Supporting Information

Oxyaapa: A Picolinate-Based Ligand with Five Oxygen Donors that Strongly Chelates Lanthanides

Aohan Hu,[†] Ivan Keresztes,[†] Samantha N. MacMillan,[†] Yang Yang,[†] Erdong Ding,[†] Warren R. Zipfel,[‡] Robert A. Distasio, Jr.,[†] John W. Babich,[§] and Justin J. Wilson*[,†]

[†]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, United States

[‡]Department of Biomedical Engineering, Cornell University, Ithaca, New York 14853, United States

[§]Department of Radiology, Weill Cornell Medicine, New York, New York 10065, United States

*email: jjw275@cornell.edu

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1. 1D NMR Spectra

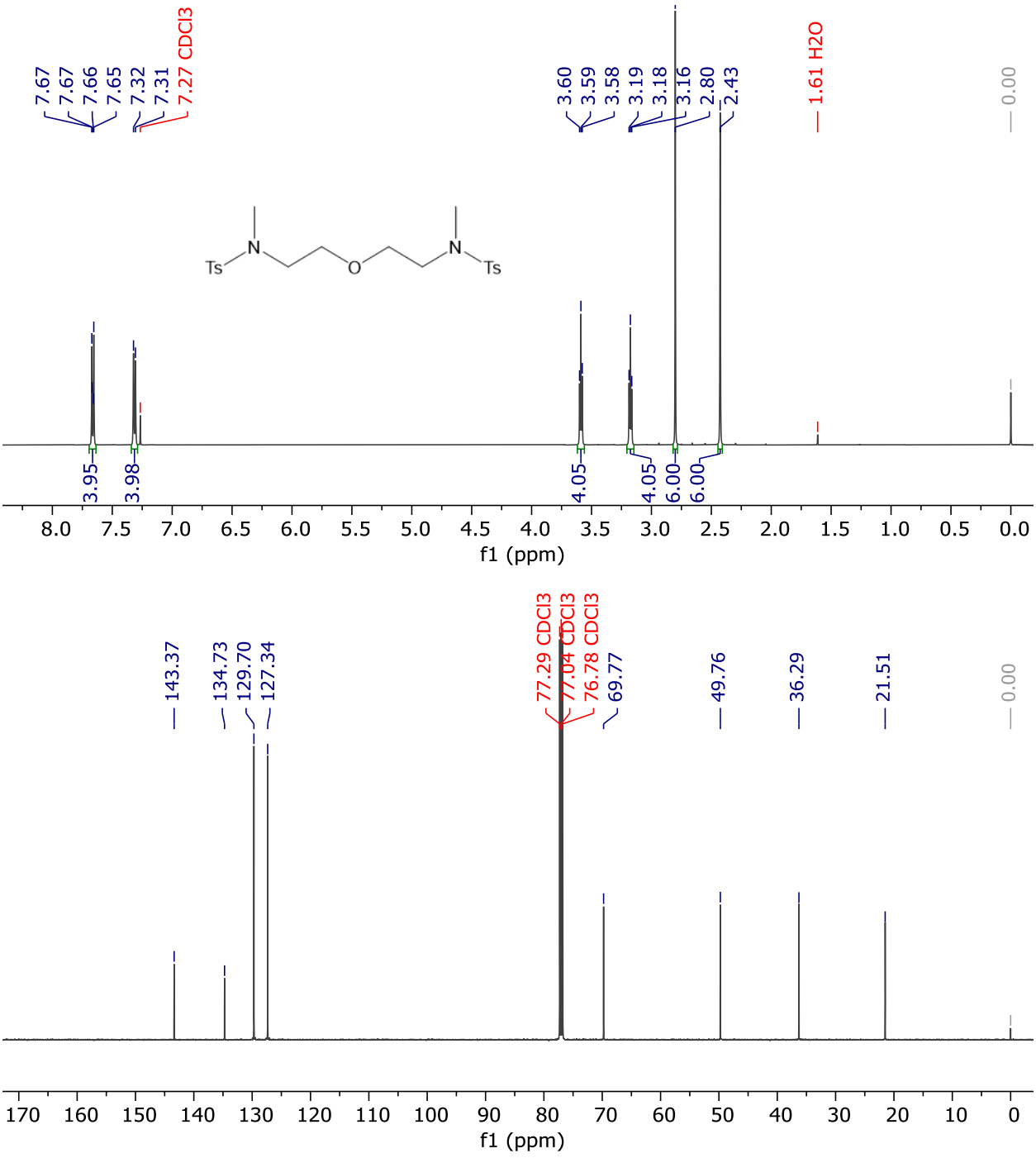

Figure S1. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 25 °C) spectra of **2**.

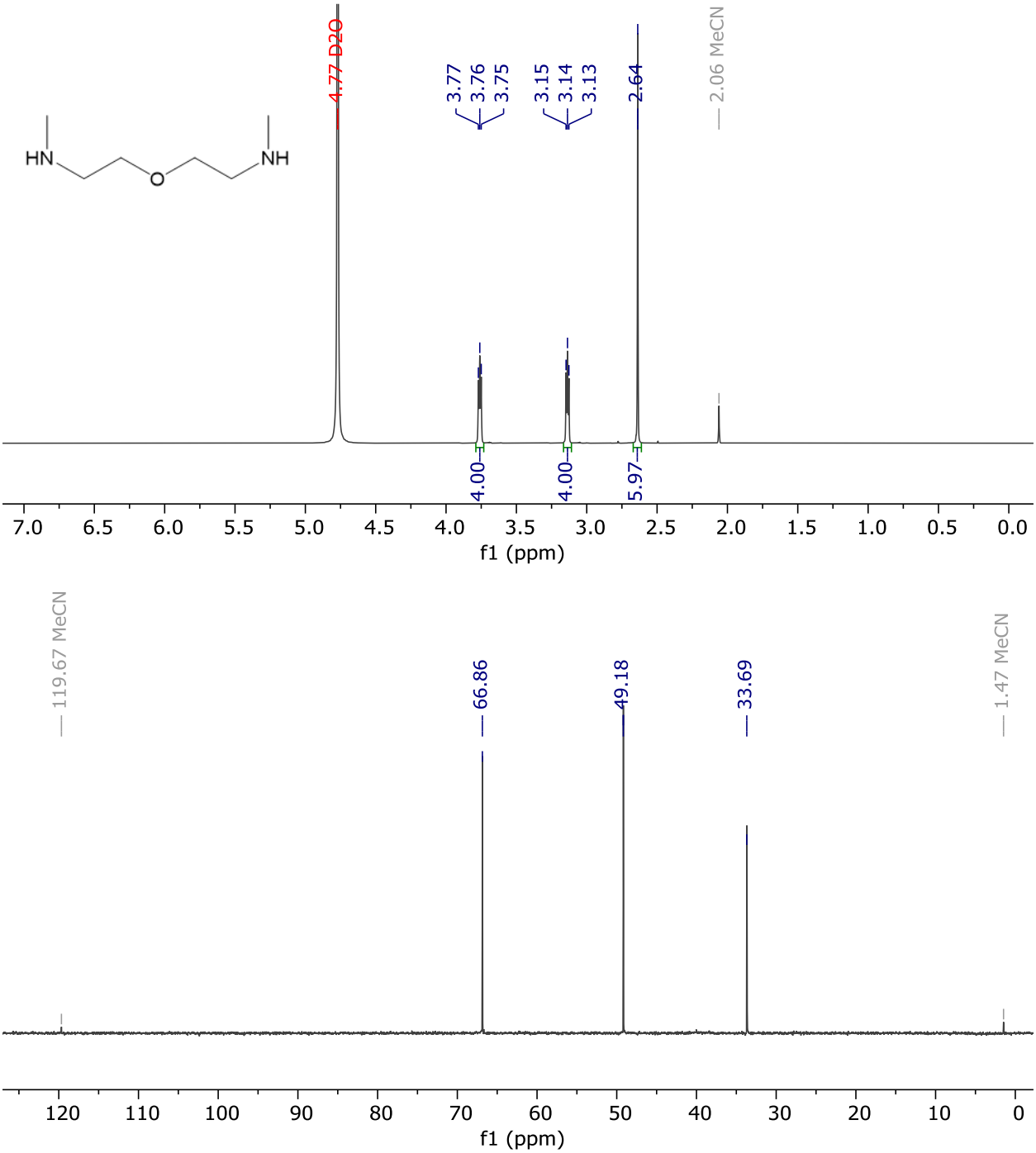

Figure S2. ^{1}H NMR (500 MHz, D_2O, pD = 9–10 by NaOD, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, D_2O, pD = 9–10 by NaOD, 25 °C) spectra of **3**. Acetonitrile was added as an internal reference.

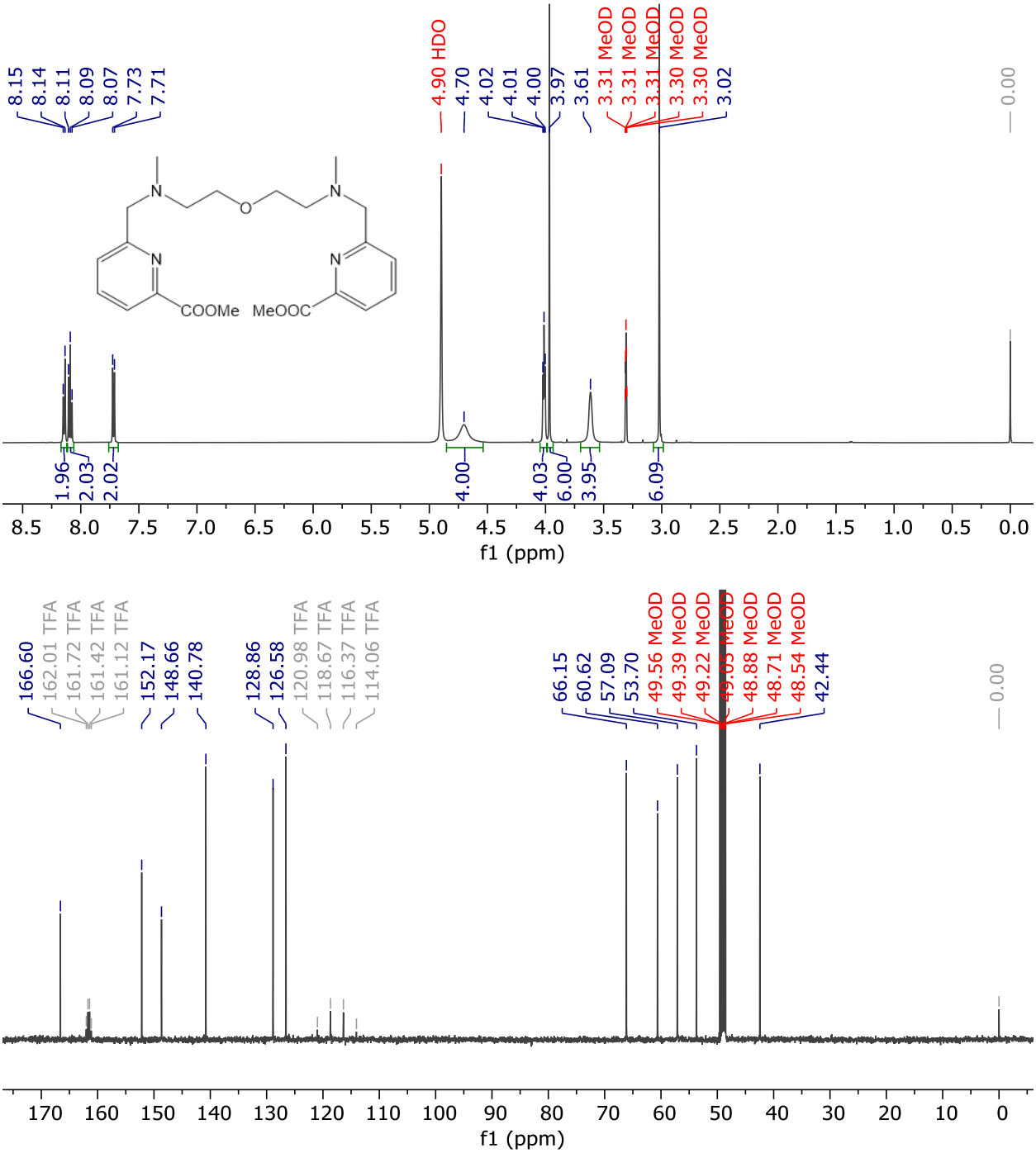

Figure S3. ^{1}H NMR (500 MHz, CD_3OD, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3OD, 25 °C) spectra of **4**.

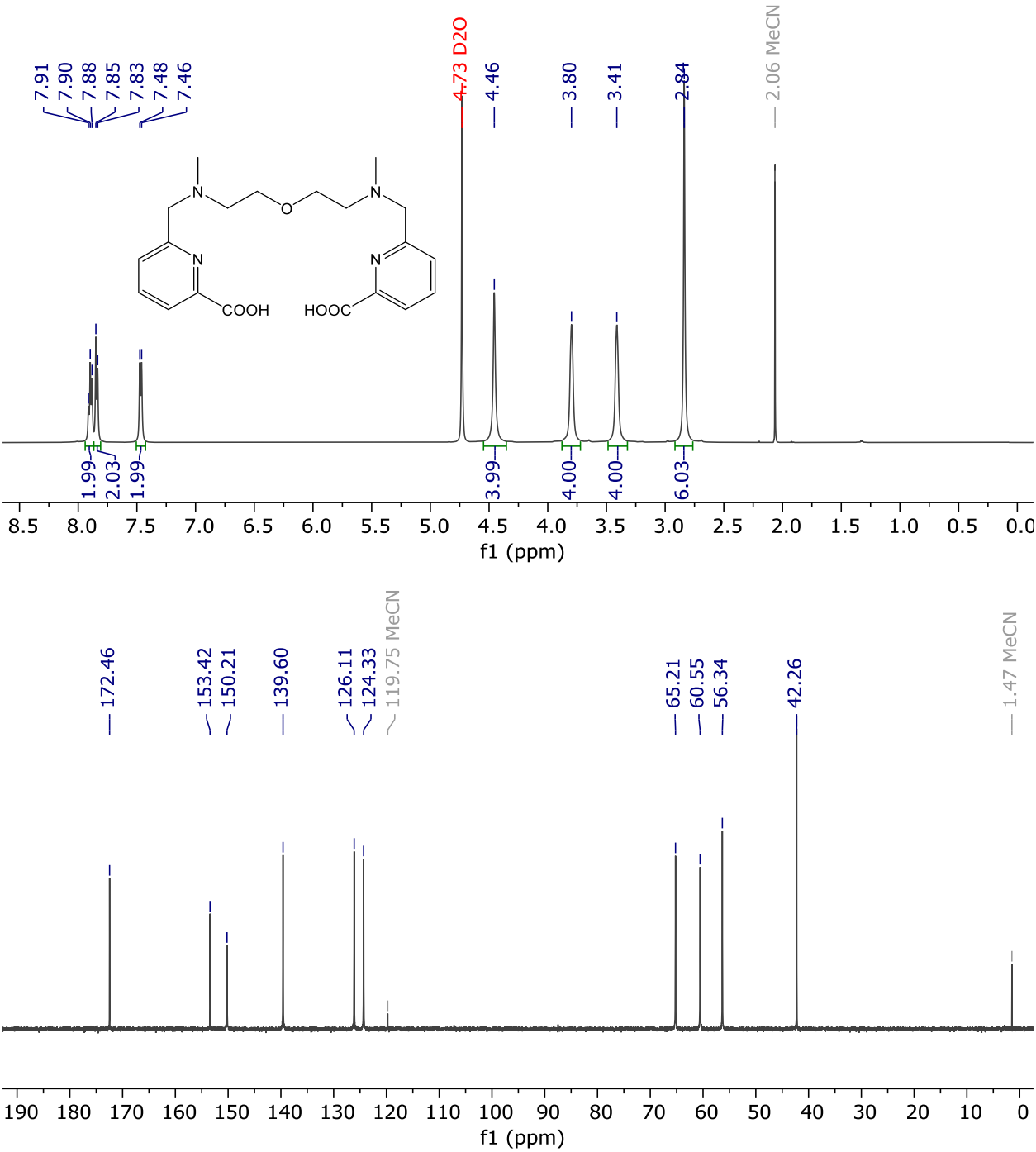

Figure S4. ^{1}H NMR (500 MHz, D_2O, pD ≈ 8 by NaOD, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, D_2O, pD ≈ 8 by NaOD, 25 °C) spectra of **OxyMepa**. Acetonitrile was added as an internal reference.

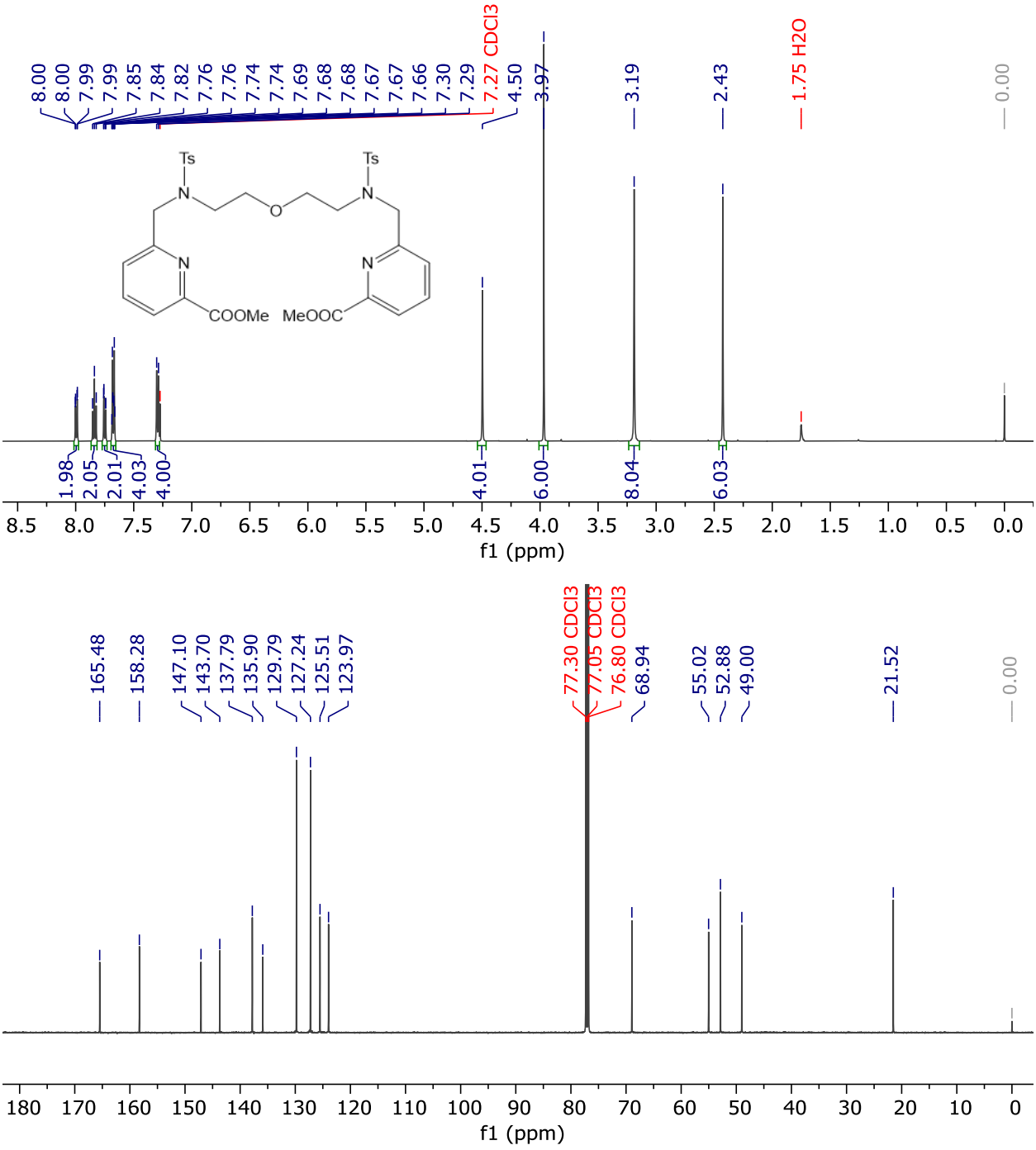

Figure S5. ^{1}H NMR ($CDCl_3$, 500 MHz, 25 °C) and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz, 25 °C) spectra of **5**.

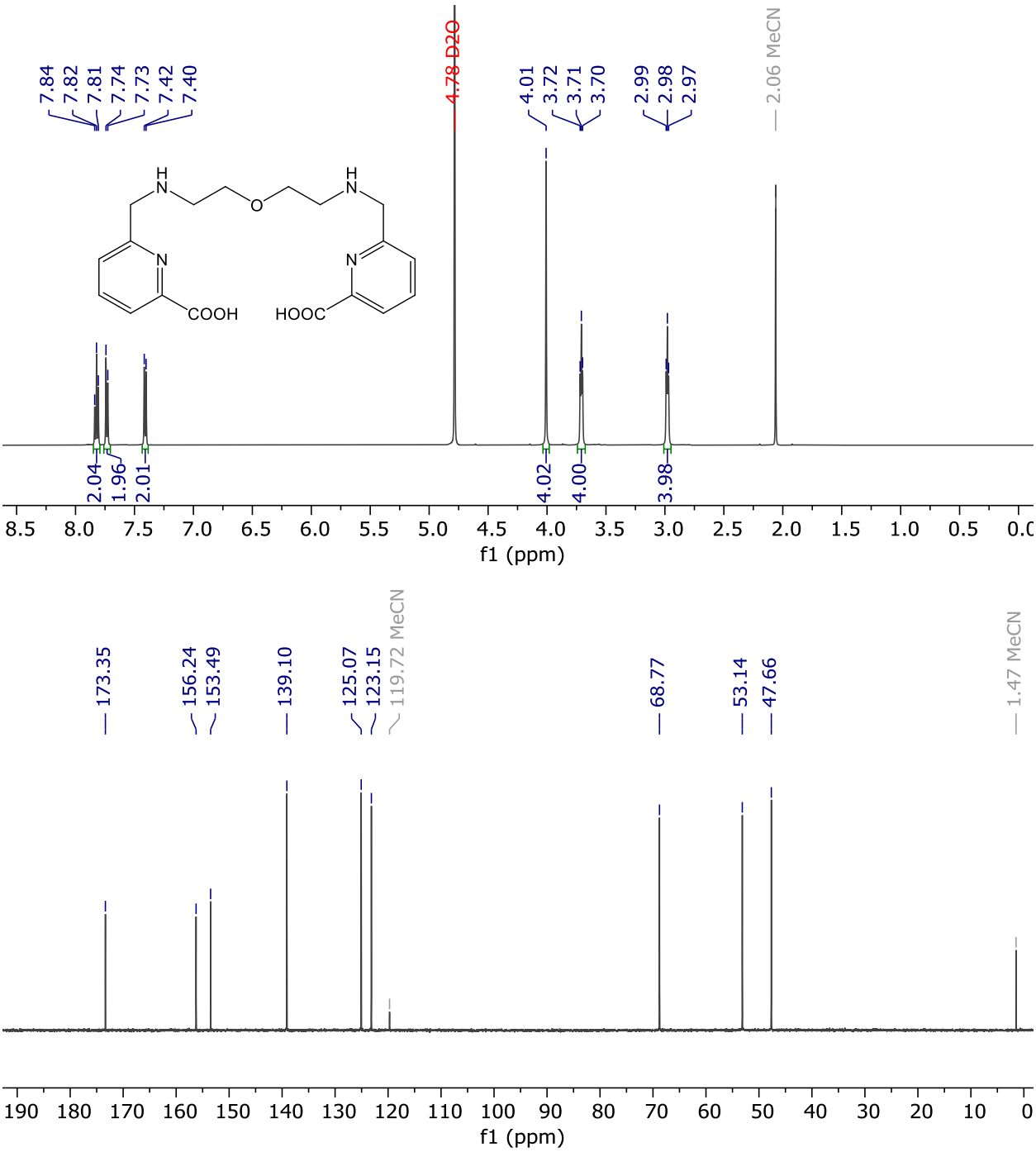

Figure S6. ^{1}H NMR (500 MHz, D_2O, pD ≈ 9 by NaOD, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, D_2O, pD ≈ 9 by NaOD, 25 °C) spectra of **6**. Acetonitrile was added as an internal reference.

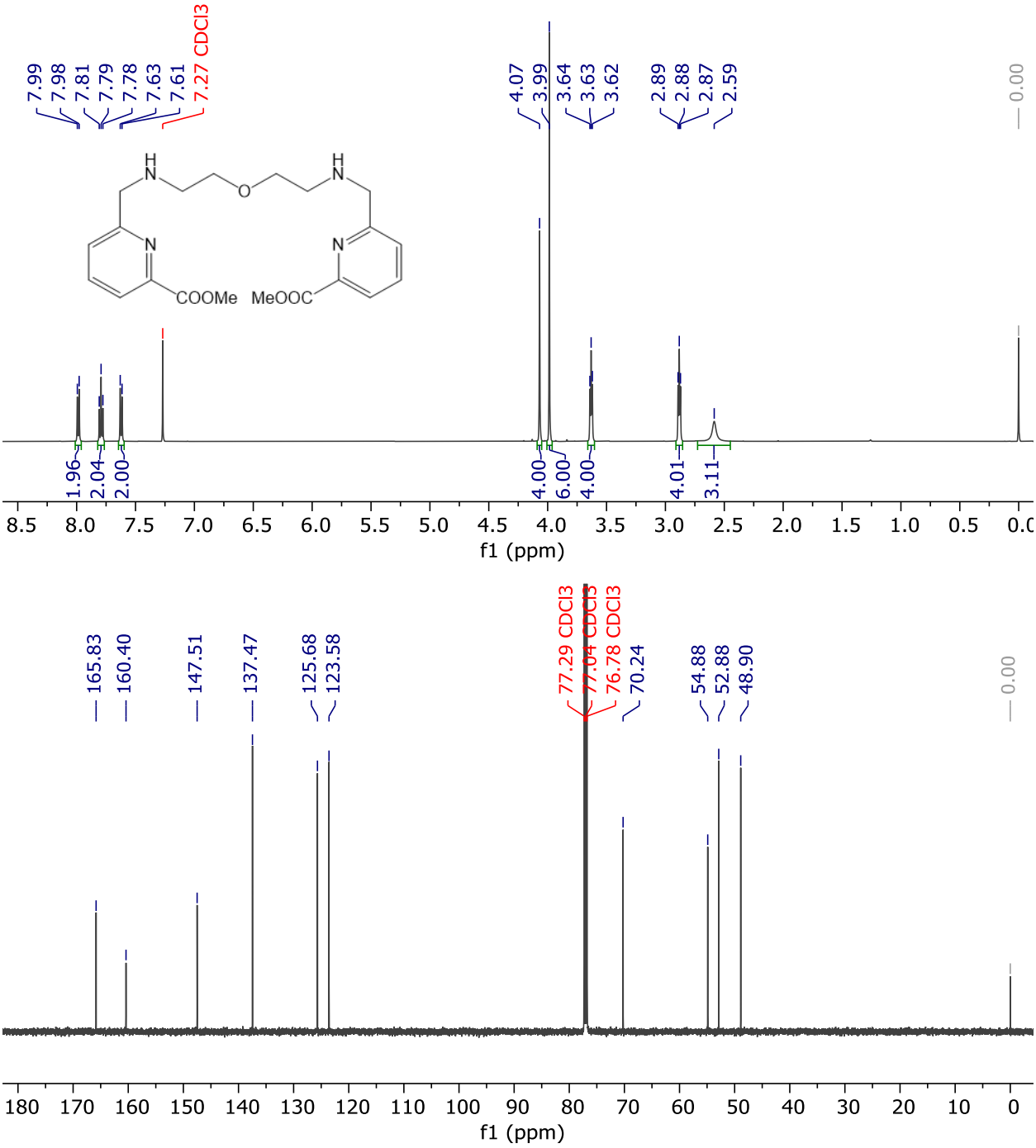

Figure S7. ^{1}H NMR (500 MHz, CDCl3, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 25 °C) spectra of **7**.

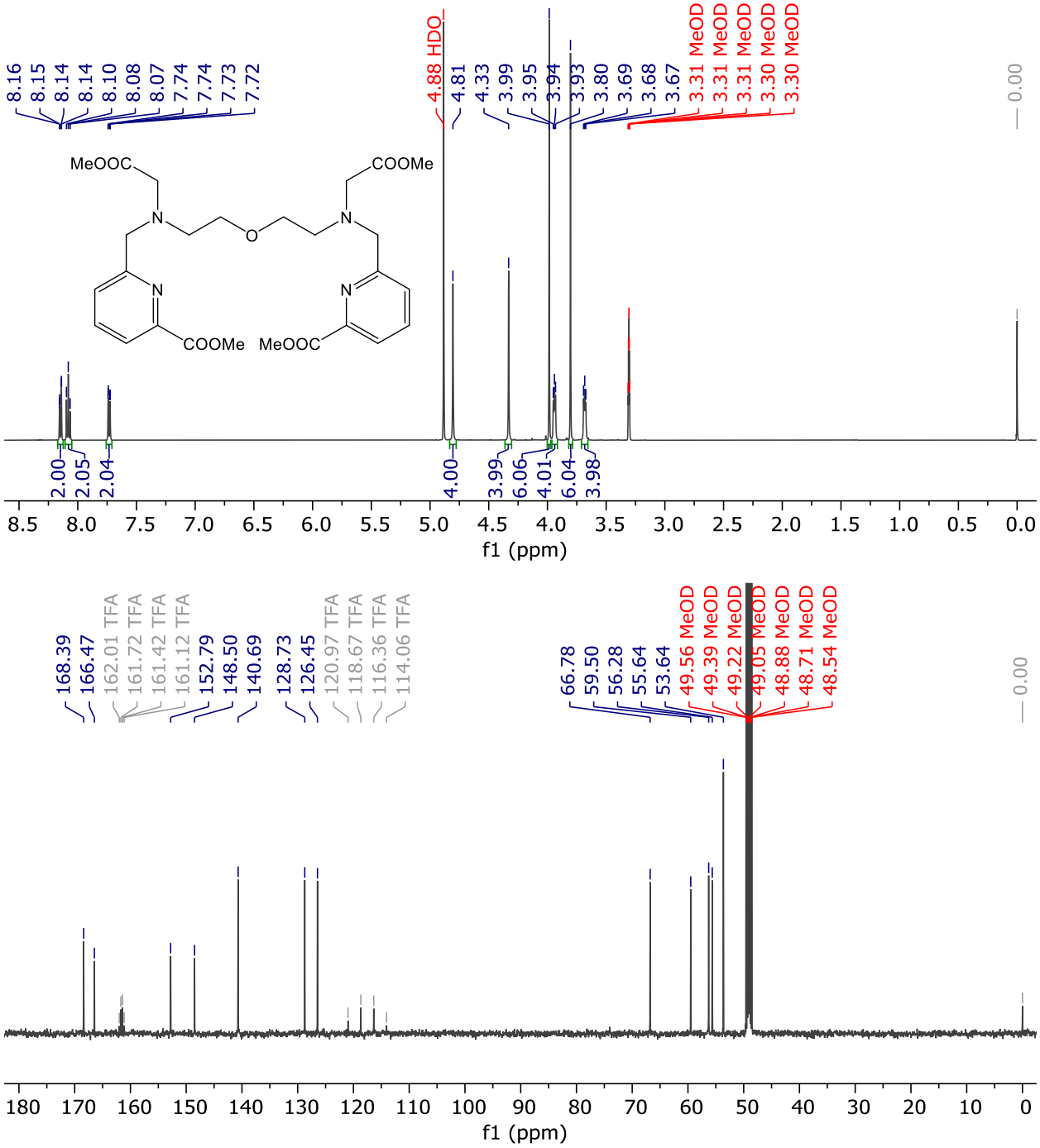

Figure S8. ^{1}H NMR (500 MHz, CD_3OD, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3OD, 25 °C) spectra of **8**.

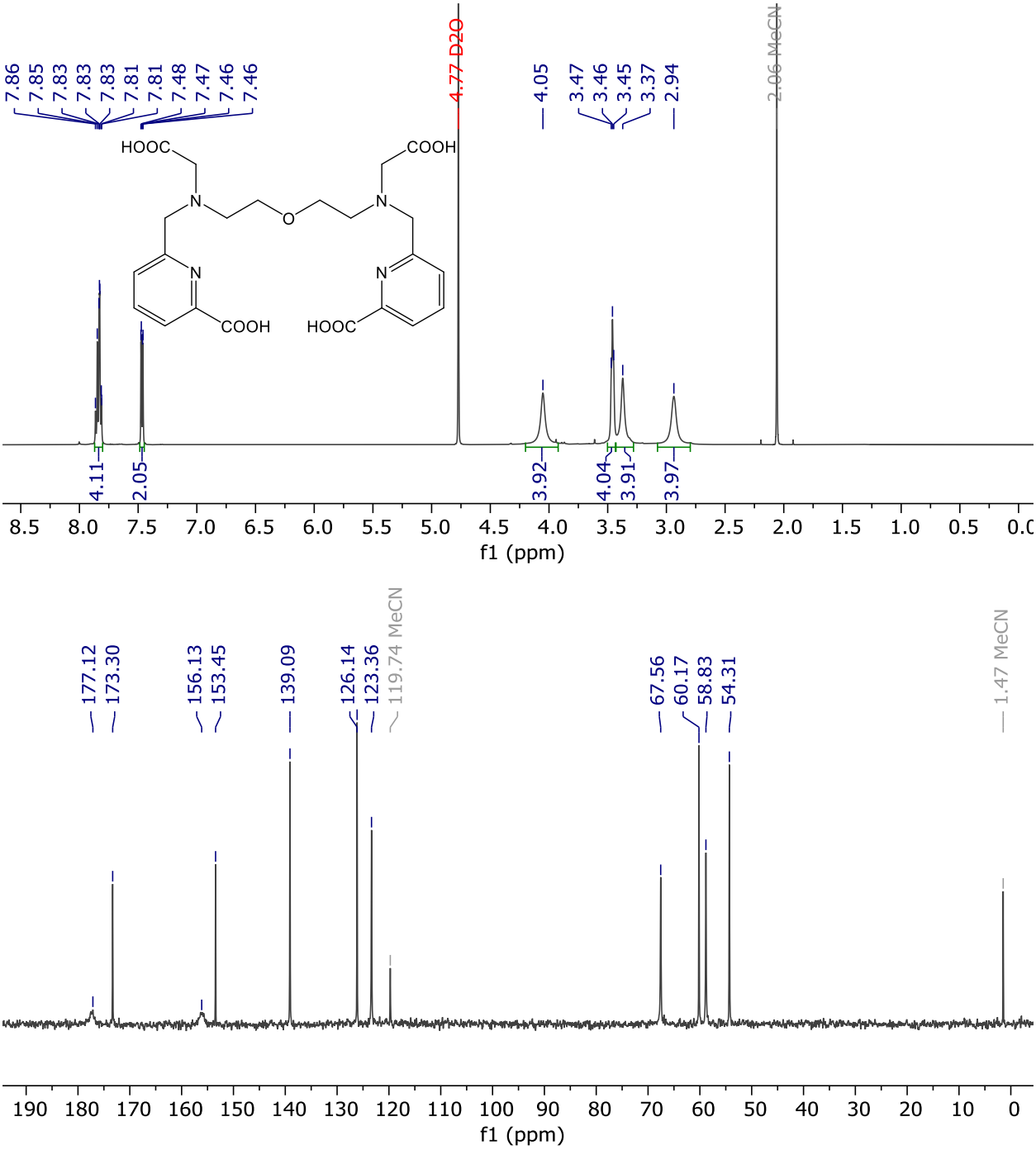

Figure S9. ^{1}H NMR (500 MHz, D_2O, pD ≈ 9 by NaOD, 25 °C) and $^{13}C\{^{1}H\}$ NMR (126 MHz, D_2O, pD ≈ 9 by NaOD, 25 °C) spectra of **Oxyaapa**. Acetonitrile was added as an internal reference.

2. High-Resolution Mass Spectra

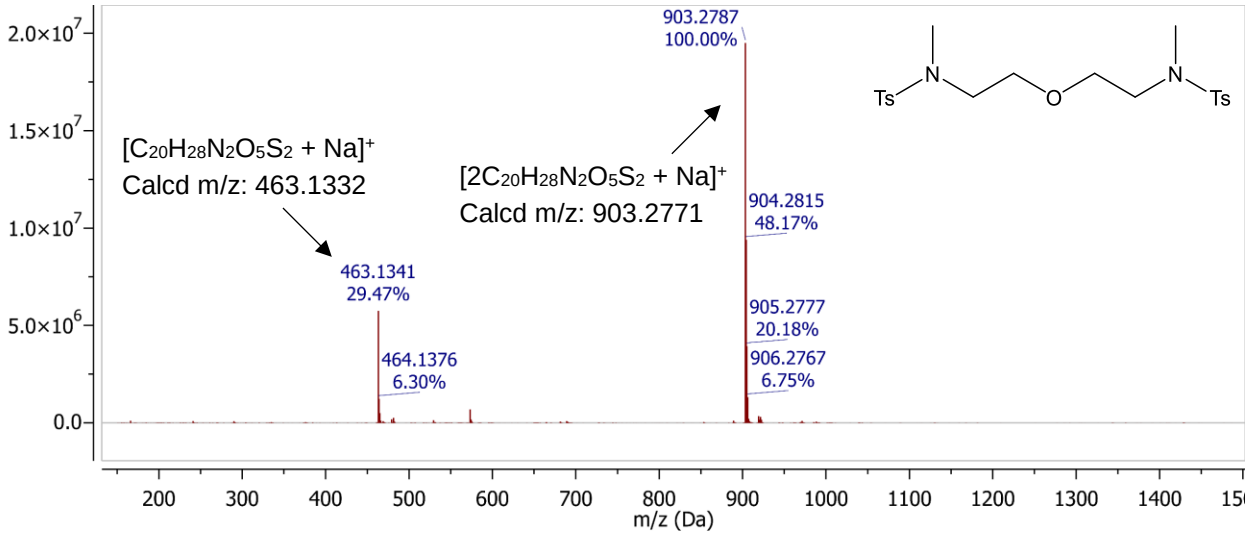

Figure S10. ESI-HRMS of **2**. MeCN was used as the mobile phase.

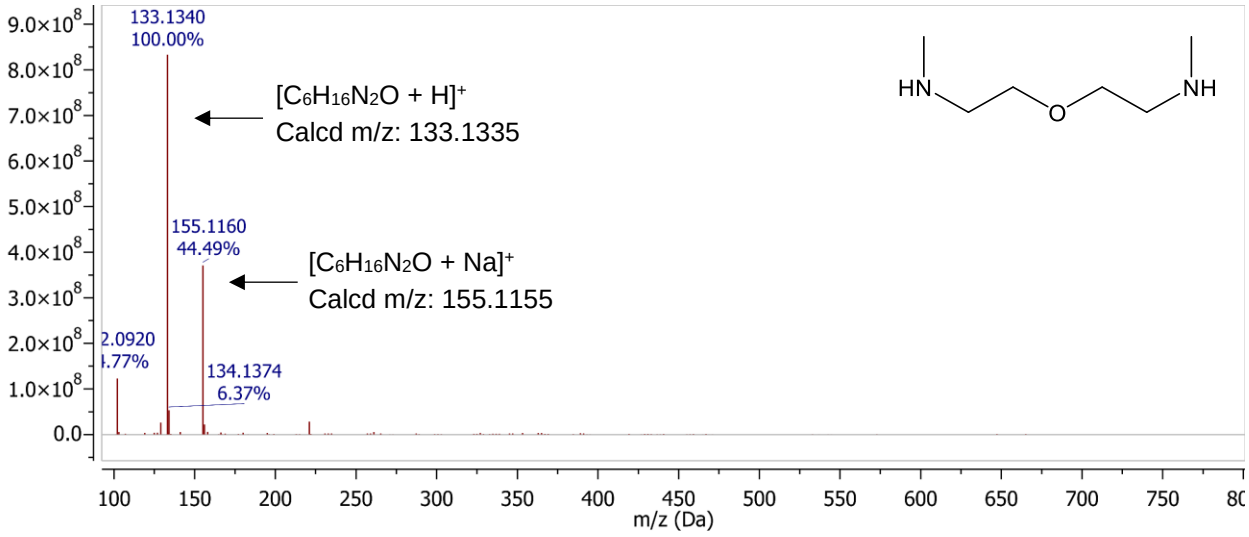

Figure S11. ESI-HRMS of **3**. MeCN was used as the mobile phase.

