0.21372600	C	-3.21704400	0.30555400	0.67550400
C	-0.59186600	2.79727900	-1.20367800	C	-3.01643300	-1.02973800	-0.01432000
O	-0.60839000	3.70116300	-2.05568500	O	-1.85000200	-1.50425800	-0.04867800
O	0.33715400	1.90810900	-1.09029700	N	-4.03989300	-1.66821000	-0.58879700
H	-2.22181400	3.63040200	-0.03363400	C	-3.77614400	-2.90087500	-1.33163900
H	-2.49398000	1.98761200	-0.68190500	H	-3.40195900	-2.67701500	-2.34450400
H	-2.88744600	2.33896800	2.37442000	H	-3.03339100	-3.50964100	-0.80374000
H	-3.07052400	0.98614400	1.23624600	H	-4.71464500	-3.46290500	-1.41611000
H	-1.19852800	1.16371600	3.66282200	C	-5.36374200	-1.08247900	-0.78255400
H	-2.57595000	0.09431600	3.47543500	H	-5.47543100	-0.15202700	-0.21913500
C	-1.58871200	-1.70487600	2.19504500	H	-5.52061700	-0.86729200	-1.85186800

C	-2.40882000	-1.63567800	0.91327200	H	-6.13518900	-1.79348800	-0.45255100
O	-2.10743300	-0.76695000	0.04394300	H	-4.17255200	0.34613500	1.22395600
N	-3.42110500	-2.47593900	0.70763300	H	-3.24496300	1.08081500	-0.10702000
C	-3.73658500	-3.60952400	1.57373500	H	-2.78657000	2.25269400	2.64242600
H	-3.11452900	-3.61133800	2.47272400	H	-2.12198700	2.57349700	1.02622900
H	-4.79490800	-3.56844400	1.87079200	H	-0.59534200	1.80671100	3.57214100
H	-3.56176700	-4.54835900	1.02532700	H	-0.51660400	3.33464100	2.71387100
C	-4.13432600	-2.42355000	-0.57030100	C	1.03574800	2.78848200	0.92227700
H	-3.53698300	-2.88961400	-1.37045400	C	0.13164300	2.98369100	-0.30276200
H	-5.07903100	-2.96960000	-0.46210200	O	0.12136100	4.07347300	-0.89368800
H	-4.34585500	-1.38328400	-0.84544200	O	-0.56956000	1.95127100	-0.65948400
H	-2.22596300	-1.89316200	3.07219900	H	1.13829800	3.74391800	1.46448900
H	-0.88710500	-2.54125700	2.09288200	H	2.02394400	2.49676900	0.54403400
O	0.12431700	-0.52803900	-1.95022800	O	-0.07385400	-0.86975800	-1.81512500
H	0.22900800	0.30995400	-2.42837500	H	-0.82037100	-1.48959200	-1.79208500

Table S50 Atomic coordinates (x,y,z) of Sc($\mathbf{L}^{\mathbf{021}}$)]$^{2+}$ isomers.

[Sc($\mathbf{L}^{\mathbf{021}}$)]$^{2+}$ Δ			[Sc($\mathbf{L}^{\mathbf{021}}$)]$^{2+}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.53145100	1.32264300	1.93061300	N	0.81723000	1.08990400	1.94775600
C	0.64285900	1.84512600	2.69743400	C	-0.25469200	1.62523900	2.85306400
C	1.95445300	1.72495200	1.93083700	C	-1.65159600	1.61506100	2.23552800
N	2.06294700	0.38891200	1.29791800	N	-1.90729600	0.34778300	1.50549300
C	2.27543400	-0.66107800	2.34098700	C	-2.08786000	-0.78418000	2.46850500
C	1.39485200	-1.88109800	2.15264500	C	-1.27694400	-2.01782700	2.11240900
N	-0.03407100	-1.53068900	1.92625500	N	0.13943800	-1.69469600	1.80307600
C	-0.66194300	-0.85811100	3.11111500	C	0.88870700	-1.15621800	2.98110200
C	-1.38859800	0.43342300	2.75146400	C	1.67672200	0.10405500	2.64553800
H	-1.71897000	0.93631000	3.67738600	H	2.09828100	0.53148100	3.57211000
H	-2.28454100	0.20774100	2.15566100	H	2.51614600	-0.13293700	1.97763600
H	0.11115400	-0.67430100	3.86628300	H	0.18149400	-0.96894200	3.79670500
H	-1.38981200	-1.53635600	3.57875000	H	1.59177600	-1.91390500	3.35661900
C	-0.76690500	-2.77751000	1.59865200	C	0.81690600	-2.90857300	1.29178300
C	-1.95542800	-2.49332700	0.73239300	C	2.01575200	-2.51070800	0.48364000
C	-3.13470800	-3.24162900	0.74181300	C	3.23695100	-3.18535800	0.46427100
C	-4.12974800	-2.94175000	-0.18936500	C	4.25276000	-2.71280900	-0.36977200
C	-3.92202600	-1.91041100	-1.11037900	C	4.02066600	-1.59452500	-1.17608500
C	-2.72450500	-1.20814400	-1.04827900	C	2.77331200	-0.98436900	-1.10464400
N	-1.77313900	-1.49101500	-0.14006300	C	2.35224100	0.19523500	-1.94417700
C	-2.35287300	-0.09176800	-1.98815600	O	3.15240900	0.74163800	-2.71156100
O	-3.13204700	0.26767200	-2.87812800	O	1.11079600	0.53144900	-1.77729300
O	-1.17843000	0.41148100	-1.76678200	N	1.80758200	-1.42838000	-0.28160100
H	-4.66324600	-1.64744600	-1.86372500	H	4.78006500	-1.19715600	-1.84811300
H	-5.06047600	-3.51095800	-0.19978600	H	5.22132400	-3.21468000	-0.39032400
H	-3.26038500	-4.04536200	1.46754300	H	3.38612100	-4.05768600	1.10065200
H	-0.09323000	-3.42701400	1.01831200	H	0.11867600	-3.43488600	0.62285100
H	-1.05009700	-3.32832300	2.50828600	H	1.08400900	-3.59654200	2.10882800
H	1.50074600	-2.53980000	3.03312200	H	-1.34572000	-2.74476800	2.94150300
H	1.72114600	-2.44810400	1.27069500	H	-1.69324400	-2.49398300	1.21392100
H	2.10214100	-0.21402600	3.32617100	H	-1.82686900	-0.42907100	3.47222400
H	3.32623700	-0.98873800	2.33568100	H	-3.14972600	-1.06942200	2.51331000
C	3.14509000	0.37162900	0.29543400	C	-3.07675400	0.48130400	0.61210500
C	2.83485100	-0.66208800	-0.76772000	C	-2.91228000	-0.42662400	-0.58976300
O	1.60321900	-0.89219200	-1.02042900	O	-1.72265500	-0.74934000	-0.92511000
N	3.78723000	-1.28422100	-1.43999400	N	-3.94282500	-0.84786700	-1.30120300
C	3.43818900	-2.27888000	-2.45851900	C	-3.72103000	-1.70846700	-2.46775100
H	2.49387100	-2.76842700	-2.19889300	H	-3.55162500	-1.09834800	-3.36889000
H	3.34593600	-1.80028600	-3.44595000	H	-2.85495900	-2.35705800	-2.29895800
H	4.24202500	-3.02515000	-2.49669900	H	-4.61759500	-2.32339900	-2.61503500
C	5.21571500	-0.98685800	-1.31319600	C	-5.32366000	-0.41062100	-1.08815300
H	5.63131500	-0.85851900	-2.32259500	H	-5.37620000	0.41774000	-0.37653700
H	5.38626500	-0.06556500	-0.75044600	H	-5.72801800	-0.06772200	-2.05127400

H	5.73259500	-1.82416400	-0.82111800	H	-5.93461100	-1.25116100	-0.72714000
H	4.12197500	0.21105100	0.77004300	H	-4.01492000	0.29257900	1.15171200
H	3.17117400	1.34435500	-0.22039500	H	-3.11407800	1.50900900	0.21842800
H	2.79516600	1.90258000	2.62448000	H	-2.39557300	1.76255600	3.03790100
H	2.01044000	2.47571600	1.13727200	H	-1.76244600	2.43606500	1.52190400
H	0.70304700	1.30621800	3.64874200	H	-0.24234800	1.03916300	3.77784300
H	0.47661700	2.90198500	2.95508100	H	-0.00746900	2.65749600	3.14421400
C	-1.30010100	2.44634000	1.35553400	C	1.61292400	2.19670900	1.37610800
C	-0.53018900	2.94866500	0.14510700	C	0.72834100	2.88820700	0.35337700
O	0.26949400	2.12758300	-0.40200400	O	-0.18139400	2.17874600	-0.17773600
N	-0.70384800	4.17145700	-0.33424700	N	0.90115200	4.15988200	0.02427600
C	-1.70161800	5.11444000	0.17113900	C	1.99225300	4.99521800	0.52530000
H	-2.39984900	4.62800200	0.85803300	H	2.75799000	4.39499900	1.02465800
H	-1.20826100	5.95642800	0.67963800	H	2.45785700	5.50704400	-0.32891100
H	-2.27392300	5.50479500	-0.68280800	H	1.60246600	5.75325700	1.22169400
C	0.04488400	4.60933900	-1.51448600	C	0.01540600	4.79046500	-0.95685000
H	-0.53160900	4.40928700	-2.43155700	H	0.45244400	4.72961000	-1.96601400
H	0.21994500	5.68979600	-1.43136700	H	-0.96171400	4.29649000	-0.95256000
H	1.00479200	4.08527900	-1.56637700	H	-0.10587600	5.84681600	-0.68369500
H	-1.48552500	3.22936800	2.10360800	H	1.97713600	2.87486600	2.16059300
H	-2.27136500	2.07303300	0.99227100	H	2.48287200	1.78137000	0.84152300

Table S51 Atomic coordinates (x,y,z) of $[ScF(\mathbf{L}^{021})]^+$ isomers.