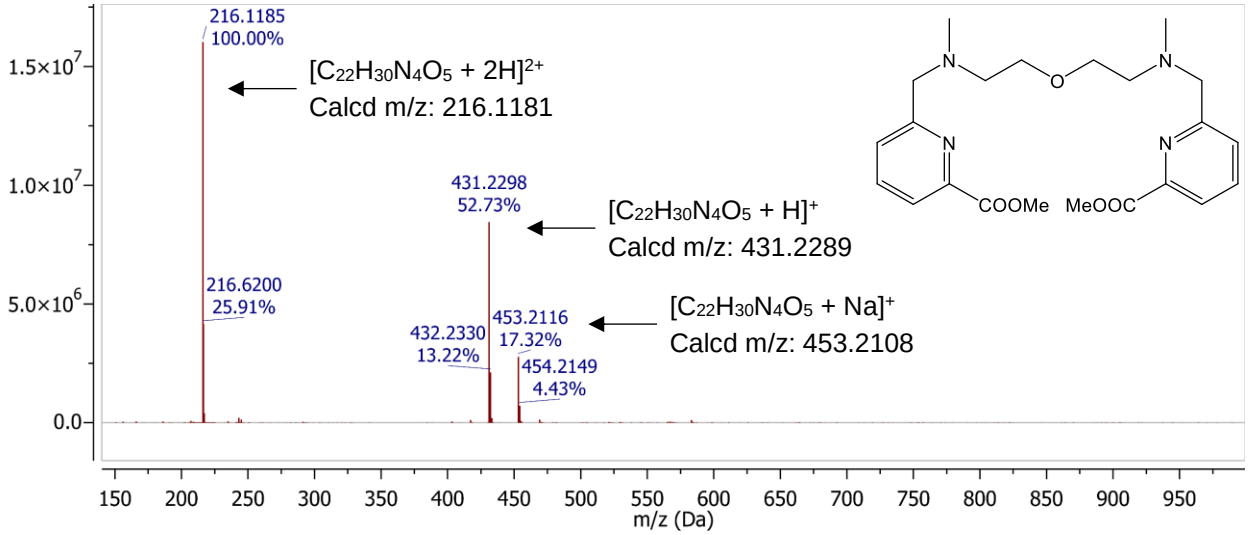

Figure S12. ESI-HRMS of **4**. MeCN was used as the mobile phase.

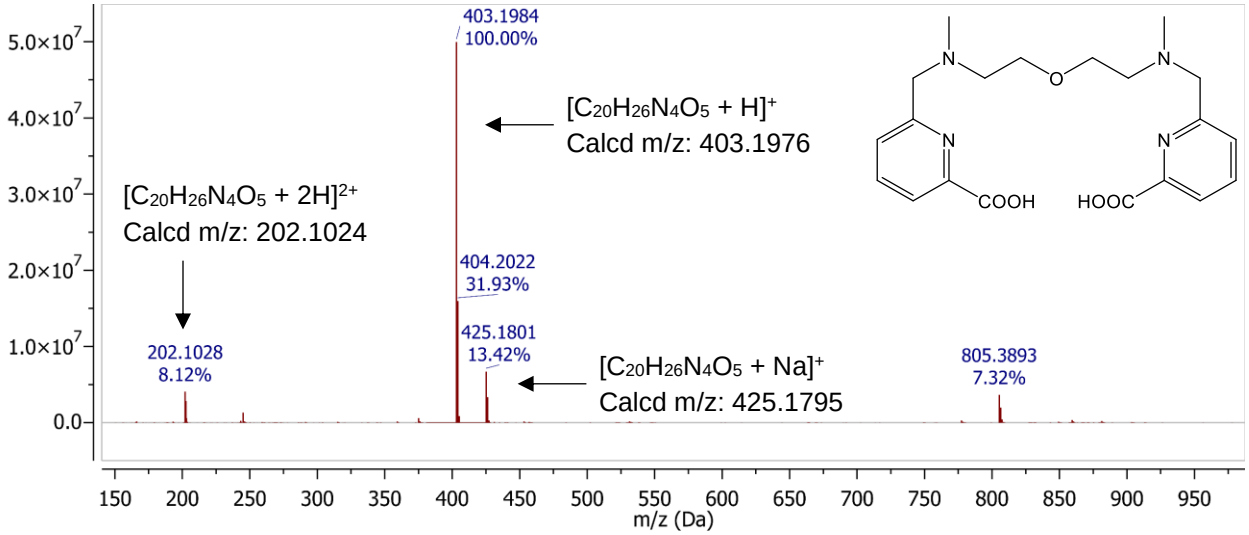

Figure S13. ESI-HRMS of **OxyMepa**. MeCN was used as the mobile phase.

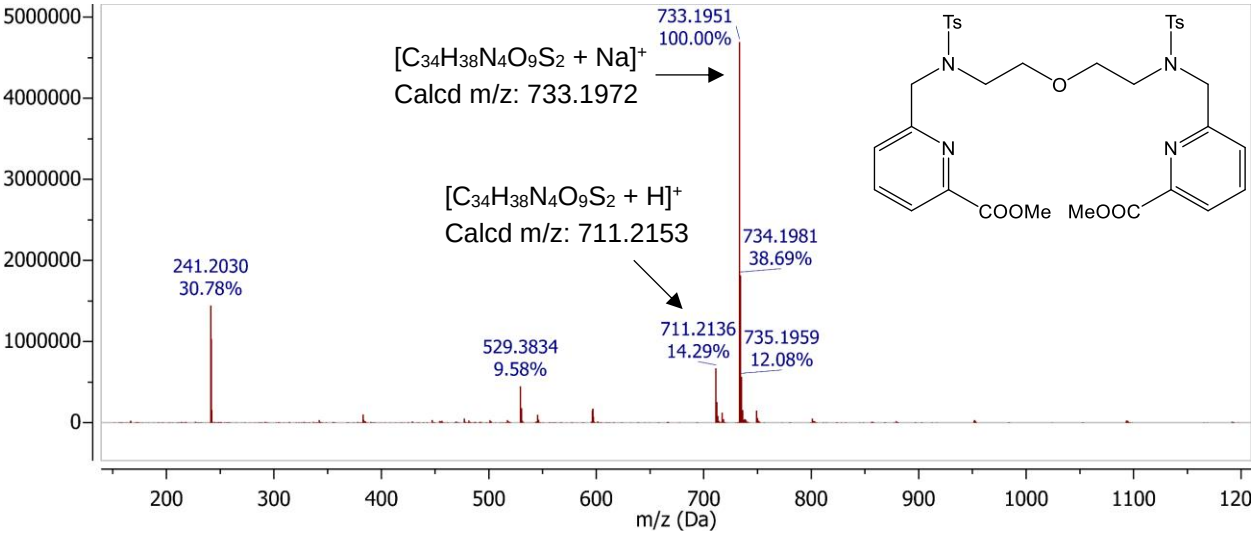

Figure S14. ESI-HRMS of **5**. MeCN was used as the mobile phase.

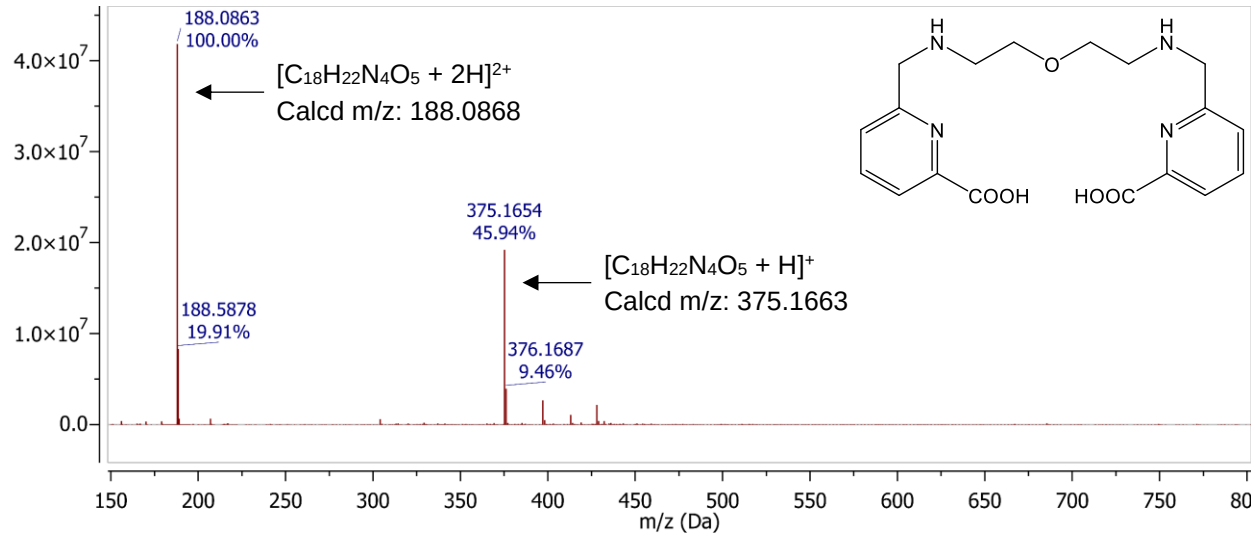

Figure S15. ESI-HRMS of **6**. MeCN was used as the mobile phase.

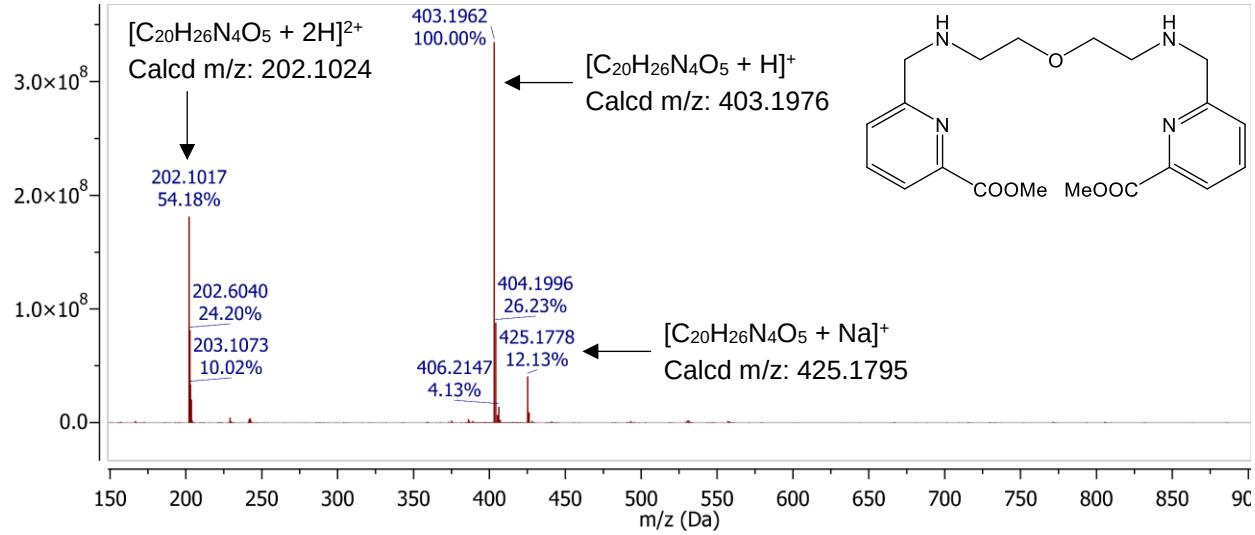

Figure S16. ESI-HRMS of **7**. MeCN was used as the mobile phase.

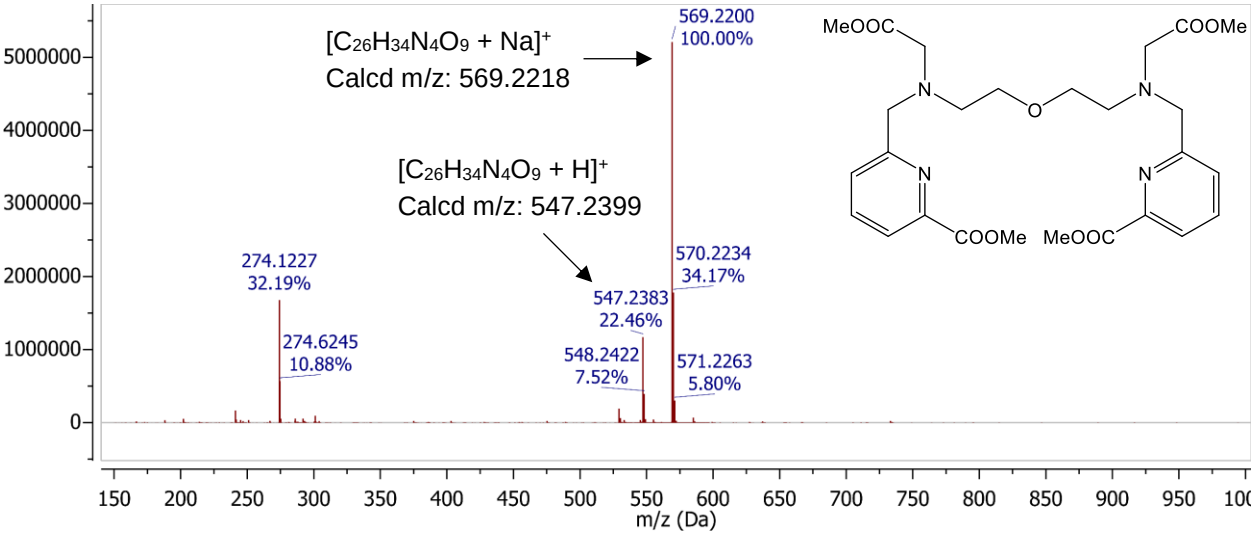

Figure S17. ESI-HRMS of **8**. MeCN was used as the mobile phase.

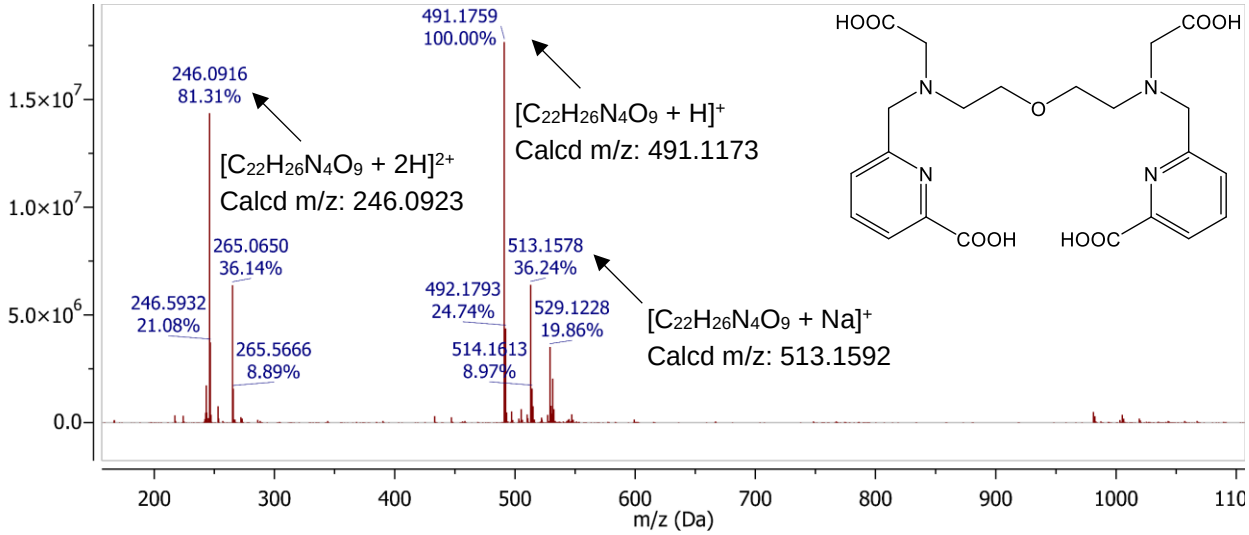

Figure S18. ESI-HRMS of **Oxyaapa**. MeCN was used as the mobile phase.

3. Analytical HPLC Chromatograms

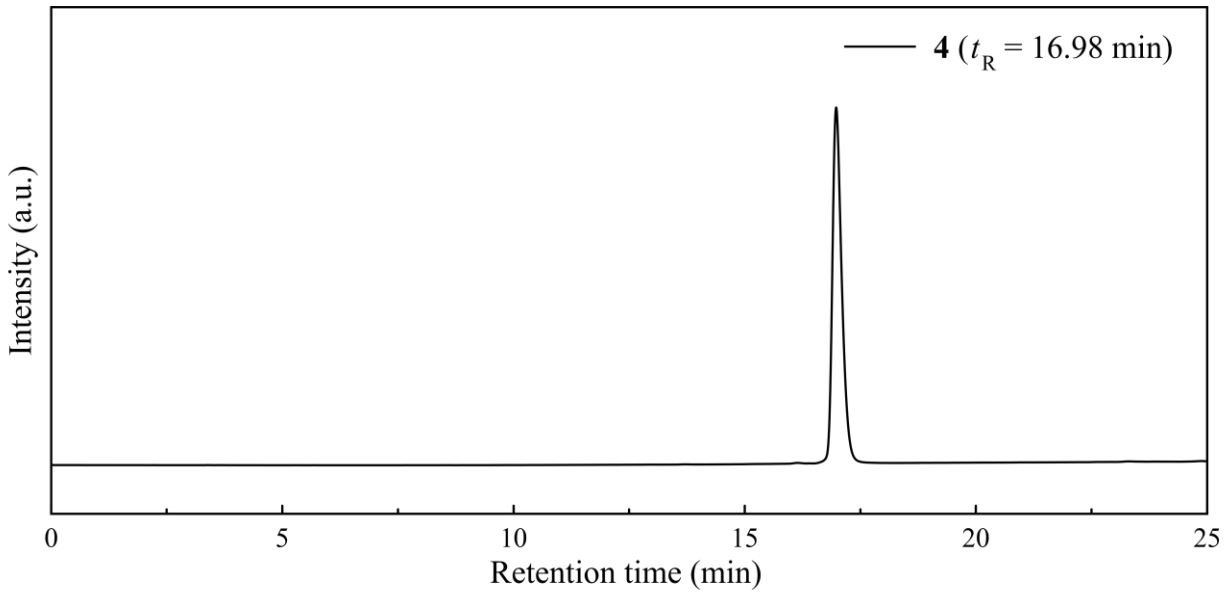

Figure S19. HPLC chromatogram of **4**. Method: 0–5 min, 90% H_2O/MeOH; 5–25 min, 90% → 0% H_2O/MeOH.

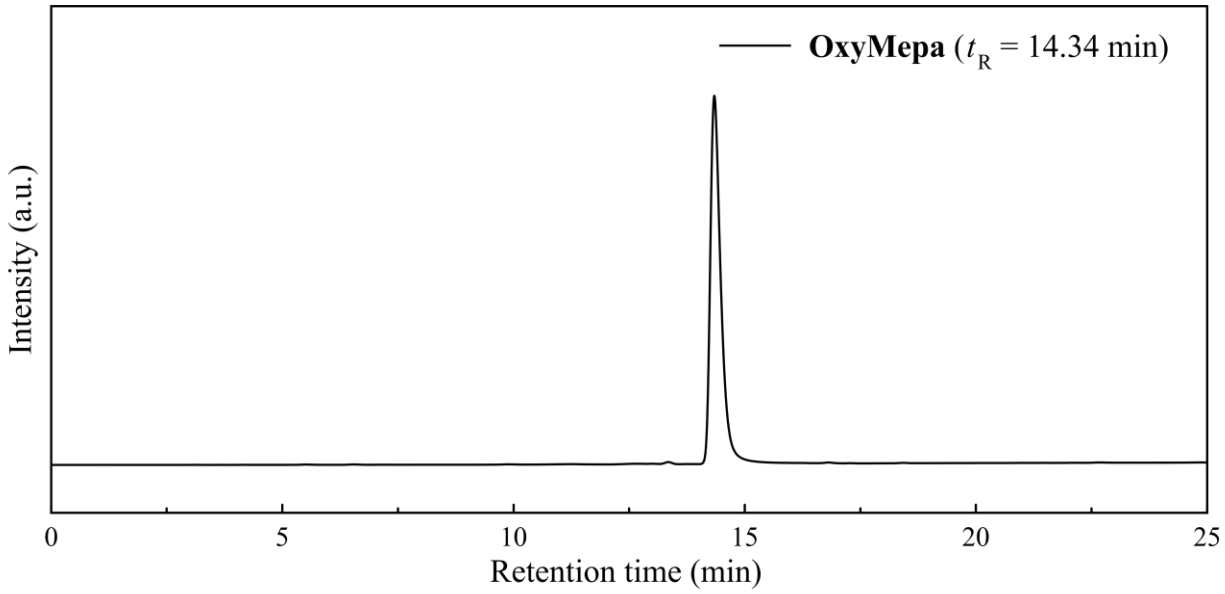

Figure S20. HPLC chromatogram of **OxyMepa**. Method: 0–5 min, 90% H_2O/MeOH; 5–25 min, 90% → 0% H_2O/MeOH.

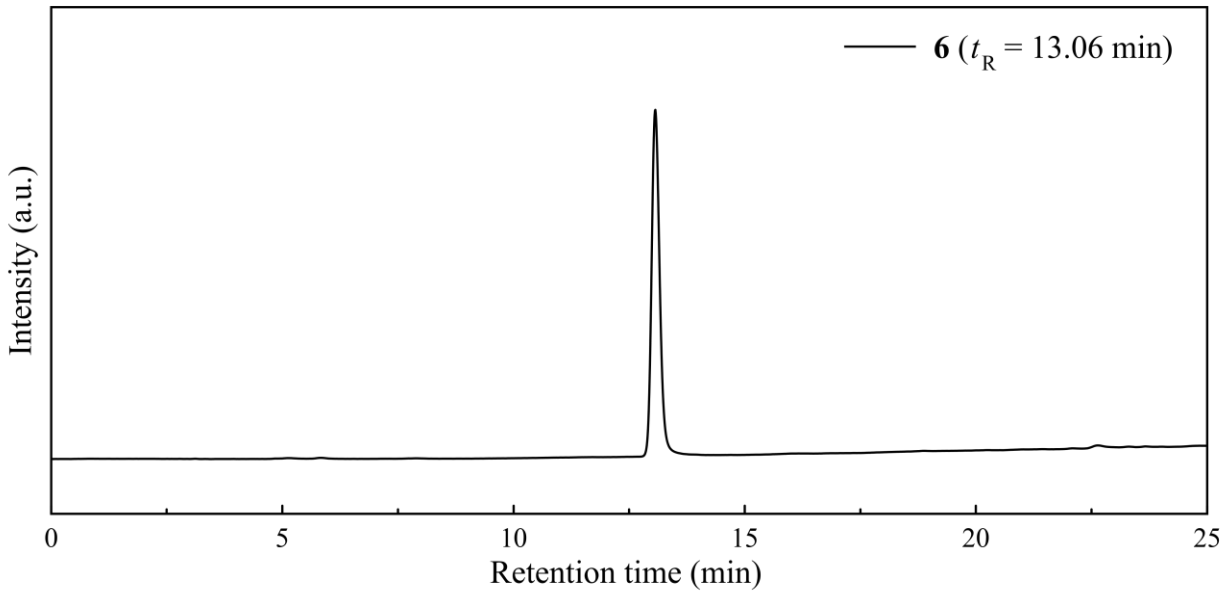

Figure S21. HPLC chromatogram of **6**. Method: 0–5 min, 90% H_2O/MeOH; 5–25 min, 90% → 0% H_2O/MeOH.

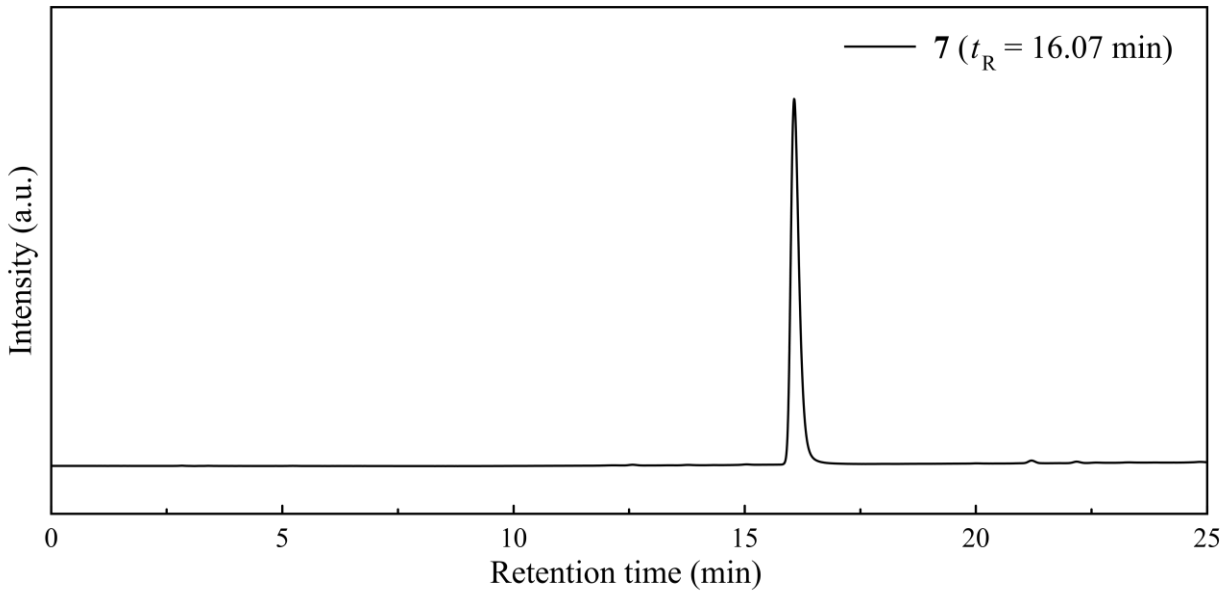

Figure S22. HPLC chromatogram of **7**. Method: 0–5 min, 90% H_2O/MeOH; 5–25 min, 90% → 0% H_2O/MeOH.

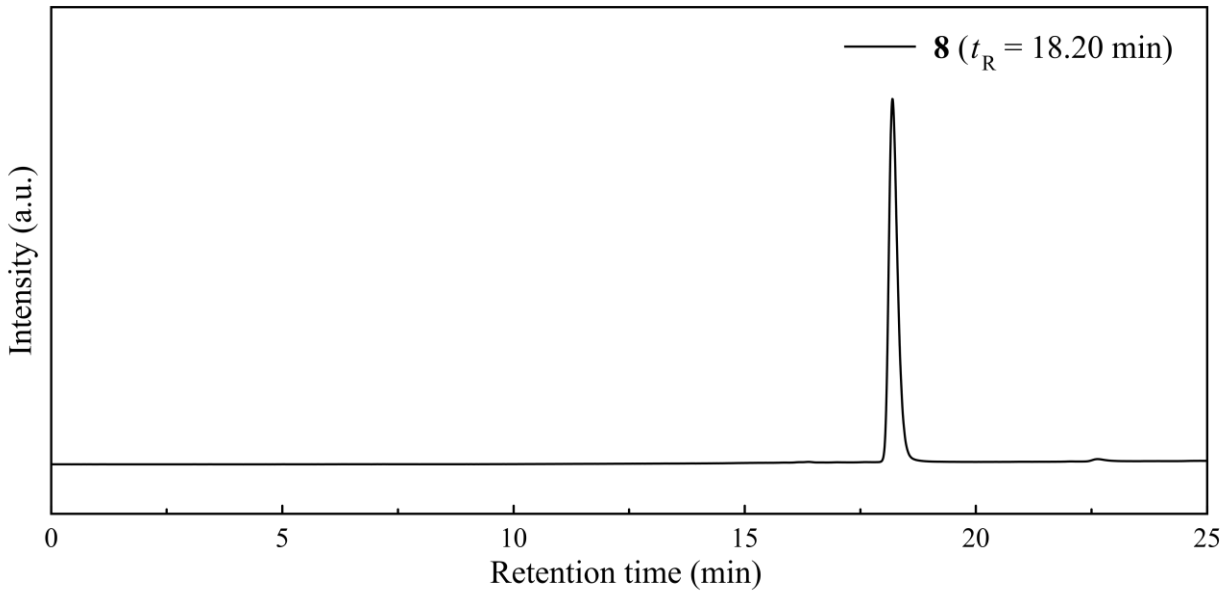

Figure S23. HPLC chromatogram of 8. Method: 0–5 min, 90% H_2O/MeOH; 5–25 min, 90% → 0% H_2O/MeOH.

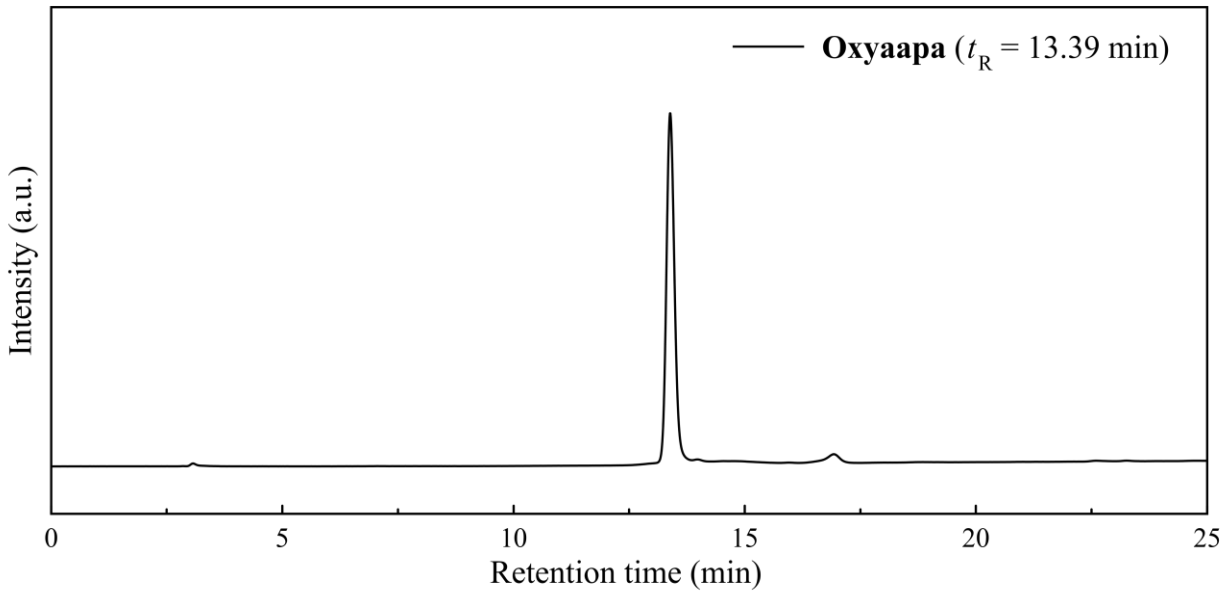

Figure S24. HPLC chromatogram of **Oxyaapa**. Method: 0–5 min, 90% H_2O/MeOH; 5–25 min, 90% → 0% H_2O/MeOH.We noticed that Oxyaapa, as a strong metal binder, was able to catch trace metal (e.g. iron from the injection syringe) under the HPLC condition, which could give chromatograms with more than one peak and strange peak shape.

4. Potentiometric Titrations

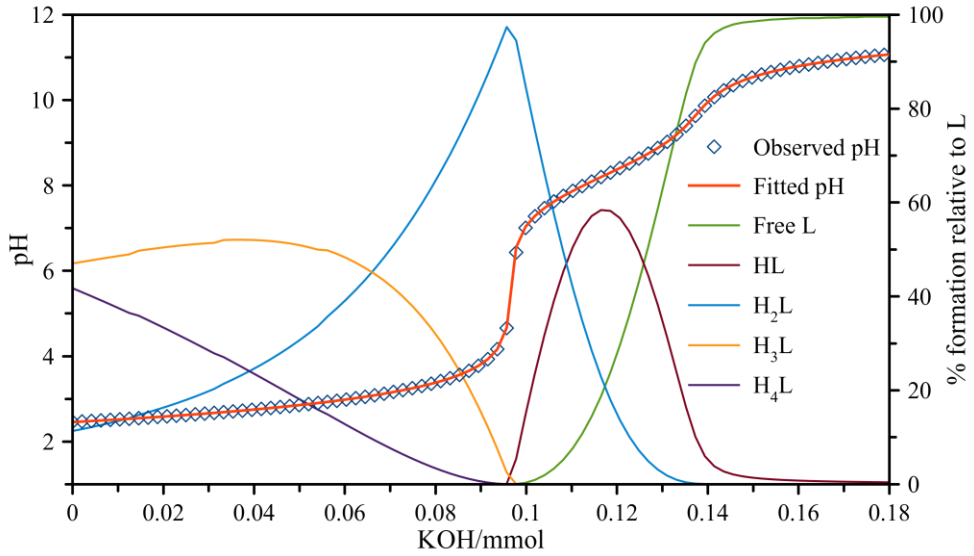

Figure S25. Representative protonation constant determination of OxyMepa by potentiometric titration. c_{OxyMepa} = 1 × 10^{-3} M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.423.

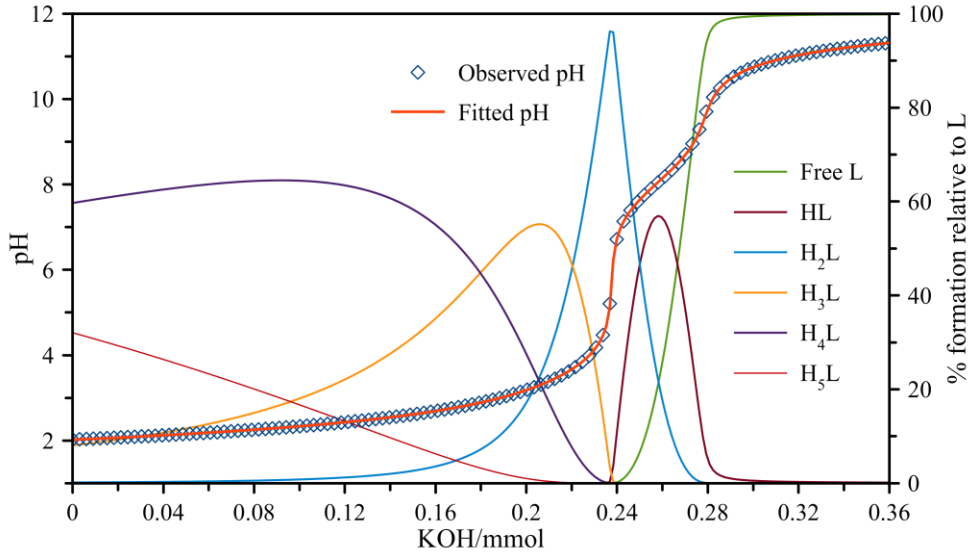

Figure S26. Representative protonation constant determination of Oxyaapa by potentiometric titration. c_{Oxyaapa} = 1 × 10^{-3} M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.847.

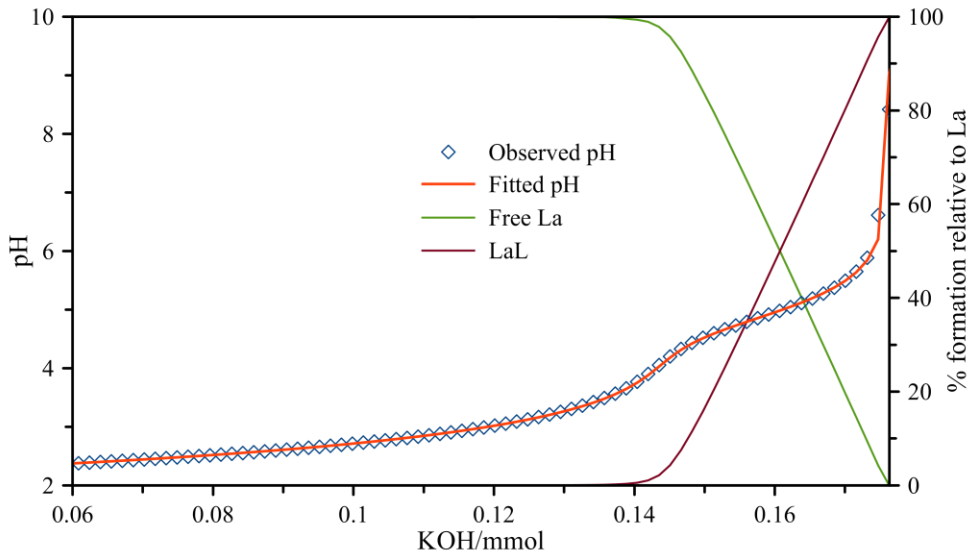

Figure S27. Representative stability constant determination of La-OxyMepa system by potentiometric titration. $c_{La} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.699.

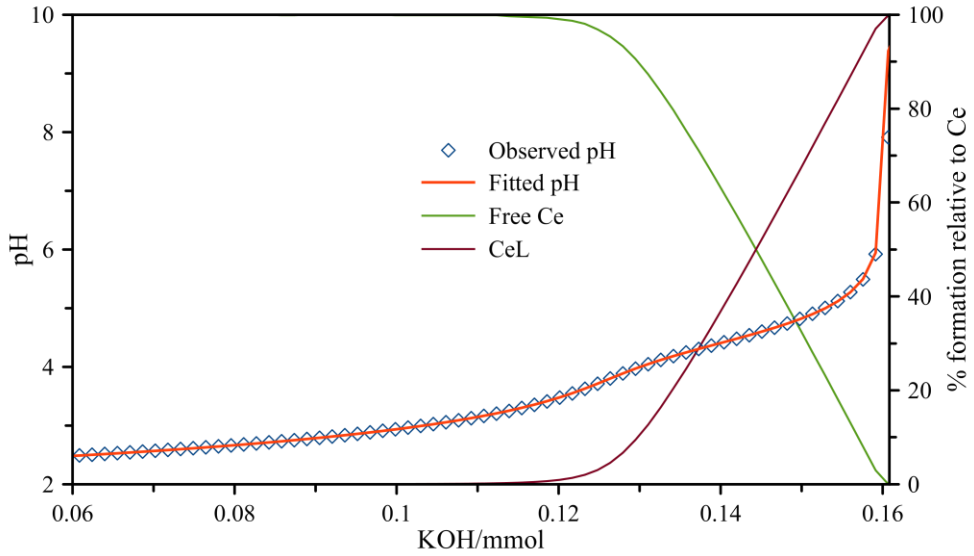

Figure S28. Representative stability constant determination of Ce-OxyMepa system by potentiometric titration. $c_{Ce} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.390.

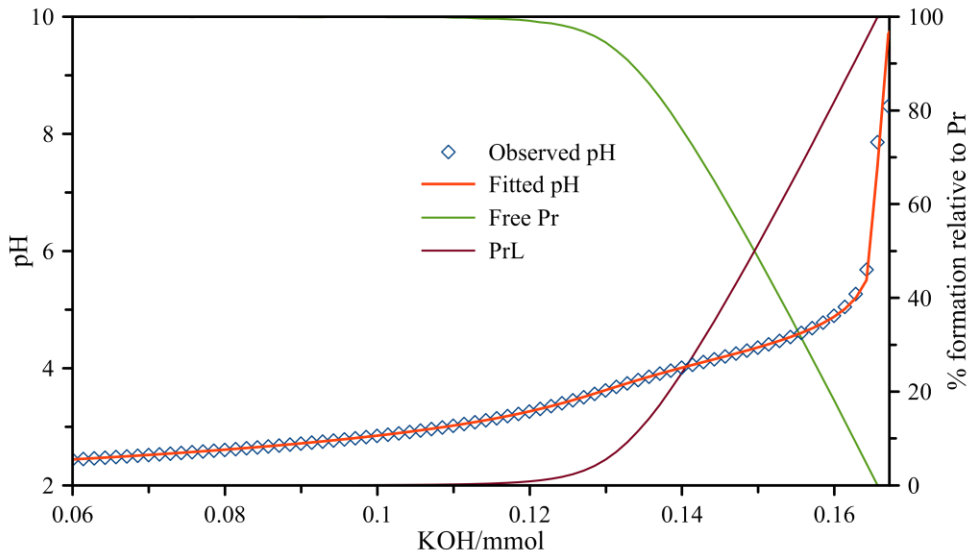

Figure S29. Representative stability constant determination of Pr-OxyMepa system by potentiometric titration. $c_{Pr} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.862.

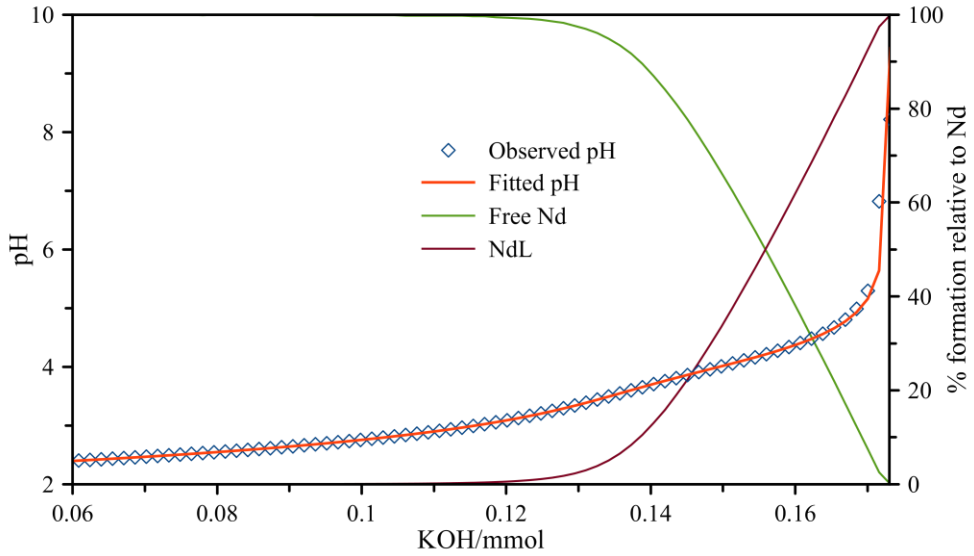

Figure S30. Representative stability constant determination of Nd-OxyMepa system by potentiometric titration. $c_{Nd} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.406.

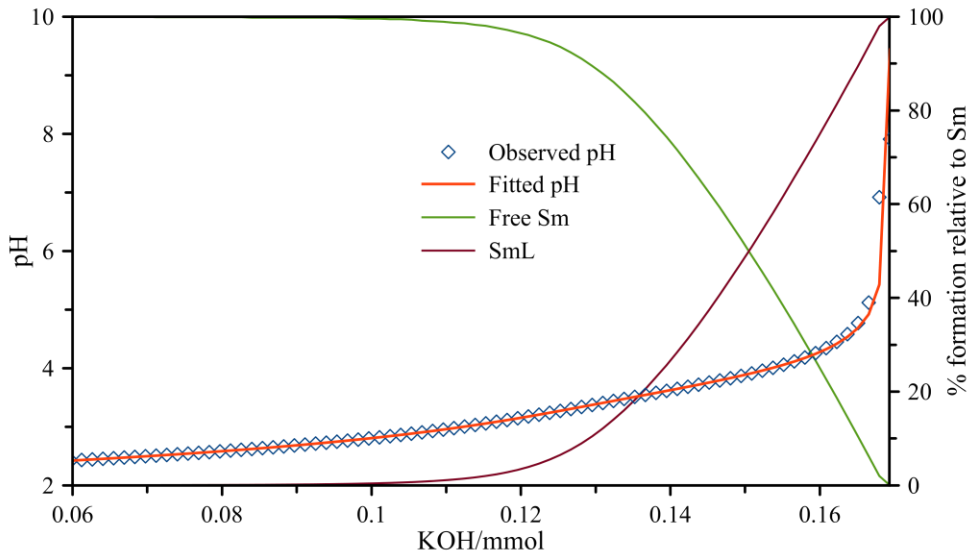

Figure S31. Representative stability constant determination of Sm-OxyMepa system by potentiometric titration. $c_{Sm} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.492.

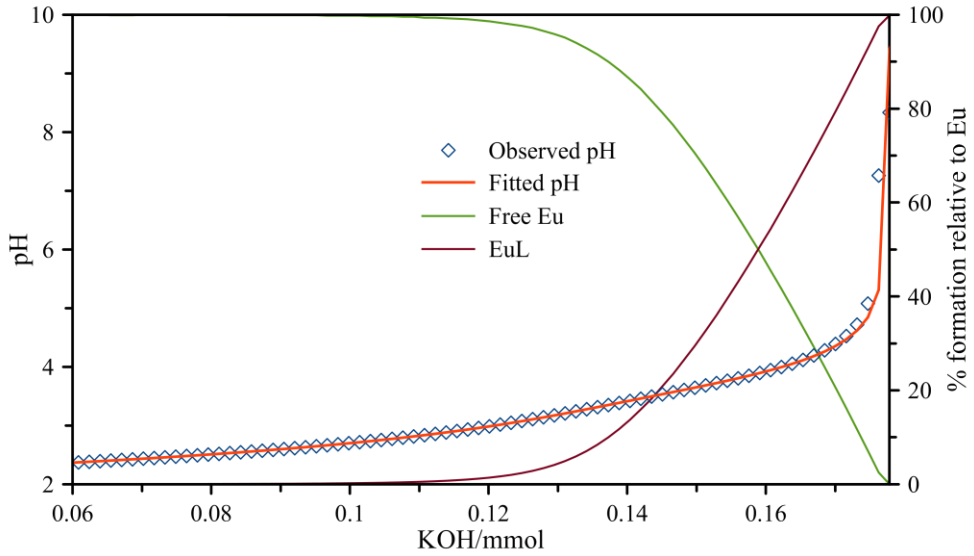

Figure S32. Representative stability constant determination of Eu-OxyMepa system by potentiometric titration. $c_{Eu} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.573.

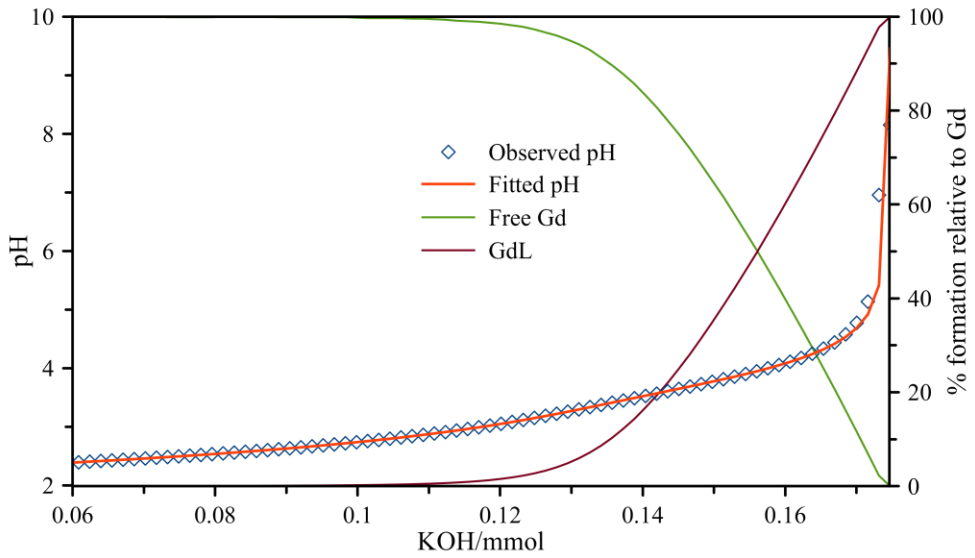

Figure S33. Representative stability constant determination of Gd-OxyMepa system by potentiometric titration. $c_{Gd} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.487.

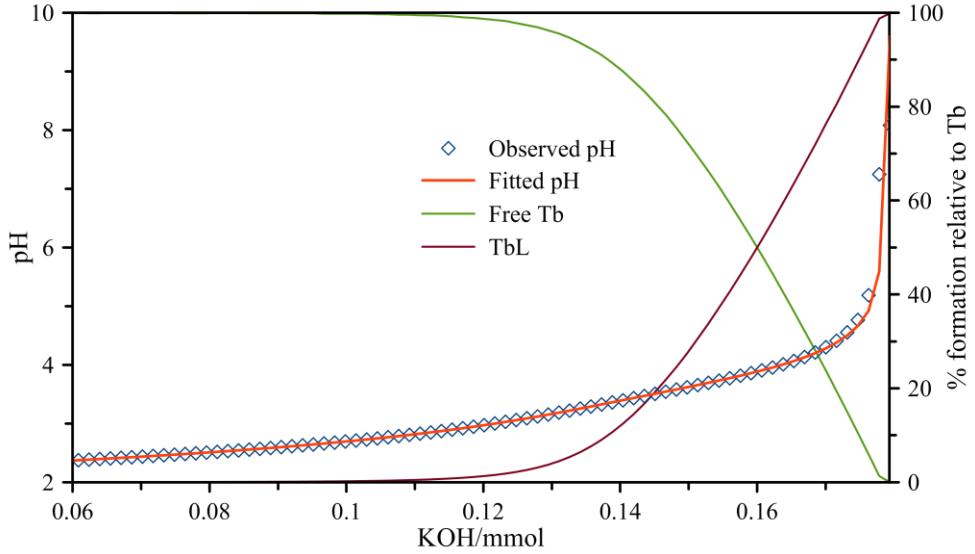

Figure S34. Representative stability constant determination of Tb-OxyMepa system by potentiometric titration. $c_{Tb} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.506.

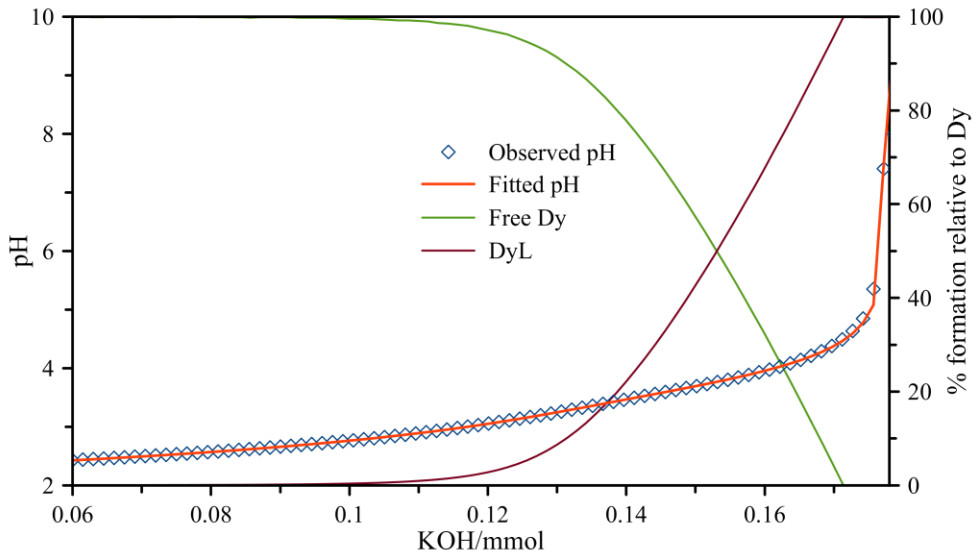

Figure S35. Representative stability constant determination of Dy-OxyMepa system by potentiometric titration. $c_{Dy} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.596.

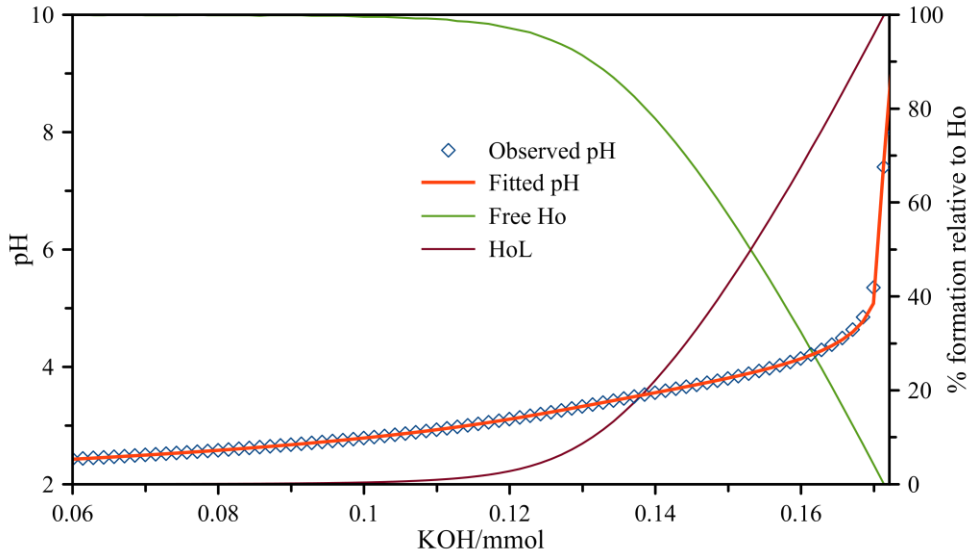

Figure S36. Representative stability constant determination of Ho-OxyMepa system by potentiometric titration. $c_{Ho} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.515.

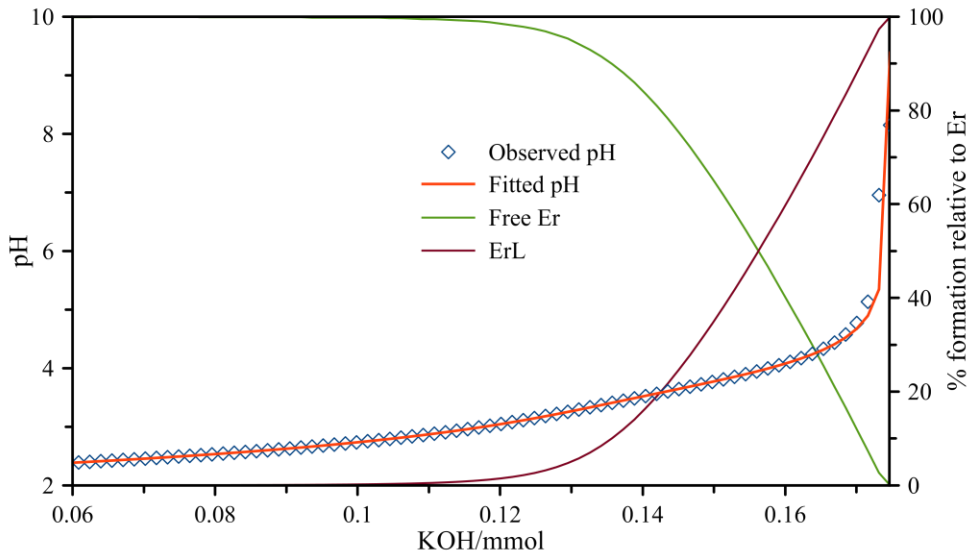

Figure S37. Representative stability constant determination of Er-OxyMepa system by potentiometric titration. $c_{Er} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.571.

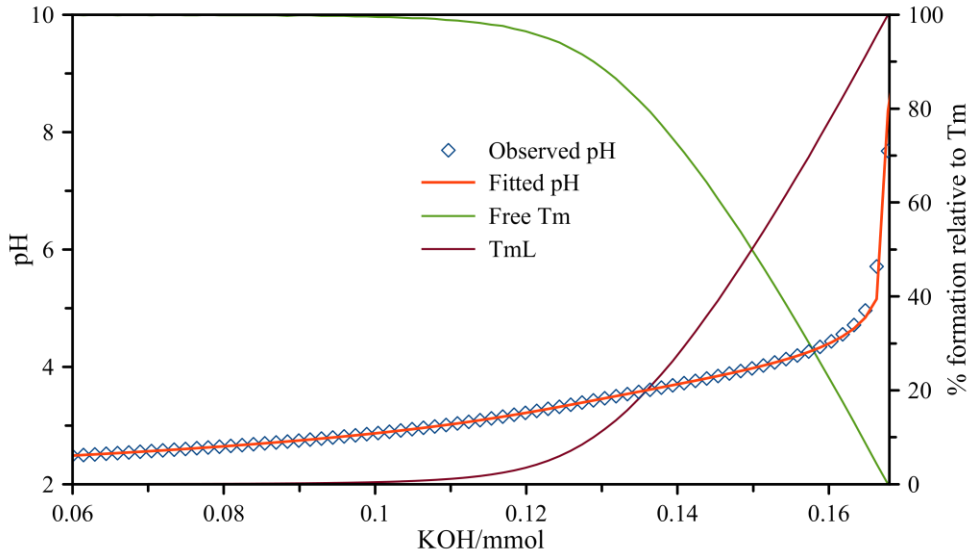

Figure S38. Representative stability constant determination of Tm-OxyMepa system by potentiometric titration. $c_{Tm} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.553.

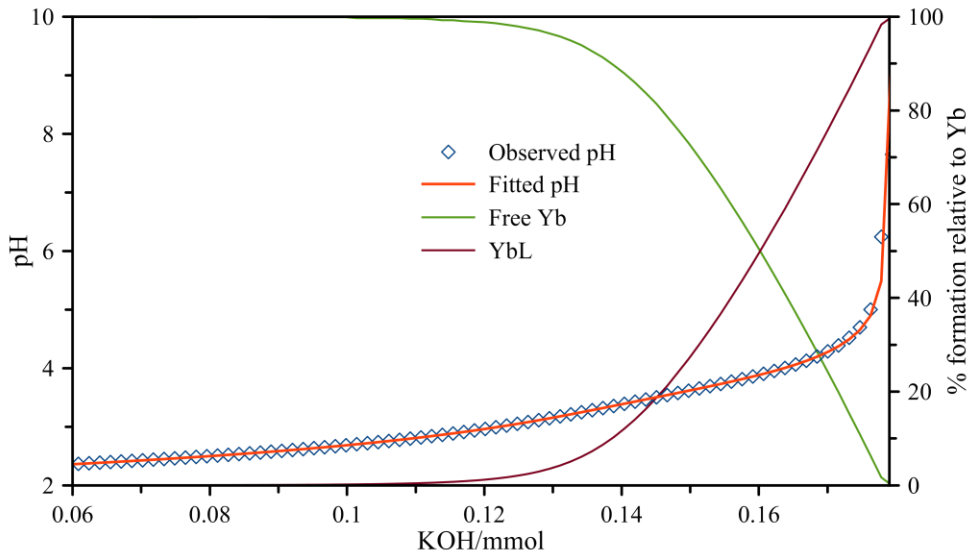

Figure S39. Representative stability constant determination of Yb-OxyMepa system by potentiometric titration. $c_{Yb} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.327.

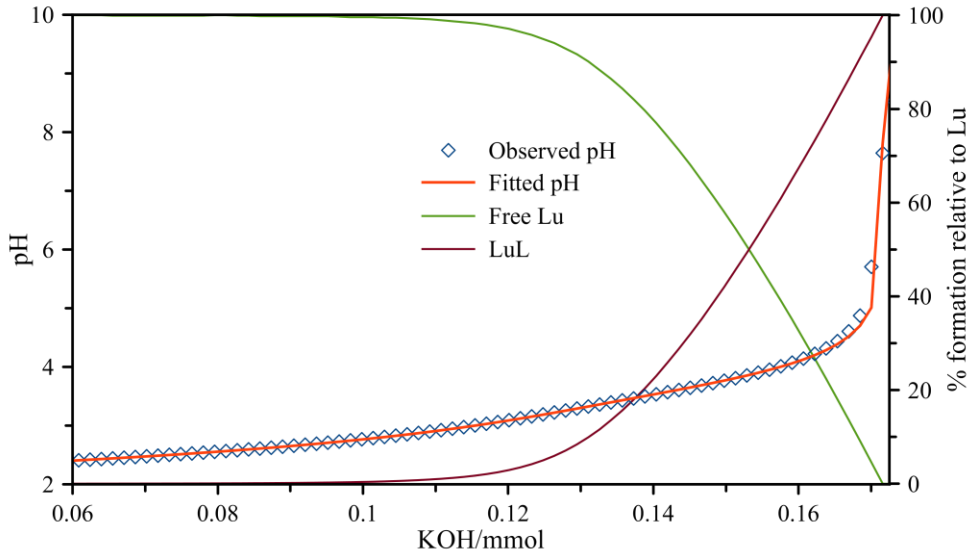

Figure 40. Representative stability constant determination of Lu-OxyMepa system by potentiometric titration. $c_{Lu} = c_{OxyMepa} = 1 \times 10^{-3}$ M. Data fitting and speciation distribution over the titration pH range are shown. Sigma value of this refinement = 0.781.

5. UV–Vis Spectroscopic Titrations

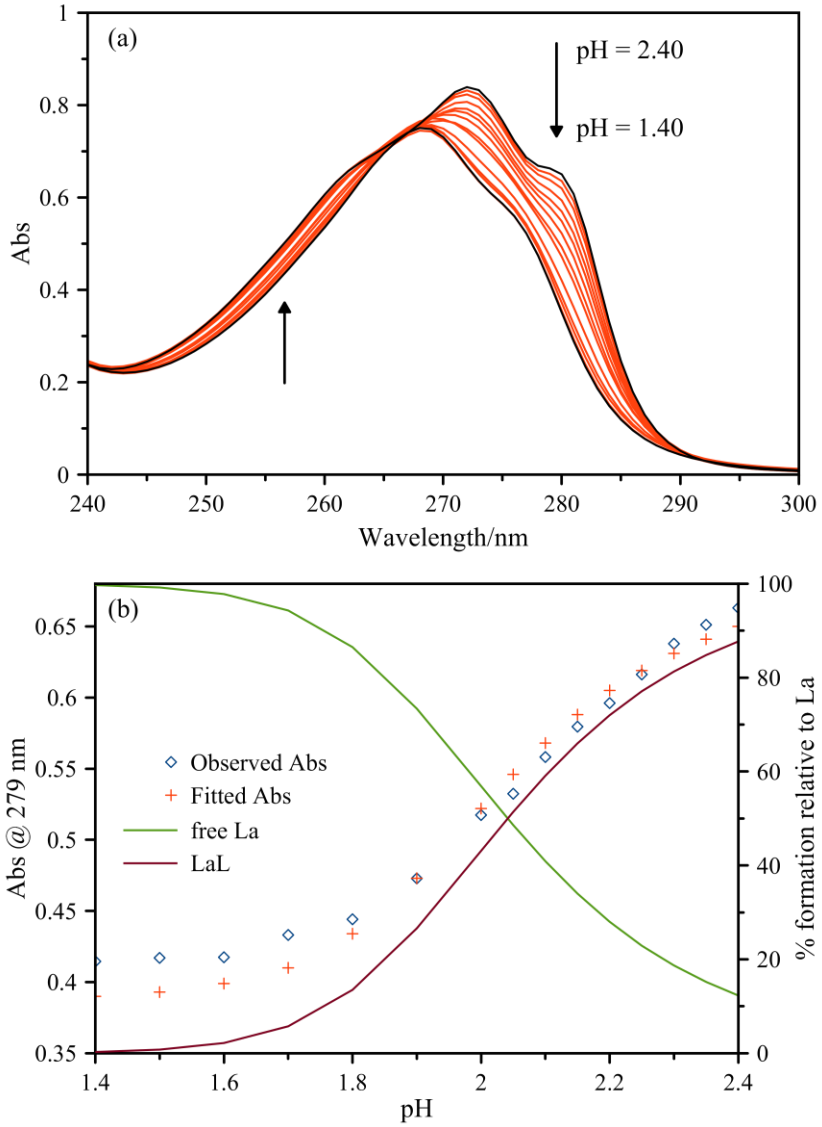

Figure S41. Representative UV–Vis spectroscopic titration of La-Oxyaapa system. $c_{La} = c_{Oxyaapa} = 1 \times 10^{-4}$ M. (a) UV–Vis spectral change over the titration pH range; (b) Data fitting at 279 nm (where the most significant spectral change occurs) and speciation distribution over the titration pH range. Sigma value of this refinement = 0.011935.

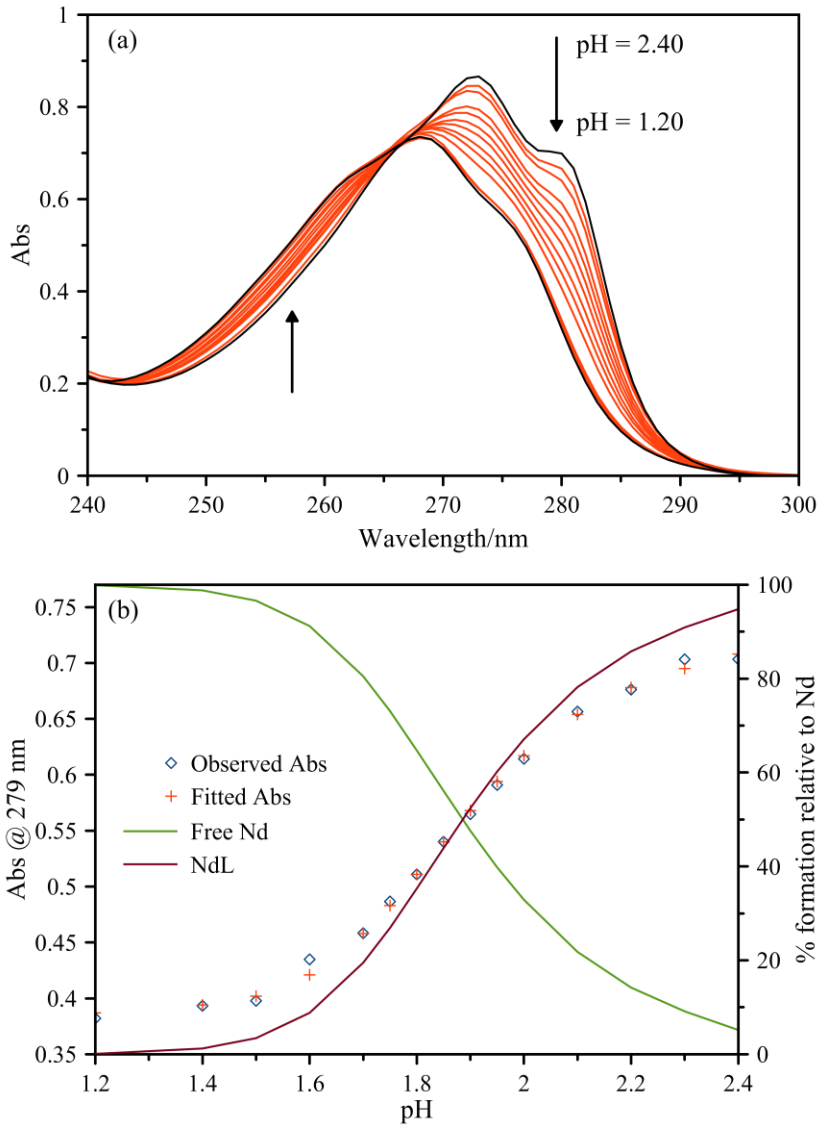

Figure S42. Representative UV–Vis spectroscopic titration of Nd-Oxyaapa system. $c_{Nd} = c_{Oxyaapa} = 1 \times 10^{-4}$ M. (a) UV–Vis spectral change over the titration pH range; (b) Data fitting at 279 nm (where the most significant spectral change occurs) and speciation distribution over the titration pH range. Sigma value of this refinement = 0.007266.

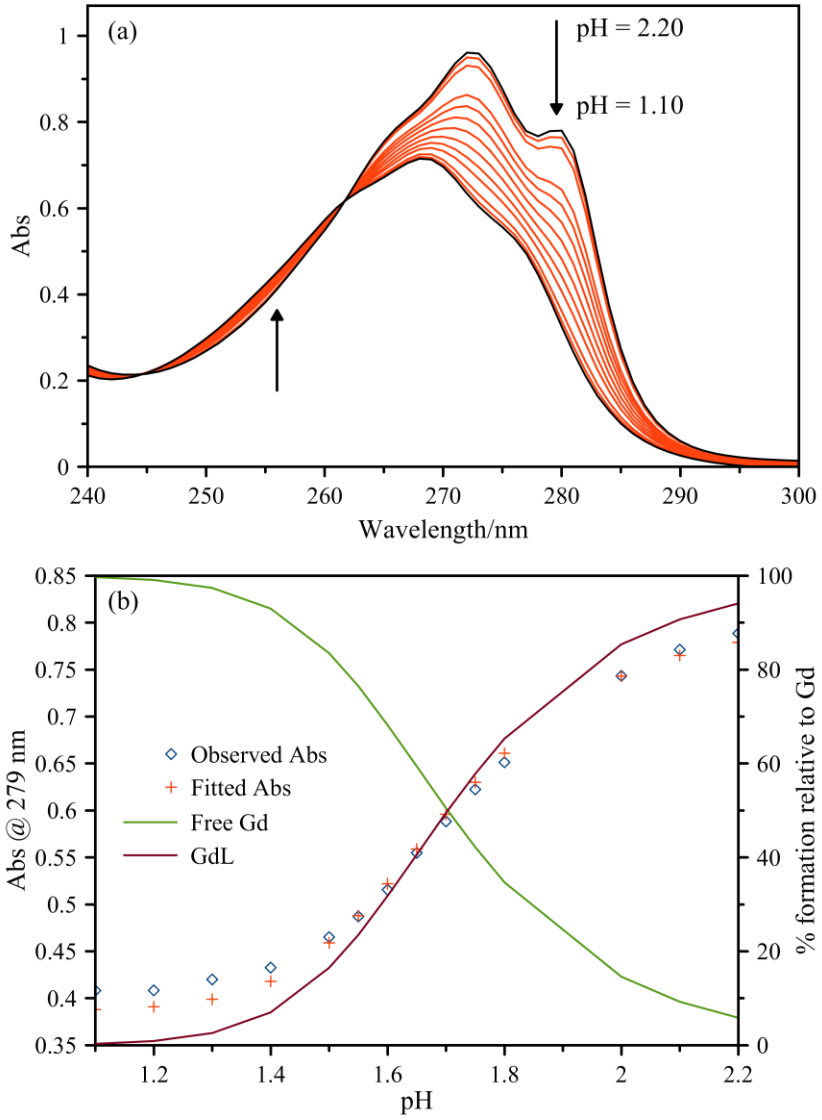

Figure S43. Representative UV–Vis spectroscopic titration of Gd-Oxyaapa system. $c_{Gd} = c_{Oxyaapa} = 1 \times 10^{-4}$ M. (a) UV–Vis spectral change over the titration pH range; (b) Data fitting at 279 nm (where the most significant spectral change occurs) and speciation distribution over the titration pH range. Sigma value of this refinement = 0.013949.

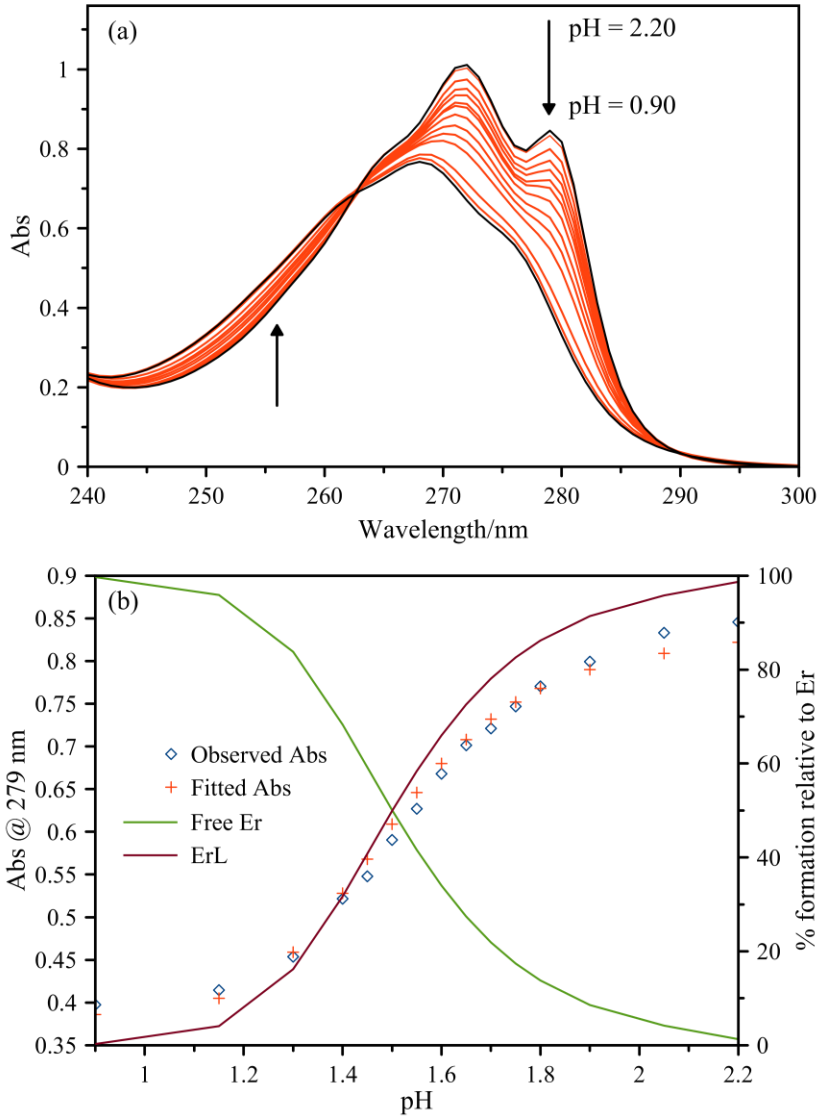

Figure S44. Representative UV–Vis spectroscopic titration of Er-Oxyaapa system. $c_{Er} = c_{Oxyaapa} = 1 \times 10^{-4}$ M. (a) UV–Vis spectral change over the titration pH range; (b) Data fitting at 279 nm (where the most significant spectral change occurs) and speciation distribution over the titration pH range. Sigma value of this refinement = 0.014679.

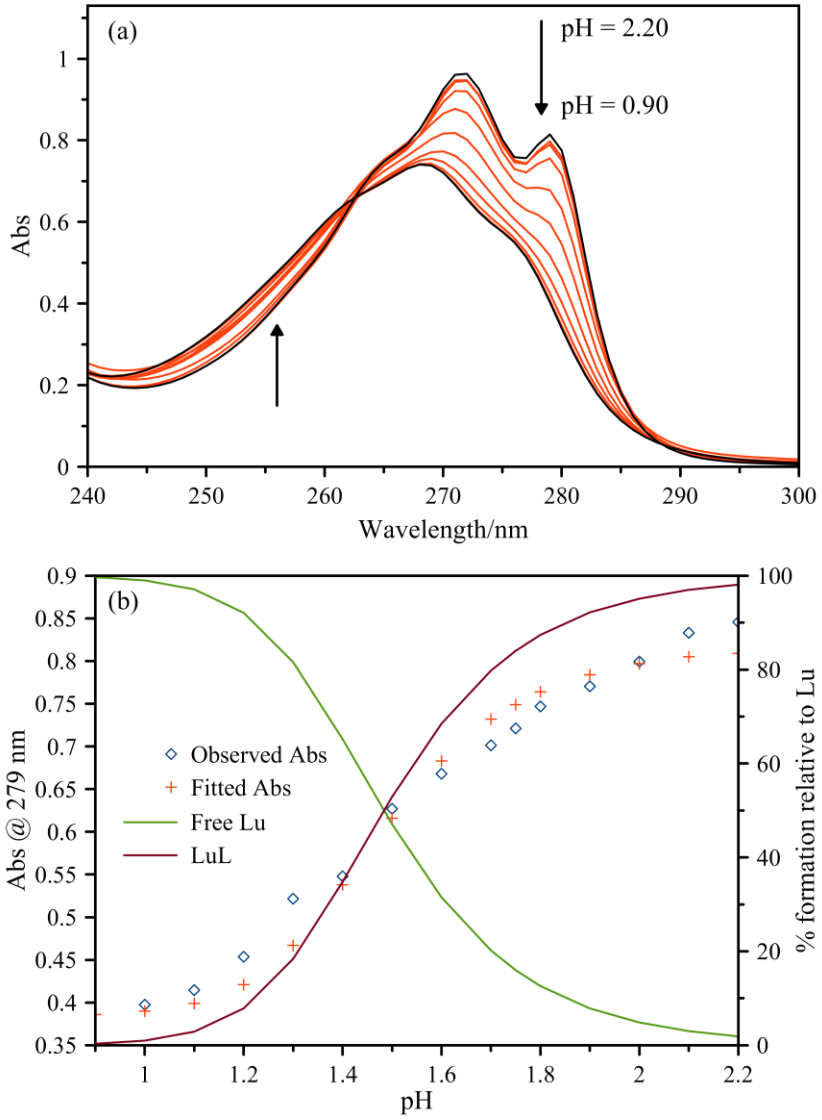

Figure S45. Representative UV–Vis spectroscopic titration of Lu-Oxyaapa system. $c_{Lu} = c_{Oxyaapa} = 1 \times 10^{-4}$ M. (a) UV–Vis spectral change over the titration pH range; (b) Data fitting at 279 nm (where the most significant spectral change occurs) and speciation distribution over the titration pH range. Sigma value of this refinement = 0.014015.

Table S1. pM values of OxyMepa and Oxyaapa complexes formed with lanthanide ions. pM is defined as the $-\log [M]_{free}$ value when $[M]_{total} = 10^{-6}$ M and $[L]_{total} = 10^{-5}$ M at pH = 7.4.

	OxyMepa	Oxyaapa
pLa	9.0	18.5
pCe	9.8	
pPr	10.3	
pNd	10.6	19.2
pSm	11.2	
pEu	11.2	
pGd	11.1	19.9
pTb	11.2	
pDy	11.3	
pHo	11.2	
pEr	11.1	20.8
pTm	11.1	
pYb	11.2	
pLu	11.3	21.1

6. DTPA Transchelation Studies

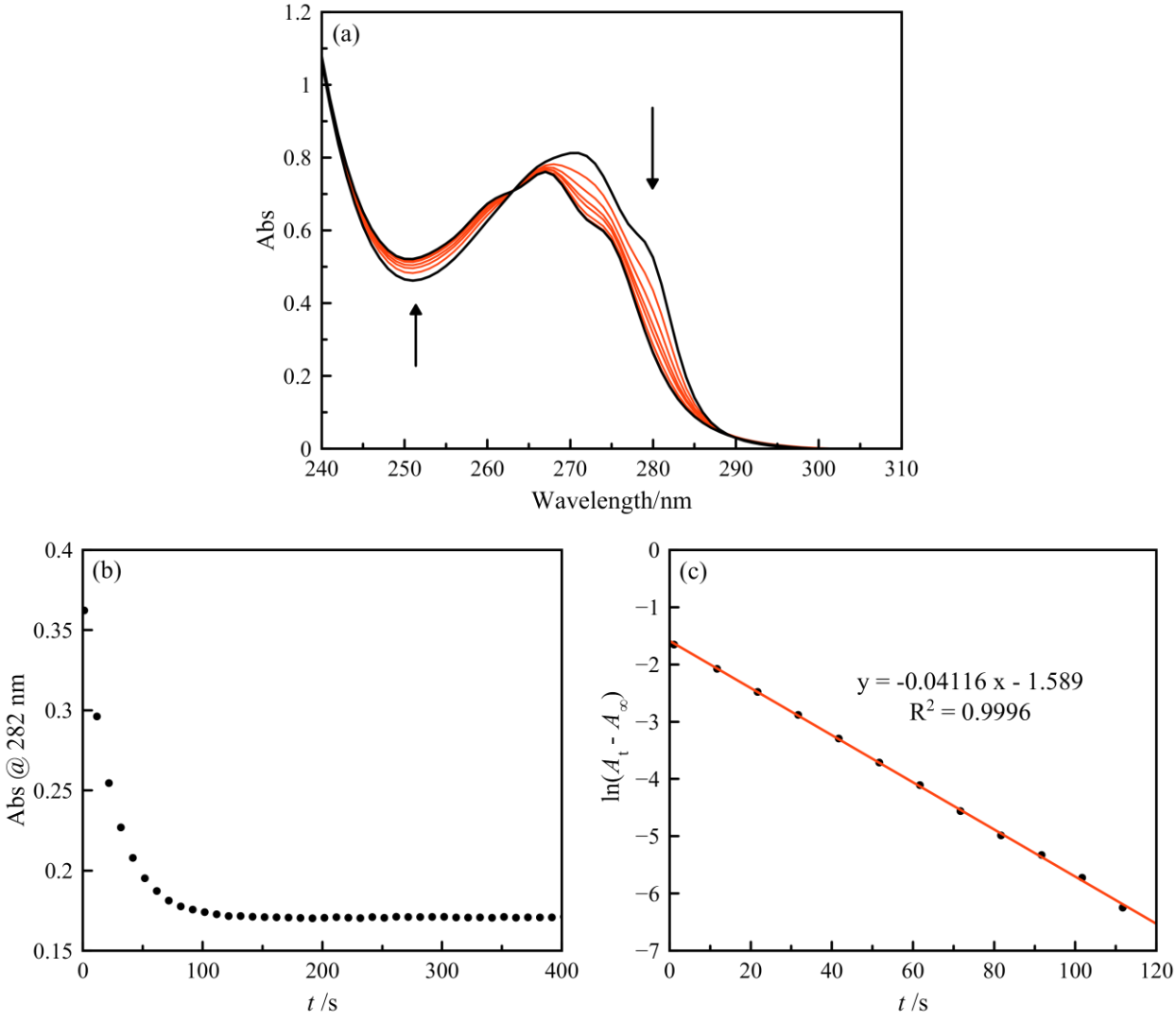

Figure S46. DTPA transchelation challenge on Gd-OxyMepa complex (100 μM complex with 10 mM DTPA). (a) UV–Vis spectral change over the transchelation reaction; (b) The absorbance change at 282 nm versus time; (c) The linear fit to the first-order kinetics model.