$[ScF(\mathbf{L}^{021})]^+$ Δ				$[ScF(\mathbf{L}^{021})]^+$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	1.01660600	-0.85258900	2.08076500	N	-1.00564000	-0.85684800	2.07925500
C	0.10273400	-1.65894300	2.95118500	C	-0.09095800	-1.66495200	2.94850000
C	-1.19168800	-2.07869500	2.25797700	C	1.20205000	-2.08423500	2.25311700
N	-1.77905500	-0.91155400	1.57463600	N	1.79139800	-0.91735600	1.57222600
C	-2.31052400	0.03946100	2.59718900	C	2.32631700	0.03266300	2.59184500
C	-1.93216700	1.49028200	2.35789800	C	1.94745700	1.48344900	2.35290900
N	-0.52387300	1.63711900	1.93440800	N	0.53823000	1.63027100	1.93161600
C	0.41403200	1.36679200	3.06957500	C	-0.39924800	1.36177900	3.06805200
C	1.52389200	0.35851800	2.76432200	C	-1.51125400	0.35385900	2.76496800
H	2.02787800	0.10052400	3.71426300	H	-2.01300100	0.09615000	3.71610600
H	2.27747100	0.80570600	2.10336900	H	-2.26629200	0.80197600	2.10615400
H	-0.17523200	1.02211800	3.92882700	H	0.18957800	1.01740500	3.92741400
H	0.89576900	2.30376000	3.39012600	H	-0.87962200	2.29966500	3.38814000
C	-0.35474600	3.00832700	1.41428500	C	0.37077700	3.00169300	1.41070700
C	0.94798900	3.13079800	0.68755300	C	-0.93457600	3.12906200	0.69020600
C	1.72469400	4.29255700	0.67507000	C	-1.70678900	4.29350200	0.68219100
C	2.92962400	4.29117100	-0.02682900	C	-2.91361200	4.29852100	-0.01677700
C	3.34212700	3.11986000	-0.66682600	C	-3.33290100	3.13008700	-0.65675100
C	2.51605200	2.00329000	-0.59486500	C	-2.51165900	2.00943000	-0.58776400
N	1.33132800	2.02035500	0.04161700	C	-2.89837400	0.66577600	-1.14564300
C	2.89218600	0.65833300	-1.15635400	O	-3.96998400	0.53385300	-1.76275400
O	3.96222100	0.52011900	-1.77567200	O	-2.05180000	-0.26480500	-0.89857600
O	2.03888100	-0.26685100	-0.91201500	N	-1.32473900	2.02058700	0.04363600
H	4.29056700	3.05191200	-1.19774100	H	-4.28279400	3.06636600	-1.18565000
H	3.55347900	5.18603700	-0.05334400	H	-3.53308700	5.19648900	-0.04065400
H	1.38640300	5.17432600	1.21985500	H	-1.36346900	5.17311600	1.22731300
H	-1.17216400	3.20229900	0.70281200	H	1.18547300	3.19091100	0.69490000
H	-0.42577200	3.76257000	2.21715800	H	0.44877800	3.75642300	2.21240500
H	-2.12285500	2.06282600	3.28485700	H	2.13957500	2.05641000	3.27921500
H	-2.55499700	1.92416300	1.57123100	H	2.56896500	1.91770300	1.56518100
H	-1.94840100	-0.27797700	3.58067800	H	1.96716600	-0.28307400	3.57686200
H	-3.40904900	-0.03641400	2.64205600	H	3.42506300	-0.04371300	2.63413500
C	-2.83443000	-1.27991600	0.62252800	C	2.84067600	-1.28461400	0.61437400
C	-3.06295900	-0.08221800	-0.29016900	C	3.06485900	-0.08519100	-0.29717100
O	-2.13646000	0.76806300	-0.38628800	O	2.13489700	0.76102500	-0.39114800
N	-4.20722000	0.03547900	-0.96381600	N	4.20887000	0.03785500	-0.97077500
C	-4.45859200	1.20034100	-1.81025000	C	4.45570100	1.20418100	-1.81662900
H	-3.73384400	1.98834800	-1.58415800	H	4.38882200	0.92695600	-2.88071800
H	-4.38169600	0.92530100	-2.87425000	H	3.72223200	1.98571100	-1.59652700
H	-5.47580600	1.56960400	-1.61480000	H	5.46835100	1.58263400	-1.61467500
C	-5.27778700	-0.95991500	-0.91240300	C	5.28338800	-0.95316200	-0.92340600
H	-5.75135800	-1.00555300	-1.90246400	H	4.89774800	-1.94920200	-0.68351100

H	-4.88594900	-1.95551200	-0.68045300	H	5.74930000	-1.00190500	-1.91713400
H	-6.04289300	-0.68143600	-0.17024400	H	6.05353300	-0.66819000	-0.18897400
H	-3.75865200	-1.59084800	1.13455300	H	3.76733200	-1.59743100	1.12075800
H	-2.48749400	-2.12155900	0.00151200	H	2.48942400	-2.12401600	-0.00732900
H	-1.88354600	-2.49195200	3.01502200	H	1.89285300	-2.50151700	3.00913600
H	-1.00625400	-2.85588100	1.51180400	H	1.01404500	-2.85938000	1.50525300
H	-0.12335700	-1.07289100	3.84882700	H	0.13698800	-1.08039600	3.84633900
H	0.62541300	-2.56128600	3.30360300	H	-0.61418100	-2.56694900	3.30076500
C	2.11552600	-1.71140000	1.61379700	C	-2.10420300	-1.71731400	1.61391100
C	1.56633000	-2.58590700	0.49885700	C	-1.55721700	-2.58517300	0.49209600
O	0.49666400	-2.22206500	-0.06510900	O	-0.48908600	-2.21745600	-0.07349600
N	2.20562200	-3.69632700	0.13747200	N	-2.19809400	-3.69346500	0.12698400
C	3.49590500	-4.10823900	0.68698700	C	-3.48383400	-4.11078500	0.68272400
H	3.98381300	-3.28899700	1.22317900	H	-3.96916700	-3.29653700	1.22856200
H	3.37358000	-4.96888300	1.36328300	H	-4.14296900	-4.40546500	-0.14664800
H	4.14911400	-4.40776200	-0.14527100	H	-3.35523300	-4.97608100	1.35186100
C	1.66898500	-4.54762100	-0.92305900	C	-1.66753800	-4.53993600	-0.94040600
H	2.17556600	-4.33879100	-1.87912300	H	-2.19565300	-4.34178000	-1.88701200
H	1.84318400	-5.59850700	-0.65288700	H	-0.59836600	-4.34820900	-1.07365400
H	0.59441000	-4.37274700	-1.03604600	H	-1.82066700	-5.59260800	-0.66402300
H	2.53141400	-2.31035000	2.43815200	H	-2.51377300	-2.32082100	2.43768300
H	2.92120600	-1.09235900	1.19777800	H	-2.91355600	-1.09951900	1.20335000
F	-0.42930000	-0.41852500	-1.85427700	F	0.40950300	-0.38102400	-1.86590900

Table S52 Atomic coordinates (x,y,z) of $[Sc(OH_2)(\mathbf{L}^{\mathbf{021}})]^{2+}$ isomers.

$[Sc(OH_2)(\mathbf{L}^{\mathbf{021}})]^{2+}$ Δ				$[Sc(OH_2)(\mathbf{L}^{\mathbf{021}})]^{2+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.73861000	1.02872500	2.04617200	N	0.73725300	1.02839400	2.04709800
C	0.30388300	1.59017700	2.96272600	C	-0.30528600	1.58908200	2.96367100
C	1.64793700	1.78493000	2.27756900	C	-1.64922600	1.78378500	2.27819600
N	1.98846300	0.55650200	1.53823400	N	-1.98926300	0.55574100	1.53806000
C	2.32373200	-0.53528000	2.49404000	C	-2.32421600	-0.53695500	2.49286100
C	1.66665900	-1.85644700	2.14746300	C	-1.66691900	-1.85772900	2.14526300
N	0.23982400	-1.70691700	1.76671000	N	-0.23987000	-1.70774100	1.76521800
C	-0.61869500	-1.30133600	2.93382500	C	0.61789900	-1.30235100	2.93302400
C	-1.50040800	-0.07179700	2.68502800	C	1.49933700	-0.07254100	2.68506500
H	-1.93447400	0.24710000	3.64940800	H	1.93362100	0.24577300	3.64954600
H	-2.33201800	-0.32326400	2.01449900	H	2.33088100	-0.32338200	2.01422600
H	0.03356600	-1.13063600	3.79881200	H	-0.03489000	-1.13219200	3.79771600
H	-1.28045700	-2.13477500	3.21209600	H	1.27969500	-2.13571700	3.21141700
C	-0.19568900	-3.01714900	1.22795900	C	0.19621600	-3.01776900	1.22630700
C	-1.50768400	-2.87201400	0.52607600	C	1.50830200	-2.87188200	0.52465700
C	-2.48500700	-3.86802100	0.46483900	C	2.48600900	-3.86753600	0.46332700
C	-3.66596600	-3.60847900	-0.23038600	C	3.66705200	-3.60725000	-0.23143200
C	-3.85069600	-2.35500300	-0.82077300	C	3.85153800	-2.35340000	-0.82114000
C	-2.83331500	-1.41511700	-0.70146200	C	2.83380800	-1.41391900	-0.70180700
N	-1.68099000	-1.68088200	-0.06208800	C	2.93213100	-0.00471000	-1.21875200
C	-2.93177100	-0.00629900	-1.21941100	O	3.93859900	0.36468700	-1.84342400
O	-3.93739300	0.36217200	-1.84599000	O	1.91460300	0.72914300	-0.93277700
O	-1.91492300	0.72821400	-0.93255200	N	1.68128500	-1.68049500	-0.06298100
H	-4.76518600	-2.09314200	-1.35113700	H	4.76613400	-2.09098200	-1.35104100
H	-4.44509600	-4.36974900	-0.29409200	H	4.44649700	-4.36818200	-0.29532600
H	-2.31705900	-4.82240700	0.96434800	H	2.31826600	-4.82217400	0.96241700
H	0.55809000	-3.34936800	0.49747100	H	-0.55738600	-3.35019900	0.49573700
H	-0.24999000	-3.77917300	2.02262000	H	0.25075400	-3.77983400	2.02089500
H	1.76448800	-2.54430300	3.00635600	H	-1.76501500	-2.54637000	3.00348800
H	2.17377000	-2.32100500	1.29487500	H	-2.17366000	-2.32152400	1.29204200
H	2.02665700	-0.21954000	3.50028700	H	-2.02729800	-0.22206500	3.49942100
H	3.41463400	-0.68480300	2.53148900	H	-3.41508900	-0.68687400	2.53027500
C	3.07944800	0.77187700	0.58084900	C	-3.08014600	0.77143700	0.58069900
C	3.00075900	-0.31641800	-0.47145100	C	-3.00107000	-0.31609700	-0.47235500
O	1.87405300	-0.87295200	-0.65375200	O	-1.87408800	-0.87202100	-0.65484400
N	4.05044400	-0.67135900	-1.19955600	N	-4.05069500	-0.67058000	-1.20074900
C	3.88792400	-1.70424100	-2.22701300	C	-3.88939500	-1.70336300	-2.22843300
H	3.25207400	-2.51438900	-1.85165500	H	-3.44495500	-1.27641400	-3.14161200
H	3.43281800	-1.27977800	-3.13607200	H	-3.24481500	-2.50851200	-1.85747200
H	4.87902200	-2.10254200	-2.47400600	H	-4.87970200	-2.10886400	-2.46696500
C	5.34705100	0.00502600	-1.16896400	C	-5.34839000	0.00367800	-1.16754100
H	5.58566900	0.35860300	-2.18309500	H	-5.33401500	0.86967200	-0.50033100

H	5.33441300	0.86664800	-0.49608600	H	-5.59246200	0.35053900	-2.18264100
H	6.12967600	-0.69801900	-0.84767800	H	-6.12831700	-0.69867400	-0.83813300
H	4.05955200	0.80529000	1.07912100	H	-4.06029200	0.80429700	1.07893100
H	2.92211000	1.73291200	0.06554800	H	-2.92304200	1.73287800	0.06608400
H	2.41167600	2.02395800	3.03981500	H	-2.41327400	2.02239500	3.04026800
H	1.61299200	2.61521500	1.56600000	H	-1.61407600	2.61441900	1.56702600
H	0.40820400	0.91651800	3.81984400	H	-0.40961300	0.91504900	3.82048700
H	-0.04057300	2.55127200	3.37177500	H	0.03877800	2.55010900	3.37326200
C	-1.59987200	2.12654600	1.56706000	C	1.59826100	2.12647700	1.56821600
C	-0.87517700	2.80767800	0.41525300	C	0.87401600	2.80741100	0.41603700
O	0.08309400	2.18009600	-0.13533300	O	-0.08405600	2.17979600	-0.13492400
N	-1.23619300	4.00863800	-0.01346700	N	1.23508000	4.00814900	-0.01317600
C	-2.41404100	4.72946400	0.46662500	C	2.41307700	4.72909200	0.46642500
H	-2.92133700	4.17884000	1.26348900	H	2.91778500	4.18090200	1.26660900
H	-2.11762000	5.71975300	0.84199300	H	3.11851700	4.85990800	-0.36824800
H	-3.11745200	4.86449300	-0.36907600	H	2.11721600	5.72119300	0.83735900
C	-0.55750000	4.58331600	-1.17819000	C	0.55672200	4.58070600	-1.17926300
H	-0.95262500	4.14609700	-2.10915500	H	0.94479200	4.13413500	-2.10871600
H	-0.73715000	5.66483900	-1.18350400	H	-0.52222200	4.39746600	-1.11708200
H	0.52008100	4.39112400	-1.12103100	H	0.74484900	5.66066200	-1.19224900
H	-1.83593300	2.82976200	2.37845000	H	1.83368800	2.82985000	2.37967800
H	-2.54174200	1.72024800	1.17665900	H	2.54058700	1.72059800	1.17846200
O	0.16530900	0.02784600	-2.31774800	O	-0.16569000	0.02977600	-2.31797300
H	1.05382600	0.25139100	-2.64195400	H	-1.05316200	0.25809700	-2.64166000
H	-0.42804300	0.72034200	-2.65612000	H	0.43079000	0.72096700	-2.65357300

Table S53 Atomic coordinates (x,y,z) of $[Sc(OH)(\mathbf{L}^{021})]^+$ isomers.