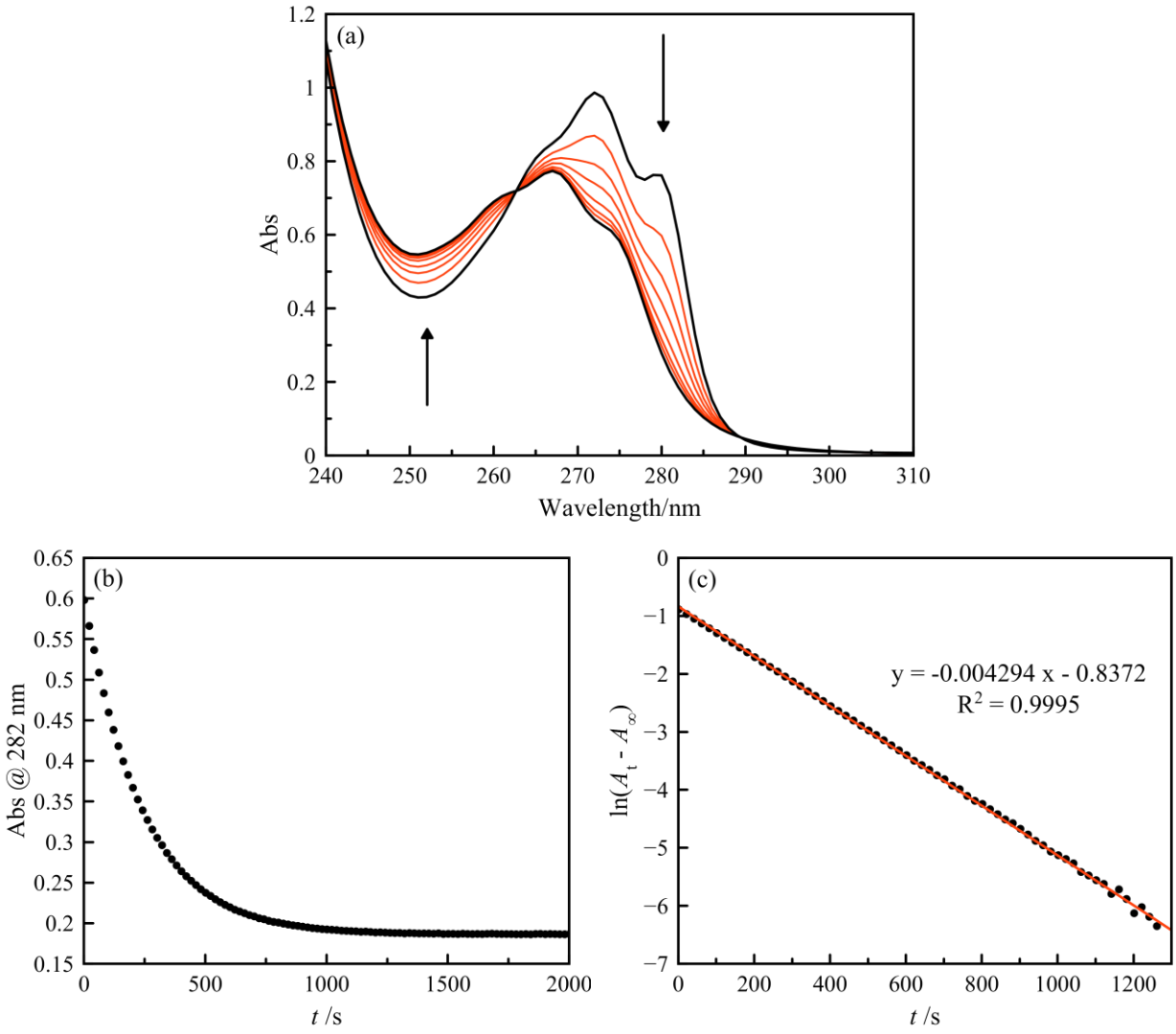

Figure S47. DTPA transchelation challenge on Lu-OxyMepa complex (100 μM complex with 10 mM DTPA). (a) UV–Vis spectral change over the transchelation reaction; (b) The absorbance change at 282 nm versus time; (c) The linear fit to the first-order kinetics model.

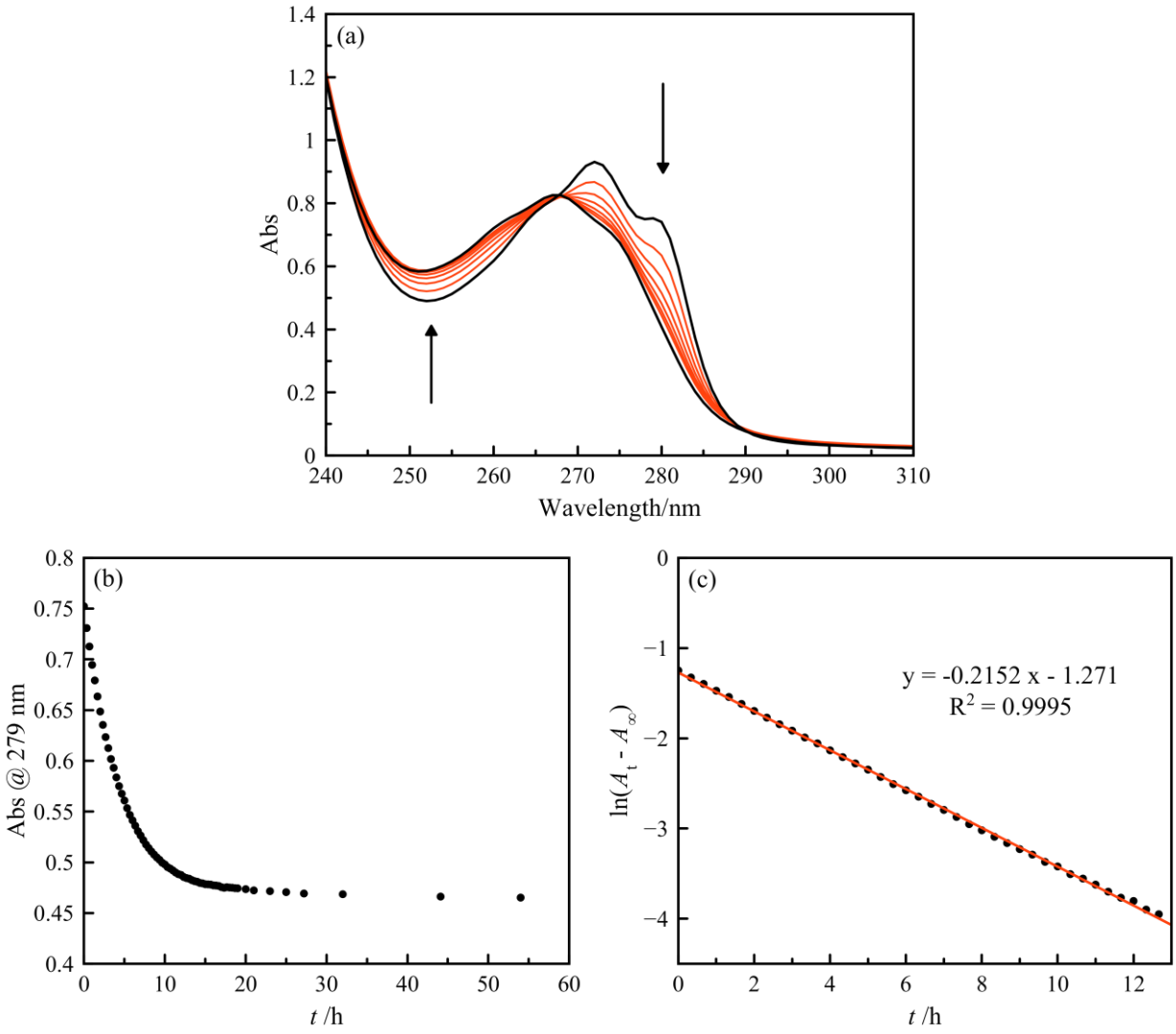

Figure S48. DTPA transchelation challenge on La-Oxyaapa complex (100 μM complex with 10 mM DTPA). (a) UV–Vis spectral change over the transchelation reaction; (b) The absorbance change at 279 nm versus time; (c) The linear fit to the first-order kinetics model.

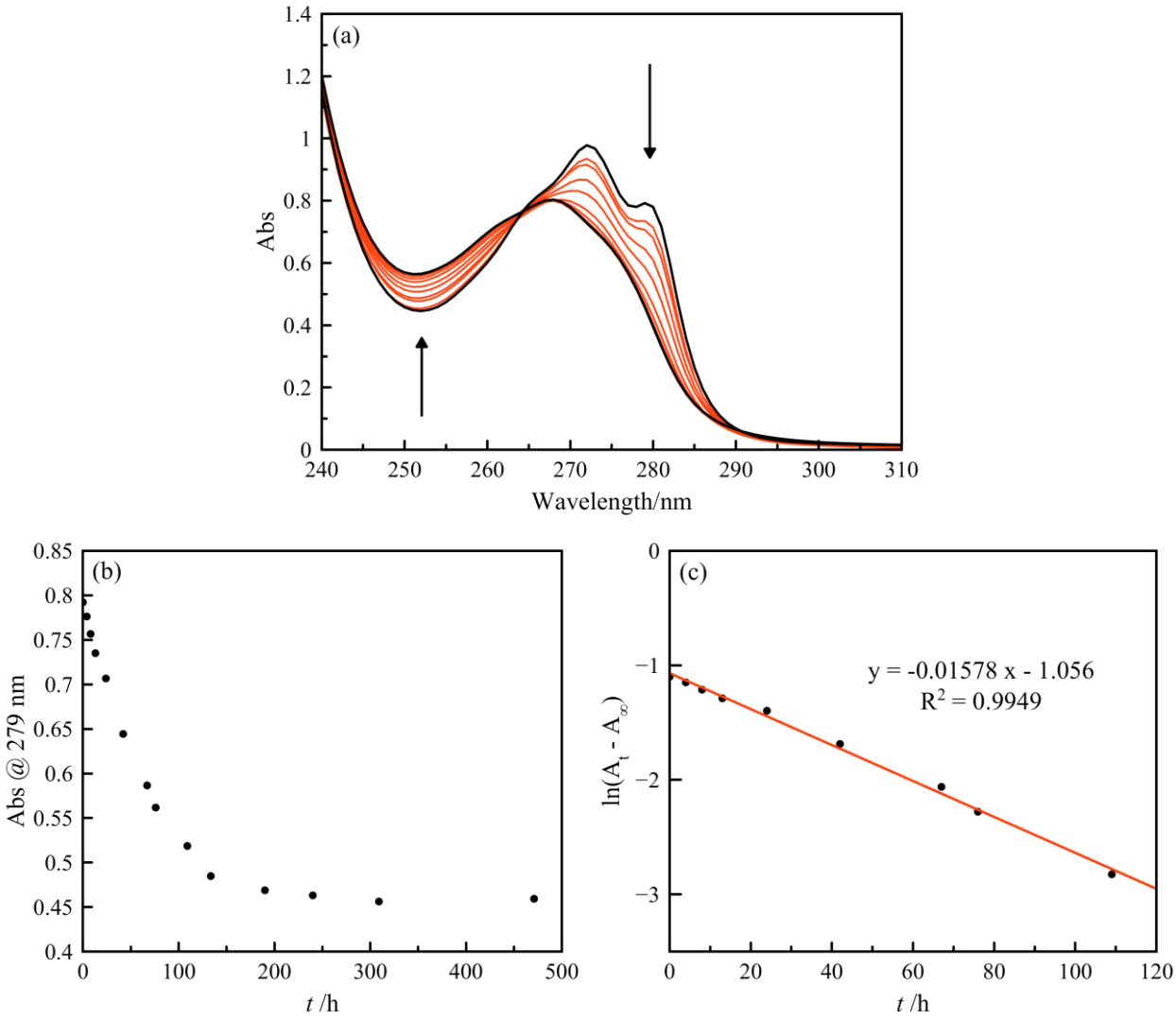

Figure S49. DTPA transchelation challenge on Gd-Oxyaapa complex (100 μM complex with 10 mM DTPA). (a) UV–Vis spectral change over the transchelation reaction; (b) The absorbance change at 279 nm versus time; (c) The linear fit to the first-order kinetics model.

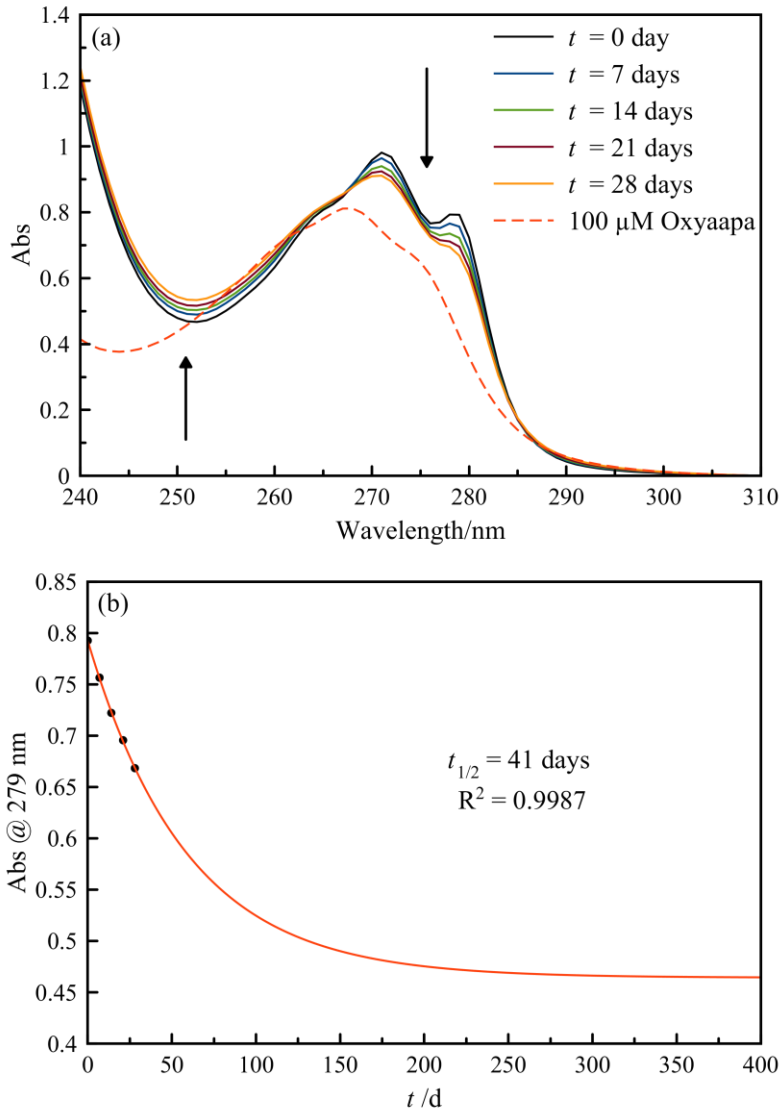

Figure S50. DTPA transchelation challenge on Lu-Oxyaapa complex (100 μM complex with 10 mM DTPA). (a) UV–Vis spectral change over the transchelation reaction (the complex showed ~65% intactness after 4 weeks); (b) The absorbance change at 279 nm versus time. The data points are fitted to a standard exponential decay model to estimate the half-life, which is about 41 days.

7. X-Ray Crystallography

Table S2. X-ray crystal data and structure refinement details for Lu-OxyMepa and Lu-Oxyaapa.

	Lu-OxyMepa	Lu-Oxyaapa
Empirical formula	$C_{20}H_{26}F_6LuN_4O_6P$	$C_{44}H_{64}ClLu_2N_8Na_3O_{30.50}$
Formula weight	738.39	1647.39
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	$P\overline{1}$
a (Å)	16.8531(4)	10.05350(10)
b (Å)	9.0126(2)	11.6225(2)
c (Å)	16.5519(4)	13.9236(2)
α (°)	90	103.0180(10)
β (°)	102.365(2)	103.8080(10)
γ (°)	90	100.8710(10)
V (Å^3)	2455.75(10)	1487.95(4)
Z	4	1
ρ_{calc} (10^3 kg·m^{-3})	1.997	1.838
μ (mm^{-1})	4.176	3.462
T (K)	252.99(10)	252.99(10)
λ (Å)	0.71073	0.71073
θ range (°)	2.474–27.103	2.158–27.876
Reflections collected	30157	66345
Independent reflections	5429	7089
R_{int}	0.0449	0.0638
Number of restraints	242	10
Number of parameters	388	436
Largest peak/hole (e·Å^{-3})	1.103/-0.800	1.357/-1.177
GoF	1.142	1.076
R1/wR2 (all data)	0.0340/0.0559	0.0246/0.0582
R1/wR2 (>2θ)	0.0274/0.0541	0.0224/0.0568

R1 = $\Sigma||F_o| - |F_c||/|F_o|$; wR2 = $\{\Sigma[w(F_o^2 - F_c^2)2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

GoF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$, where n is the number of data and p is the number of refined parameters.

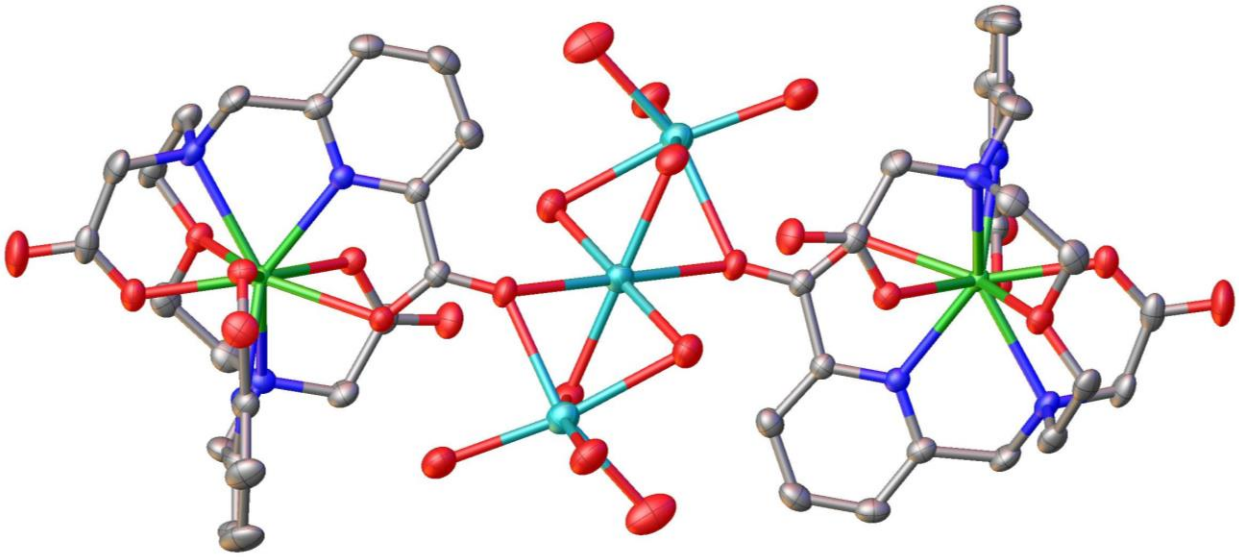

Figure S51. Crystal structure of Lu-Oxyaapa complex with the trisodium cationic moiety included. Solvent, counterions, and hydrogen atoms are omitted for clarity. Different types of atoms are drawn in different colors. Gray: C; Blue: N; Red: O; Cyan: Na; Green: Lu.

8. 2D NMR Spectra for Complex Solution Studies

(1) La-OxyMepa complex

Table S3. Peak assignments of NMR spectra on La-OxyMepa complex. See Chart 2 for the numbering scheme.

Carbon/Hydrogen Number	Symmetric, *anti*-		Asymmetric, *syn*-	
	δ_C (ppm)	δ_H (ppm)	δ_C (ppm)	δ_H (ppm)
1	55.97	3.01, 2.83		3.13, 2.53
2	69.27	3.80, 3.76		3.61, 3.36
3	69.27	3.80, 3.76		4.08, 3.41
4	55.97	3.01, 2.83		3.34, 2.79
5	44.71	2.42	45.58	2.77
6	44.71	2.42	40.72	2.25
7	61.90	4.23, 3.94		4.42, 4.06
8	157.68			
9	126.01	7.69		7.71
10	141.31	8.13		8.14
11	123.99	8.05		8.05
12	151.29			
13	173.09			
14	61.90	4.23, 3.94		4.71, 3.75
15	157.68			
16	126.01	7.69		7.71
17	141.31	8.13		8.14
18	123.99	8.05		8.05
19	151.29			
20	173.09			

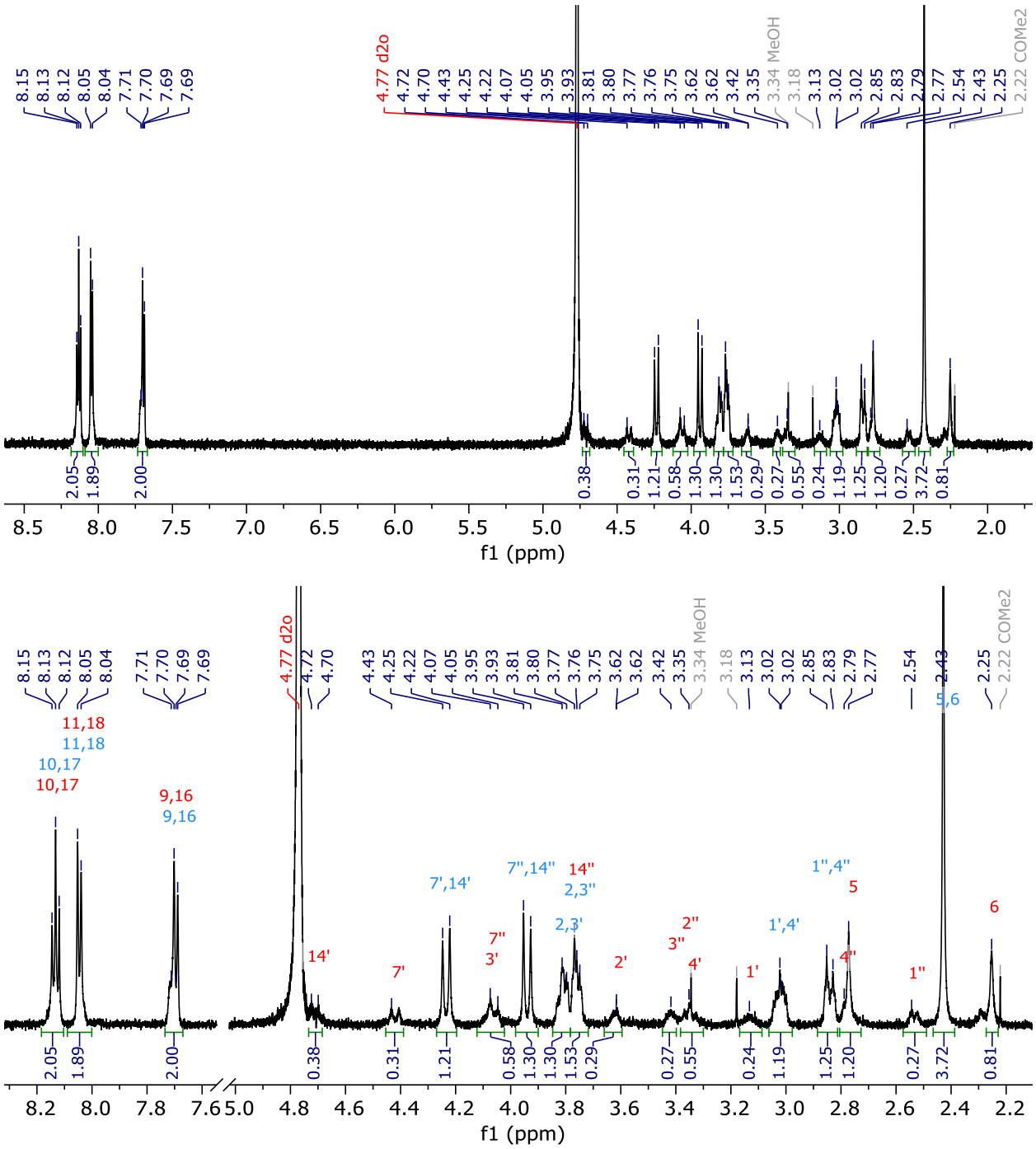

Figure S52. Full (top) as well as properly expanded and labeled (bottom) ^{1}H NMR spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

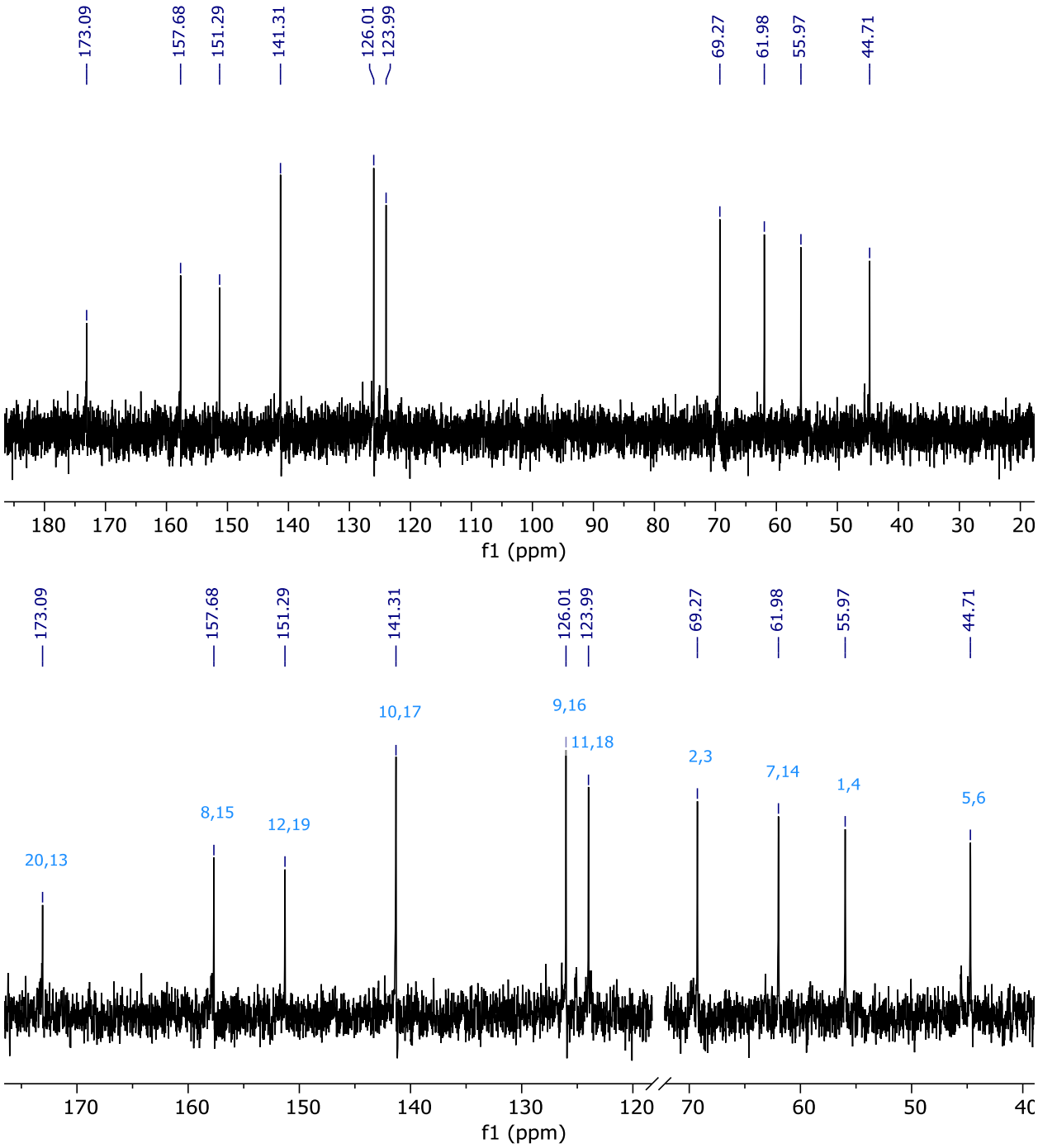

Figure S53. Full (top) as well as properly expanded and labeled (bottom) $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

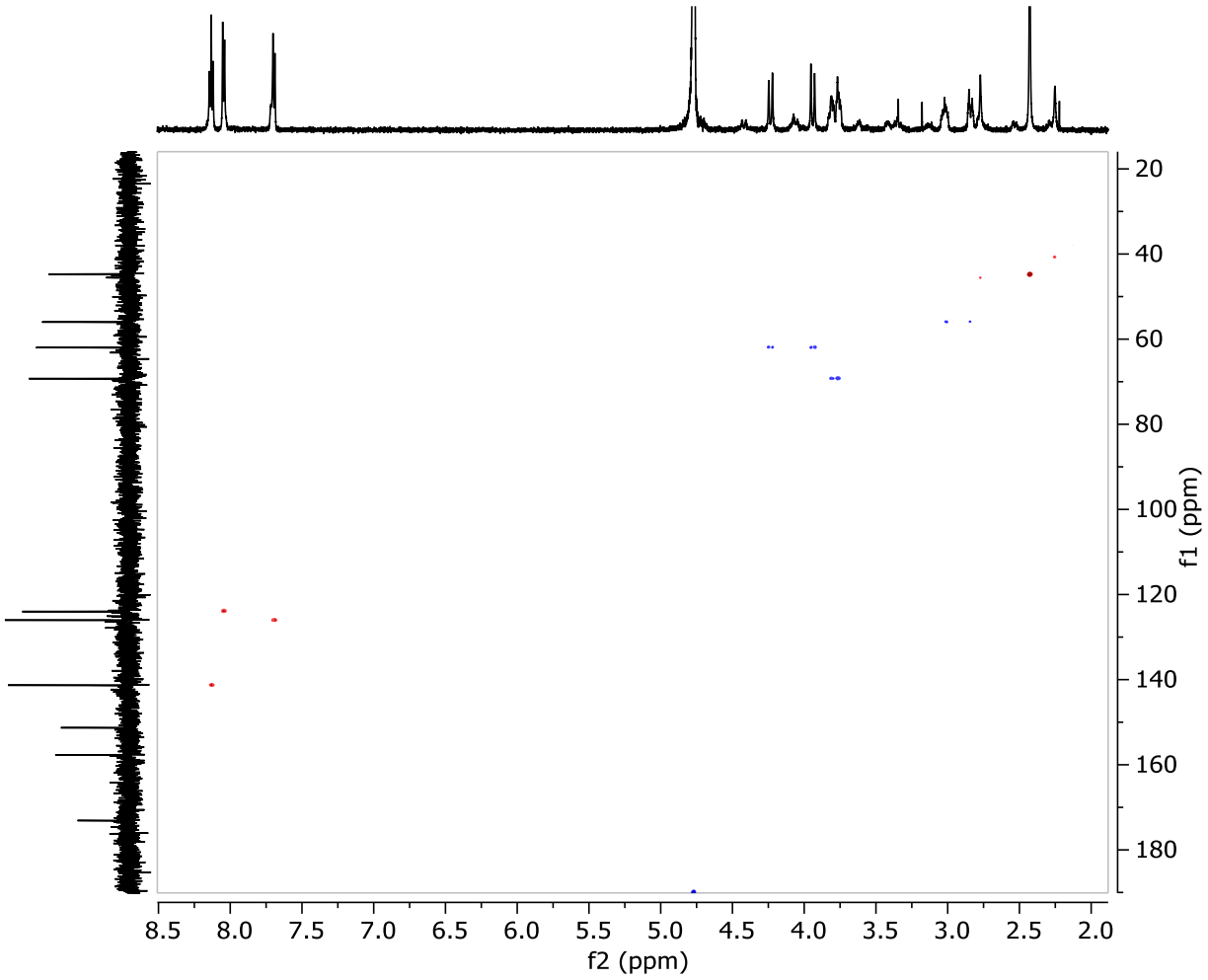

Figure S54. Full HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

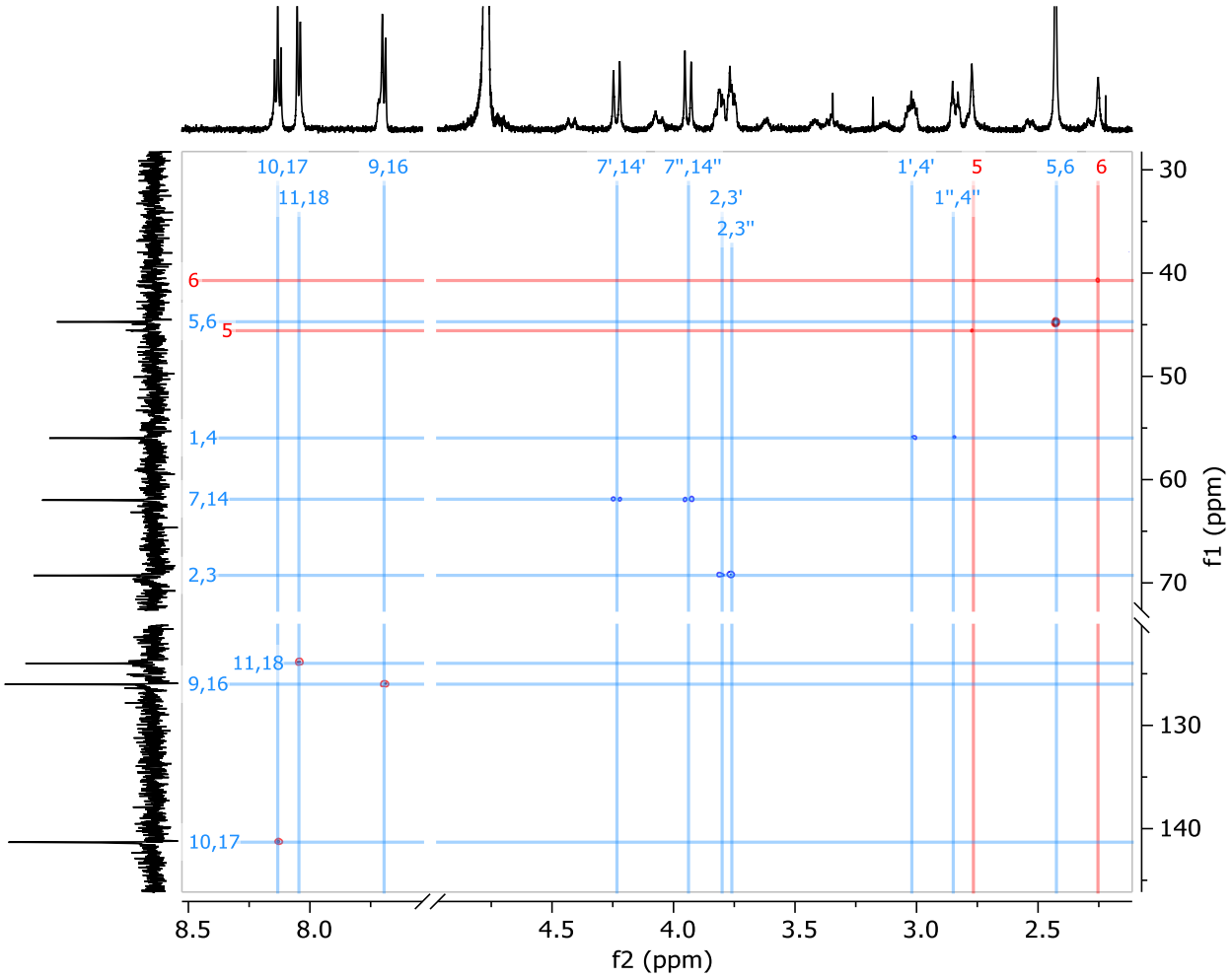

Figure S55. Properly expanded and labeled HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