$[Sc(OH)(\mathbf{L}^{021})]^+$ Δ				$[Sc(OH)(\mathbf{L}^{021})]^+$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.77705600	1.06537200	2.11689900	N	0.77720400	1.06343200	2.11917900
C	0.26843200	1.62552800	3.02069200	C	-0.26817600	1.61985400	3.02534100
C	1.60561100	1.83317600	2.32407200	C	-1.60582500	1.82739700	2.32982300
N	1.97654900	0.60361000	1.60228700	N	-1.97538100	0.59896000	1.60562300
C	2.32485200	-0.46603800	2.57922100	C	-2.32058400	-0.47360600	2.58047900
C	1.66025200	-1.80379500	2.29927200	C	-1.65423600	-1.80981700	2.29707200
N	0.24452500	-1.67784600	1.88211700	N	-0.23900400	-1.68111900	1.87902900
C	-0.63929200	-1.25943600	3.02153600	C	0.64530700	-1.26383000	3.01853200
C	-1.52843000	-0.03862600	2.75056400	C	1.53146400	-0.04033000	2.74973100
H	-1.97986100	0.27351200	3.71119100	H	1.98291400	0.27060700	3.71074500
H	-2.34872400	-0.30432300	2.07171600	H	2.35183800	-0.30262200	2.06967900
H	-0.00535100	-1.07075600	3.89714000	H	0.01203900	-1.07893400	3.89545600
H	-1.30046600	-2.09339800	3.30294500	H	1.30870900	-2.09708500	3.29671400
C	-0.16746700	-2.99673300	1.35349400	C	0.17454100	-2.99827200	1.34711700
C	-1.47800600	-2.88393900	0.63910500	C	1.48495900	-2.88180200	0.63294700
C	-2.42712900	-3.90807100	0.57797600	C	2.43567600	-3.90431400	0.56856600
C	-3.61258000	-3.68460300	-0.12174000	C	3.62064000	-3.67682300	-0.13066700
C	-3.83235500	-2.43590700	-0.71010400	C	3.83854600	-2.42593700	-0.71519100
C	-2.84253400	-1.46649400	-0.58816900	C	2.84717900	-1.45855000	-0.59021800
N	-1.68123900	-1.70067900	0.04628900	C	2.99170800	-0.04478000	-1.08932100
C	-2.99056900	-0.05445100	-1.09157400	O	4.00833300	0.28747900	-1.72585900
O	-4.00710800	0.27228900	-1.73105300	O	2.01390100	0.72231400	-0.77707700
O	-2.01621500	0.71701500	-0.77943300	N	1.68640300	-1.69658300	0.04361700
H	-4.75419800	-2.19873600	-1.23944000	H	4.76000100	-2.18594800	-1.24394600
H	-4.36884500	-4.46854600	-0.18801300	H	4.37804600	-4.45943000	-0.19962300
H	-2.23415400	-4.85591100	1.08128700	H	2.24424300	-4.85404500	1.06890000
H	0.59692000	-3.32469800	0.63183100	H	-0.58943800	-3.32535400	0.62461700
H	-0.21900900	-3.75688600	2.15178600	H	0.22705500	-3.76031800	2.14353800
H	1.74176900	-2.43750600	3.20184300	H	-1.73408500	-2.44538800	3.19848600
H	2.18391100	-2.31774700	1.48804200	H	-2.17791000	-2.32297400	1.48534000
H	2.05773500	-0.11952100	3.58413700	H	-2.05268700	-0.12894300	3.58582300
H	3.41630300	-0.62020100	2.59569900	H	-3.41175300	-0.62964400	2.59801100
C	3.08118800	0.83951100	0.66865800	C	-3.08141600	0.83521200	0.67387500
C	3.13135900	-0.31768400	-0.31270300	C	-3.13025500	-0.31972600	-0.30987800
O	2.08998300	-1.01553000	-0.45432700	O	-2.08725100	-1.01511900	-0.45364000
N	4.24083600	-0.56514500	-1.00986800	N	-4.23766700	-0.57271000	-1.00810200
C	4.27777600	-1.68369900	-1.95101700	C	-4.25439600	-1.68444800	-1.95857500
H	3.58488300	-2.46812600	-1.62890200	H	-3.89682800	-1.35888500	-2.94924900
H	4.00308600	-1.35018300	-2.96512200	H	-3.61751800	-2.49902000	-1.59665400
H	5.29934000	-2.08646500	-1.97601900	H	-5.28692600	-2.04466600	-2.05506400
C	5.42486100	0.29202000	-0.99016100	C	-5.42107400	0.28495600	-1.00765800
H	5.74846900	0.46395000	-2.02703100	H	-5.23089300	1.23071200	-0.49225400

H	5.20782500	1.26452300	-0.53851200	H	-5.69123800	0.51286100	-2.04952200
H	6.24847800	-0.19198700	-0.44219600	H	-6.27052400	-0.22751200	-0.52997100
H	4.04015300	0.97420000	1.19459500	H	-4.03966500	0.96666300	1.20189700
H	2.87672300	1.75733300	0.09404300	H	-2.87953700	1.75490600	0.10142300
H	2.36695200	2.10381500	3.07968400	H	-2.36721300	2.09551000	3.08632900
H	1.54910200	2.65178800	1.60013600	H	-1.55059100	2.64766300	1.60763400
H	0.38971100	0.94986800	3.87433200	H	-0.38805400	0.94171700	3.87722200
H	-0.07211800	2.58452300	3.44116200	H	0.07142700	2.57816000	3.44809200
C	-1.63726500	2.15708200	1.64071600	C	1.63501200	2.15759600	1.64407900
C	-0.93283600	2.83573400	0.47252000	C	0.92897900	2.83642600	0.47737300
O	0.02063700	2.22580200	-0.09634900	O	-0.02427200	2.22633400	-0.09184300
N	-1.31737000	4.03903500	0.05694600	N	1.30897500	4.04036000	0.05941100
C	-2.50306800	4.73483500	0.55314000	C	2.49825300	4.73828300	0.54308100
H	-3.02032900	4.14811500	1.31733400	H	2.97440400	4.19492600	1.36377900
H	-2.21930200	5.71012600	0.97591200	H	3.22338000	4.83378400	-0.28008600
H	-3.19734400	4.90322100	-0.28426500	H	2.22522400	5.74587300	0.88946800
C	-0.65937500	4.64003100	-1.10478100	C	0.65276200	4.62135300	-1.11414300
H	-1.08313900	4.24130900	-2.04067800	H	1.01592900	4.14511900	-2.03908100
H	-0.82093500	5.72450000	-1.07177900	H	-0.43345200	4.48671500	-1.04746600
H	0.41605600	4.43040600	-1.08099100	H	0.88563800	5.69224800	-1.14548300
H	-1.86103300	2.87178100	2.44735100	H	1.85813600	2.87143700	2.45152000
H	-2.58561500	1.75215700	1.26642200	H	2.58398500	1.75531500	1.26859700
O	0.17766500	-0.16842500	-1.99159300	O	-0.17476100	-0.17042200	-1.99251700
H	1.02788700	-0.60136500	-2.16965000	H	-1.02694300	-0.59969800	-2.17012300

Table S54 Atomic coordinates (x,y,z) of [Sc($\mathbf{L}^{102}$)] isomers.

[Sc($\mathbf{L}^{102}$)] Δ				[Sc($\mathbf{L}^{102}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.05421900	-0.32354700	2.44259900	N	0.76152600	2.07767200	1.11714600
C	-0.77990200	0.70236100	3.16071300	C	-0.25871800	3.04348800	1.61715900
C	-1.60079500	1.60739800	2.23402300	C	-1.63983100	2.81212700	1.03506700
N	-0.76148400	2.07774300	1.11705700	N	-1.99526500	1.38526100	1.10750000
C	0.25874600	3.04355000	1.61717900	C	-2.20904300	0.95908100	2.51826000
C	1.63989500	2.81218100	1.03520100	C	-1.46901200	-0.31753400	2.88886900
N	1.99526900	1.38529400	1.10761300	N	-0.05431200	-0.32361700	2.44258600
C	2.20907000	0.95906600	2.51834200	C	0.77973500	0.70227700	3.16078700
C	1.46887000	-0.31747100	2.88900100	C	1.60073500	1.60725300	2.23415300
H	1.52978400	-0.45972400	3.98359900	H	1.99898000	2.44969600	2.82963800
H	1.94898900	-1.18673600	2.42121400	H	2.45647500	1.06859400	1.81281300
H	1.90724000	1.77574800	3.18485900	H	0.11494600	1.30806200	3.78755600
H	3.28203200	0.79664700	2.71011000	H	1.46881800	0.19654200	3.85308000
C	3.19082600	1.12777100	0.29349000	C	0.50287800	-1.67152700	2.69990400
C	3.33859900	-0.34776900	0.07610300	C	1.83428700	-1.78919900	2.02155700
C	4.56194300	-1.02073900	0.11185700	C	2.90092700	-2.56588700	2.47996100
C	4.58421400	-2.39840400	-0.10717900	C	4.06648900	-2.62164100	1.71384500
C	3.38417300	-3.06547700	-0.36083200	C	4.12823800	-1.91775800	0.50783500
C	2.20977900	-2.31999200	-0.38822500	C	3.01656200	-1.17496700	0.12224200
N	2.18639700	-0.99366400	-0.16774900	C	2.90429700	-0.44804100	-1.19179000
C	0.86088600	-2.91605000	-0.69278400	O	3.88094500	-0.39061100	-1.95839500
O	0.73528000	-4.14087800	-0.84304300	O	1.74106100	0.05251900	-1.41706900
O	-0.08389600	-2.04506400	-0.78623700	N	1.91200900	-1.09957800	0.87817700
H	3.34276000	-4.13899200	-0.53970400	H	5.00764400	-1.94445600	-0.13440000
H	5.52713500	-2.94660200	-0.07626500	H	4.91802400	-3.21479400	2.05112600
H	5.47668600	-0.46485000	0.31876800	H	2.81213000	-3.11163400	3.41962200
H	3.04681600	1.61096000	-0.68551000	H	-0.17994600	-2.41584900	2.25885900
H	4.10310500	1.55148600	0.74818400	H	0.57781000	-1.87965800	3.77994700
H	2.37048000	3.43570500	1.58498300	H	-1.53001700	-0.45988600	3.98344900
H	1.67546600	3.11197600	-0.01678500	H	-1.94912300	-1.18674100	2.42096700
H	0.29685300	2.97353100	2.70926100	H	-1.90703300	1.77572800	3.18473700
H	-0.06260600	4.07269500	1.39084400	H	-3.28202200	0.79686400	2.71009600
C	-1.49246500	2.68256600	-0.00648600	C	-3.19085600	1.12773700	0.29345100
C	-0.63768500	2.59929800	-1.27934700	C	-3.33854500	-0.34780600	0.07599700
O	-0.84343500	3.37991100	-2.21671600	C	-4.56187300	-1.02082700	0.11169300
O	0.26741900	1.66516000	-1.28573700	C	-4.58407000	-2.39849100	-0.10732500
H	-1.77017600	3.73151700	0.18912800	C	-3.38398800	-3.06552200	-0.36092600
H	-2.41399200	2.11458200	-0.19321300	C	-2.20963000	-2.31998500	-0.38831900
H	-1.99900000	2.44987400	2.82948400	N	-2.18632700	-0.99364800	-0.16783800
H	-2.45655700	1.06881300	1.81263500	C	-0.86070900	-2.91594200	-0.69291000
H	-0.11518900	1.30811000	3.78759200	O	-0.73498600	-4.14078400	-0.84300800
H	-1.46906900	0.19661600	3.85291600	O	0.08394600	-2.04485500	-0.78665400

C	-0.50305200	-1.67142300	2.69996800	H	-3.34253400	-4.13904000	-0.53976700
C	-1.83440900	-1.78905600	2.02151400	H	-5.52696400	-2.94673700	-0.07644400
C	-2.90113500	-2.56567000	2.47983900	H	-5.47664700	-0.46497100	0.31856000
C	-4.06663000	-2.62138400	1.71361600	H	-4.10313400	1.55134200	0.74825000
C	-4.12822800	-1.91754400	0.50757200	H	-3.04698600	1.61101900	-0.68552500
C	-3.01647200	-1.17482600	0.12206100	H	-2.37044500	3.43570800	1.58474700
N	-1.91199900	-1.09946200	0.87810800	H	-1.67525100	3.11186900	-0.01694000
C	-2.90403400	-0.44799800	-1.19201500	H	-0.29687900	2.97353000	2.70925100
O	-3.88061600	-0.39048200	-1.95866900	H	0.06261500	4.07263000	1.39078100
O	-1.74071900	0.05247000	-1.41724300	C	1.49267000	2.68246400	-0.00630600
H	-5.00756700	-1.94421600	-0.13475700	C	0.63812500	2.59912600	-1.27930800
H	-4.91822800	-3.21447400	2.05084700	O	0.84424600	3.37945000	-2.21682800
H	-2.81246600	-3.11138300	3.41953100	O	-0.26712400	1.66511900	-1.28567200
H	-0.57809100	-1.87945000	3.78002400	H	1.77034900	3.73142100	0.18933600
H	0.17977400	-2.41581500	2.25904800	H	2.41424300	2.11450500	-0.19287300

Table S55 Atomic coordinates (x,y,z) of [ScF($\mathbf{L}^{102}$)]$^-$ isomers.

[ScF($\mathbf{L}^{102}$)]$^-$ Δ				[ScF($\mathbf{L}^{102}$)]$^-$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.17648800	-0.52597700	2.74970400	N	1.30411400	1.67281300	1.63272000
C	-0.79118400	0.23623600	3.58417500	C	0.48001900	2.83165000	2.08503000
C	-1.87180700	0.95791800	2.78539200	C	-0.90796600	2.92891200	1.45621200
N	-1.30416300	1.67222800	1.63296800	N	-1.59282300	1.62816900	1.44307300
C	-0.48017500	2.83122600	2.08507000	C	-1.95122300	1.19300200	2.82202200
C	0.90772000	2.92868800	1.45606000	C	-1.55791800	-0.24268600	3.15391800
N	1.59275800	1.62802900	1.44284800	N	-0.17589100	-0.52559600	2.74982900
C	1.95144600	1.19293900	2.82174500	C	0.79178600	0.23685600	3.58408100
C	1.55850700	-0.24283800	3.15364500	C	1.87215100	0.95865400	2.78504000
H	1.70432100	-0.39850000	4.24186300	H	2.40535700	1.65191700	3.46578600
H	2.21034600	-0.95640200	2.63763000	H	2.61461400	0.25005900	2.40343900
H	1.47787200	1.87694800	3.53615000	H	0.23605100	0.96394500	4.18821400
H	3.03691700	1.30161100	2.98031300	H	1.28308900	-0.43618200	4.30674400
C	2.80225100	1.67507700	0.61040200	C	0.11708700	-1.95816900	2.83177300
C	3.29821500	0.27059100	0.39694400	C	1.43708000	-2.23098800	2.16629400
C	4.64895700	-0.08440100	0.36096900	C	2.35908700	-3.16510200	2.64574100
C	4.98943600	-1.42102600	0.14443900	C	3.55561300	-3.35347300	1.95217800
C	3.97314400	-2.35881600	-0.04705900	C	3.78837800	-2.61488800	0.79115300
C	2.65100200	-1.91814900	-0.00855300	C	2.80828400	-1.71433000	0.37530100
N	2.32857400	-0.63985000	0.23205800	C	2.90800600	-0.93533800	-0.91242300
C	1.47708800	-2.82421200	-0.29454600	O	3.98047500	-0.92560200	-1.54592200
O	1.67009900	-4.04903300	-0.43296000	O	1.82488300	-0.34298600	-1.26410900
O	0.34861700	-2.22756000	-0.39319300	N	1.67534900	-1.51189500	1.06061500
H	4.18324900	-3.41137200	-0.23250000	H	4.69886900	-2.73027300	0.20477500
H	6.03693600	-1.72646800	0.12290900	H	4.29610400	-4.06933700	2.31312400
H	5.41419600	0.67832900	0.50901200	H	2.13787200	-3.72547300	3.55490700
H	2.53717600	2.11106600	-0.36606000	H	-0.67155400	-2.51024700	2.29761500
H	3.59361300	2.30529200	1.05537400	H	0.13083700	-2.32409400	3.87545500
H	1.49128400	3.68403300	2.01943700	H	-1.70356800	-0.39833200	4.24216100
H	0.83177700	3.26755600	0.41875400	H	-2.20967800	-0.95640300	2.63800800
H	-0.38507200	2.78391600	3.17702400	H	-1.47771700	1.87713300	3.53636200
H	-1.01432700	3.77264900	1.87441200	H	-3.03670000	1.30141700	2.98073600
C	-2.35576000	2.13278200	0.72469800	C	-2.80239600	1.67513500	0.61076100
C	-1.74039000	2.54003500	-0.61035000	C	-3.29832300	0.27064900	0.39727100
O	-2.37138700	3.30260400	-1.37006300	C	-4.64906300	-0.08433200	0.36114600
O	-0.58987000	2.03044000	-0.86241000	C	-4.98953100	-1.42093600	0.14449000
H	-2.93899500	2.97470300	1.14160100	C	-3.97322700	-2.35873300	-0.04691500
H	-3.05782800	1.30648700	0.53508300	C	-2.65108400	-1.91807400	-0.00821500
H	-2.40498700	1.65106700	3.46627500	N	-2.32867100	-0.63978700	0.23243500
H	-2.61424000	0.24922900	2.40391200	C	-1.47715200	-2.82415900	-0.29393800
H	-0.23547100	0.96336100	4.18828000	O	-1.67025700	-4.04890100	-0.43299800
H	-1.28225400	-0.43694400	4.30686800	O	-0.34860400	-2.22759000	-0.39229800

C	-0.11620900	-1.95860500	2.83159000	H	-4.18333900	-3.41127400	-0.23242000
C	-1.43622600	-2.23162100	2.16624900	H	-6.03703600	-1.72635200	0.12279800
C	-2.35801000	-3.16593300	2.64575300	H	-5.41431200	0.67840200	0.50911200
C	-3.55460400	-3.35443300	1.95234900	H	-3.59376200	2.30530400	1.05579800
C	-3.78765500	-2.61576900	0.79143100	H	-2.53743400	2.11115800	-0.36571800
C	-2.80777600	-1.71500700	0.37552100	H	-1.49155400	3.68416800	2.01969200
N	-1.67475200	-1.51247000	1.06067400	H	-0.83223000	3.26785300	0.41891200
C	-2.90792800	-0.93579200	-0.91204900	H	0.38506000	2.78421200	3.17699300
O	-3.98038900	-0.92657500	-1.54555900	H	1.01400100	3.77317100	1.87437800
O	-1.82493800	-0.34335200	-1.26394500	C	2.35532900	2.13354200	0.72410700
H	-4.69823300	-2.73120200	0.20519600	C	1.73948400	2.54047000	-0.61081300
H	-4.29495000	-4.07042200	2.31334500	O	2.37004300	3.30317600	-1.37076500
H	-2.13658000	-3.72632600	3.55485200	O	0.58908000	2.03046400	-0.86260100
H	-0.12976300	-2.32459300	3.87525100	H	2.93846800	2.97566500	1.14073900
H	0.67248400	-2.51050000	2.29731500	H	3.05756700	1.30741300	0.53439000
F	0.85323000	0.11578800	-1.76461400	F	-0.85332900	0.11506800	-1.76463200

Table S56 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{102})]$^{-}$ isomers.

[Sc(OH)(**L**^{102})]$^{-}$ Δ			[Sc(OH)(**L**^{102})]$^{-}$ Λ		
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.21758500	-0.58811100	2.72302400	N	1.30352900	1.61196700	1.64207300
C	-0.75222500	0.15172400	3.57472200	C	0.48359900	2.77421200	2.09971900
C	-1.84548900	0.87489400	2.79578100	C	-0.90036500	2.88964900	1.46519800
N	-1.30351500	1.61196200	1.64209500	N	-1.60128700	1.59733300	1.44116000
C	-0.48358800	2.77422000	2.09971800	C	-1.96895000	1.15189800	2.81372500
C	0.90036100	2.88966300	1.46517400	C	-1.59831600	-0.29434100	3.12451400
N	1.60130700	1.59736400	1.44118800	N	-0.21753700	-0.58814300	2.72297000
C	1.96894300	1.15196700	2.81377300	C	0.75228100	0.15168700	3.57467400
C	1.59835300	-0.29428300	3.12456900	C	1.84552800	0.87487700	2.79573300
H	1.75182900	-0.46626700	4.20922600	H	2.37618400	1.55576100	3.49049300
H	2.25723100	-0.99001600	2.59325600	H	2.58667300	0.16463900	2.41504600
H	1.48522900	1.81872700	3.53747700	H	0.20036400	0.87447200	4.18738300
H	3.05275400	1.27586200	2.97242400	H	1.23297300	-0.53746300	4.28935200
C	2.80696000	1.65990900	0.60460000	C	0.05634100	-2.02577500	2.78405600
C	3.30301200	0.25993500	0.36647000	C	1.37851600	-2.31158400	2.12680700
C	4.65329400	-0.09467500	0.32076800	C	2.26901300	-3.28502800	2.58800300
C	4.99342300	-1.42706100	0.07700100	C	3.46661200	-3.48692200	1.89999300
C	3.97713800	-2.36128900	-0.13081600	C	3.73230600	-2.72150900	0.76343600
C	2.65541800	-1.92006300	-0.08177200	C	2.78209900	-1.78185100	0.36496400
N	2.33324800	-0.64752000	0.18446600	C	2.91644000	-0.96740600	-0.89767400
C	1.47685000	-2.81368400	-0.38522100	O	3.99689100	-0.96844100	-1.51886700
O	1.65793600	-4.03862100	-0.53424500	O	1.85451900	-0.33609800	-1.24305100
O	0.35575900	-2.20276400	-0.48763600	N	1.64827500	-1.56849000	1.04490500
H	4.18702800	-3.40986600	-0.33793800	H	4.64536600	-2.84561100	0.18275300
H	6.04102200	-1.73144500	0.04663900	H	4.18259400	-4.23431900	2.24623200
H	5.41914900	0.66484400	0.48167600	H	2.02295900	-3.86586600	3.47778200
H	2.53542100	2.10704600	-0.36465600	H	-0.73593400	-2.55805300	2.23460600
H	3.59877200	2.28459600	1.05626800	H	0.05361600	-2.40863100	3.82184600
H	1.47695500	3.65005900	2.02905700	H	-1.75179600	-0.46633500	4.20916800
H	0.81264600	3.23163500	0.42953800	H	-2.25717600	-0.99008600	2.59319200
H	-0.38377900	2.71904000	3.19111100	H	-1.48529400	1.81867100	3.53745200
H	-1.02588300	3.71257700	1.89826100	H	-3.05277200	1.27575200	2.97233300
C	-2.39192700	2.07949600	0.77776100	C	-2.80694300	1.65988900	0.60458100
C	-1.84252700	2.52332100	-0.57304000	C	-3.30300200	0.25991800	0.36645200
O	-2.54321700	3.24736700	-1.30915500	C	-4.65328500	-0.09468700	0.32073500
O	-0.67309400	2.08332400	-0.86120100	C	-4.99341500	-1.42706900	0.07695400
H	-2.96925900	2.90325300	1.23670100	C	-3.97713100	-2.36129900	-0.13086300
H	-3.09128600	1.24892100	0.59848000	C	-2.65541000	-1.92007900	-0.08180400
H	-2.37613100	1.55579500	3.49053500	N	-2.33324100	-0.64754100	0.18445400
H	-2.58664400	0.16464700	2.41512900	C	-1.47684400	-2.81368900	-0.38528400
H	-0.20028900	0.87452500	4.18739800	O	-1.65791100	-4.03863800	-0.53423900
H	-1.23289800	-0.53741000	4.28942700	O	-0.35574500	-2.20277200	-0.48764400
C	-0.05627800	-2.02574600	2.78410700	H	-4.18702700	-3.40987200	-0.33800300