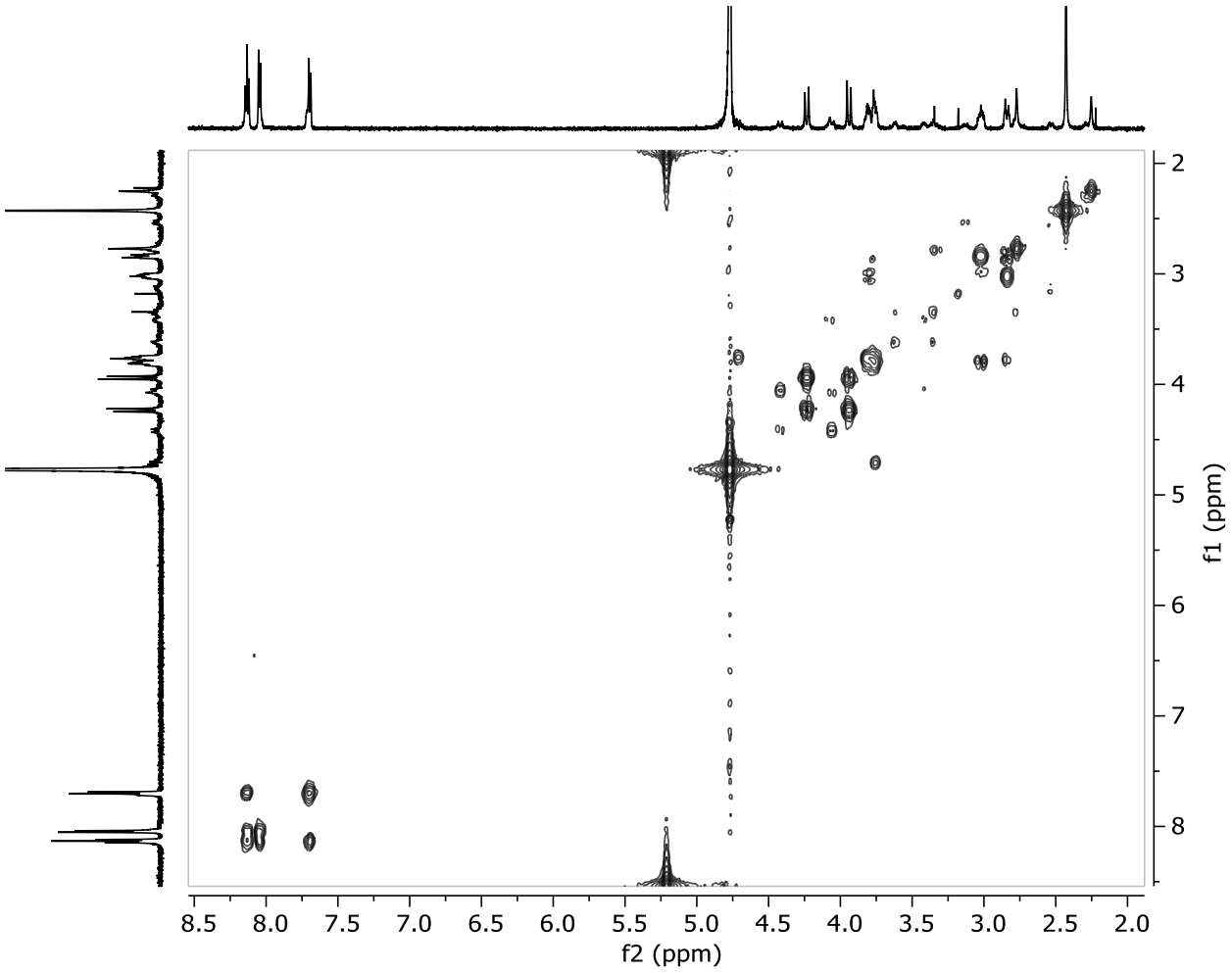

Figure S56. Full COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

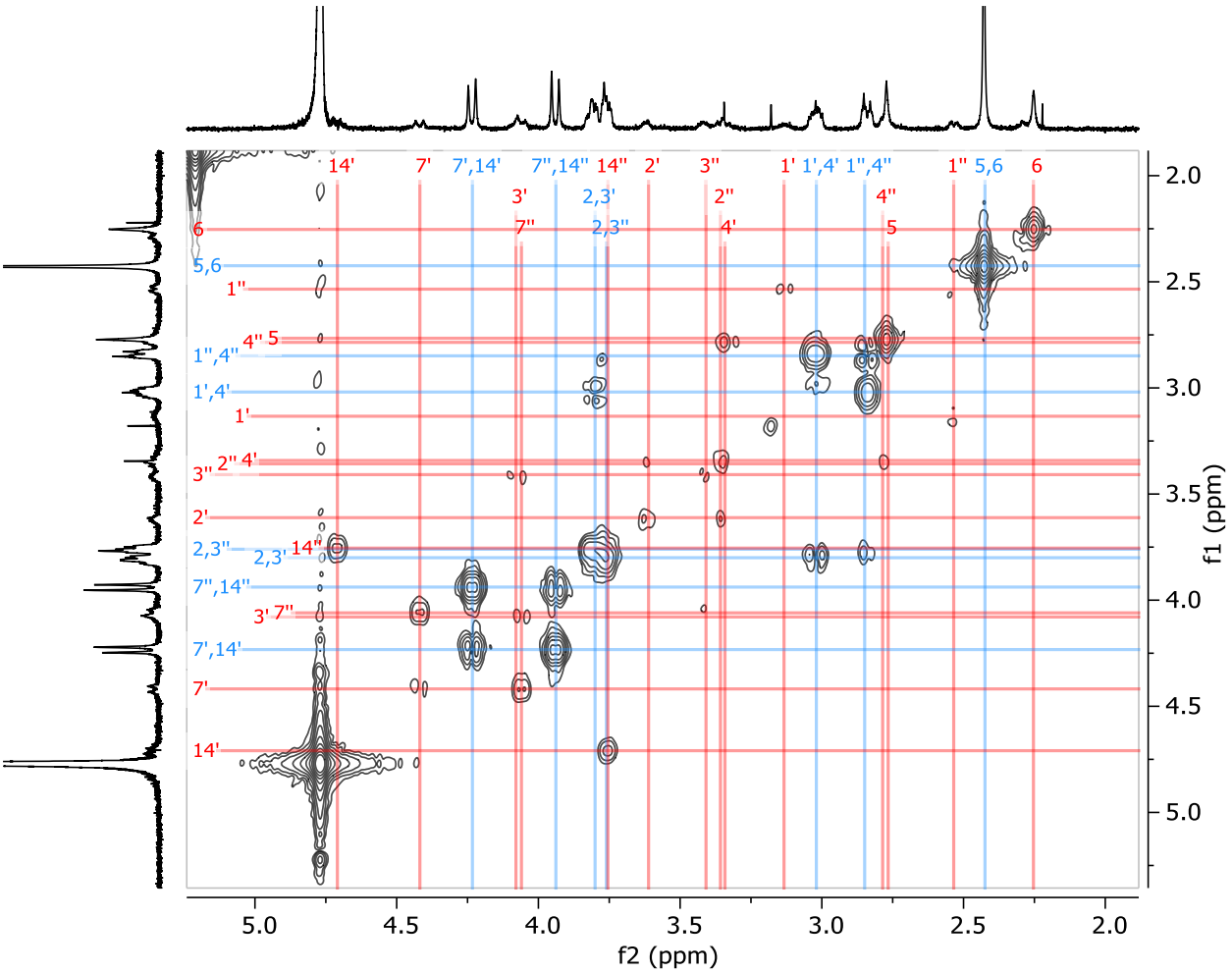

Figure S57. Expanded (aliphatic region) and labeled COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

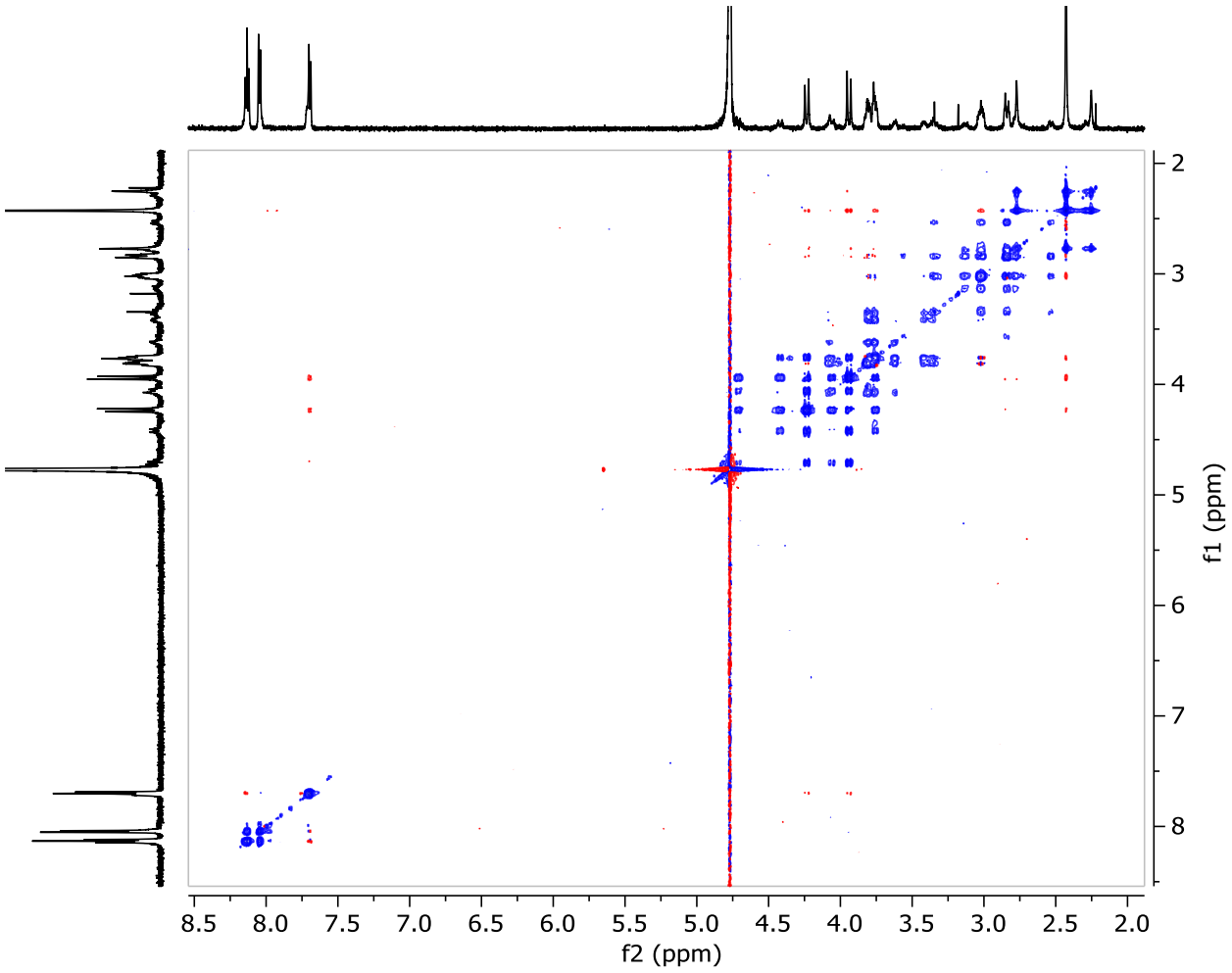

Figure S58. Full ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

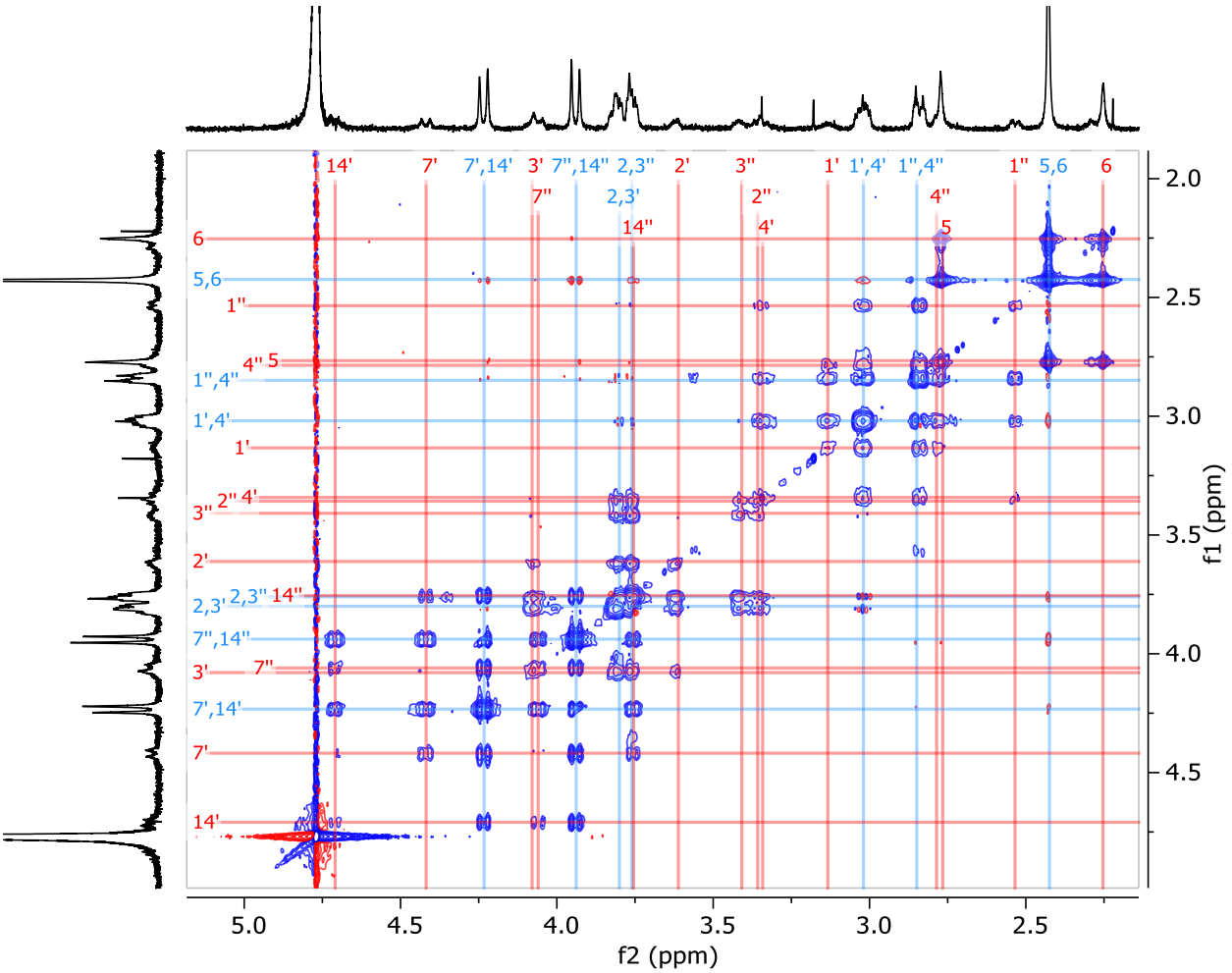

Figure S59. Expanded (aliphatic region) and labeled ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-OxyMepa complex.

(2) Lu-OxyMepa complex

Table S4. Peak assignments of NMR spectra on Lu-OxyMepa complex. See Chart 2 for the numbering scheme.

Carbon/Hydrogen Number	Symmetric, *anti*-		Asymmetric, *syn*-	
	δ_C (ppm)	δ_H (ppm)	δ_C (ppm)	δ_H (ppm)
1		3.22, 2.96	55.62	3.03, 2.55
2		4.27, 4.08	70.30	4.33, 3.86
3		4.27, 4.08	72.19	4.39, 4.14
4		3.22, 2.96	55.13	3.79, 2.84
5	45.61	2.52	44.49	2.73
6	45.61	2.52	43.07	2.46
7		4.42, 3.98	63.22	4.72, 4.08
8			158.21 or 156.45	
9		7.74	126.76 or 126.59	7.79
10		8.16	142.44 or 142.16	8.20 or 8.17
11		7.98	123.31 or 122.92	7.94
12			149.71 or 149.48	
13			173.14 or 173.08	
14		4.42, 3.98	63.72	4.99, 4.02
15			158.21 or 156.45	
16		7.74	126.76 or 126.59	7.79
17		8.16	142.44 or 142.16	8.20 or 8.17
18		7.98	123.31 or 122.92	7.94
19			149.71 or 149.48	
20			173.14 or 173.08	

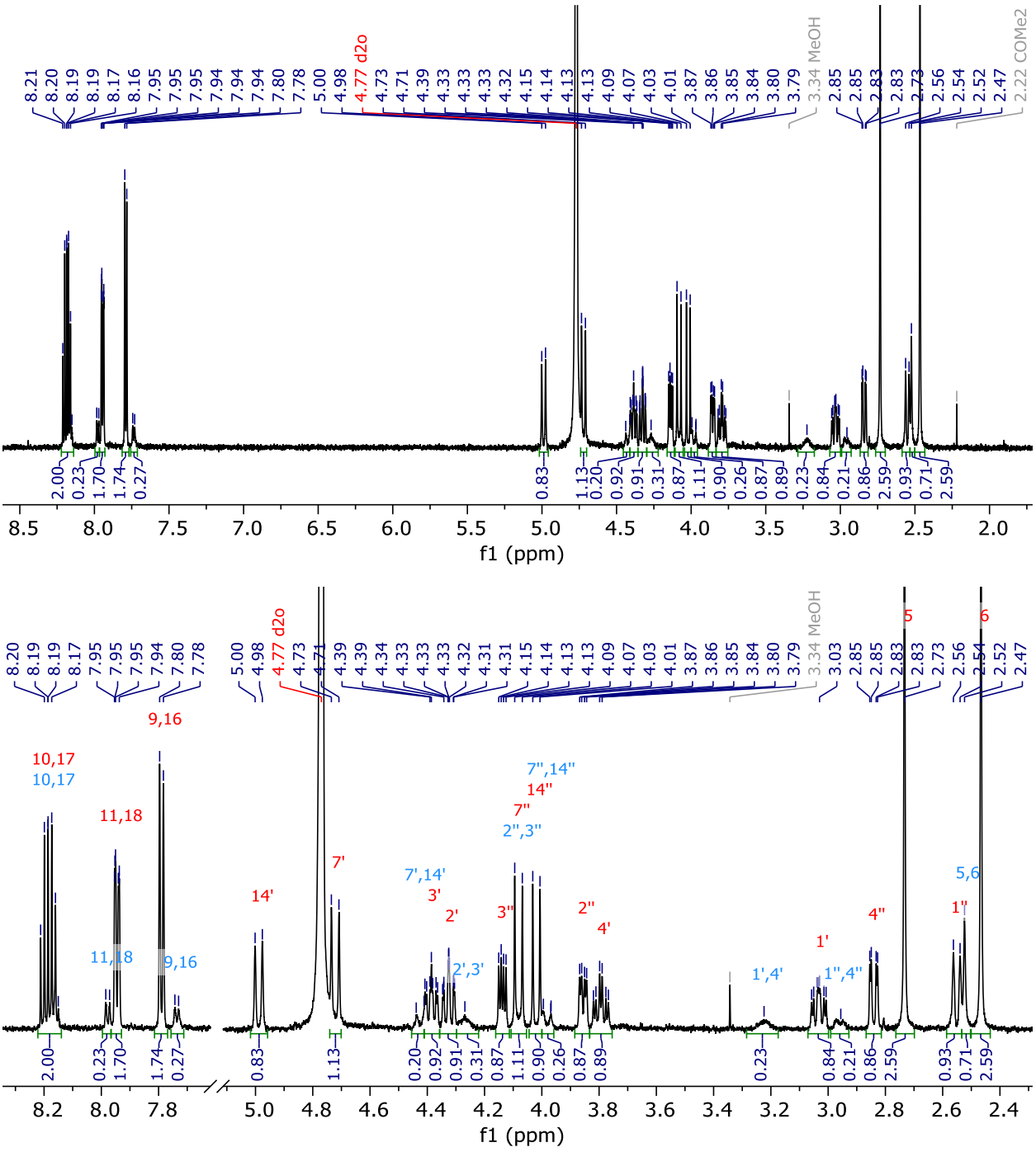

Figure S60. Full (top) as well as properly expanded and labeled (bottom) ^{1}H NMR spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

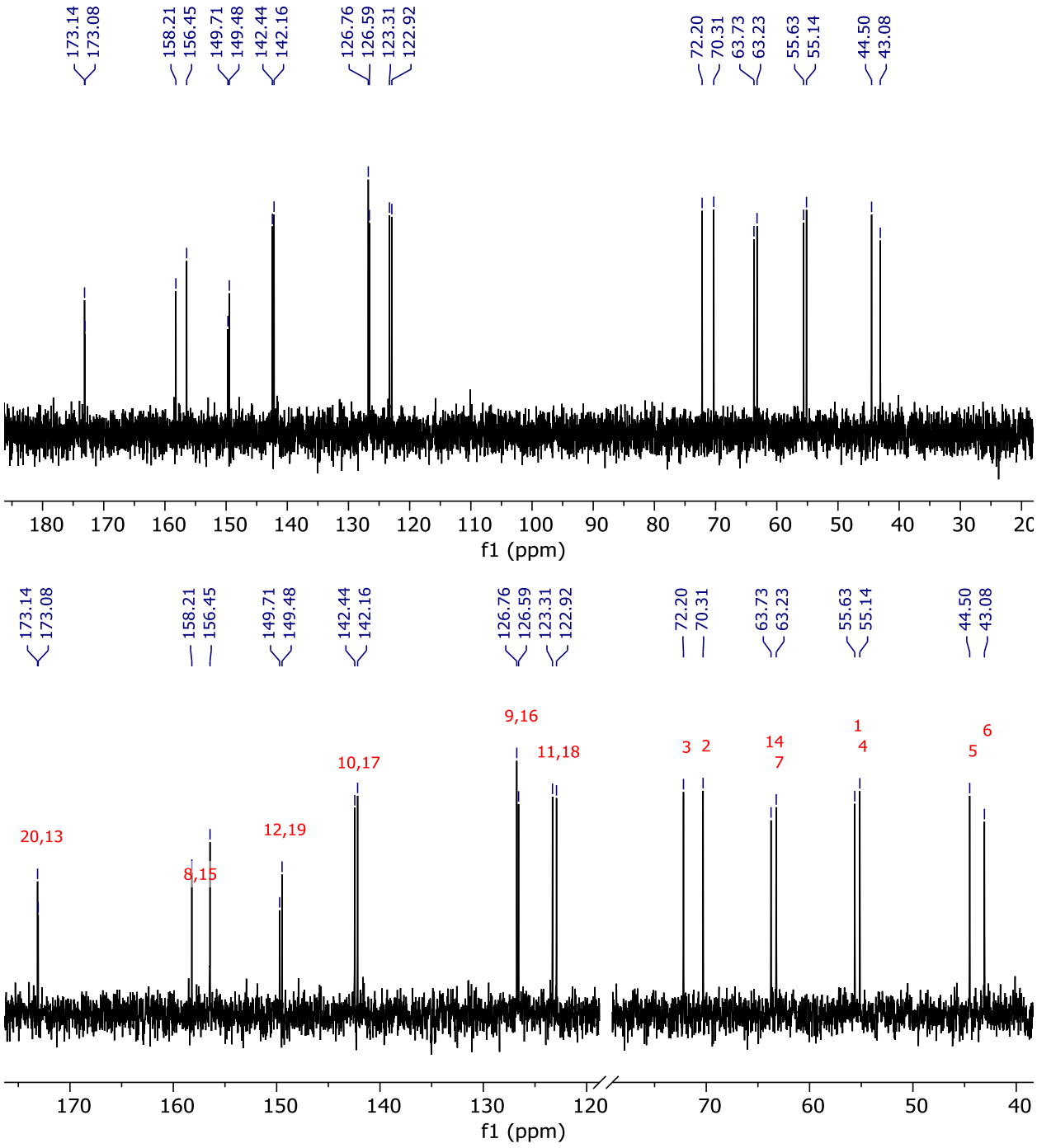

Figure S61. Full (top) as well as properly expanded and labeled (bottom) $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

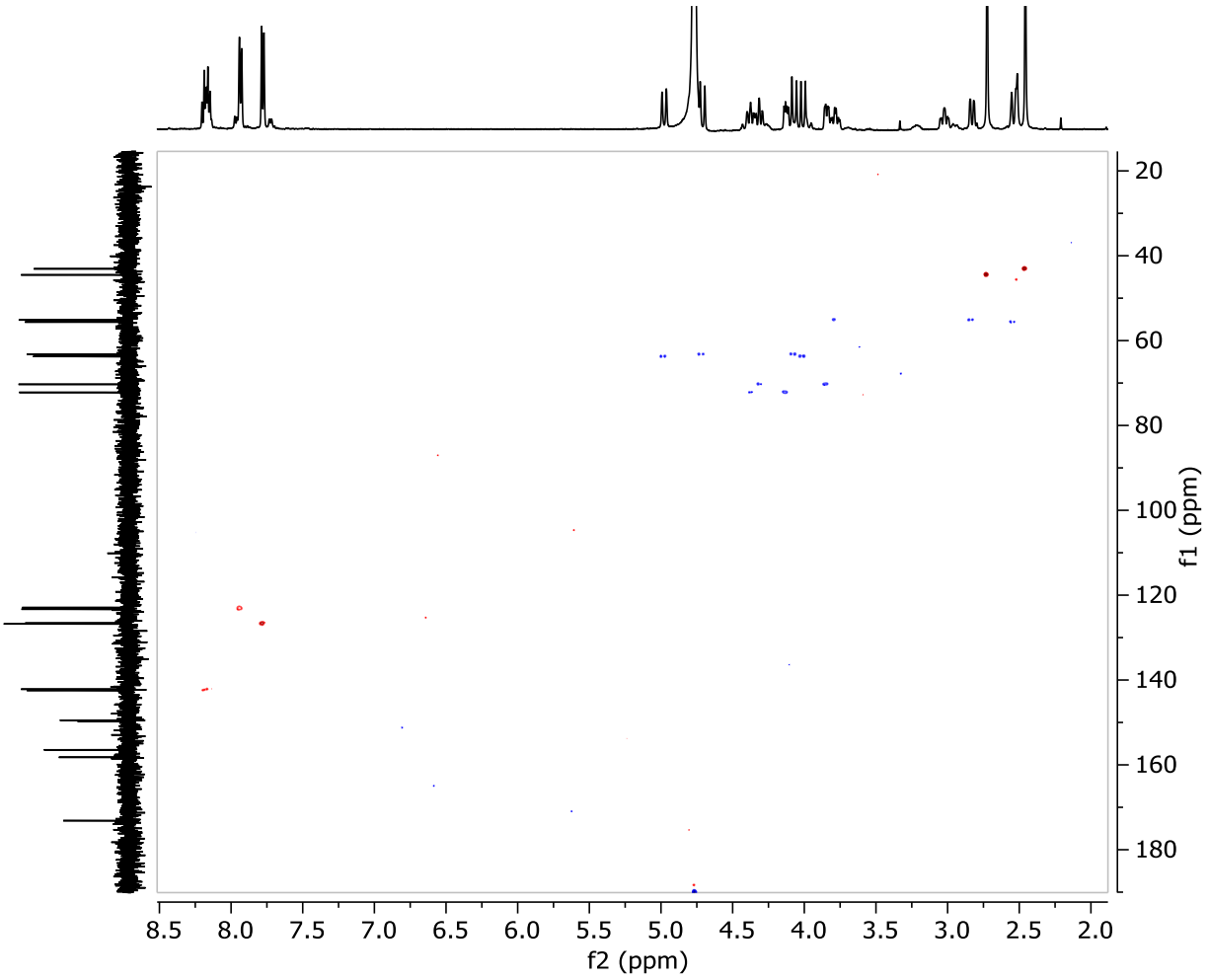

Figure S62. Full HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

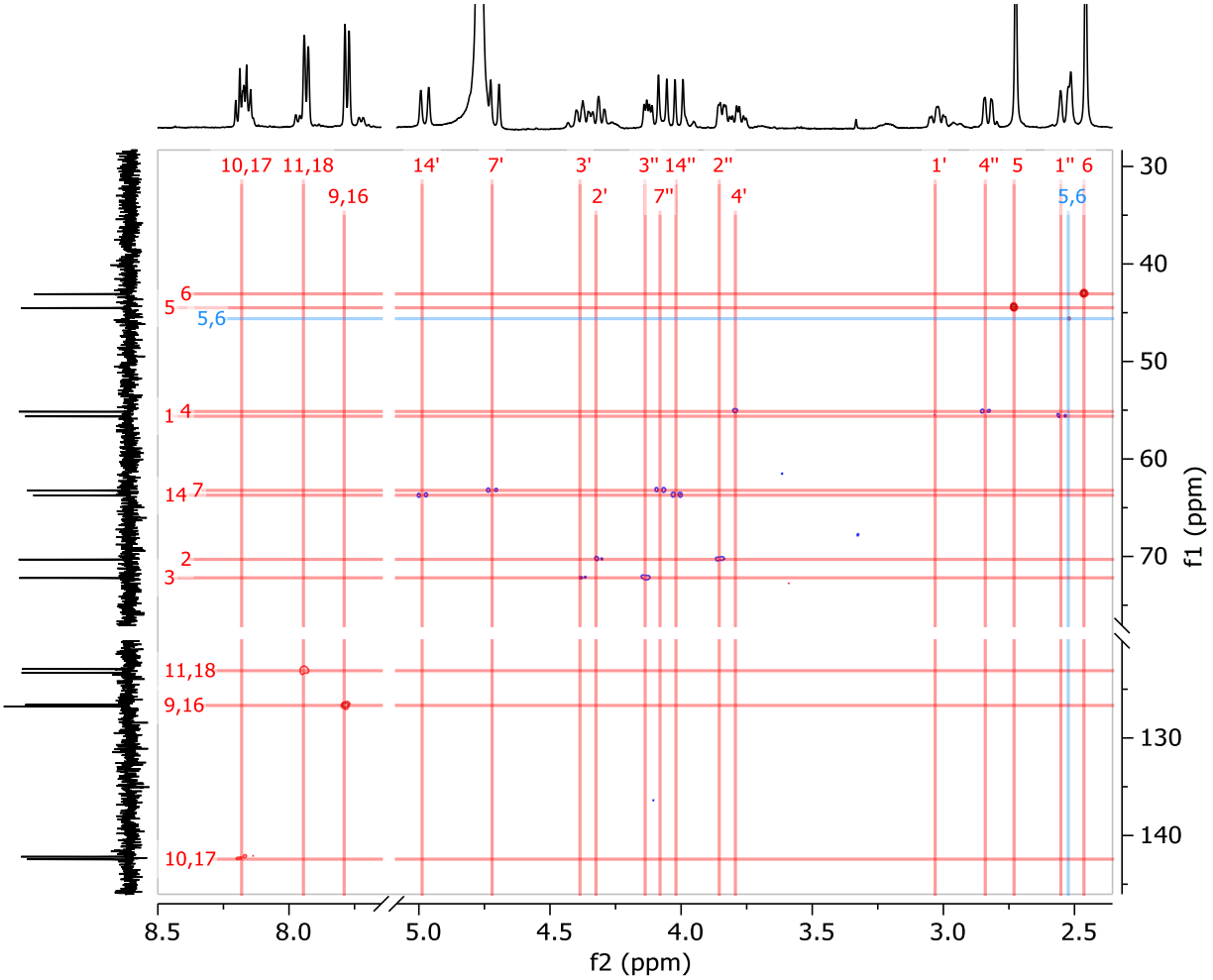

Figure S63. Properly expanded and labeled HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

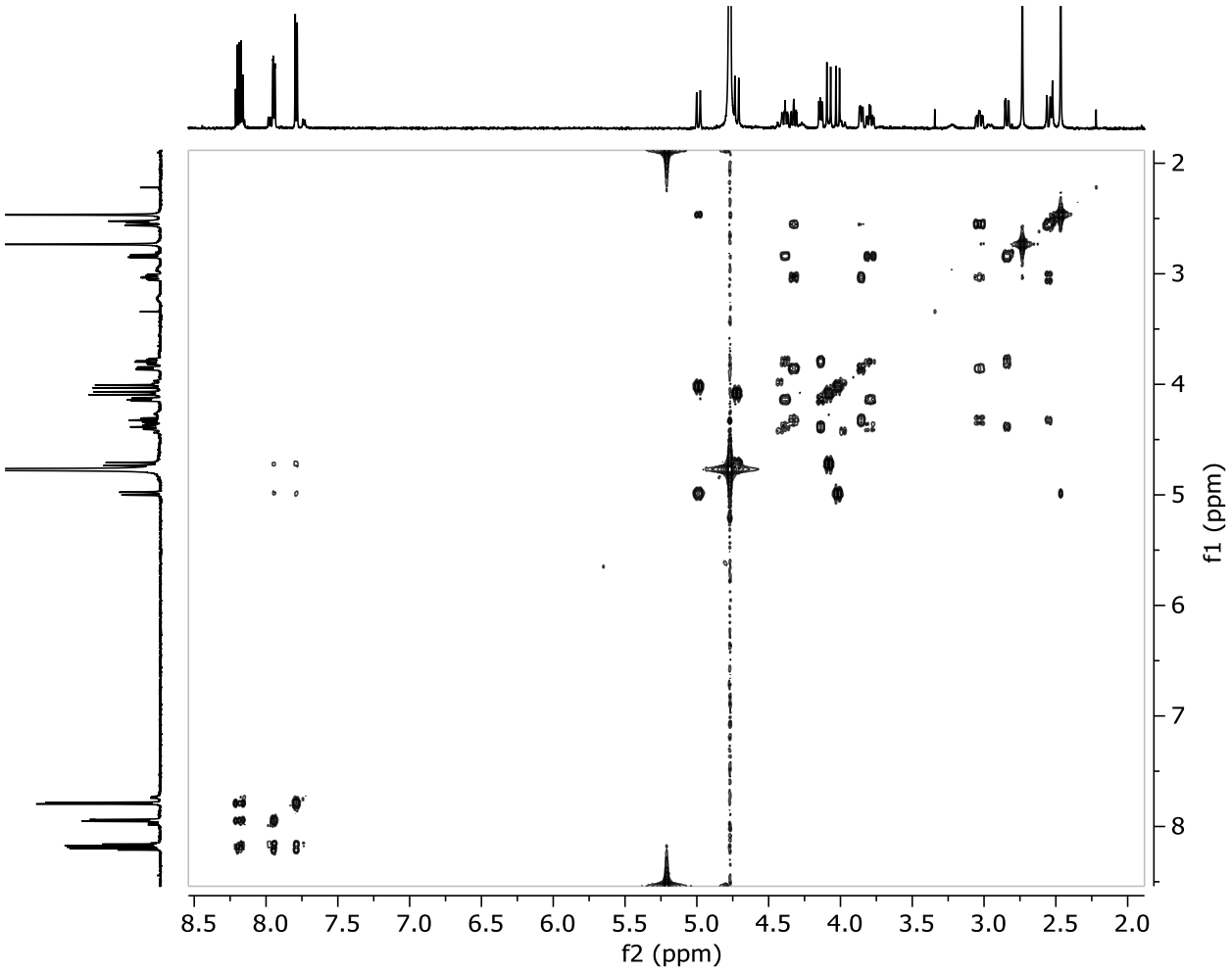

Figure S64. Full COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

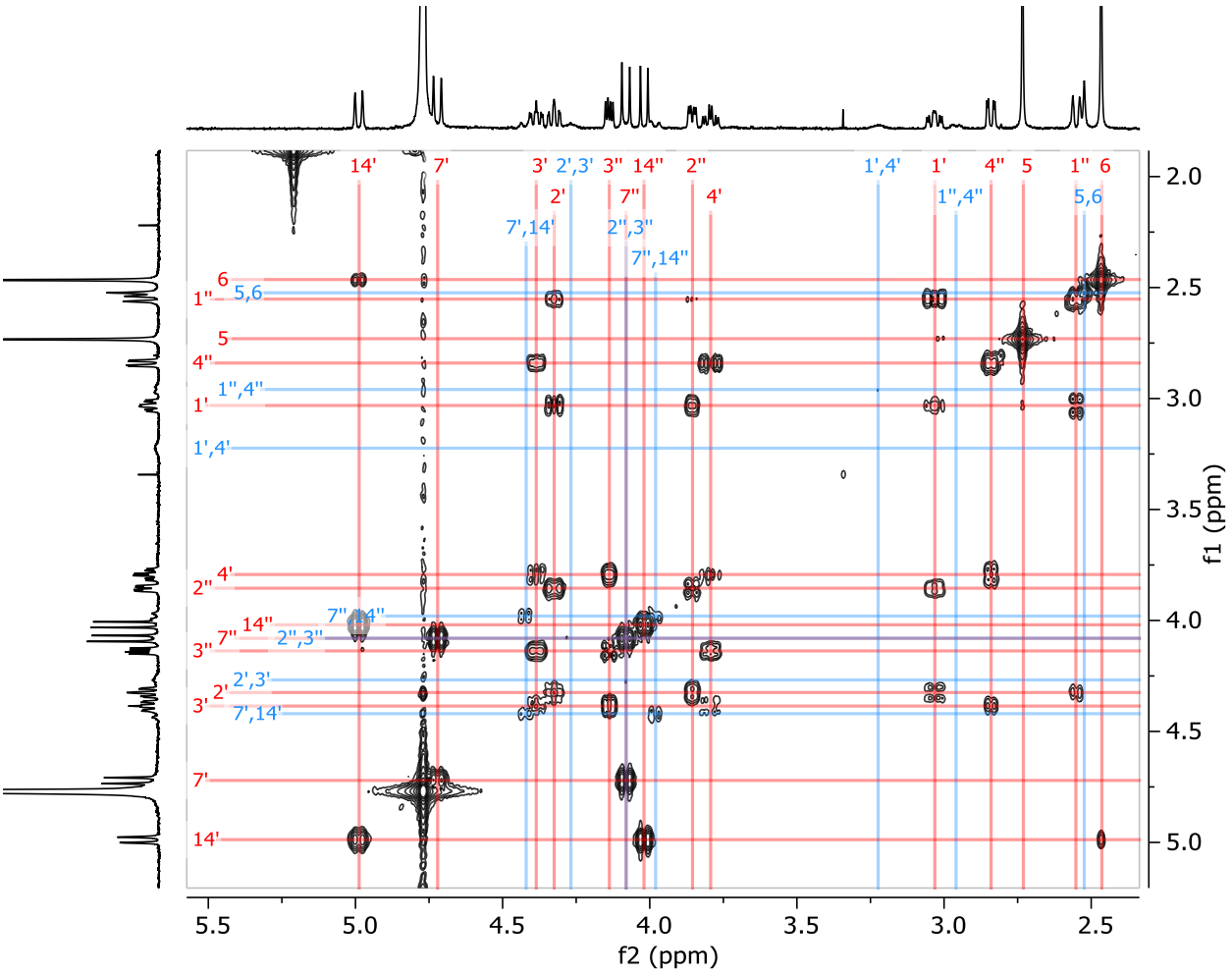

Figure S65. Expanded (aliphatic region) and labeled COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

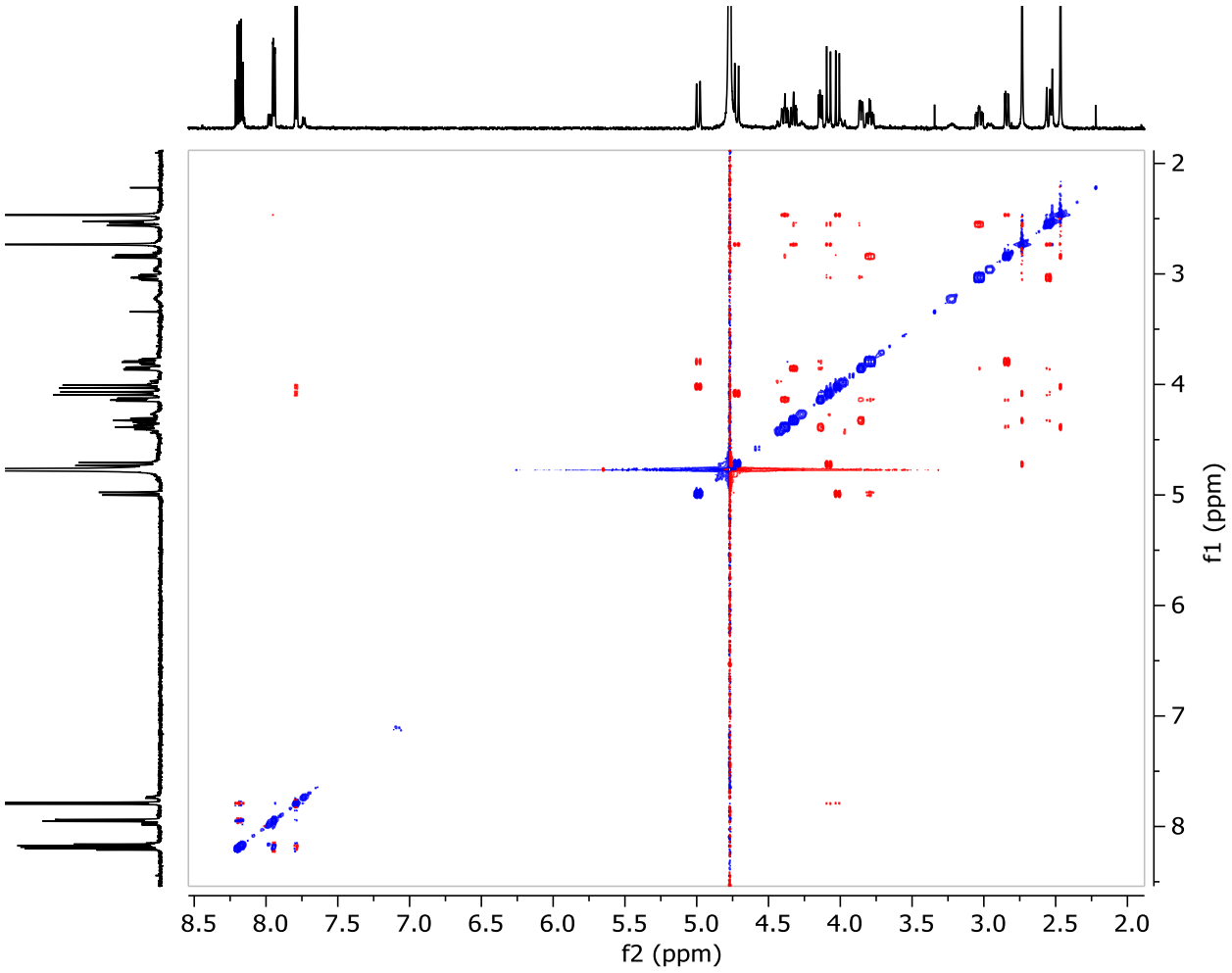

Figure S66. Full ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

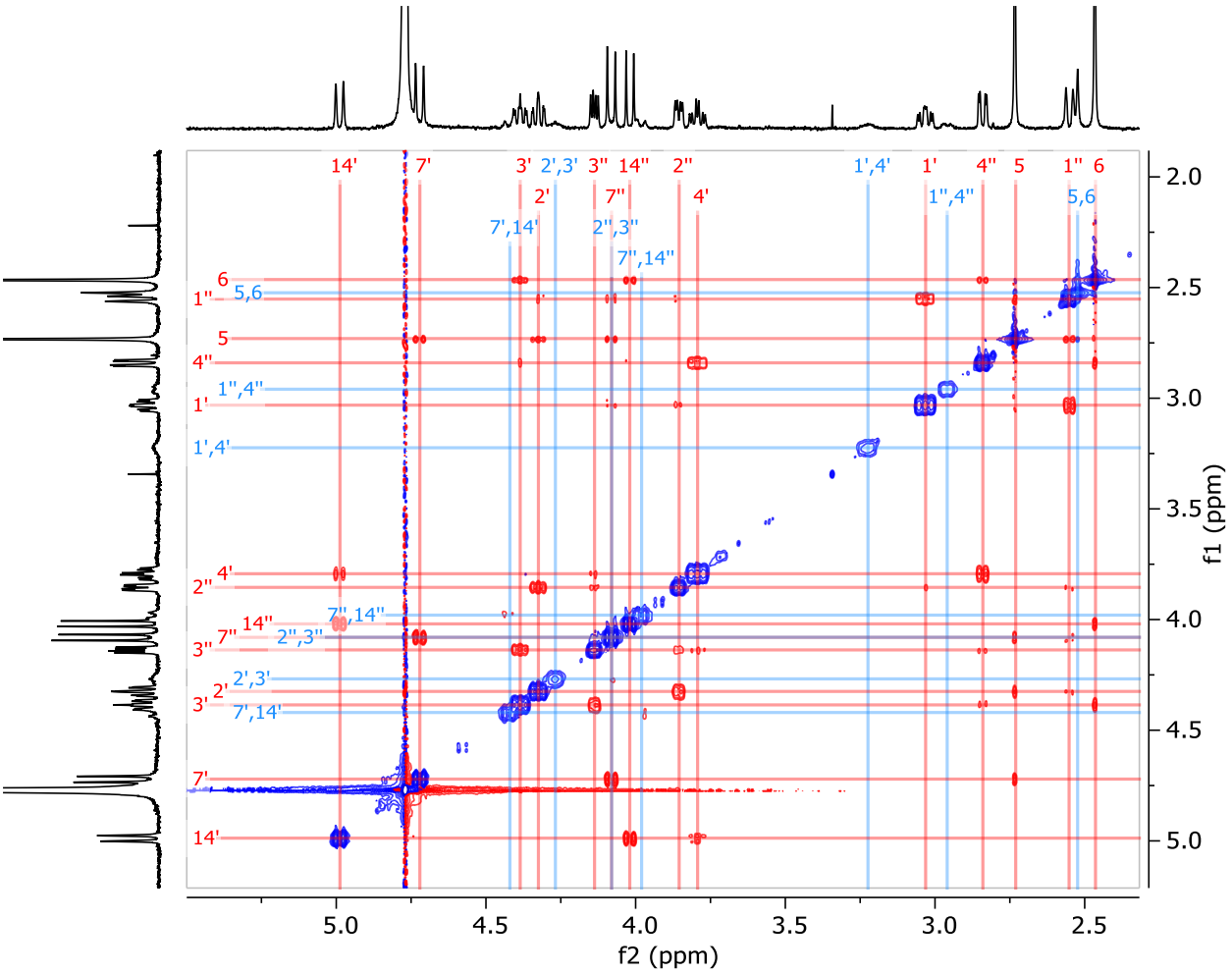

Figure S67. Expanded (aliphatic region) and labeled ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-OxyMepa complex.