C	-1.37845300	-2.31157100	2.12686300	H	-6.04101500	-1.73144900	0.04658000
C	-2.26894000	-3.28501400	2.58808000	H	-5.41913900	0.66483500	0.48163800
C	-3.46654800	-3.48692200	1.90009000	H	-3.59874700	2.28457600	1.05626300
C	-3.73226200	-2.72152400	0.76352900	H	-2.53540600	2.10703400	-0.36467200
C	-2.78206300	-1.78186900	0.36503100	H	-1.47697200	3.65001100	2.02911300
N	-1.64822900	-1.56849300	1.04495100	H	-0.81266900	3.23166000	0.42957500
C	-2.91644700	-0.96741900	-0.89760200	H	0.38381200	2.71901900	3.19111300
O	-3.99689800	-0.96850700	-1.51879200	H	1.02588400	3.71257700	1.89826800
O	-1.85452900	-0.33613200	-1.24302500	C	2.39192400	2.07950700	0.77772300
H	-4.64533300	-2.84562700	0.18286400	C	1.84250500	2.52333600	-0.57306600
H	-4.18252300	-4.23431600	2.24635000	O	2.54320100	3.24735400	-1.30920500
H	-2.02287400	-3.86583700	3.47786500	O	0.67306100	2.08335400	-0.86120500
H	-0.05354400	-2.40860800	3.82189500	H	2.96926100	2.90326600	1.23665300
H	0.73600000	-2.55801200	2.23465300	H	3.09128500	1.24893400	0.59842800
O	0.86205100	0.25612000	-1.83096700	O	-0.86206400	0.25613700	-1.83096300
H	0.36812400	1.01415900	-2.18329700	H	-0.36815300	1.01419800	-2.18326800

Table S57 Atomic coordinates (x,y,z) of [Sc($\mathbf{L}^{012}$)]$^{+}$ isomers.

[Sc($\mathbf{L}^{012}$)]$^{+}$ Δ				[Sc($\mathbf{L}^{012}$)]$^{+}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	0.64757900	-0.91819700	2.16082400	N	1.54353200	0.88464300	1.75560500
C	-0.43542400	-0.77719900	3.19748500	C	1.10051800	2.06680600	2.55379000
C	-1.77265600	-0.26815400	2.64934600	C	-0.06078300	2.81398000	1.92827400
N	-1.54374100	0.88408800	1.75610600	N	-1.10744700	1.87444100	1.48456300
C	-1.10087700	2.06661800	2.55389100	C	-1.79430200	1.25543800	2.65620600
C	0.06032800	2.81387900	1.92825000	C	-1.91259900	-0.25927600	2.56928100
N	1.10718000	1.87454200	1.48457100	N	-0.64729400	-0.91838600	2.16045000
C	1.79428400	1.25575100	2.65620400	C	0.43597200	-0.77738700	3.19684800
C	1.91284800	-0.25896600	2.56945000	C	1.77294800	-0.26778700	2.64850100
H	2.25241800	-0.64623600	3.54715000	H	2.42126500	0.00192700	3.50213600
H	2.66861400	-0.54248700	1.82538500	H	2.28844100	-1.04551000	2.07576000
H	1.25613700	1.53938900	3.56859900	H	0.07144300	-0.10995900	3.98581500
H	2.80913400	1.67020100	2.76362300	H	0.60935300	-1.74942500	3.68099500
C	2.06770800	2.59537800	0.63231700	C	-0.91820400	-2.35922200	1.93912100
C	2.92880000	1.61468600	-0.10227900	C	0.27197900	-2.97596900	1.26710800
C	4.29549900	1.79247600	-0.32837400	C	0.69077500	-4.29884200	1.42406800
C	4.99850500	0.81284000	-1.03010200	C	1.78705700	-4.74598000	0.68387500
C	4.31812000	-0.31894300	-1.48436200	C	2.42067700	-3.87072700	-0.20309700
C	2.95578500	-0.41701000	-1.22116900	C	1.93319300	-2.57134600	-0.30399700
N	2.27764400	0.52818200	-0.54729300	C	2.44274600	-1.55126500	-1.28751200
C	2.10800700	-1.57755400	-1.66689300	O	3.44466100	-1.79474100	-1.97875400
O	2.62149800	-2.54393400	-2.24818000	O	1.74257200	-0.47002500	-1.33363400
O	0.85456600	-1.44528500	-1.39074700	N	0.90328900	-2.13902100	0.43634400
H	4.81815800	-1.11764200	-2.03044600	H	3.26505300	-4.17994200	-0.81789300
H	6.06809900	0.92695300	-1.21335200	H	2.13983100	-5.77288000	0.79153200
H	4.79332600	2.68429100	0.05278400	H	0.16416700	-4.95887100	2.11374800
H	1.49548100	3.17612300	-0.10762400	H	-1.78503800	-2.44634700	1.26404200
H	2.68330400	3.30325300	1.21306300	H	-1.16668100	-2.87280300	2.88188700
H	0.46078400	3.53465900	2.66538200	H	-2.25205700	-0.64673200	3.54694500
H	-0.26627100	3.38662700	1.05474000	H	-2.66837900	-0.54279700	1.82523000
H	-0.82685400	1.72329400	3.55665700	H	-1.25610500	1.53905700	3.56857100
H	-1.94579700	2.75933800	2.69167200	H	-2.80922200	1.66967400	2.76378100
C	-2.70498900	1.25445400	0.93480400	C	-2.06816000	2.59511800	0.63241700
C	-2.18364100	2.01407400	-0.28017900	C	-2.92883400	1.61435600	-0.10253500
O	-0.96606100	1.85771200	-0.60615500	C	-4.29550600	1.79202500	-0.32888500
N	-2.98788000	2.81713300	-0.96362300	C	-4.99823400	0.81252200	-1.03105900
C	-2.48008800	3.58329000	-2.10275900	C	-4.31758400	-0.31902100	-1.48550500
H	-1.39687100	3.71282600	-2.01301900	C	-2.95529900	-0.41700500	-1.22201400
H	-2.71145700	3.06705800	-3.04786500	N	-2.27740000	0.52805600	-0.54768300
H	-2.96770000	4.56746300	-2.10578900	C	-2.10736600	-1.57733300	-1.66796500
C	-4.41449900	2.96547800	-0.66871500	O	-2.62074100	-2.54353700	-2.24969500
H	-4.94919500	3.08512700	-1.62031800	O	-0.85400200	-1.44512000	-1.39155200

H	-4.81135200	2.07675300	-0.16784600	H	-4.81738600	-1.11759800	-2.03197700
H	-4.59668000	3.85582700	-0.04693700	H	-6.06779800	0.92655400	-1.21453100
H	-3.43009600	1.85328500	1.50644200	H	-4.79352400	2.68367200	0.05241900
H	-3.21682900	0.34971900	0.57832600	H	-2.68407300	3.30263300	1.21327100
H	-2.42084300	0.00161900	3.50306200	H	-1.49607200	3.17624600	-0.10733000
H	-2.28808500	-1.04616400	2.07694000	H	-0.46136000	3.53463900	2.66545900
H	-0.07088200	-0.10936900	3.98609700	H	0.26570500	3.38684600	1.05480100
H	-0.60836200	-1.74912400	3.68202500	H	0.82650100	1.72308900	3.55642200
C	0.91841100	-2.35904000	1.93951200	H	1.94533600	2.75960100	2.69182500
C	-0.27193900	-2.97578800	1.26777600	C	2.70443600	1.25560700	0.93405700
C	-0.69087300	-4.29856200	1.42514800	C	2.18256000	2.01494800	-0.28091400
C	-1.78728200	-4.74579900	0.68519100	O	0.96497300	1.85807300	-0.60669700
C	-2.42085000	-3.87074900	-0.20200400	N	2.98631600	2.81830500	-0.96458400
C	-1.93322600	-2.57144800	-0.30332900	C	4.41297100	2.96732000	-0.67022200
N	-0.90325900	-2.13899600	0.43684200	H	4.81015700	2.07940000	-0.16821300
C	-2.44266700	-1.55167400	-1.28724800	H	4.94743100	3.08579200	-1.62211700
O	-3.44462900	-1.79528700	-1.97836100	H	4.59508000	3.85858200	-0.04973500
O	-1.74234900	-0.47054000	-1.33381900	C	2.47799300	3.58415100	-2.10368400
H	-3.26528000	-4.18005400	-0.81668400	H	2.70998600	3.06821700	-3.04879800
H	-2.14017300	-5.77262200	0.79319300	H	1.39465200	3.71271600	-2.01409800
H	-0.16427600	-4.95845600	2.11496500	H	2.96475100	4.56875400	-2.10654800
H	1.16705700	-2.87260200	2.88224400	H	3.42931000	1.85481400	1.50559000
H	1.78509300	-2.44620600	1.26423900	H	3.21666100	0.35112700	0.57750600

Table S58 Atomic coordinates (x,y,z) of [ScF($\mathbf{L}^{012}$)] isomers.