Table S5. Diagnostic ROESY (Lu-OxyMepa) interactions that verify the asymmetric conformation belongs to *syn*- conformer. The atomic distances are taken from the Lu-OxyMepa crystal structure.

Hydrogen Pairs	Atomic Distance (Å)	Interaction Intensity
H1A–H7A	3.534	
H1A–H7B	2.494	medium
H1B–H7A	3.420	
H1B–H7B	2.609	medium
H4A–H14A	2.739	
H4A–H14B	2.676	weak
H4B–H14A	2.260	strong
H4B–H14B	3.067	
H2A–H5	3.054/2.272[a]	very strong
H2B–H5	4.212/3.634[a]	
H3A–H6	4.125/3.546[a]	
H3B–H6	2.905/2.167[a]	very strong

[a]For hydrogen pairs involving methyl groups, the atomic distance is listed as (averaged distance considering 3 hydrogens on the methyl group)/(shortest distance among the 3 hydrogens on the methyl group).

(3) La-Oxyaapa complex

Table S6. Peak assignments of NMR spectra on La-Oxyaapa complex. See Chart 2 for the numbering scheme.

Carbon/Hydrogen Number	Asymmetric, *syn*-	
	δ_C (ppm)	δ_H (ppm)
1	53.45	2.78, 2.75
2	68.99	3.92, 3.49
3	69.71	3.84, 3.68
4	57.79	3.28, 2.89
5	59.38	4.01, 3.36
6	180.22	
7	61.30	3.55, 3.32
8	180.22	
9	61.21	4.44, 3.94
10	157.35	
11	124.71	7.64
12	140.90	8.09
13	123.57	7.93
14	150.94	
15	173.03	
16	62.68	4.57, 4.06
17	156.61	
18	125.59	7.62
19	140.19	8.04
20	123.18	7.94
21	150.81	
22	172.53	

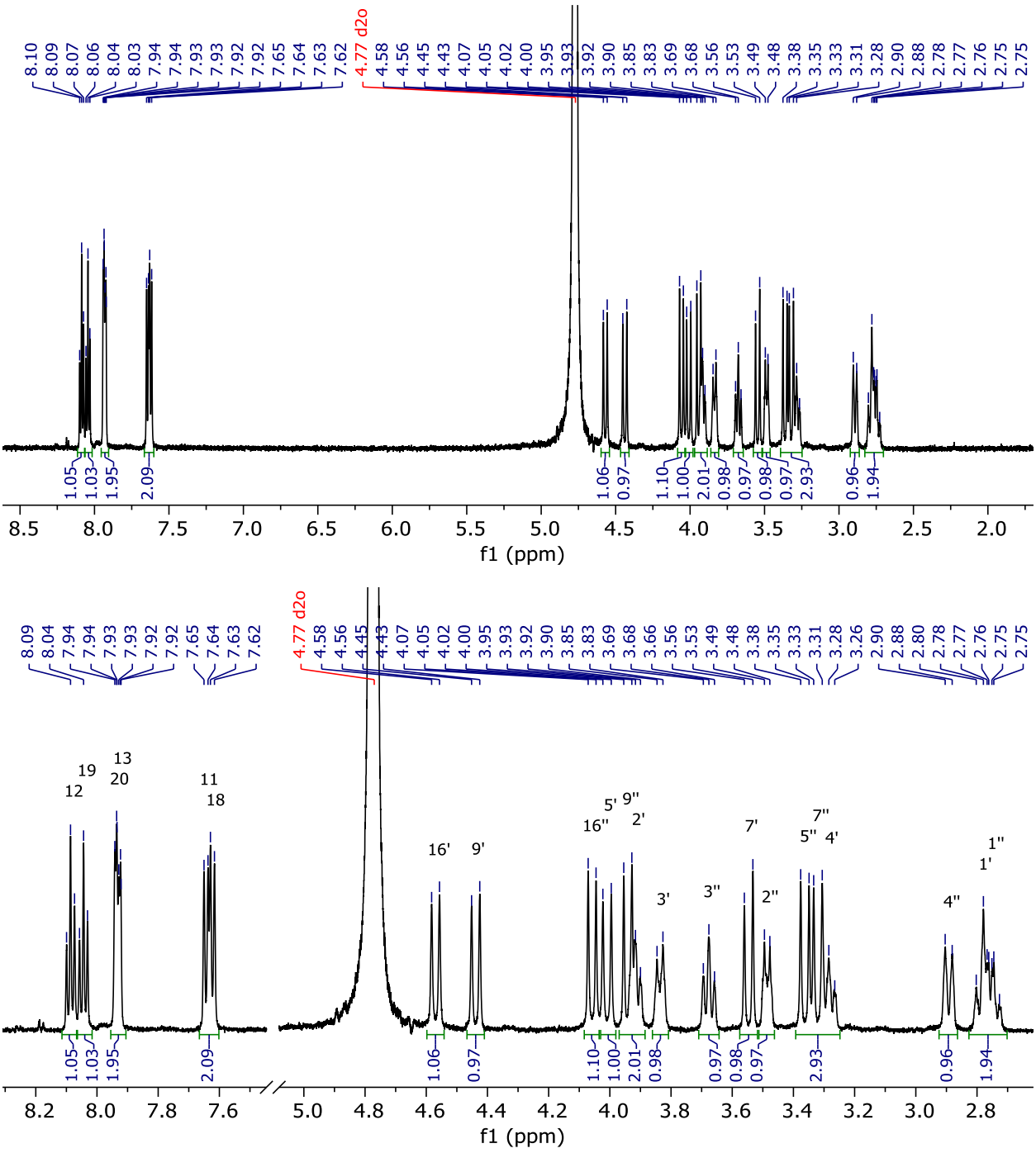

Figure S68. Full (top) as well as properly expanded and labeled (bottom) ^{1}H NMR spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

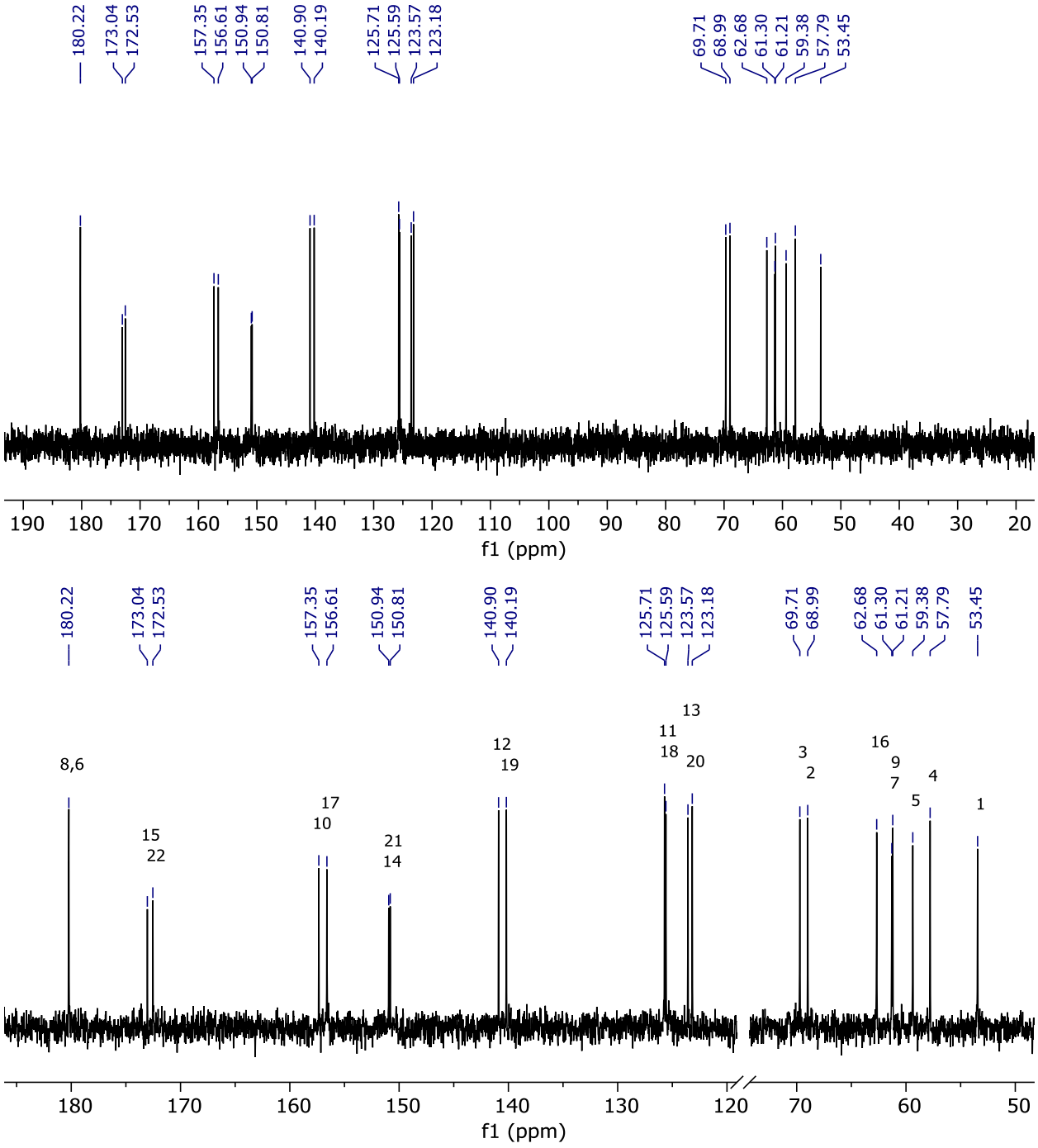

Figure S69. Full (top) as well as properly expanded and labeled (bottom) $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

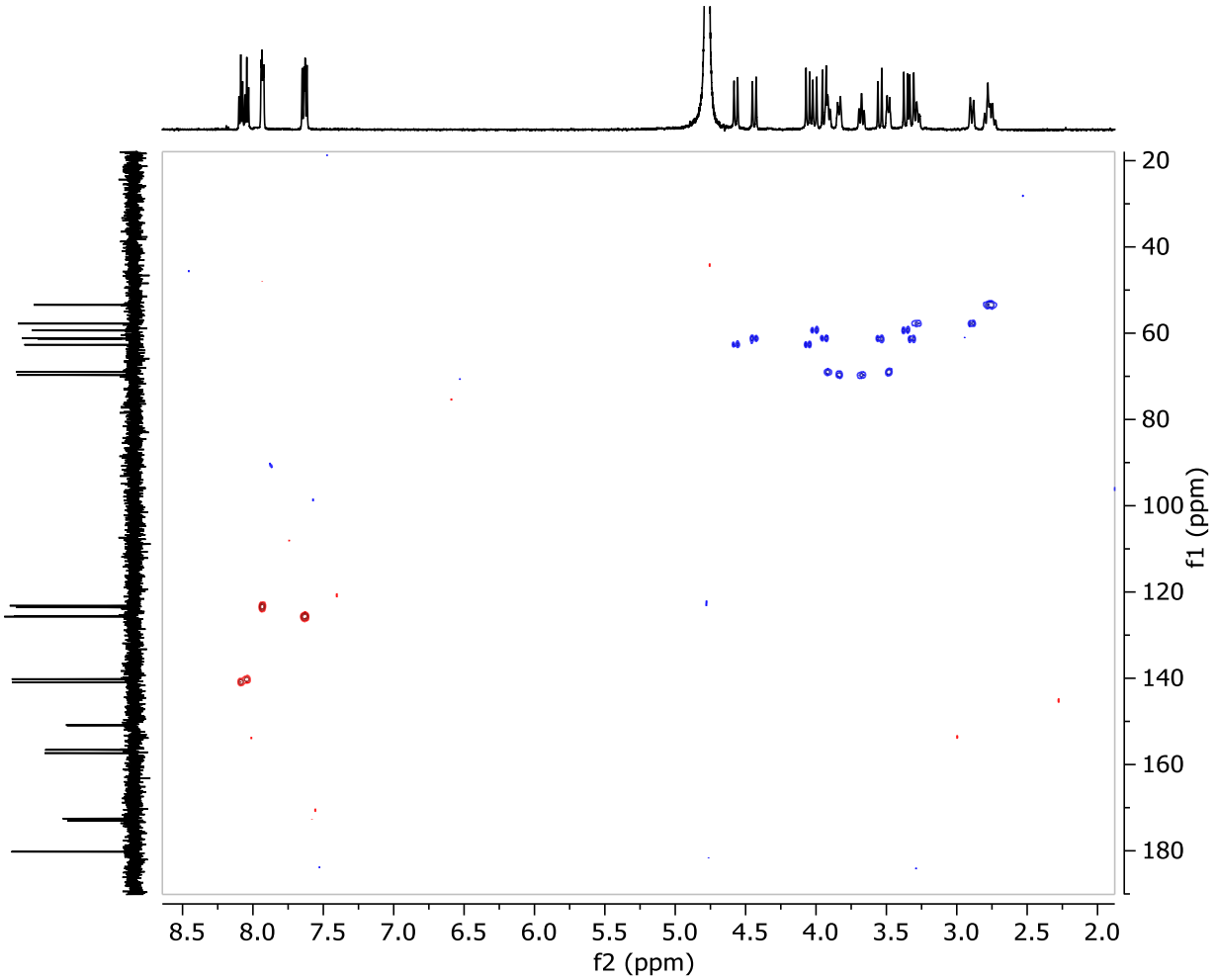

Figure S70. Full HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

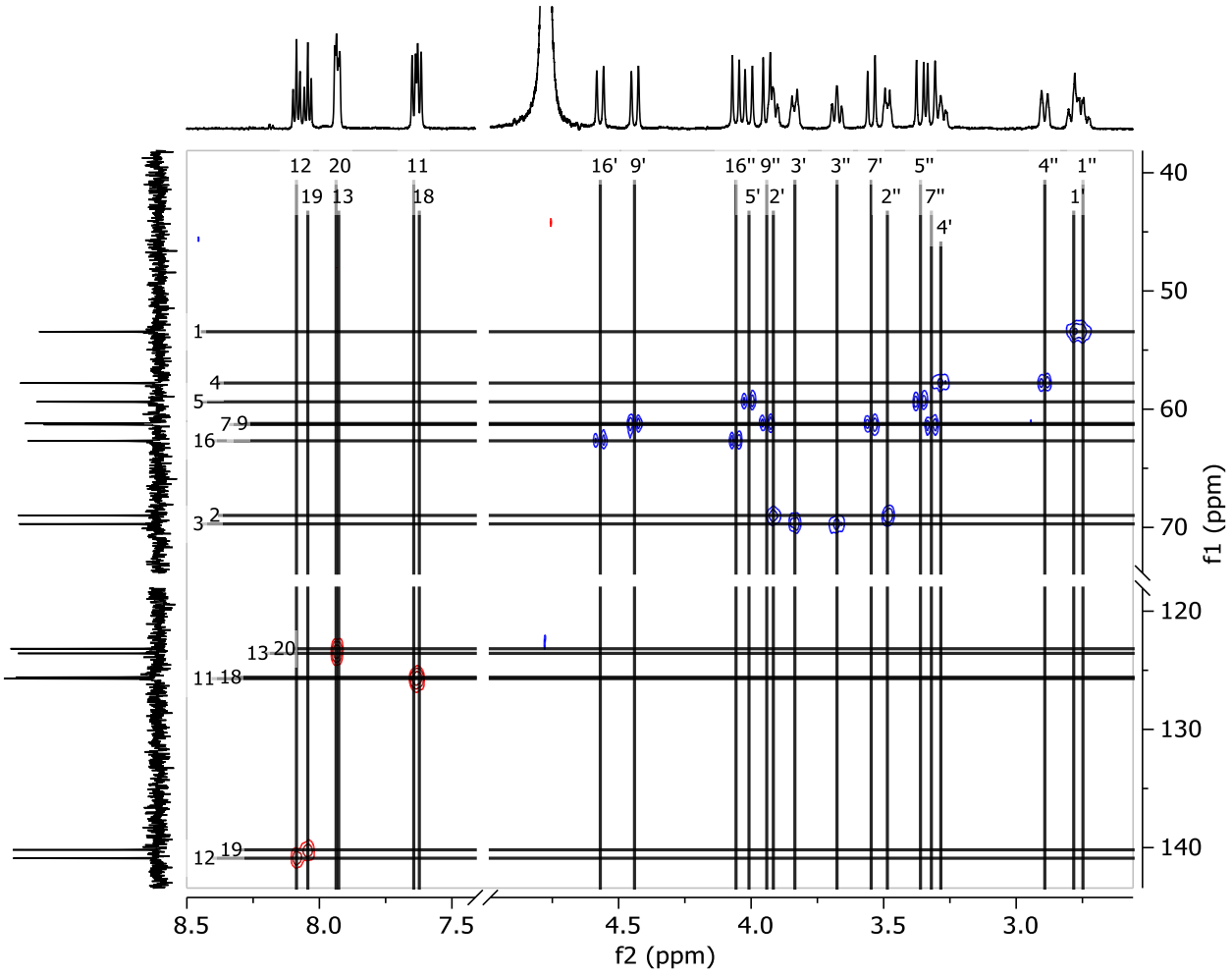

Figure S71. Properly expanded and labeled HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

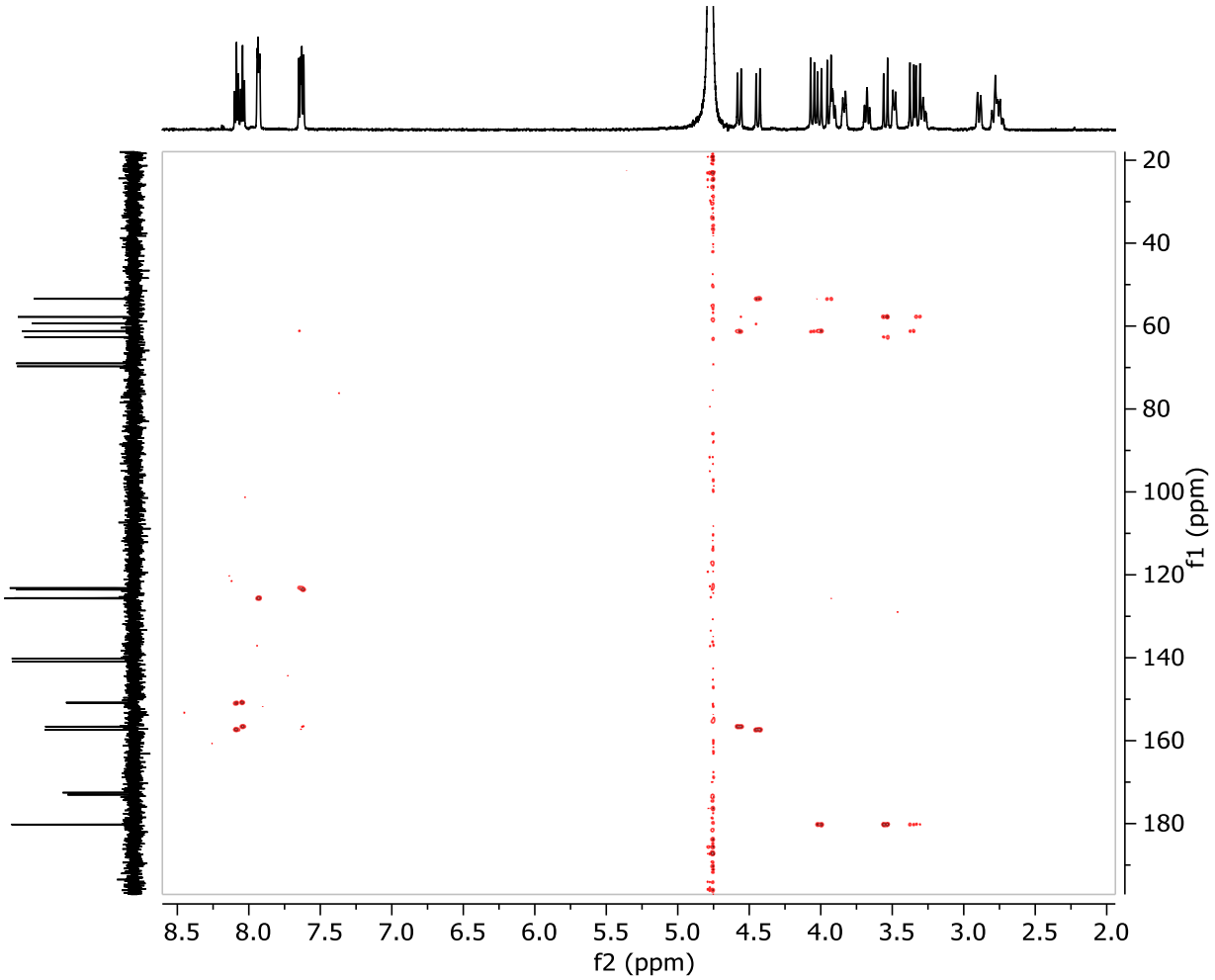

Figure S72. Full HMBC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

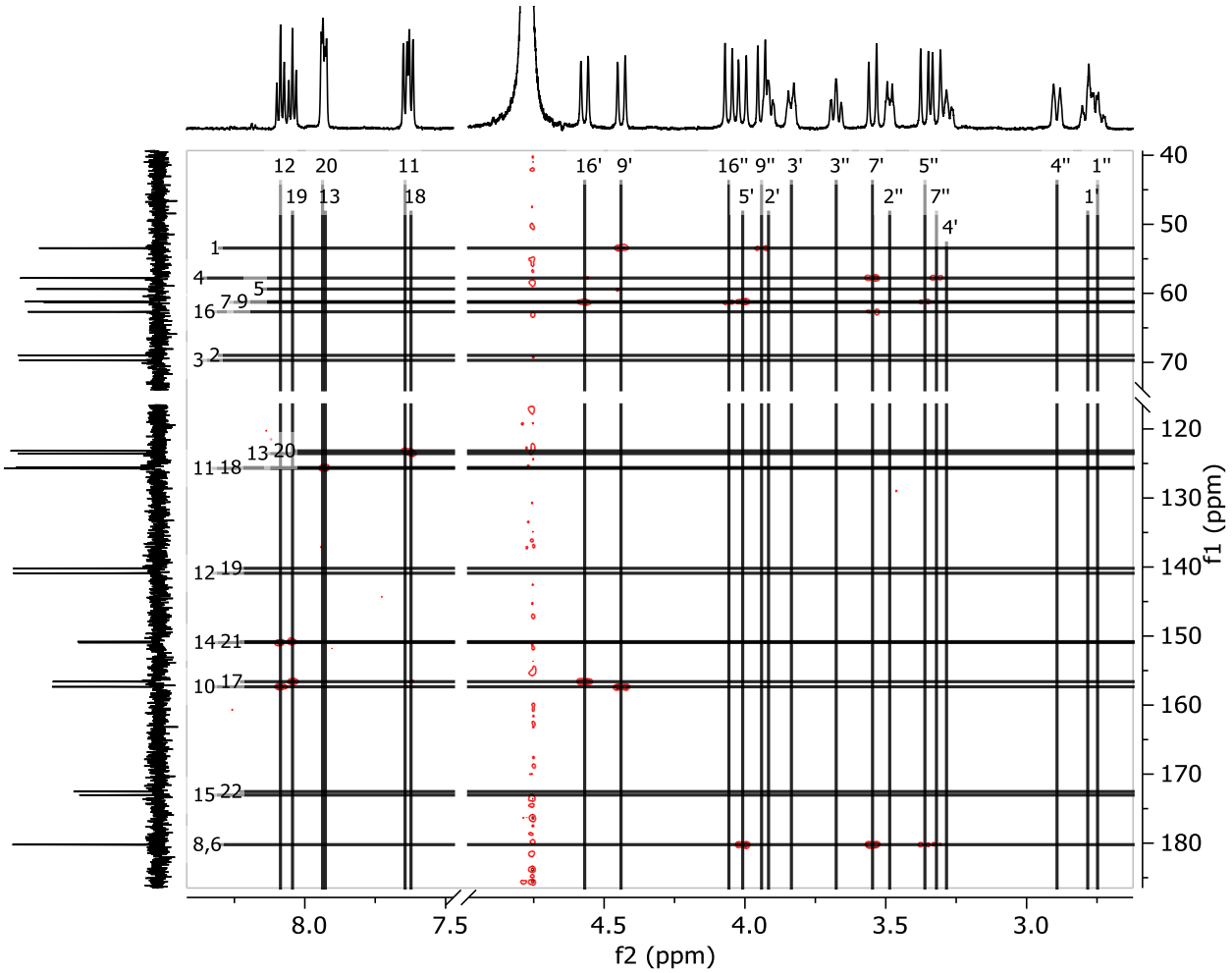

Figure S73. Properly expanded and labeled HMBC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

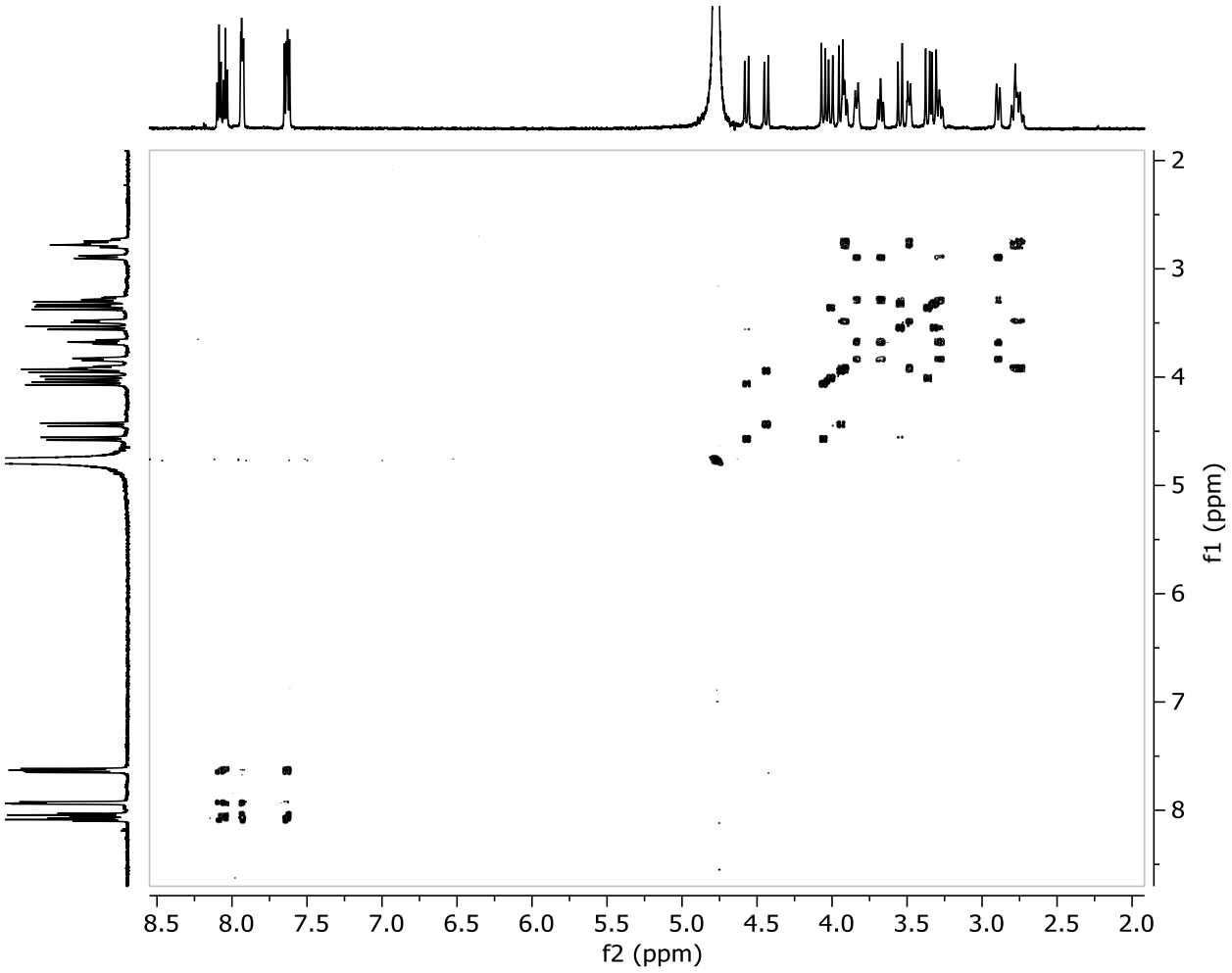

Figure S74. Full COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

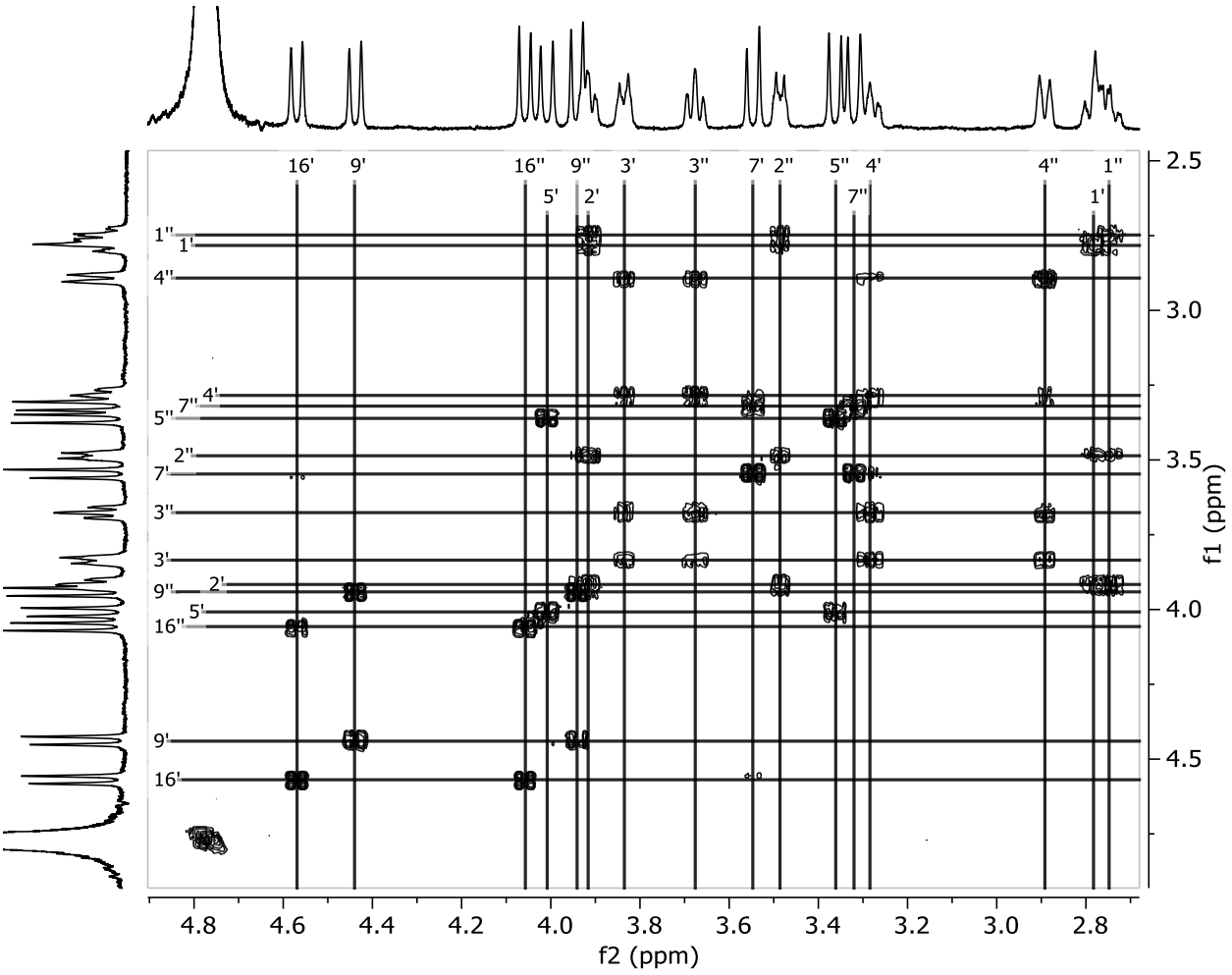

Figure 75. Expanded (aliphatic region) and labeled COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

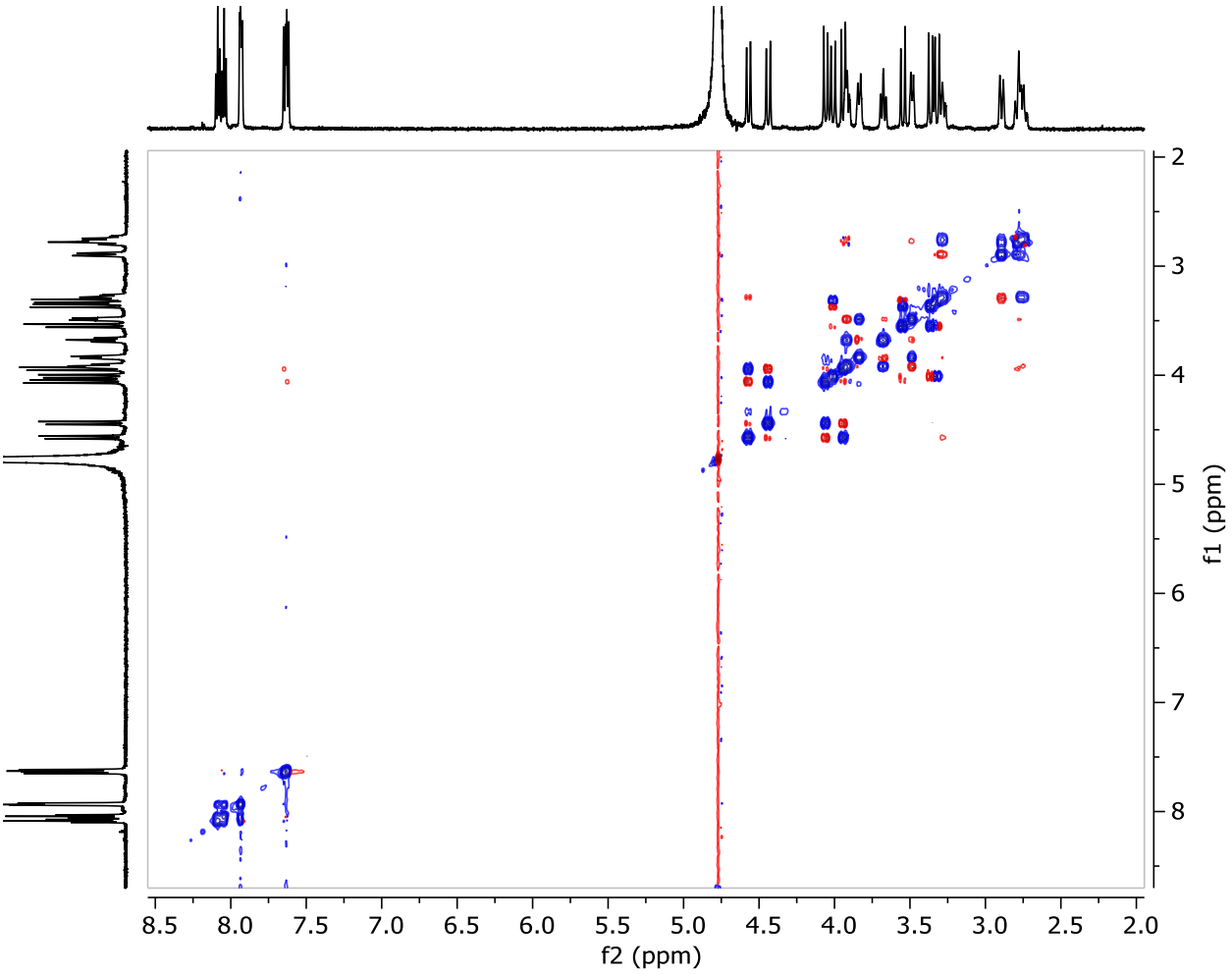

Figure S76. Full ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

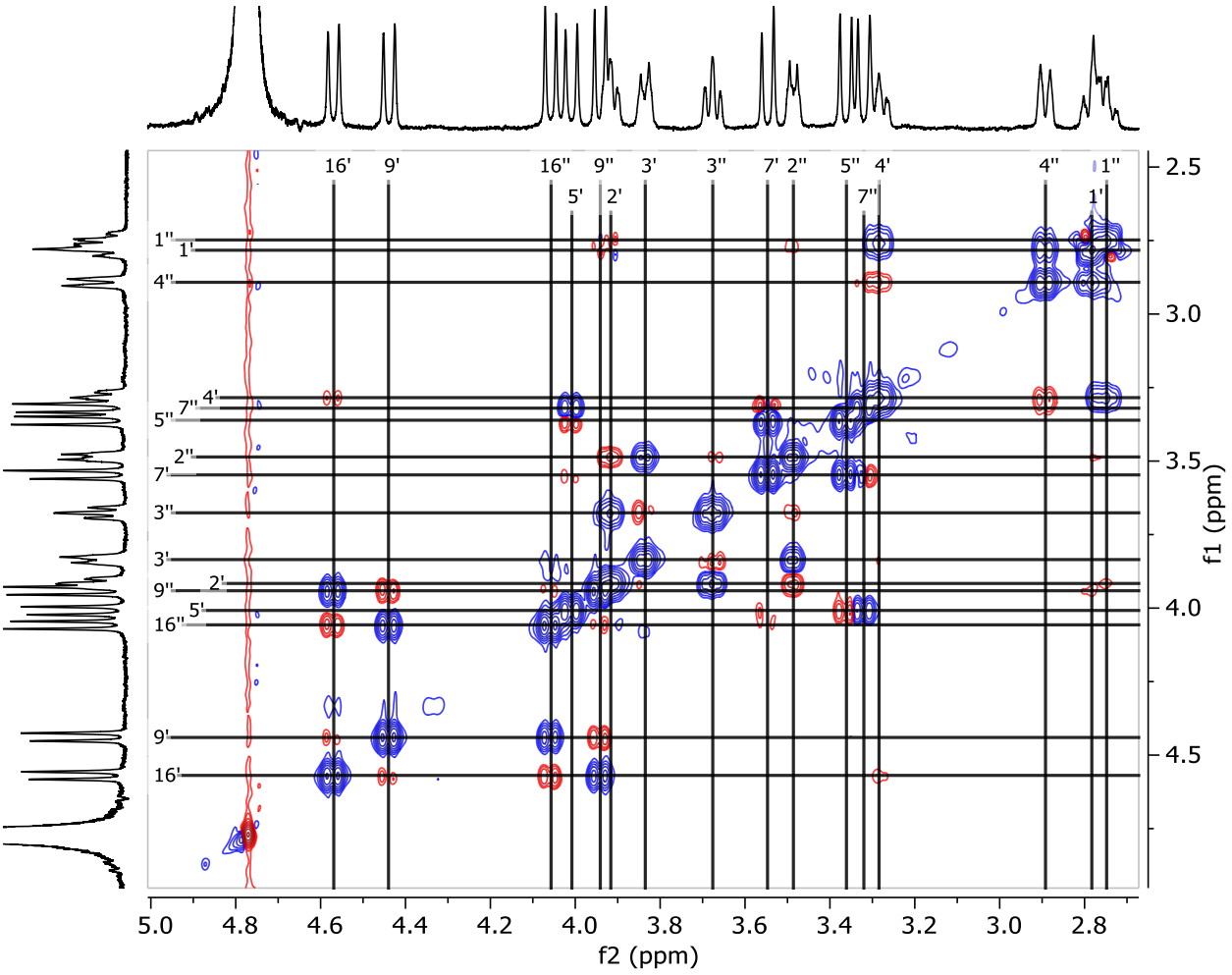

Figure S77. Expanded (aliphatic region) and labeled ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of La-Oxyaapa complex.