[ScF($\mathbf{L}^{012}$)] Δ				[ScF($\mathbf{L}^{012}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.77484600	0.67278200	2.34824900	N	-1.71232600	-0.81189700	1.76531600
C	0.26592600	0.46912600	3.39784800	C	-1.32718800	-2.16421500	2.29250600
C	1.66117300	0.19227600	2.86490000	C	-0.19506200	-2.84543000	1.53354800
N	1.71236800	-0.81189900	1.76543100	N	0.96662700	-1.96355800	1.30493900
C	1.32725500	-2.16416800	2.29276100	C	1.67521200	-1.60677600	2.56795900
C	0.19515200	-2.84546600	1.53384700	C	1.97684400	-0.11613500	2.67561000
N	-0.96651500	-1.96361100	1.30512700	N	0.77490600	0.67276000	2.34820900
C	-1.67513400	-1.60674400	2.56809100	C	-0.26587000	0.46908000	3.39780400
C	-1.97678400	-0.11610000	2.67565100	C	-1.66111500	0.19220200	2.86486900
H	-2.33437200	0.10628600	3.69868300	H	-2.28685300	-0.14808800	3.71149100
H	-2.77265700	0.17730200	1.98123300	H	-2.11429400	1.11344200	2.48653900
H	-1.06535600	-1.93449000	3.41783100	H	0.05086000	-0.35024700	4.05128600
H	-2.62119600	-2.16493300	2.64423700	H	-0.32333300	1.35934800	4.04446700
C	-1.92432700	-2.60838700	0.38576500	C	1.09422700	2.10811500	2.22465200
C	-2.87571200	-1.56853000	-0.13564100	C	-0.09374500	2.82549500	1.63957300
C	-4.23844000	-1.77210100	-0.36474900	C	-0.47773600	4.12833800	1.96604500
C	-4.99934700	-0.72153500	-0.88371600	C	-1.59538200	4.67778100	1.33330700
C	-4.37874000	0.49366700	-1.18466000	C	-2.29369100	3.92108500	0.38805100
C	-3.01274200	0.60735000	-0.93983900	C	-1.84023900	2.63284000	0.11590200
N	-2.29685300	-0.38933800	-0.40241100	C	-2.45475400	1.71712500	-0.91609300
C	-2.17918500	1.80629600	-1.31800400	O	-3.47367600	2.07436100	-1.53333100
O	-2.72193900	2.84706100	-1.72108600	O	-1.83255600	0.60115400	-1.07680400
O	-0.90880000	1.61228000	-1.20551900	N	-0.77997300	2.10707200	0.74257800
H	-4.92491700	1.33377900	-1.61195700	H	-3.16664400	4.31114400	-0.13372800
H	-6.06821300	-0.85350900	-1.05997200	H	-1.92029400	5.69050600	1.57750100
H	-4.69052300	-2.73693400	-0.13321800	H	0.08714400	4.69376200	2.70782800
H	-1.36180600	-3.01278200	-0.46683400	H	1.94812500	2.21500700	1.53619500
H	-2.46481400	-3.43689900	0.87350300	H	1.38461900	2.55057100	3.19323600
H	-0.09928900	-3.75566900	2.09111400	H	2.33441000	0.10621600	3.69865800
H	0.55625200	-3.15261400	0.54730800	H	2.77272800	0.17730400	1.98122400
H	1.06553900	-2.06225700	3.35448300	H	1.06540100	-1.93458800	3.41764400
H	2.19643500	-2.83523800	2.25817300	H	2.62126700	-2.16497500	2.64409200
C	3.12285800	-0.79089000	1.31993700	C	1.92449100	-2.60826800	0.38558300
C	3.46082700	-1.64598000	0.11148100	C	2.87580100	-1.56833300	-0.13581400
O	2.68401500	-2.50982500	-0.32690200	C	4.23854300	-1.77179100	-0.36495800
N	4.69130800	-1.43615900	-0.42355900	C	4.99935700	-0.72113900	-0.88388200
C	5.05033300	-2.08263600	-1.68060300	C	4.37865100	0.49403300	-1.18476100
H	4.34641800	-2.89452000	-1.88762400	C	3.01264700	0.60759400	-0.93993000
H	5.01787500	-1.35615700	-2.51098400	N	2.29684600	-0.38918000	-0.40252700
H	6.07023600	-2.49040300	-1.61456200	C	2.17897000	1.80646200	-1.31804700
C	5.57201900	-0.35120800	0.00571700	O	2.72162000	2.84731300	-1.72107200
H	5.24900700	0.62217100	-0.39819900	O	0.90860400	1.61227200	-1.20567000

H	5.62663600	-0.28742500	1.09970300	H	4.92476300	1.33420700	-1.61201800
H	6.58345600	-0.56419800	-0.36437100	H	6.06823100	-0.85301700	-1.06016300
H	3.78047700	-1.10932100	2.15266500	H	4.69070400	-2.73660000	-0.13348100
H	3.38533300	0.25026100	1.10514800	H	2.46503000	-3.43674400	0.87332200
H	2.28694200	-0.14792700	3.71153400	H	1.36200600	-3.01271300	-0.46701600
H	2.11431200	1.11350700	2.48649200	H	0.09935400	-3.75569800	2.09072300
H	-0.05078500	-0.35022300	4.05131600	H	-0.55613100	-3.15247300	0.54696300
H	0.32336500	1.35939200	4.04451600	H	-1.06550800	-2.06242400	3.35424700
C	-1.09417800	2.10813300	2.22464400	H	-2.19635500	-2.83529600	2.25781300
C	0.09380300	2.82549600	1.63957100	C	-3.12282700	-0.79085600	1.31988100
C	0.47786000	4.12830500	1.96608200	C	-3.46082800	-1.64577600	0.11133000
C	1.59551500	4.67772800	1.33333500	O	-2.68405800	-2.50965500	-0.32710000
C	2.29376600	3.92104100	0.38803700	N	-4.69129400	-1.43583100	-0.42365100
C	1.84025400	2.63282000	0.11585700	C	-5.57201400	-0.35099400	0.00589600
N	0.77997600	2.10707700	0.74252400	H	-5.62642600	-0.28732500	1.09989800
C	2.45474700	1.71709900	-0.91615700	H	-5.24913600	0.62244700	-0.39798100
O	3.47362400	2.07435300	-1.53344800	H	-6.58350300	-0.56402000	-0.36403100
O	1.83258200	0.60109900	-1.07679900	C	-5.05048200	-2.08215900	-1.68072700
H	3.16672500	4.31107200	-0.13375500	H	-5.01845600	-1.35547800	-2.51094500
H	1.92047000	5.69043200	1.57756100	H	-4.34638400	-2.89379000	-1.88810800
H	-0.08697400	4.69372700	2.70790100	H	-6.07025400	-2.49023200	-1.61450400
H	-1.38459900	2.55062000	3.19320400	H	-3.78042000	-1.10939800	2.15259200
H	-1.94805400	2.21498900	1.53615000	H	-3.38534000	0.25031700	1.10523800
F	0.05955300	-1.35605200	-1.38154900	F	-0.05959500	-1.35612200	-1.38150600

Table S59 Atomic coordinates (x,y,z) of [Sc(OH)($\mathbf{L}^{012}$)] isomers.

[Sc(OH)($\mathbf{L}^{012}$)] Δ				[Sc(OH)($\mathbf{L}^{012}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
N	-0.86374700	0.66652700	2.36029700	N	-1.66643000	-0.80456800	1.80574100
C	0.18700100	0.50225100	3.40591200	C	-1.29488100	-2.14958600	2.35877900
C	1.58927800	0.22597000	2.87988900	C	-0.17281800	-2.86080600	1.61277300
N	1.66640800	-0.80453200	1.80570700	N	0.99551500	-1.99661900	1.36864400
C	1.29487800	-2.14958300	2.35869300	C	1.70835500	-1.63351700	2.62168900
C	0.17282900	-2.86079900	1.61266200	C	2.04456000	-0.15001300	2.69300800
N	-0.99552200	-1.99662100	1.36855200	N	0.86369700	0.66656800	2.36031100
C	-1.70838700	-1.63357700	2.62160800	C	-0.18705900	0.50228100	3.40591700
C	-2.04460600	-0.15007600	2.69297000	C	-1.58932500	0.22597300	2.87988400
H	-2.42116400	0.08634500	3.70666100	H	-2.21561300	-0.08137200	3.73902700
H	-2.84070600	0.10666700	1.98336300	H	-2.02928100	1.14403800	2.47910400
H	-1.08879100	-1.92419400	3.47795000	H	0.11789200	-0.30028000	4.08611300
H	-2.64113500	-2.21260300	2.71549000	H	-0.24219800	1.41108700	4.02687200
C	-1.93915500	-2.64816900	0.44473700	C	1.24283200	2.08402400	2.22369900
C	-2.86876000	-1.61301200	-0.12259000	C	0.08513500	2.86194900	1.65949500
C	-4.23631500	-1.80662400	-0.33234400	C	-0.20300000	4.19225000	1.97696100
C	-4.99153600	-0.76524200	-0.87598900	C	-1.30259600	4.80382300	1.37145300
C	-4.36106800	0.43443800	-1.21490700	C	-2.08229400	4.07622200	0.46780500
C	-2.99106200	0.53978000	-0.98969400	C	-1.72136300	2.75716300	0.20411500
N	-2.27536200	-0.45196100	-0.43925000	C	-2.44745800	1.86335000	-0.77252000
C	-2.16314100	1.73811200	-1.38666600	O	-3.48869800	2.26987200	-1.32203200
O	-2.71481300	2.76754400	-1.80692300	O	-1.89938800	0.71602200	-0.95763700
O	-0.89191900	1.56001900	-1.26331000	N	-0.67048600	2.17494700	0.79598500
H	-4.90360100	1.27136500	-1.65272900	H	-2.94957500	4.51100700	-0.02743400
H	-6.06379000	-0.89019400	-1.03614000	H	-1.55246300	5.83981000	1.60640000
H	-4.69688200	-2.75717900	-0.06172800	H	0.42180500	4.73009500	2.69085000
H	-1.36318700	-3.08075500	-0.38455800	H	2.09109400	2.14723200	1.52206400
H	-2.50386700	-3.45910100	0.93603400	H	1.57231800	2.51649900	3.18523400
H	-0.10759200	-3.76497900	2.18796500	H	2.42110400	0.08643400	3.70669800
H	0.53952800	-3.18099800	0.63262600	H	2.84066400	0.10672000	1.98340300
H	1.03069100	-2.02848200	3.41804800	H	1.08875500	-1.92411200	3.47803900
H	2.17301100	-2.81033200	2.34165600	H	2.64111400	-2.21252200	2.71561000
C	3.07851200	-0.78368900	1.36714600	C	1.93915900	-2.64817600	0.44485200
C	3.41158200	-1.62133100	0.14456100	C	2.86876000	-1.61303800	-0.12251400
O	2.62340100	-2.47246600	-0.31435100	C	4.23629800	-1.80669600	-0.33232900
N	4.63867900	-1.41925700	-0.38733800	C	4.99152800	-0.76535500	-0.87604000
C	5.00063900	-2.06129600	-1.64665000	C	4.36108200	0.43433500	-1.21495800
H	4.26666000	-2.83635000	-1.88635700	C	2.99109000	0.53972500	-0.98967500
H	5.02185300	-1.31773300	-2.46134200	N	2.27538100	-0.45197400	-0.43917100
H	5.99970900	-2.51469000	-1.56234200	C	2.16319300	1.73807000	-1.38665000
C	5.53949600	-0.36032600	0.06593700	O	2.71486400	2.76747300	-1.80697200
H	5.23592900	0.62424100	-0.32548700	O	0.89196500	1.56000200	-1.26326000

H	5.58749900	-0.31526400	1.16089800	H	4.90361800	1.27123300	-1.65283100
H	6.54814500	-0.58759500	-0.30264800	H	6.06376900	-0.89035000	-1.03624200
H	3.73312600	-1.11981600	2.19527800	H	4.69684900	-2.75725900	-0.06171200
H	3.34911200	0.25728400	1.16396600	H	2.50388100	-3.45908700	0.93617500
H	2.21555800	-0.08140000	3.73902900	H	1.36320300	-3.08079400	-0.38443500
H	2.02923200	1.14405300	2.47914600	H	0.10761600	-3.76496300	2.18810600
H	-0.11793900	-0.30031800	4.08610100	H	-0.53951100	-3.18104600	0.63274800
H	0.24211600	1.41105400	4.02687500	H	-1.03068900	-2.02843600	3.41812900
C	-1.24289400	2.08398200	2.22369800	H	-2.17300100	-2.81035300	2.34176900
C	-0.08519900	2.86192500	1.65951500	C	-3.07852500	-0.78376100	1.36714600
C	0.20290600	4.19223000	1.97700200	C	-3.41153400	-1.62143200	0.14456200
C	1.30249500	4.80382900	1.37151000	O	-2.62330800	-2.47254700	-0.31431000
C	2.08221300	4.07625200	0.46785900	N	-4.63860500	-1.41938400	-0.38740400
C	1.72131600	2.75718900	0.20415100	C	-5.53950100	-0.36051700	0.06585600
N	0.67044400	2.17494500	0.79601200	H	-5.58750900	-0.31543700	1.16081500
C	2.44743400	1.86340100	-0.77249100	H	-5.23600800	0.62406800	-0.32558500
O	3.48865000	2.26997200	-1.32201400	H	-6.54813300	-0.58786400	-0.30272700
O	1.89941500	0.71605000	-0.95759200	C	-5.00050600	-2.06143100	-1.64672600
H	2.94948600	4.51106300	-0.02737200	H	-5.02207500	-1.31778800	-2.46133300
H	1.55234500	5.83981800	1.60646800	H	-4.26628900	-2.83620700	-1.88660000
H	-0.42191700	4.73005300	2.69089000	H	-5.99941000	-2.51518400	-1.56235300
H	-1.57240000	2.51643900	3.18523400	H	-3.73315300	-1.11988700	2.19526600
H	-2.09115200	2.14718700	1.52205700	H	-3.34914000	0.25720400	1.16393300
O	0.23816000	-1.42369700	-1.34807700	O	-0.23808800	-1.42372500	-1.34808200
H	1.09545700	-1.85033700	-1.15022300	H	-1.09535900	-1.85040400	-1.15019900

Table S60 Atomic coordinates (x,y,z) of [Sc($\mathbf{L}^{003}$)] isomers.

[Sc($\mathbf{L}^{003}$)] Δ				[Sc($\mathbf{L}^{003}$)] Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
O	0.82720600	-1.41901300	-1.47600200	O	-0.82682800	-1.41938800	-1.47574300
C	2.06448300	-1.75604100	-1.59519800	C	-2.06406100	-1.75646100	-1.59516800
O	2.49621900	-2.68817700	-2.29395700	O	-2.49563600	-2.68851700	-2.29413500
C	3.01599900	-0.88333900	-0.82008300	C	-3.01574800	-0.88393600	-0.82004900
C	4.39767500	-0.90158600	-0.99517300	C	-4.39741700	-0.90253900	-0.99510400
H	4.84708600	-1.62784400	-1.67119700	C	-5.16157800	0.03863800	-0.30147000
C	5.16160600	0.03978500	-0.30155600	C	-4.52006200	0.95964900	0.52880800
C	4.51987300	0.96061000	0.52876200	C	-3.13059100	0.89921400	0.65729600
H	5.08181600	1.71811200	1.07594700	N	-2.40838800	-0.02315500	0.00704100
C	3.13042600	0.89981100	0.65728900	C	-2.31725200	1.84992700	1.48758100
N	2.40844100	-0.02272300	0.00701500	N	-1.18483800	1.11721600	2.07818000
C	2.31686800	1.85032400	1.48758800	C	-1.70454700	0.15113800	3.09560000
N	1.18459800	1.11737600	2.07815700	H	-1.12897900	0.27556900	4.02011200
C	1.70446800	0.15137200	3.09558000	H	-2.74394100	0.40615500	3.35542200
H	1.12884800	0.27564300	4.02008300	C	-1.66274500	-1.30802000	2.65820800
H	2.74380300	0.40658800	3.35543400	N	-0.36214800	-1.64887500	2.05944800
C	1.66298700	-1.30778400	2.65816500	C	0.71812600	-1.62712600	3.09042700
N	0.36247700	-1.64887800	2.05937900	H	0.31003400	-1.19760300	4.01259600
C	-0.71779100	-1.62735600	3.09035000	H	1.01283900	-2.65730900	3.34704200
H	-0.30974500	-1.19774500	4.01250400	C	1.96578500	-0.85892300	2.67339000
H	-1.01227900	-2.65760100	3.34697900	N	1.62303200	0.44286600	2.07674800
C	-1.96560100	-0.85942700	2.67329400	C	1.05880600	1.36674100	3.10634700
N	-1.62315500	0.44245600	2.07669200	H	1.80001400	2.14095900	3.36115900
C	-1.05911500	1.36646800	3.10626000	H	0.89338700	0.80062600	4.03027200
H	-1.80048200	2.14055300	3.36104600	C	-0.23307000	2.06036900	2.69140500
H	-0.89358900	0.80044800	4.03022000	H	-0.03661700	2.85277100	1.96144600
C	0.23263500	2.06034000	2.69136100	H	-0.67244100	2.54251500	3.58570300
H	0.03606300	2.85272200	1.96141400	C	2.81124700	1.05706900	1.46737600
H	0.67187300	2.54256000	3.58568400	H	3.56120400	1.34905600	2.22379000
C	-2.81149800	1.05637300	1.46733500	H	3.28349400	0.32083900	0.79810600
H	-3.56152500	1.34819200	2.22375100	C	2.38215600	2.24521400	0.65538500
H	-3.28362100	0.32005800	0.79806500	N	1.20491900	2.09724400	0.03284900
C	-2.38267700	2.24463200	0.65537300	C	0.75516300	3.06667600	-0.77587300
N	-1.20533700	2.09701000	0.03294800	C	1.43705400	4.26780900	-0.95479400
C	-0.75580600	3.06657500	-0.77573800	C	2.65215500	4.44138700	-0.28836100
C	-1.43802700	4.26751200	-0.95470700	C	3.13807900	3.41221200	0.51958600
C	-2.65324700	4.44072400	-0.28838900	H	4.08888100	3.50527600	1.04524500
C	-3.13894200	3.41139900	0.51950000	H	3.22021200	5.36588700	-0.40377000
H	-4.08983100	3.50415400	1.04505000	H	1.02379500	5.02975600	-1.61438500
H	-3.22157800	5.36504500	-0.40386100	C	-0.49330200	2.70185000	-1.53542500
H	-1.02493600	5.02957800	-1.61425900	O	-1.08385000	3.55657900	-2.21715000
C	0.49277000	2.70206800	-1.53523900	O	-0.83446900	1.46529700	-1.42536700

O	1.08317900	3.55697300	-2.21685900	H	2.54494300	-1.42179400	1.93349300
O	0.83415700	1.46555400	-1.42531000	H	2.61125700	-0.73157100	3.56390600
H	-2.54460600	-1.42241900	1.93337200	C	-0.40740900	-2.97462600	1.42527700
H	-2.61113900	-0.73226600	3.56379700	H	-0.51311900	-3.78618100	2.16667300
C	0.40801100	-2.97459000	1.42512300	H	-1.28229900	-3.01501400	0.75785300
H	0.51394000	-3.78616200	2.16646200	C	0.83696300	-3.15980900	0.60365200
H	1.28289000	-3.01472700	0.75767900	C	1.51389900	-4.37393700	0.46919300
C	-0.83632900	-3.15999200	0.60351300	C	2.64820300	-4.42825400	-0.34306300
N	-1.25555100	-2.05298500	-0.02560500	C	3.06165500	-3.27576100	-1.01473800
C	-2.31915200	-2.11059700	-0.83793400	C	2.31958400	-2.11017700	-0.83784200
C	-3.06105200	-3.27630300	-1.01478800	N	1.25603200	-2.05272800	-0.02543100
C	-2.64740700	-4.42872400	-0.34311300	C	2.57922900	-0.83495700	-1.59760900
C	-1.51309900	-4.37421500	0.46912900	O	3.61753700	-0.70760800	-2.26886900
H	-1.15330200	-5.25636000	0.99955600	O	1.63946800	0.03871500	-1.49617900
H	-3.19846500	-5.36371600	-0.45655600	H	3.92697800	-3.26937600	-1.67624800
H	-3.92639300	-3.27005400	-1.67627100	H	3.19940900	-5.36315900	-0.45652900
C	-2.57908200	-0.83538300	-1.59761900	H	1.15424200	-5.25615600	0.99959900
O	-3.61741800	-0.70820700	-2.26886600	H	-2.43819900	-1.51853900	1.91369900
O	-1.63949800	0.03846400	-1.49613700	H	-1.87590400	-1.94229400	3.54035500
H	2.43851600	-1.51813700	1.91368400	H	-2.94217400	2.33509700	2.25754900
H	1.87623900	-1.94202100	3.54031800	H	-1.91941000	2.64083600	0.83278400
H	2.94167700	2.33563400	2.25755900	H	-5.08219700	1.71700300	1.07600700
H	1.91886100	2.64116000	0.83279200	H	-6.24691600	0.06056100	-0.41229500
H	6.24693200	0.06201100	-0.41241900	H	-4.84665400	-1.62893300	-1.67110200

Table S61 Atomic coordinates (x,y,z) of [ScF($\mathbf{L}^{003}$)]$^-$ isomers.

[ScF($\mathbf{L}^{003}$)]$^-$ Δ				[ScF($\mathbf{L}^{003}$)]$^-$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
F	-0.01769400	-0.20135900	-1.91641700	O	1.97325800	0.62047400	-0.41883900
N	-1.36818400	1.23087700	3.69626700	C	3.07784400	-0.01142800	-0.21424800
C	-2.10668600	0.10568300	4.24868300	O	4.17140000	0.29988600	-0.71151000
C	-1.19855200	-1.03869200	4.73278800	C	2.99360300	-1.18703400	0.73333900
N	-0.18479600	-1.44954500	3.76328600	C	4.13416000	-1.93770700	1.02029500
C	1.17306400	-1.50187300	4.28707100	C	4.02872700	-2.97285200	1.94556900
C	1.72889300	-0.13000100	4.70844700	C	2.80223200	-3.17996100	2.57387200
N	1.57010400	0.92352900	3.70663500	C	1.70358600	-2.37399200	2.24853500
C	0.93411700	2.13753000	4.19861400	N	1.79545400	-1.41550800	1.30345300
C	-0.52163800	1.93729500	4.65508900	C	0.41187100	-2.51378500	3.02262600
H	-0.52708800	1.38258400	5.60368000	N	0.13587900	-1.32723100	3.82018900
H	-0.93509700	2.93619300	4.89922400	C	1.18015300	-0.97760200	4.78068000
H	0.97049600	2.87627600	3.38751500	H	0.70310900	-0.63792200	5.71062600
H	1.48842900	2.58861700	5.05471700	H	1.78078500	-1.86279000	5.06811000
C	2.76142200	1.18862000	2.91650800	C	2.15094300	0.10950000	4.28700100
H	3.60304900	1.58217000	3.52768500	N	1.47545700	1.27612100	3.73825300
H	2.51388400	1.96418200	2.17574900	C	0.68101400	2.03110300	4.70551900
C	3.25375900	-0.04238300	2.18690300	H	0.65967500	1.47407300	5.65230900
N	2.40599700	-0.67813700	1.35761700	H	1.15858600	3.00132700	4.94786600
C	2.80572000	-1.82186400	0.77967500	C	-0.76249000	2.32650100	4.26381300
C	4.08201600	-2.36382900	0.95510500	N	-1.49004300	1.16020200	3.78096900
C	4.97585900	-1.69060400	1.78423800	C	-1.68949500	0.10992500	4.78163800
C	4.54921700	-0.52388300	2.41758500	H	-2.75692900	0.02611400	5.06360700
H	5.20572200	0.01251900	3.10365900	H	-1.16908600	0.39731200	5.70644500
H	5.98216800	-2.07828900	1.95271000	C	-1.21872000	-1.29280400	4.35324500
H	4.34381600	-3.29499100	0.45563500	H	-1.88505500	-1.67809100	3.57124300
C	1.77656800	-2.55732000	-0.04847200	H	-1.34500400	-1.96497700	5.23398700
O	2.08296900	-3.62783900	-0.59856800	C	-2.68657100	1.52162700	3.03905600
O	0.60320600	-2.02393400	-0.09881500	H	-3.47072900	1.97647200	3.68329800
H	2.79421600	-0.27152600	4.97576600	H	-2.40638700	2.28209300	2.29231600
H	1.23759400	0.18825800	5.63897600	C	-3.30083800	0.34215000	2.31746100
H	1.80827600	-1.92994300	3.50089300	N	-2.51262400	-0.38249400	1.50516200
H	1.26332200	-2.18052800	5.16724900	C	-3.02141900	-1.47858500	0.92193200
C	-0.53902300	-2.61673400	2.97230900	C	-4.35236100	-1.87874600	1.07275000
H	-0.66032700	-3.53331200	3.58980600	C	-5.18327500	-1.11018900	1.88489300
H	0.27576700	-2.80385400	2.25977900	C	-4.64473800	0.00440400	2.52728100
C	-1.82087500	-2.40449300	2.19785800	H	-5.25141800	0.60974800	3.20189300
N	-1.87188300	-1.41188100	1.28659400	H	-6.22854700	-1.38682800	2.03393800
C	-3.04737400	-1.14884500	0.68832500	H	-4.70507000	-2.77765600	0.56981100
C	-4.20930300	-1.88657800	0.92068300	C	-2.06550800	-2.32892400	0.11456400
H	-5.12710900	-1.61661100	0.40115000	O	-2.47271300	-3.37950200	-0.40597000
C	-4.15012600	-2.94376800	1.82509200	O	-0.84474300	-1.91116900	0.04048600