(4) Lu-Oxyaapa complex

Table S7. Peak assignments of NMR spectra on Lu-Oxyaapa complex. See Chart 2 for the numbering scheme.

Carbon/Hydrogen Number	Symmetric, *anti*-	
	δ_C (ppm)	δ_H (ppm)
1	57.50	3.32, 2.84
2	67.49	3.81, 3.77
3	67.49	3.81, 3.77
4	57.50	3.32, 2.84
5	62.65	3.88, 3.55
6	179.34	
7	62.65	3.88, 3.55
8	179.34	
9	63.93	4.51, 4.45
10	156.59	
11	125.26	7.71
12	141.51	8.16
13	123.92	7.99
14	150.28	
15	172.71	
16	63.93	4.51, 4.45
17	156.59	
18	125.26	7.71
19	141.51	8.16
20	123.92	7.99
21	150.28	
22	172.71	

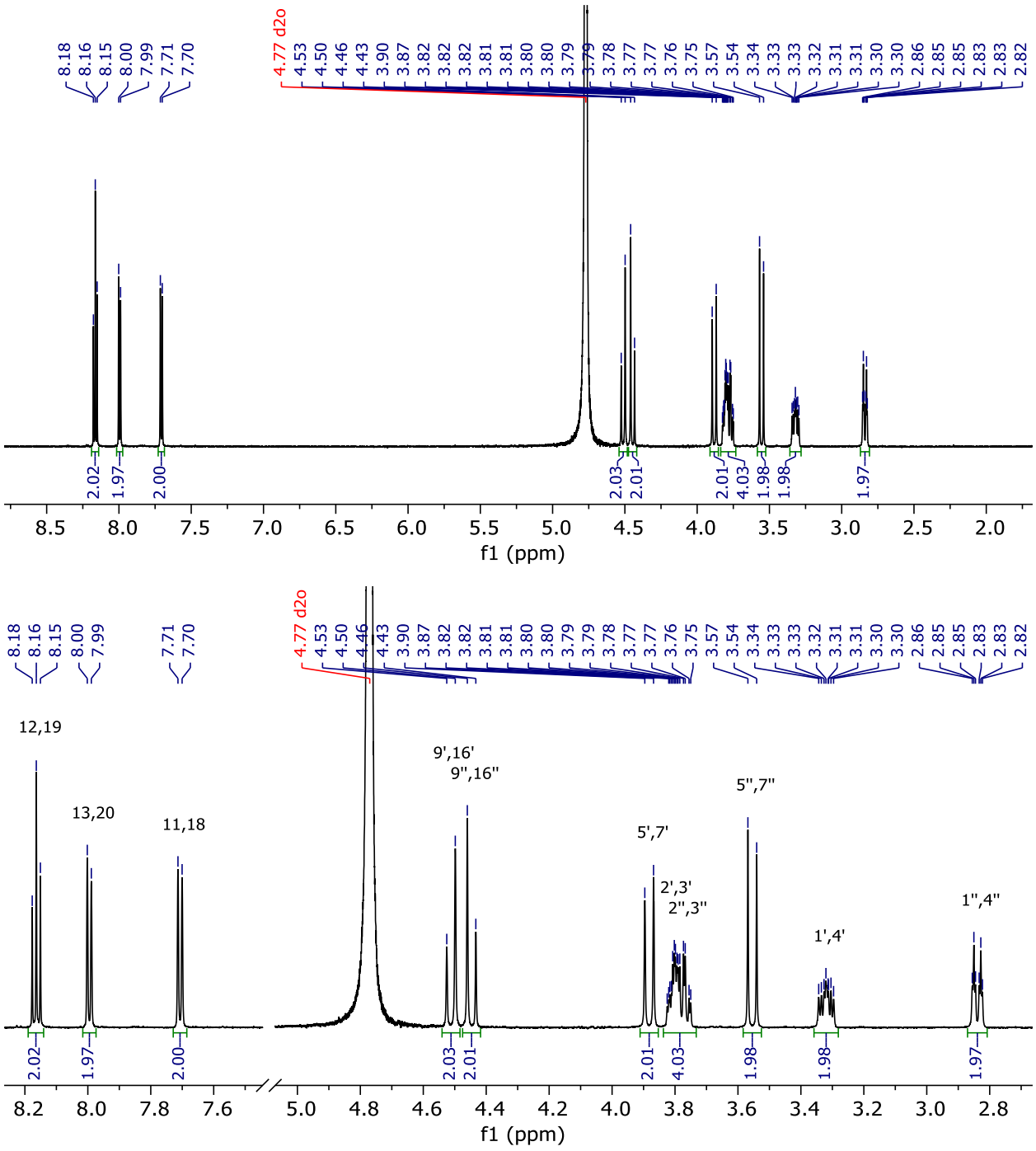

Figure S78. Full (top) as well as properly expanded and labeled (bottom) ^{1}H NMR spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

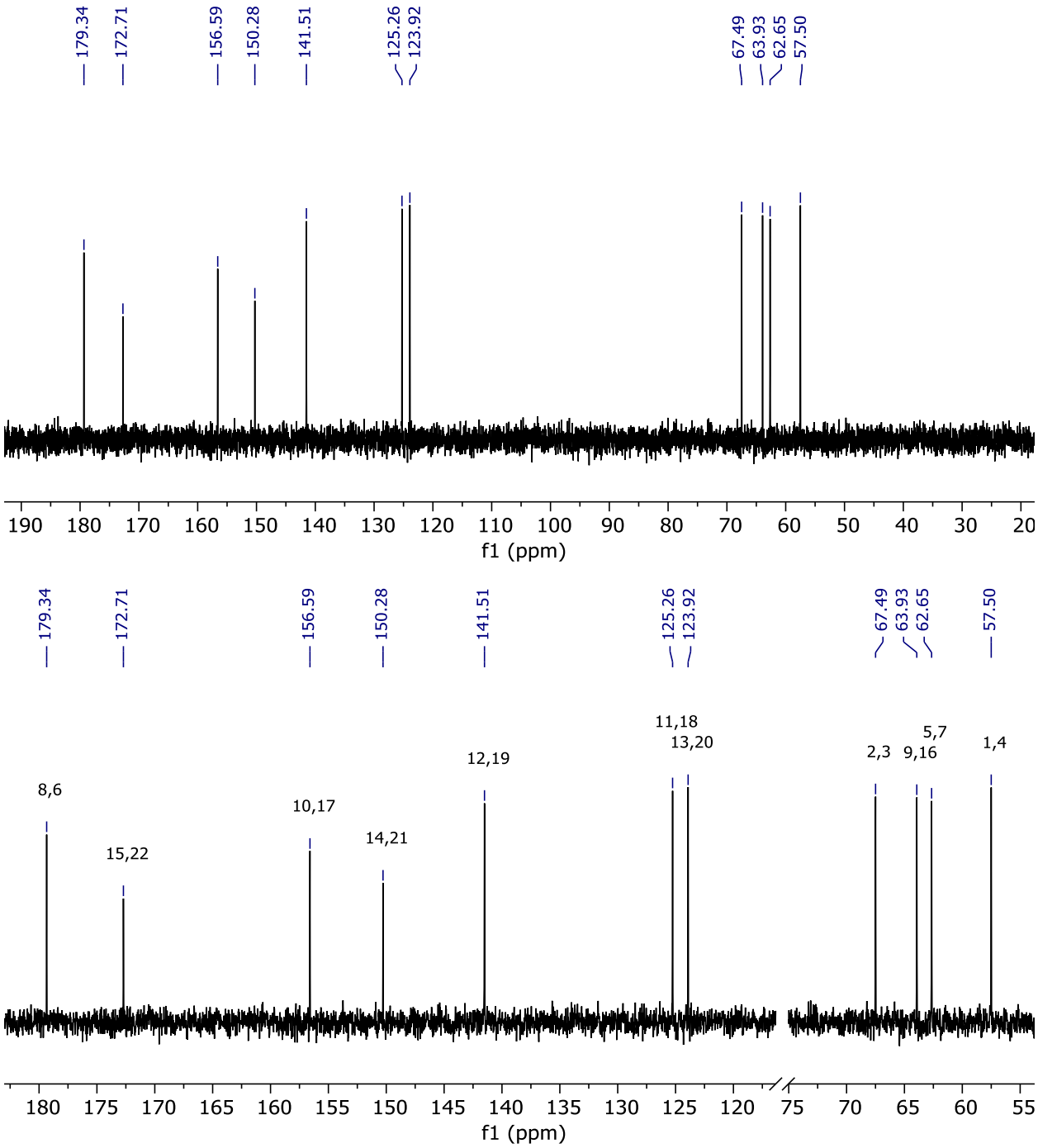

Figure S79. Full (top) as well as properly expanded and labeled (bottom) $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

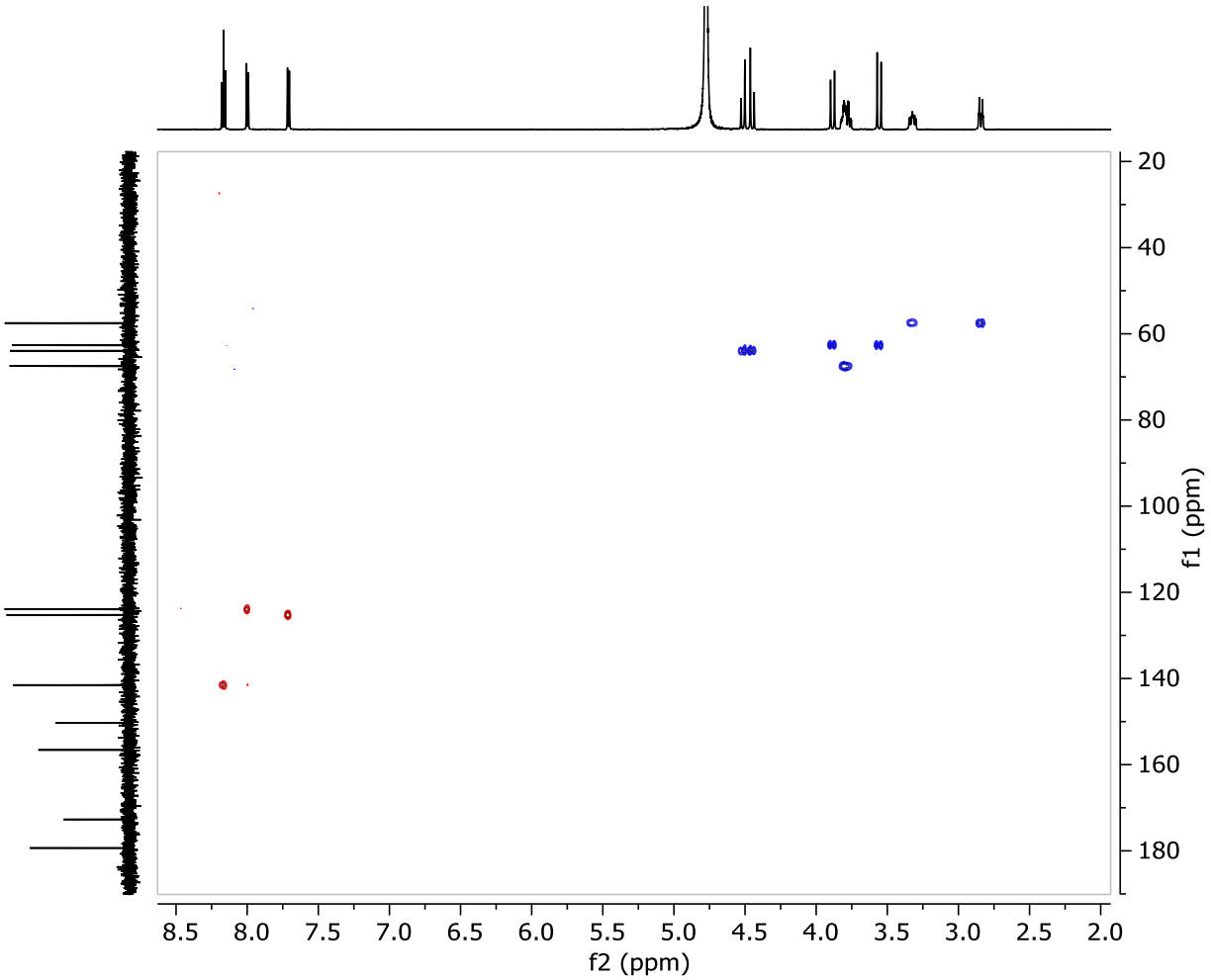

Figure S80. Full HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

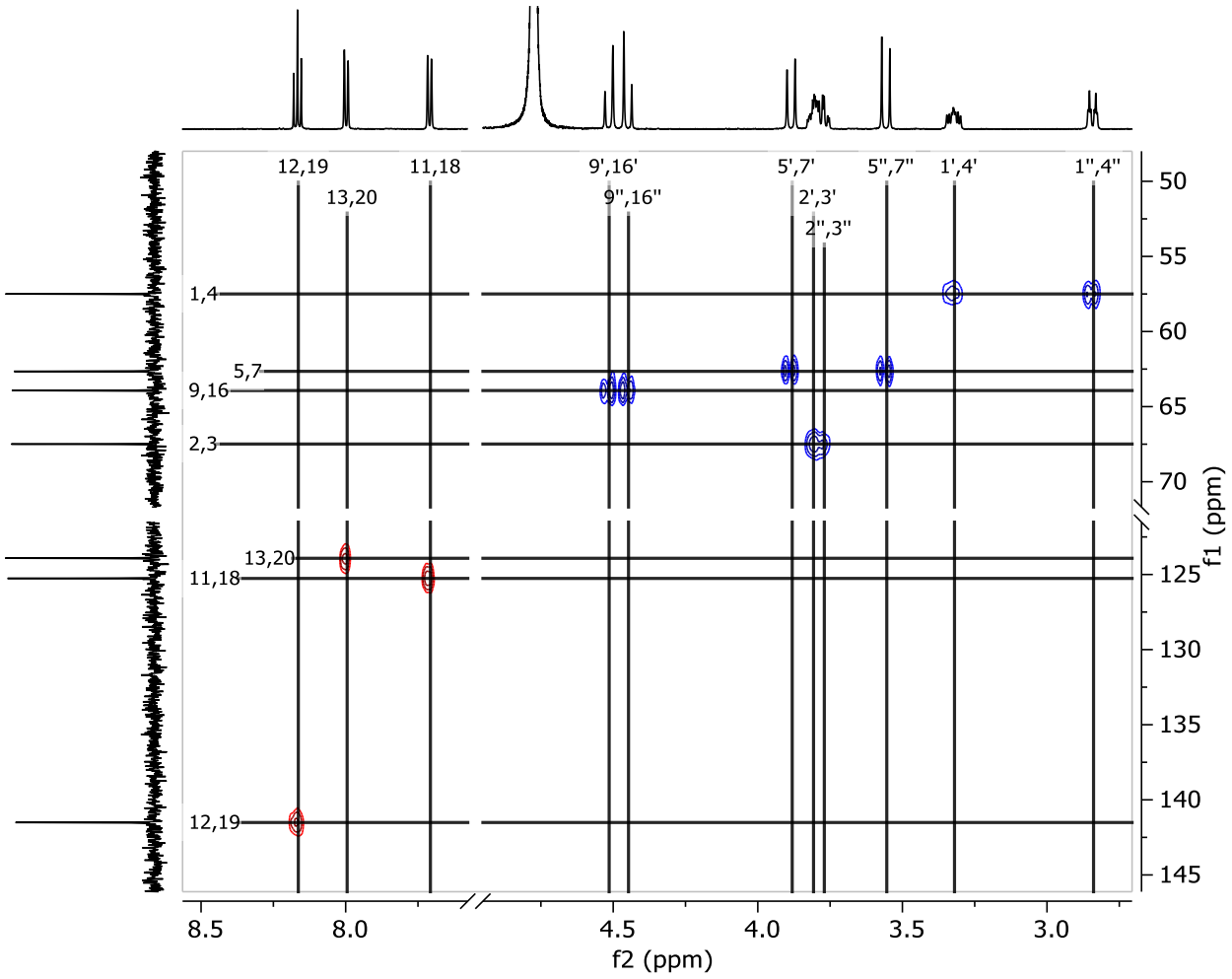

Figure S81. Properly expanded and labeled HSQC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

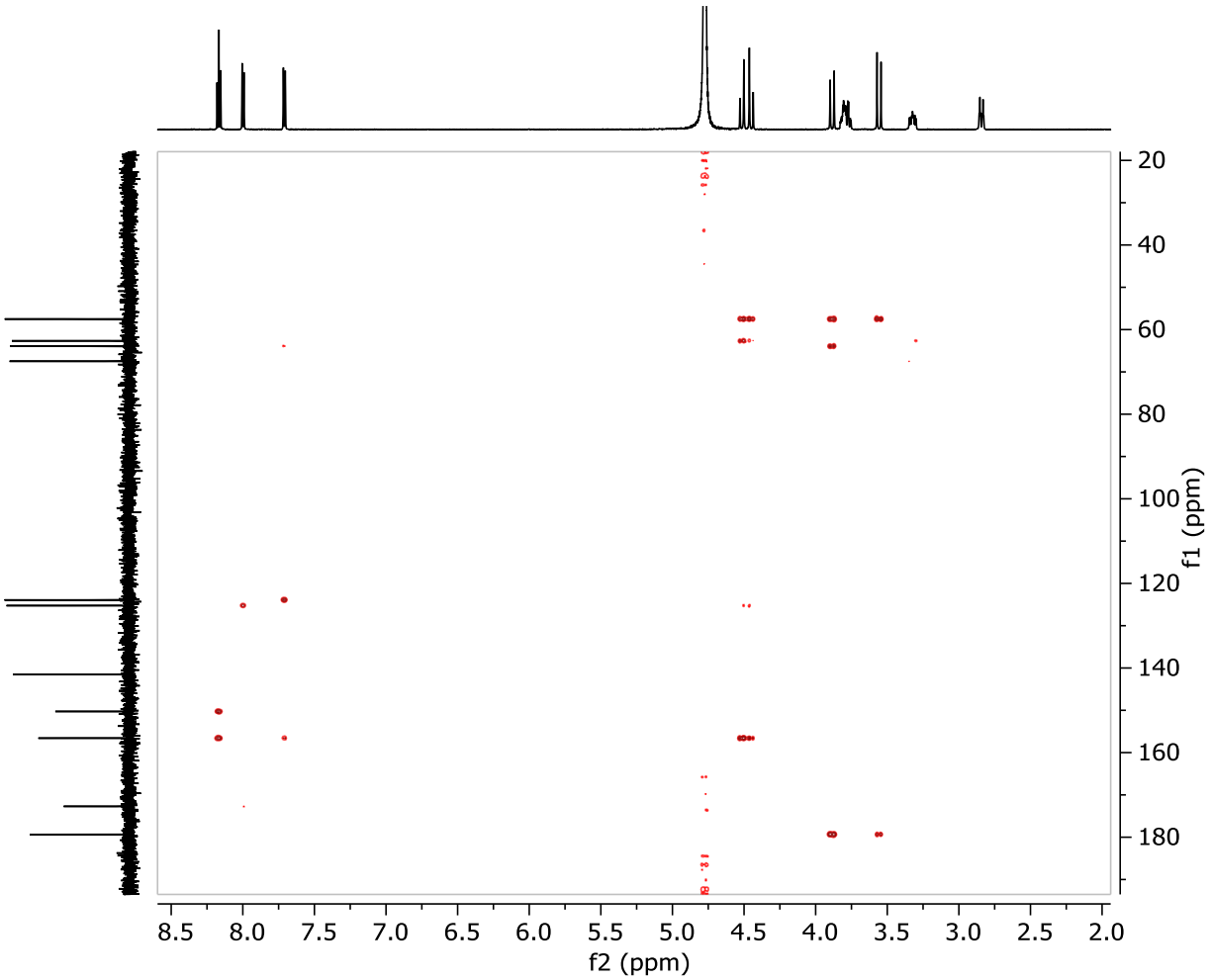

Figure S82. Full HMBC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

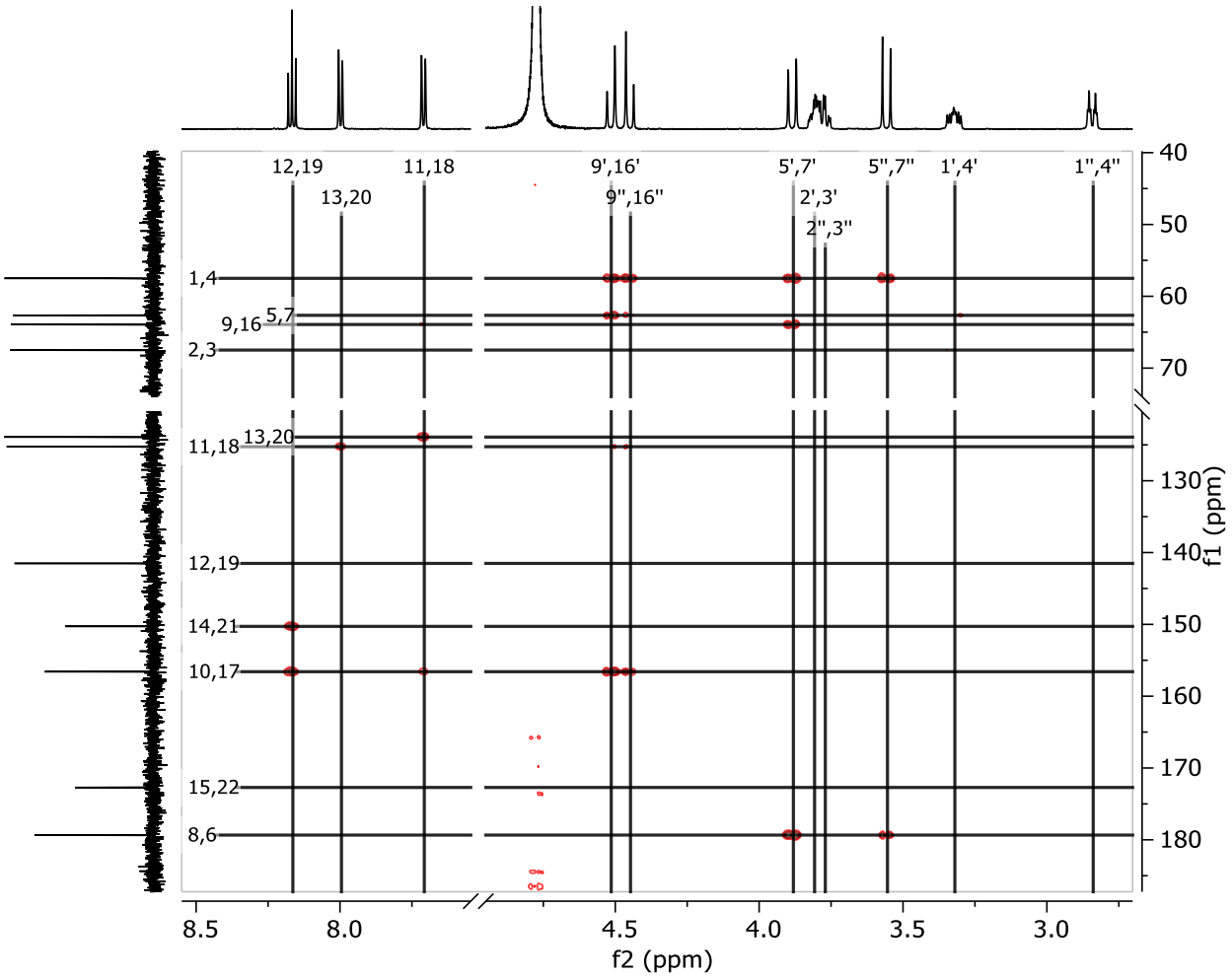

Figure S83. Properly expanded and labeled HMBC spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

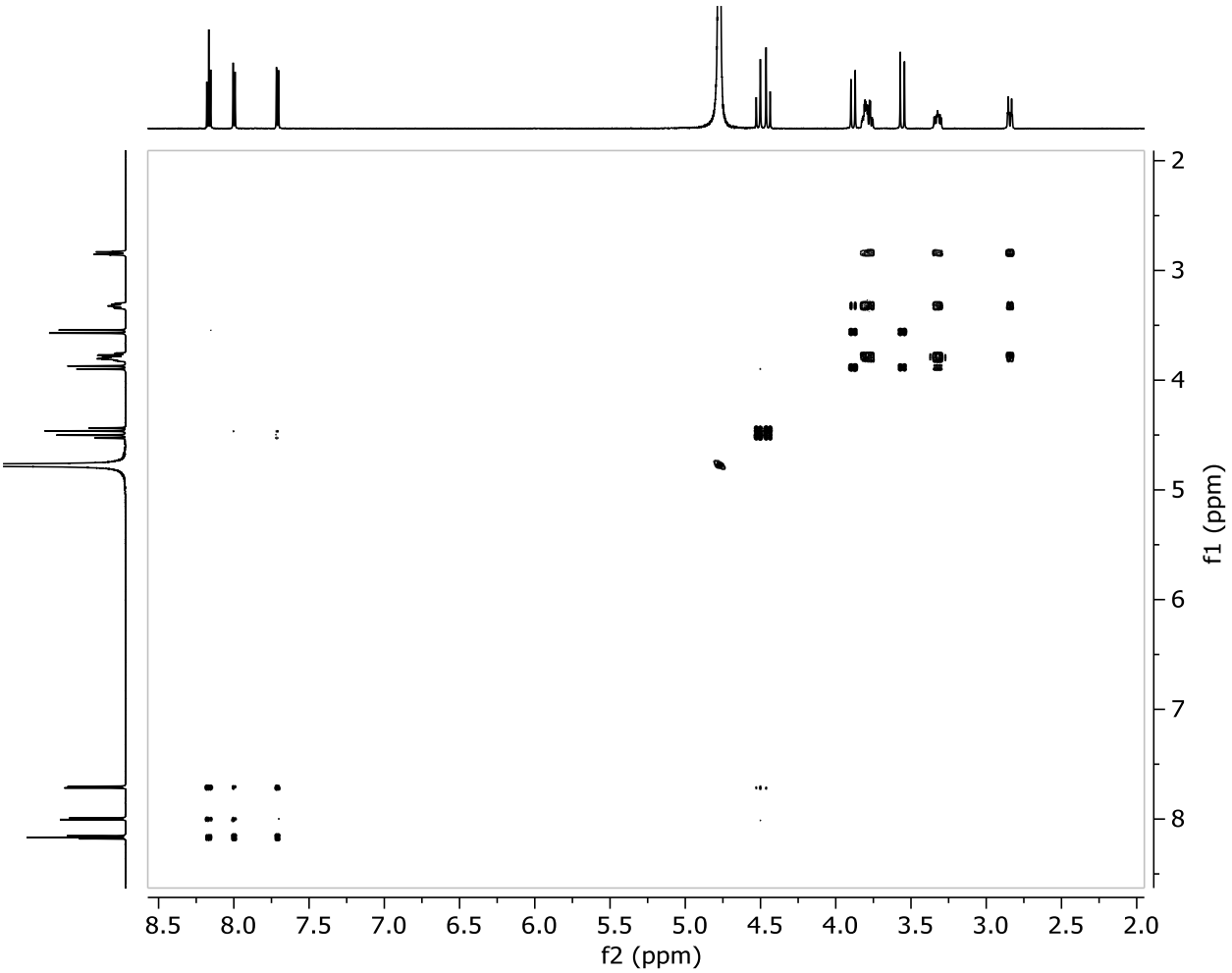

Figure S84. Full COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

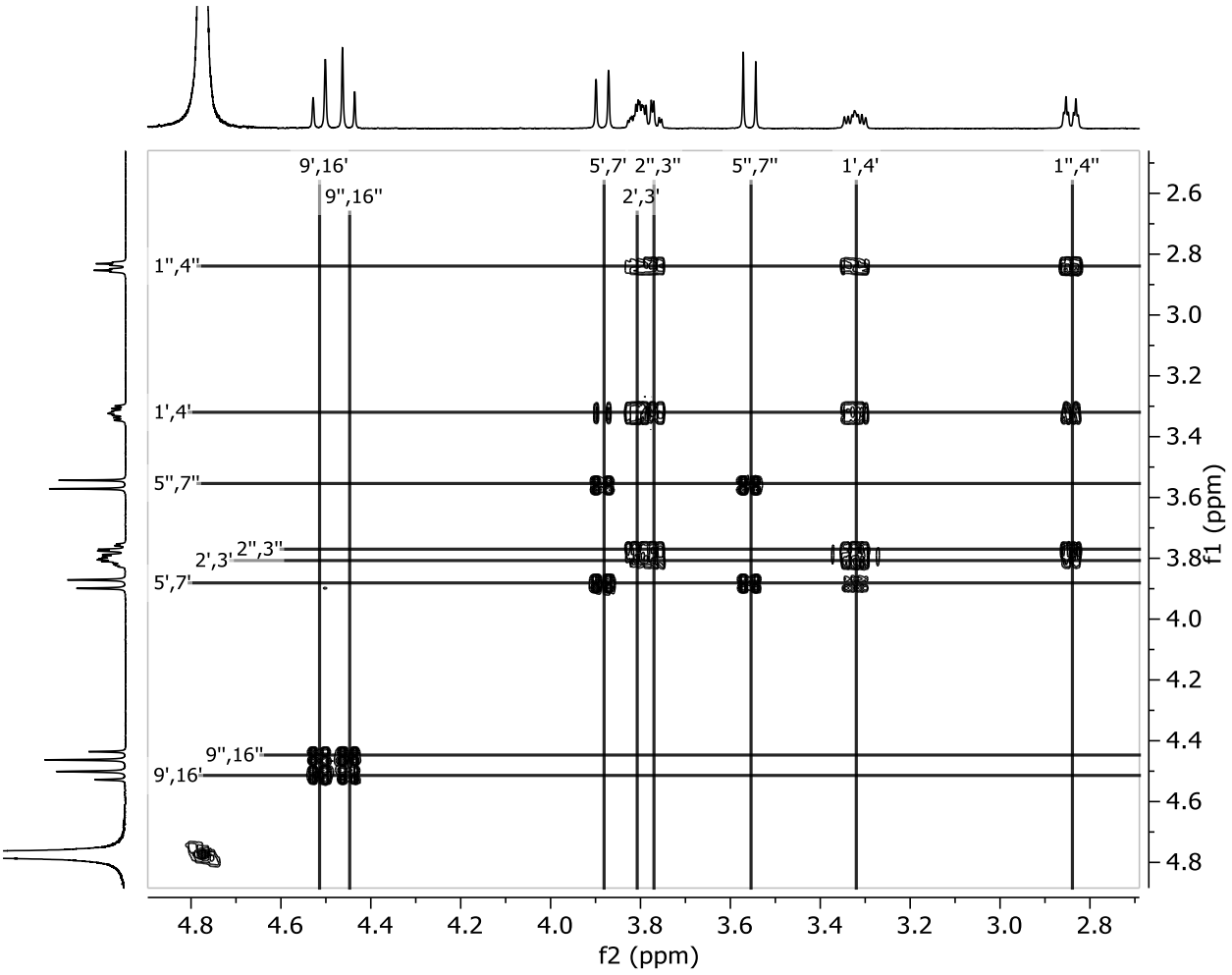

Figure S85. Expanded (aliphatic region) and labeled COSY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

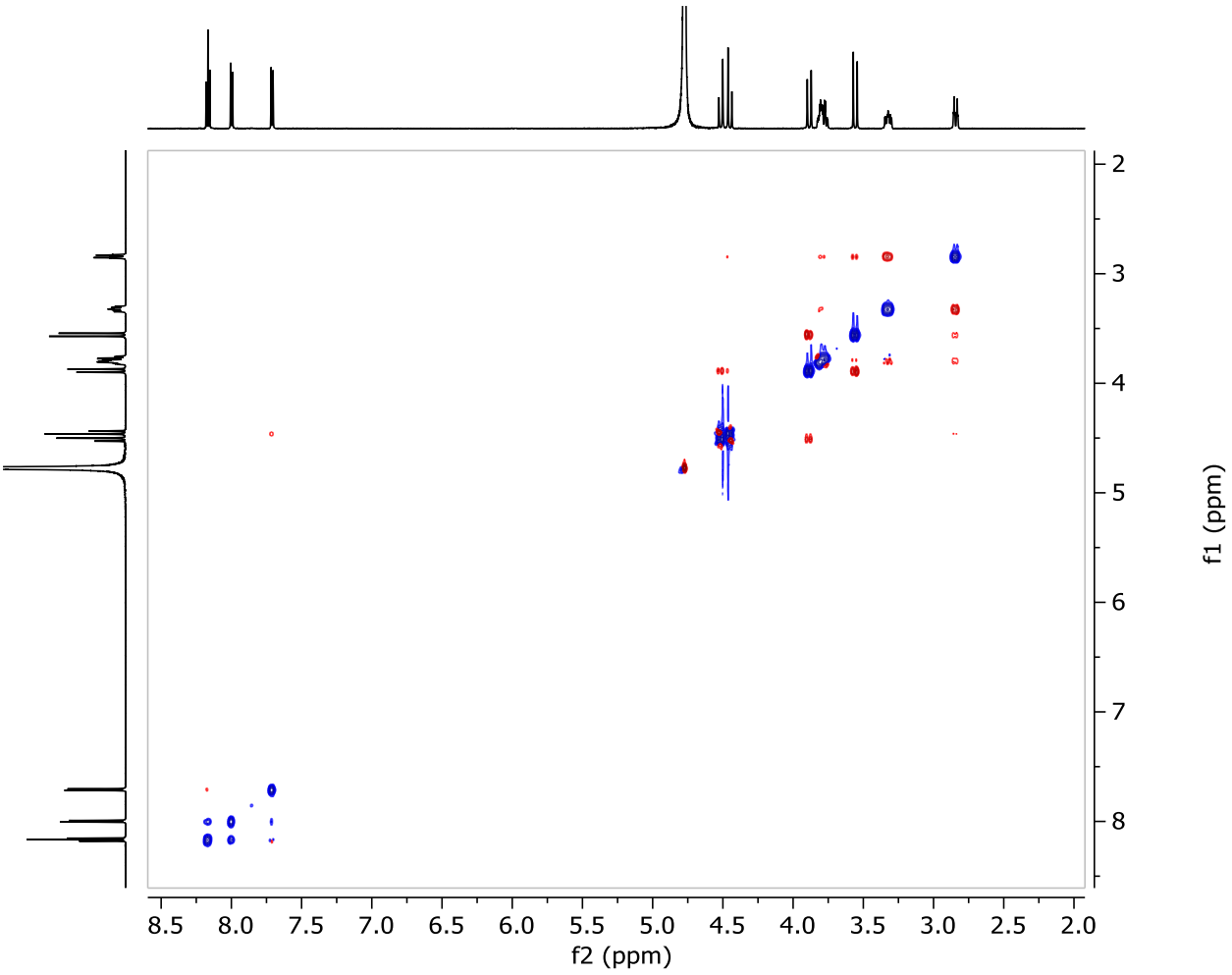

Figure S86. Expanded (aliphatic region) and labeled ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

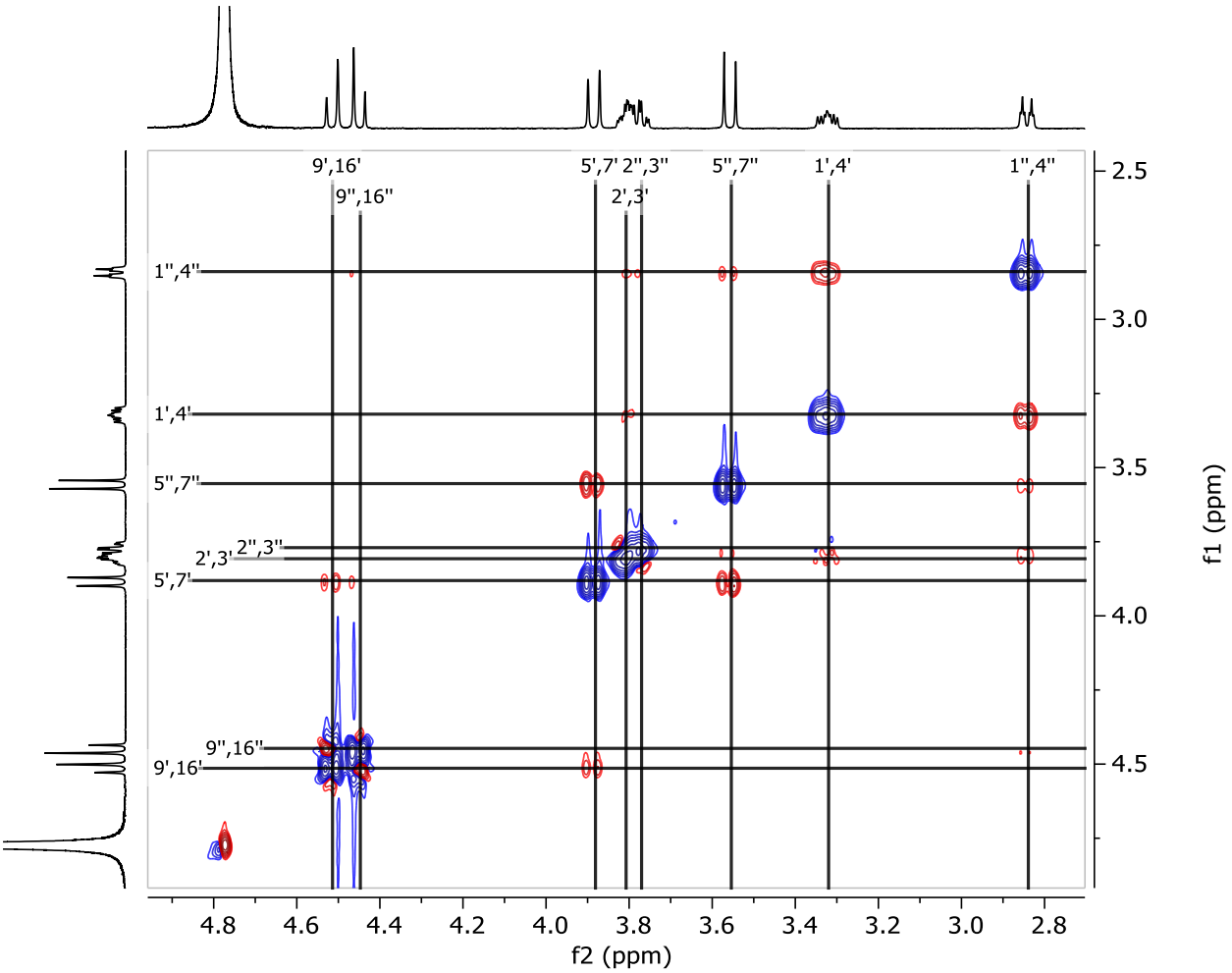

Figure S87. Expanded (aliphatic region) and labeled ROESY spectrum (600 MHz, D_2O, pD = 7, 25 °C) of Lu-Oxyaapa complex.