C	-2.94411400	-3.19322600	2.47804000	H	-0.75661200	3.06457900	3.45045400
H	-2.86471000	-3.98621300	3.22219300	H	-1.27463100	2.81733400	5.12459800
H	-5.03282600	-3.54999900	2.03579800	C	2.32195100	2.09377500	2.88458700
C	-3.07724900	0.04680400	-0.23526200	H	3.08863900	2.66254300	3.45461700
O	-4.13887100	0.37051200	-0.79050200	H	2.85794900	1.42624700	2.19383900
O	-1.96201600	0.68230100	-0.35920800	C	1.50588400	3.07818800	2.07657000
H	-0.69508100	-0.73012900	5.65956500	C	1.66757700	4.45681500	2.26595600
H	-1.84925000	-1.88746800	5.02171600	C	0.84272000	5.34824500	1.58038000
H	-2.77814300	-0.26292700	3.46192900	C	-0.13547100	4.83277400	0.73367800
H	-2.75981100	0.39934200	5.10350200	C	-0.22315800	3.44467600	0.59029000
C	-2.16838200	2.09263000	2.84330000	N	0.58691200	2.58553800	1.22672000
H	-2.91161700	2.69399800	3.41129700	C	-1.30264900	2.84802800	-0.28433800
H	-2.73063200	1.45389700	2.14619000	O	-2.12850200	3.59448700	-0.83250800
C	-1.30413700	3.04495800	2.04623100	O	-1.31177700	1.56085000	-0.39127800
N	-0.38963700	2.52602600	1.20497400	H	-0.82993700	5.47342700	0.19272800
C	0.45272400	3.36293000	0.57899000	H	0.94893400	6.42543600	1.72088800
C	0.40665200	4.75226500	0.72533400	H	2.42318400	4.81672000	2.96522900
C	-0.56541700	5.29531000	1.56126400	H	2.79381400	-0.29856100	3.49551800
C	-1.42396200	4.42772600	2.23545600	H	2.82714200	0.36490700	5.13587500
H	-2.17725500	4.80907300	2.92567400	H	0.47969000	-3.43754000	3.63746700
H	-0.64298300	6.37497700	1.70135300	H	-0.41542400	-2.64476000	2.31337500
H	1.12478400	5.37188800	0.19114000	H	2.68858100	-3.94943300	3.33780400
C	1.51363600	2.73164300	-0.29224500	H	4.89311100	-3.59110100	2.19377300
O	2.39018300	3.44504000	-0.80597800	H	5.07241100	-1.69422900	0.52463600
O	1.44330100	1.45204500	-0.43740300	F	-0.03662400	-0.27326700	-1.90414100

Table S62 Atomic coordinates (x,y,z) of [Sc(OH)(**L**^{003})]$^{-}$ isomers.

[Sc(OH)(**L**^{003})]$^{-}$ Δ				[Sc(OH)(**L**^{003})]$^{-}$ Λ			
Sc	0.00000000	0.00000000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
O	0.68415200	1.12232400	-1.48921600	O	1.88426100	0.89076900	-0.35538900
H	0.15253100	1.93218900	-1.55768000	C	3.04877400	0.38903100	-0.12375500
N	0.02349300	0.06021200	3.98251200	O	4.10736900	0.79768400	-0.62653600
C	-1.26352500	0.33217100	4.61382200	C	3.07939800	-0.75260700	0.86594600
C	-2.16953900	-0.89698300	4.80626400	C	4.29720700	-1.33962800	1.21089600
N	-2.45602200	-1.67167700	3.59718900	C	4.29937100	-2.33920400	2.17956300
C	-2.12404900	-3.08912900	3.66958500	C	3.09073600	-2.67548200	2.78505700
C	-0.64152700	-3.39918300	3.93393000	C	1.90649000	-2.03650200	2.39453600
N	0.31250400	-2.66426000	3.11041000	N	1.90003200	-1.10986900	1.41137700
C	1.38661600	-2.03445400	3.86195100	C	0.62453900	-2.33615600	3.13865600
C	0.87854900	-0.86723300	4.72490900	N	0.14130400	-1.17921900	3.87897900
H	0.31654900	-1.26785500	5.57968700	C	1.08893100	-0.63659200	4.85093500
H	1.75332500	-0.35418700	5.16679400	H	0.53977000	-0.35399100	5.75995600
H	2.12618500	-1.66663000	3.14010500	H	1.82012300	-1.40163200	5.17739800
H	1.92361500	-2.74767300	4.52806700	C	1.87480000	0.58196600	4.33956400
C	0.72948300	-3.32949900	1.88593700	N	1.02359700	1.59622100	3.73601400
H	1.17346000	-4.33213000	2.06849800	C	0.08752400	2.23692100	4.65858300
H	1.49112500	-2.70539100	1.40268300	H	0.13636000	1.71716300	5.62551700
C	-0.43555300	-3.49330100	0.93555100	H	0.38745300	3.28157700	4.87462500
N	-0.93614500	-2.39387600	0.33213700	C	-1.37518500	2.26991600	4.18116400
C	-2.08518200	-2.51194800	-0.36046800	N	-1.88849500	0.98098900	3.73736500
C	-2.75934200	-3.72211200	-0.52751800	C	-1.91987700	-0.05294200	4.77201000
C	-2.19444900	-4.87451500	0.01384500	H	-2.96116300	-0.30985700	5.04745600
C	-1.02214000	-4.75241600	0.75695300	H	-1.46866500	0.34905000	5.69050600
H	-0.56757300	-5.62119000	1.23385400	C	-1.20961800	-1.36431100	4.39267300
H	-2.67014700	-5.84735800	-0.12130200	H	-1.78553200	-1.87917000	3.61348600
H	-3.69291700	-3.73919700	-1.08745600	H	-1.23311800	-2.02510600	5.29055000
C	-2.63354500	-1.24679300	-0.97833800	C	-3.11548100	1.09830200	2.96550000
O	-3.80995700	-1.21674300	-1.36841100	H	-3.98319500	1.41772400	3.58359400
O	-1.80115200	-0.26376500	-1.07031700	H	-2.96404600	1.87859600	2.20201200
H	-0.51221400	-4.49514300	3.81986600	C	-3.48654900	-0.19297600	2.26653100
H	-0.41710600	-3.18804300	4.98882300	N	-2.56140600	-0.76894600	1.48137800
H	-2.42685400	-3.53340700	2.71173900	C	-2.83752900	-1.95152200	0.91329400
H	-2.70782100	-3.62407600	4.45605600	C	-4.07154000	-2.59507700	1.05252400
C	-3.78878400	-1.45712400	3.05956300	C	-5.04635800	-1.98713700	1.84101500
H	-4.59277900	-1.69059200	3.79182200	C	-4.74362000	-0.77839700	2.46843300
H	-3.92444200	-2.15071000	2.21207800	H	-5.46674700	-0.29011900	3.12306600
C	-4.01144900	-0.05616000	2.52824700	H	-6.02092900	-2.45770800	1.98359300
N	-3.00812400	0.49473100	1.83561800	H	-4.23948600	-3.55286400	0.56246100
C	-3.15818000	1.72529000	1.33144800	C	-1.71684800	-2.62009400	0.14429700
C	-4.34387700	2.45703100	1.45788200	O	-1.93127600	-3.70290900	-0.42700900
H	-4.42083400	3.45050900	1.01811000	O	-0.57030400	-2.02843700	0.16648800

C	-5.39512200	1.88631600	2.17649500	H	-1.47420300	2.96701000	3.33815500
C	-5.22409800	0.61785900	2.73197300	H	-1.97914700	2.70291600	5.01322200
H	-6.01609700	0.15022200	3.31937500	C	1.74364600	2.51528300	2.86798500
H	-6.33184100	2.42964900	2.31520600	H	2.39571900	3.21965200	3.42932000
C	-1.95477000	2.33172500	0.63922500	H	2.39203200	1.92081300	2.20726100
O	-2.09988900	3.36489800	-0.03669700	C	0.78785500	3.32109200	2.01862300
O	-0.81912000	1.74664600	0.83841800	C	0.68081700	4.70787500	2.18337400
H	-1.72871000	-1.56058700	5.56511800	C	-0.28923300	5.41327900	1.47142700
H	-3.10974900	-0.52606900	5.25803000	C	-1.14080800	4.70590000	0.62641400
H	-1.78310500	1.06589200	3.98334300	C	-0.95273300	3.32643400	0.50011300
H	-1.14158100	0.80311600	5.61788800	N	0.00004000	2.65021300	1.15883600
C	0.69478000	1.28662900	3.56258000	C	-1.87557900	2.51597400	-0.38050800
H	0.97481100	1.92987500	4.42449100	O	-2.86474800	3.06238600	-0.89469100
H	-0.00075800	1.85334500	2.92964500	O	-1.57733100	1.27035600	-0.53212400
C	1.95543500	1.00258700	2.77624600	H	-1.94068800	5.19175500	0.06999800
N	1.86967100	0.34679700	1.59772700	H	-0.39250500	6.49315100	1.59190800
C	3.01165600	-0.03832100	0.98744900	H	1.34301400	5.21701200	2.88450700
C	4.27929800	0.27961700	1.47060800	H	2.59565900	0.26292400	3.57435400
C	4.37388600	1.01377200	2.65051000	H	2.47730600	0.97682400	5.19038700
C	3.19917900	1.35864900	3.31432600	H	0.81104800	-3.21394500	3.79475800
H	3.23127800	1.88964100	4.26571200	H	-0.14792300	-2.61909100	2.41290100
H	5.34648500	1.28842400	3.06211700	H	3.05294100	-3.42011100	3.58052900
H	5.15771800	-0.06077100	0.92508500	H	5.22759500	-2.83008400	2.47695500
C	2.86519500	-0.91051800	-0.24232300	H	5.20930500	-0.99749600	0.72499100
O	3.87810700	-1.29633100	-0.84409300	O	-0.00536300	-0.35699700	-1.95882200
O	1.65215200	-1.22213400	-0.55784200	H	0.57804100	-1.10302700	-2.17546000

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