9. Luminescence Lifetime Measurements

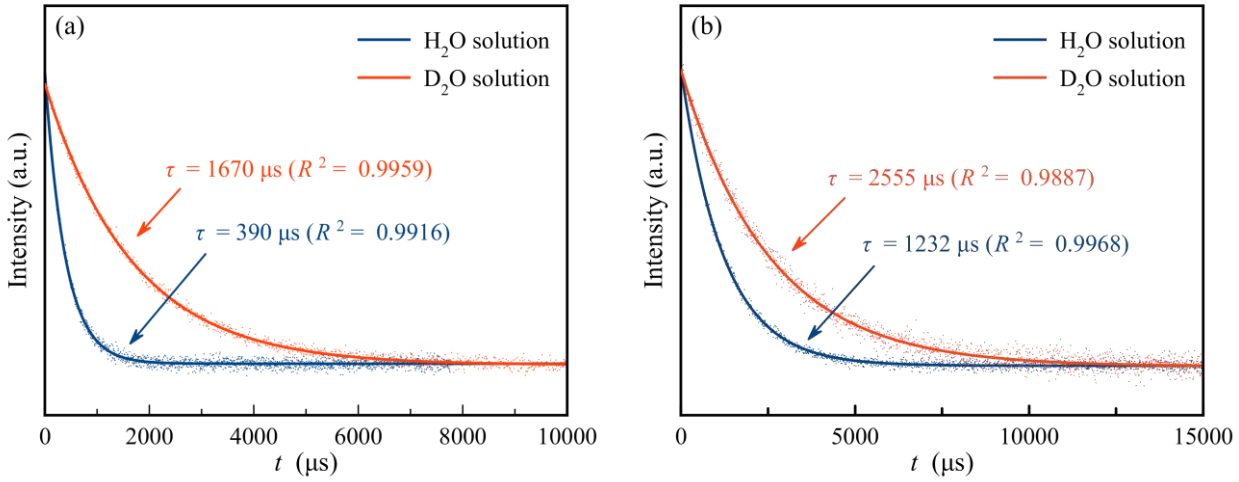

Figure S88. (a) Luminescence decay curve of Eu(III)-OxyMepa complex in H_2O and D_2O; (b) Luminescence decay curve of Tb(III)-OxyMepa complex in H_2O and D_2O.

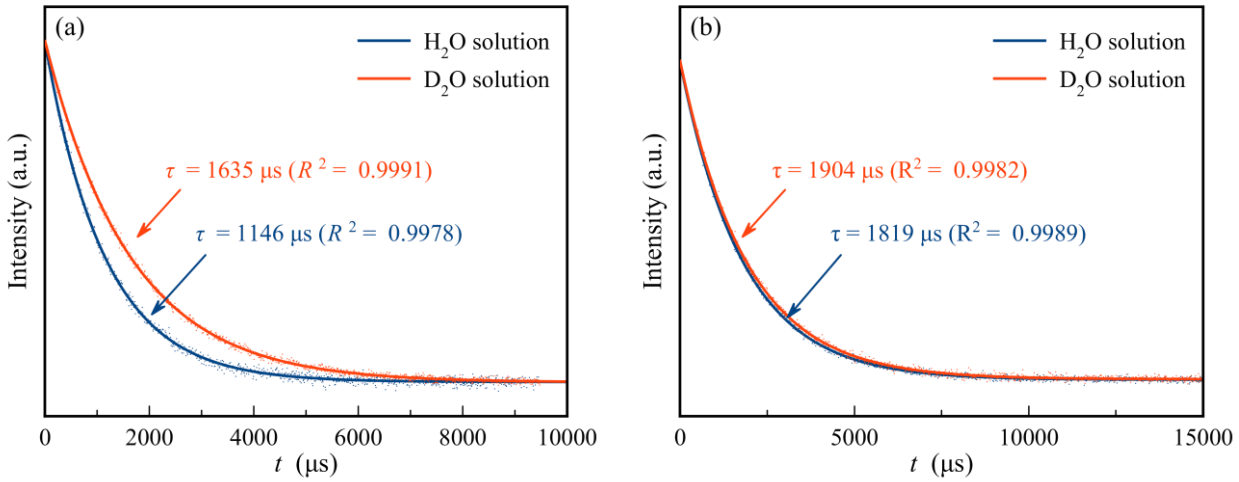

Figure S89. (a) Luminescence decay curve of Eu(III)-Oxyaapa complex in H_2O and D_2O; (b) Luminescence decay curve of Tb(III)-Oxyaapa complex in H_2O and D_2O.

10. DFT Calculations

(1) Lu-OxyMepa, N1^{S}N2^{S}($\delta\delta$), enantiomer of N1^{R}N2^{R}($\lambda\lambda$)

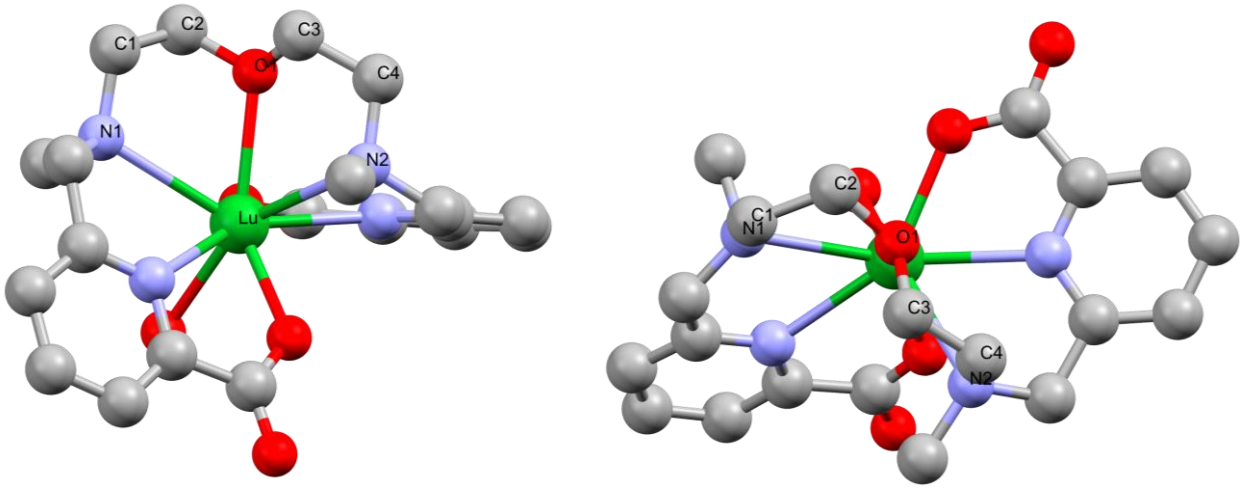

Figure S90. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in N1^{S}N2^{S}($\delta\delta$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.583201	-0.481928	2.786760
6	-2.804427	0.041115	2.064235
6	-4.017065	0.282013	2.718948
6	-5.094215	0.776044	1.986897
6	-4.950064	0.991591	0.614933
6	-3.715656	0.720907	0.032767
6	-3.467427	0.869584	-1.455200
8	-4.383462	1.276470	-2.187336
6	-1.378293	-2.590582	1.600270
8	-1.127793	-2.302166	-0.765377
6	-0.819757	-2.838108	-2.070214
6	0.674706	-2.791990	-2.340180
7	1.204348	-1.416201	-2.202307
6	2.627517	-1.433470	-1.822688
6	3.066455	-0.155695	-1.150047
6	4.381722	0.310558	-1.250877
6	4.760412	1.431690	-0.518011
6	3.819755	2.058590	0.300075
6	2.526576	1.545014	0.333230
6	1.443316	2.169115	1.189104
8	1.724027	3.137183	1.914605
6	1.037685	-0.668523	-3.467745

8	0.276694	1.623588	1.095120
7	2.159337	0.465107	-0.382166
8	-2.285374	0.531792	-1.855883
7	-2.669443	0.276424	0.751735
1	0.875368	-3.202361	-3.341006
1	1.188964	-3.435480	-1.622920
1	-1.189919	-3.866943	-2.141465
1	-1.378406	-2.220928	-2.777743
1	4.068477	2.928872	0.894914
1	5.775067	1.811841	-0.582526
1	5.087839	-0.205119	-1.893045
1	-5.768653	1.350182	0.002818
1	-6.042642	0.973918	2.476389
1	-4.107421	0.077729	3.780560
71	-0.434856	0.132800	-0.509608
7	-0.727488	-1.295356	1.900250
1	-0.989679	0.368965	3.137837
1	-1.894721	-1.045768	3.678437
6	0.589942	-1.495438	2.528522
1	1.223757	-2.111164	1.886559
1	1.077874	-0.528477	2.669568
1	0.504036	-1.993562	3.506490
6	-0.860300	-3.212766	0.320928
1	0.212503	-3.425220	0.380887
1	-1.386377	-4.155764	0.132108
1	-1.235818	-3.303214	2.426758
1	-2.453634	-2.426806	1.496249
8	-0.079692	2.200010	-1.780568
1	-0.060064	2.957118	-1.175472
1	-0.938944	2.252950	-2.231754
1	1.573625	-1.158755	-4.294417
1	1.427444	0.345622	-3.357774
1	-0.020548	-0.600995	-3.731155
1	2.781623	-2.244232	-1.101523
1	3.276044	-1.647587	-2.684053

Output energies:

Zero-point correction= 0.458399 (Hartree/Particle)
Thermal correction to Energy= 0.488502
Thermal correction to Enthalpy= 0.489446
Thermal correction to Gibbs Free Energy= 0.397998
Sum of electronic and zero-point Energies= -1487.882825
Sum of electronic and thermal Energies= -1487.852722
Sum of electronic and thermal Enthalpies= -1487.851778
Sum of electronic and thermal Free Energies= -1487.943226

(2) Lu-OxyMepa, $N1^{S}N2^{S}(\delta\lambda)$, enantiomer of $N1^{R}N2^{R}(\lambda\delta)$

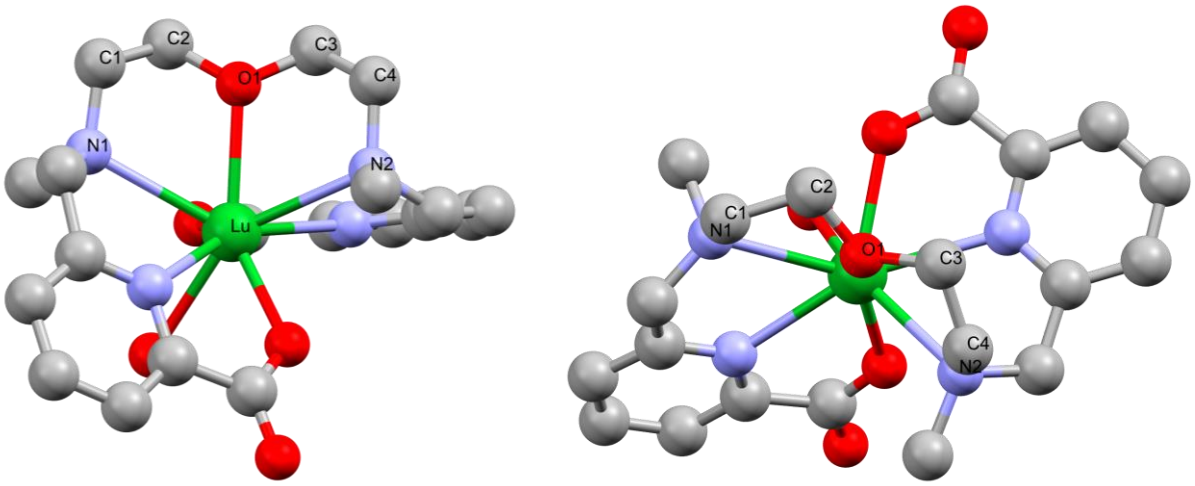

Figure S91. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in $N1^{S}N2^{S}(\delta\lambda)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.673938	-0.596452	2.830880
6	-2.847348	-0.137754	2.002114
6	-4.145934	-0.037560	2.510474
6	-5.165367	0.406434	1.670803
6	-4.872628	0.709878	0.340300
6	-3.556908	0.574483	-0.092664
6	-3.150801	0.802798	-1.532622
8	-3.990268	1.231077	-2.341713
6	-1.203228	-2.752183	1.724710
8	-0.729161	-2.385742	-0.571225
6	-0.748932	-2.821160	-1.946761
6	0.674816	-2.692393	-2.460931
7	1.211485	-1.315899	-2.302458
6	2.661758	-1.338394	-2.033451
6	3.151219	-0.094343	-1.330500
6	4.432601	0.419907	-1.554625
6	4.867229	1.507970	-0.802437
6	4.013982	2.059659	0.153747
6	2.748336	1.502896	0.310277
6	1.755055	2.056563	1.314032
8	2.099563	2.994010	2.051915
6	0.927260	-0.499494	-3.498907
8	0.593476	1.492309	1.322917
7	2.331721	0.448518	-0.417074

8	-1.925796	0.505092	-1.812450
7	-2.569087	0.188016	0.732766
1	0.716555	-3.019071	-3.509331
1	1.298989	-3.375424	-1.879605
1	-1.062013	-3.869150	-1.993929
1	-1.462143	-2.213613	-2.514743
1	4.307166	2.906538	0.761888
1	5.857512	1.923169	-0.961126
1	5.069500	-0.032762	-2.307020
1	-5.638491	1.029475	-0.355964
1	-6.181318	0.494393	2.042657
1	-4.346477	-0.312622	3.540288
71	-0.177690	-0.006373	-0.240169
7	-0.699679	-1.377160	2.032970
1	-1.155600	0.289512	3.213535
1	-2.026243	-1.168134	3.700179
6	0.571642	-1.472385	2.786618
1	1.313417	-2.001834	2.183919
1	0.945522	-0.469067	2.997876
1	0.445183	-2.010592	3.737005
6	-1.740594	-2.915134	0.308062
1	-0.365890	-3.444403	1.839356
1	-1.975438	-3.054192	2.442906
8	0.049080	2.300231	-1.484391
1	-0.162723	2.922997	-0.773202
1	-0.802096	2.109394	-1.919171
1	1.442839	-0.898982	-4.385189
1	1.259158	0.528865	-3.337497
1	-0.146105	-0.487719	-3.696896
1	2.874800	-2.183435	-1.369497
1	3.242249	-1.500561	-2.952525
1	-1.884817	-3.980584	0.099394
1	-2.688389	-2.394707	0.139839

Output energies:

Zero-point correction= 0.458510 (Hartree/Particle)
Thermal correction to Energy= 0.489367
Thermal correction to Enthalpy= 0.490311
Thermal correction to Gibbs Free Energy= 0.397110
Sum of electronic and zero-point Energies= -1487.876643
Sum of electronic and thermal Energies= -1487.845787
Sum of electronic and thermal Enthalpies= -1487.844843
Sum of electronic and thermal Free Energies= -1487.938043

(3) Lu-OxyMepa, $N1^{S}N2^{S}(\lambda\delta)$, enantiomer of $N1^{R}N2^{R}(\delta\lambda)$

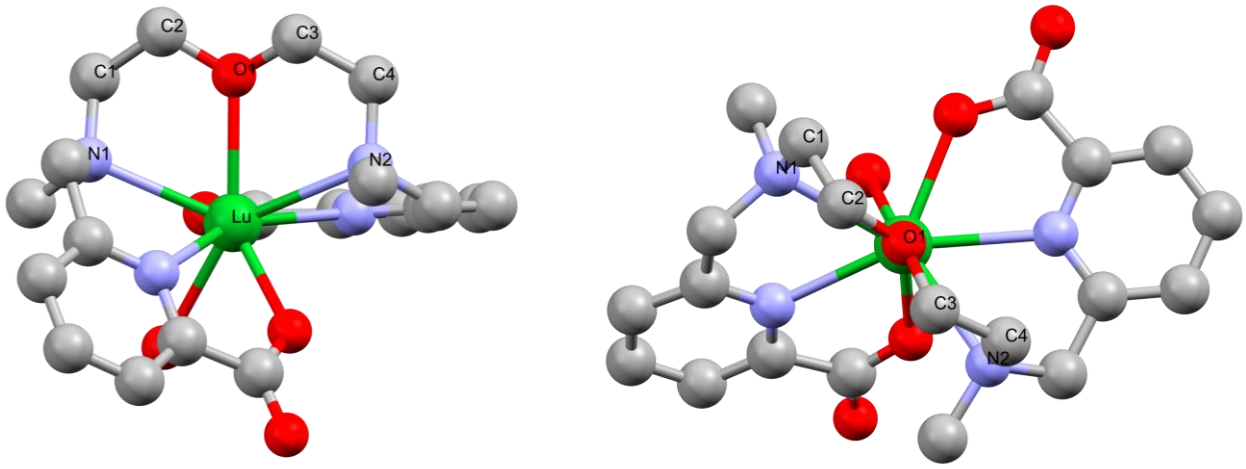

Figure S92. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in $N1^{S}N2^{S}(\lambda\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.735560	-0.348118	2.838917
6	-2.919764	0.074731	2.001003
6	-4.194578	0.261534	2.545349
6	-5.234719	0.657860	1.707638
6	-4.985729	0.839277	0.346301
6	-3.691378	0.630735	-0.119993
6	-3.325004	0.762259	-1.582155
8	-4.193281	1.111282	-2.398805
6	-1.373126	-2.507546	1.802037
8	-0.609217	-2.476000	-0.481151
6	-0.065293	-3.224027	-1.585127
6	0.124310	-2.307408	-2.776754
7	0.904973	-1.091381	-2.455740
6	2.312141	-1.402697	-2.120095
6	2.956287	-0.285104	-1.334505
6	4.301674	0.063779	-1.482416
6	4.829455	1.072163	-0.678700
6	4.004305	1.715545	0.244927
6	2.672865	1.320095	0.327441
6	1.687054	1.982812	1.270234
8	2.084098	2.881886	2.029225
6	0.863909	-0.166398	-3.608140
8	0.474243	1.546840	1.199356
7	2.171204	0.335640	-0.440399

8	-2.097611	0.483270	-1.868970
7	-2.685093	0.272260	0.695975
1	-0.852744	-1.976367	-3.140313
1	0.597844	-2.886581	-3.584258
1	0.874933	-3.689424	-1.267987
1	-0.760132	-4.028596	-1.853626
1	4.369327	2.513219	0.880334
1	5.870837	1.361439	-0.778609
1	4.914041	-0.445578	-2.218649
1	-5.768448	1.124498	-0.346070
1	-6.232775	0.806876	2.107538
1	-4.361513	0.087606	3.602956
71	-0.323503	0.027298	-0.344420
7	-0.782263	-1.177582	2.070140
1	-1.203883	0.548077	3.176012
1	-2.086360	-0.873238	3.739024
6	0.481272	-1.299926	2.822949
1	1.205164	-1.887115	2.254126
1	0.901287	-0.306645	2.988687
1	0.327287	-1.788237	3.796733
6	-0.635366	-3.268436	0.723133
1	0.394229	-3.511034	1.010828
1	-1.163474	-4.208245	0.524071
1	-1.389742	-3.121023	2.715953
1	-2.409471	-2.369554	1.484991
8	-0.100514	2.327470	-1.562966
1	-0.275019	2.933335	-0.827322
1	-0.966662	2.174208	-1.980591
1	1.278353	-0.640391	-4.510038
1	1.448882	0.728822	-3.389432
1	-0.167784	0.126739	-3.809897
1	2.342625	-2.301660	-1.497089
1	2.897228	-1.621574	-3.023498

Output energies:

Zero-point correction= 0.457373 (Hartree/Particle)
Thermal correction to Energy= 0.488143
Thermal correction to Enthalpy= 0.489087
Thermal correction to Gibbs Free Energy= 0.394741
Sum of electronic and zero-point Energies= -1487.888635
Sum of electronic and thermal Energies= -1487.857865
Sum of electronic and thermal Enthalpies= -1487.856920
Sum of electronic and thermal Free Energies= -1487.951267

(4) Lu-OxyMepa, $N1^{S}N2^{S}(\lambda\lambda)$, enantiomer of $N1^{R}N2^{R}(\delta\delta)$

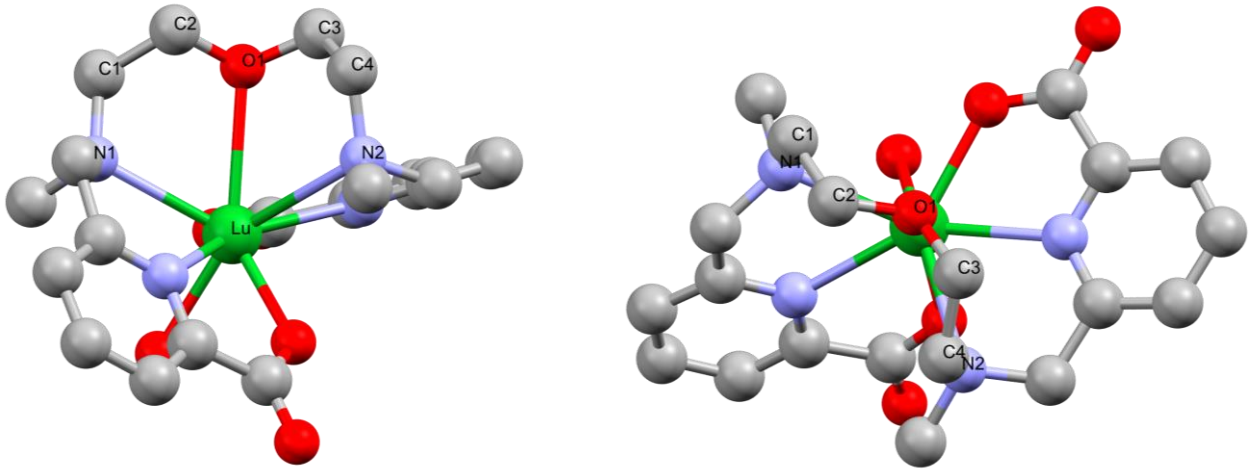

Figure S93. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in $N1^{S}N2^{S}(\lambda\lambda)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.635049	-0.502474	2.775730
6	-2.858647	-0.188641	1.945588
6	-4.142779	-0.267525	2.497375
6	-5.242823	0.066066	1.713133
6	-5.040614	0.449953	0.387581
6	-3.736788	0.497306	-0.094892
6	-3.443306	0.840277	-1.540480
8	-4.374542	1.185187	-2.284730
6	-0.752806	-2.593260	1.804805
8	-1.261469	-2.389117	-0.603383
6	-0.310009	-3.199633	-1.306779
6	0.138149	-2.457434	-2.554059
7	0.906894	-1.212317	-2.287492
6	2.277858	-1.528846	-1.824737
6	2.922646	-0.370402	-1.100605
6	4.301150	-0.135605	-1.131609
6	4.823955	0.909517	-0.372972
6	3.965459	1.697173	0.396405
6	2.604888	1.408250	0.368016
6	1.586444	2.208203	1.157289
8	1.975668	3.128640	1.893822
6	0.982331	-0.413246	-3.530087
8	0.354295	1.854609	0.992342
7	2.106168	0.397126	-0.365374

8	-2.206667	0.727331	-1.897151
7	-2.669679	0.207690	0.676285
1	-0.019415	-0.095176	-3.827848
1	1.425689	-0.996960	-4.349849
1	1.598507	0.472246	-3.363571
1	2.909365	-1.851510	-2.663836
1	2.229800	-2.367887	-1.123150
1	-0.749942	-2.175762	-3.127497
1	0.726577	-3.145140	-3.179633
1	-0.788488	-4.139462	-1.611957
1	0.533672	-3.453672	-0.654613
1	4.329984	2.520012	0.999249
1	5.890337	1.111708	-0.383823
1	4.943603	-0.761538	-1.741529
1	-5.864526	0.695292	-0.271162
1	-6.246319	0.010038	2.122999
1	-4.266769	-0.596327	3.523512
71	-0.413184	0.277076	-0.510922
7	-0.529209	-1.146609	2.037807
1	-1.255825	0.449395	3.165310
1	-1.933296	-1.103284	3.647900
6	0.711630	-0.978782	2.820303
1	1.549820	-1.428184	2.283937
1	0.918549	0.082341	2.969908
1	0.640322	-1.459471	3.808736
6	-1.696404	-2.929182	0.655283
1	-1.780381	-4.020115	0.578172
1	-2.700076	-2.535368	0.823221
1	0.223486	-3.038630	1.593936
1	-1.134931	-3.080871	2.716747
8	0.048650	2.295714	-1.826225
1	0.043323	3.029688	-1.192232
1	-0.797827	2.358484	-2.300088

Output energies:

Zero-point correction= 0.458884 (Hartree/Particle)
Thermal correction to Energy= 0.488684
Thermal correction to Enthalpy= 0.489628
Thermal correction to Gibbs Free Energy= 0.399653
Sum of electronic and zero-point Energies= -1487.881164
Sum of electronic and thermal Energies= -1487.851364
Sum of electronic and thermal Enthalpies= -1487.850420
Sum of electronic and thermal Free Energies= -1487.940394

(5) Lu-OxyMepa, N1^{S}N2^{R}($\delta\delta$), enantiomer of N1^{R}N2^{S}($\lambda\lambda$)

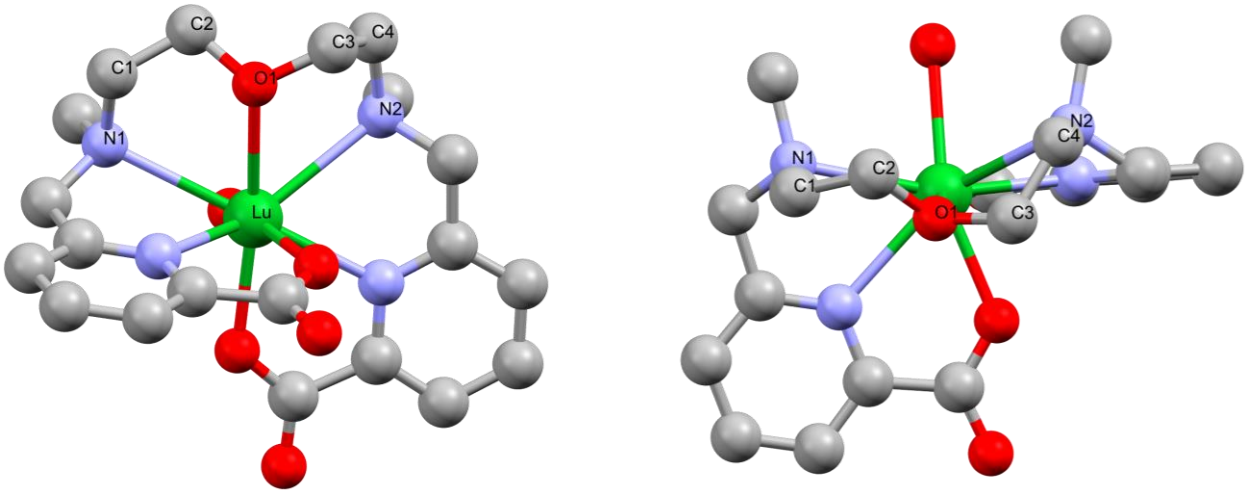

Figure S94. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in N1^{S}N2^{R}($\delta\delta$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.065152	1.757074	-0.451147
6	3.495793	0.365611	-0.046385
6	4.837810	-0.025569	-0.016526
6	5.157436	-1.313949	0.406956
6	4.133773	-2.182904	0.786078
6	2.821445	-1.721493	0.729229
6	1.643793	-2.584649	1.137488
8	1.844267	-3.760027	1.483599
6	1.247688	3.097854	-1.373124
8	-0.631541	2.616528	0.118902
6	-1.806557	2.800752	-0.697698
6	-2.911880	1.936474	-0.124287
7	-2.597509	0.484561	-0.179186
6	-3.374634	-0.244851	0.846530
6	-2.881213	0.064338	2.239698
6	-3.725260	0.100910	3.353987
6	-3.179095	0.383664	4.604385
6	-1.811949	0.644149	4.712752
6	-1.040083	0.598223	3.555994
6	0.441140	0.912647	3.550151
8	1.017838	1.156973	4.621965
6	-2.925321	-0.058547	-1.511723
8	0.999787	0.913074	2.385057
7	-1.567886	0.300177	2.356458

8	0.489449	-2.005561	1.091483
7	2.518742	-0.477488	0.319725
1	-2.368605	0.476495	-2.283431
1	-2.653206	-1.114699	-1.555845
1	-3.999560	0.037608	-1.730963
1	-4.449341	-0.025094	0.771574
1	-3.253150	-1.318121	0.658573
1	-3.064218	2.225341	0.918400
1	-3.847651	2.149585	-0.661947
1	-2.108436	3.853535	-0.655996
1	-1.586087	2.545326	-1.740155
1	-1.348716	0.888298	5.661054
1	-3.814864	0.417284	5.483524
1	-4.787809	-0.081351	3.233967
1	4.334176	-3.194069	1.118681
1	6.192469	-1.639451	0.434948
1	5.609711	0.670830	-0.325810
71	0.085730	0.182419	0.392819
7	1.806722	1.732439	-1.227889
1	3.871057	2.245884	-1.017648
1	2.906270	2.347411	0.457601
6	2.082983	1.184359	-2.572315
1	1.150194	1.064615	-3.128009
1	2.575615	0.212702	-2.491357
1	2.746977	1.847764	-3.146615
6	0.447164	3.532202	-0.157581
1	0.041652	4.537964	-0.313487
1	1.058068	3.546156	0.748367
1	0.593919	3.095081	-2.249340
1	2.040594	3.835682	-1.568840
8	0.083465	-1.240303	-1.740306
1	0.101299	-2.107365	-1.304761
1	0.917750	-1.197496	-2.229789

Output energies:

Zero-point correction= 0.457243 (Hartree/Particle)
Thermal correction to Energy= 0.486403
Thermal correction to Enthalpy= 0.487348
Thermal correction to Gibbs Free Energy= 0.396726
Sum of electronic and zero-point Energies= -1487.884527
Sum of electronic and thermal Energies= -1487.855366
Sum of electronic and thermal Enthalpies= -1487.854422
Sum of electronic and thermal Free Energies= -1487.945043

(6) Lu-OxyMepa, N1^{S}N2^{R}($\delta\lambda$), enantiomer of N1^{R}N2^{S}($\lambda\delta$)

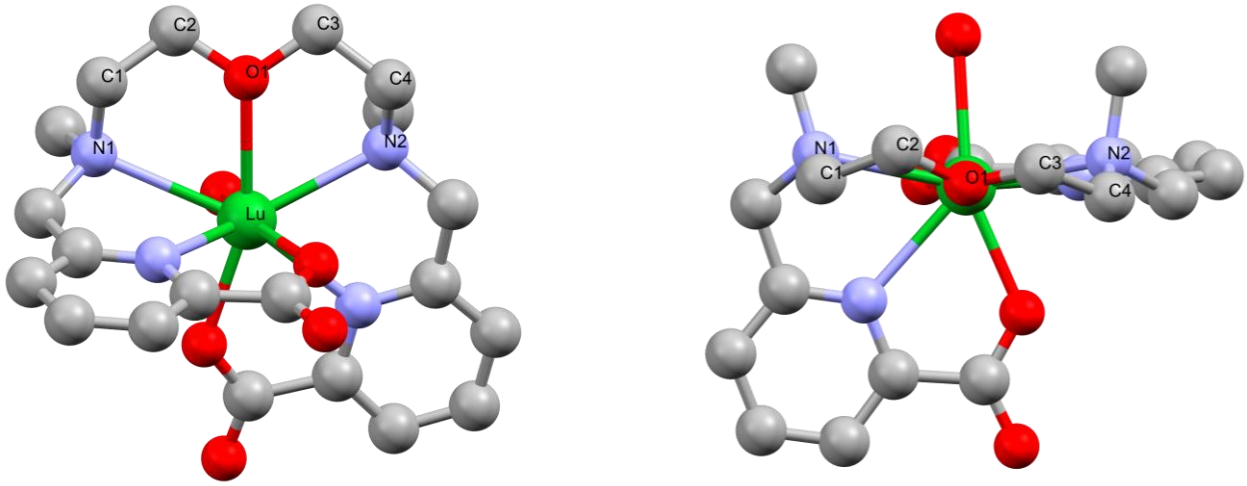

Figure S95. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in N1^{S}N2^{R}($\delta\lambda$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.303512	1.661250	-0.200285
6	3.561649	0.198536	0.074006
6	4.847196	-0.349566	0.117076
6	4.994593	-1.695843	0.443410
6	3.862211	-2.464653	0.718902
6	2.616362	-1.847890	0.655810
6	1.325632	-2.581050	0.968610
8	1.361493	-3.799179	1.204417
6	1.549343	3.270702	-0.673540
8	-0.736773	2.548496	-0.556865
6	-2.069063	2.597003	-1.106935
6	-2.993665	1.749744	-0.256523
7	-2.592543	0.322691	-0.195574
6	-3.244254	-0.337010	0.954170
6	-2.675740	0.118562	2.277010
6	-3.435110	0.115978	3.452018
6	-2.836531	0.515764	4.643975
6	-1.502410	0.926562	4.635034
6	-0.816250	0.909777	3.425014
6	0.623350	1.360610	3.300568
8	1.232195	1.744374	4.312874
6	-2.988859	-0.375713	-1.433709
8	1.115909	1.311461	2.108300
7	-1.392904	0.505421	2.279339

8	0.259832	-1.847987	0.975999
7	2.480389	-0.548614	0.335890
1	-2.533066	0.102557	-2.301657
1	-2.654211	-1.414939	-1.393441
1	-4.081265	-0.366257	-1.567381
1	-4.332604	-0.178063	0.943917
1	-3.080767	-1.416682	0.856753
1	-2.997268	2.155938	0.757594
1	-4.016697	1.849083	-0.650779
1	-2.424816	3.633675	-1.090016
1	-2.035295	2.264499	-2.151188
1	-0.999745	1.258632	5.535258
1	-3.406488	0.519543	5.567668
1	-4.474907	-0.191569	3.421844
1	3.933147	-3.514023	0.978076
1	5.982897	-2.142989	0.481247
1	5.708199	0.272197	-0.103772
71	0.150218	0.346164	0.242671
7	1.987546	1.865174	-0.845128
1	4.114280	2.085675	-0.807623
1	3.305470	2.192460	0.756937
6	2.093875	1.515698	-2.281205
6	0.143677	3.495577	-1.190336
1	0.078263	3.375525	-2.277411
1	-0.178700	4.513419	-0.941356
1	2.226396	3.965145	-1.193170
1	1.584074	3.501991	0.394507
8	0.086561	-0.938853	-1.947781
1	-0.377037	-1.764541	-1.739557
1	0.984946	-1.216142	-2.182573
1	2.523845	0.517618	-2.386490
1	1.110397	1.514911	-2.751952
1	2.741137	2.228459	-2.811628

Output energies:

Zero-point correction= 0.459308 (Hartree/Particle)
Thermal correction to Energy= 0.490090
Thermal correction to Enthalpy= 0.491034
Thermal correction to Gibbs Free Energy= 0.397404
Sum of electronic and zero-point Energies= -1487.891713
Sum of electronic and thermal Energies= -1487.860932
Sum of electronic and thermal Enthalpies= -1487.859987
Sum of electronic and thermal Free Energies= -1487.953618

(7) Lu-OxyMepa, $N1^{S}N2^{R}(\lambda\delta)$, enantiomer of $N1^{R}N2^{S}(\delta\lambda)$

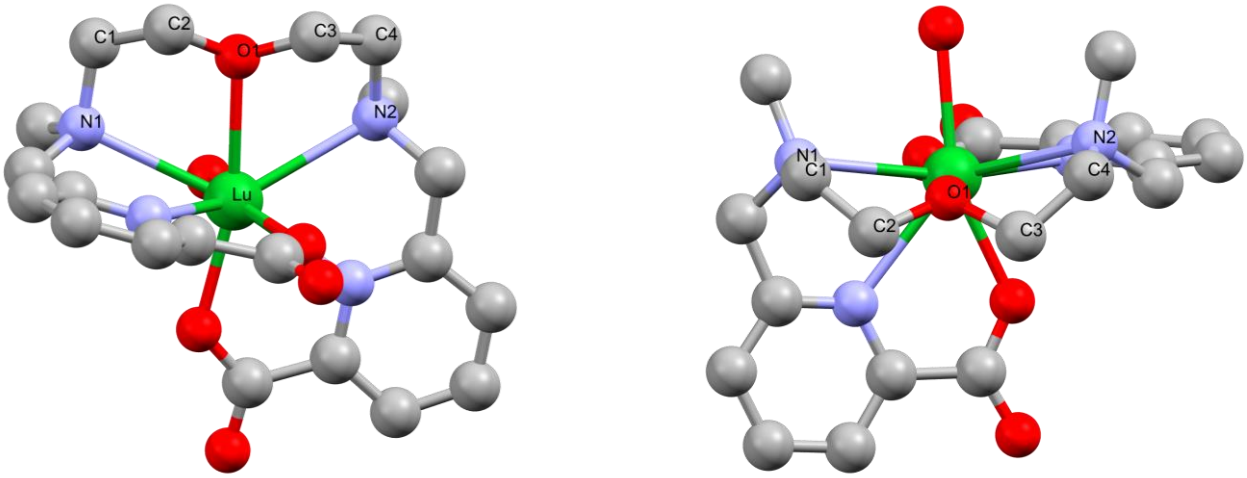

Figure S96. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in $N1^{S}N2^{R}(\lambda\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.125371	1.761589	-0.193704
6	3.522254	0.322118	0.059056
6	4.856658	-0.075642	0.188866
6	5.140860	-1.407115	0.486930
6	4.091498	-2.311447	0.654592
6	2.789192	-1.842309	0.509235
6	1.580798	-2.734148	0.720833
8	1.748946	-3.946931	0.921048
6	1.329830	3.222163	-1.031604
8	-0.803245	2.331226	-0.433200
6	-2.164150	2.567834	-0.017247
6	-3.036311	1.503887	-0.668946
7	-2.665698	0.095159	-0.349677
6	-3.401843	-0.415870	0.828231
6	-2.877040	0.118631	2.133805
6	-3.712784	0.408179	3.217238
6	-3.144545	0.872015	4.401456
6	-1.763495	1.056849	4.466500
6	-1.003329	0.757332	3.338972
6	0.488856	0.999168	3.290550
8	1.076825	1.389578	4.314788
6	-3.001230	-0.771358	-1.501002
8	1.045283	0.786632	2.148975
7	-1.549547	0.276374	2.209088

8	0.434168	-2.134134	0.689440
7	2.522634	-0.560127	0.206257
1	-2.489361	-0.414790	-2.395651
1	-2.679116	-1.795396	-1.292793
1	-4.083148	-0.783960	-1.702060
1	-4.477884	-0.208199	0.741251
1	-3.286024	-1.506014	0.843151
1	-2.944632	1.629019	-1.750922
1	-4.085869	1.700972	-0.407947
1	-2.483172	3.550627	-0.383715
1	-2.225267	2.572119	1.075217
1	-1.278671	1.439907	5.356187
1	-3.771446	1.106372	5.256105
1	-4.785582	0.279690	3.121665
1	4.264944	-3.353277	0.895416
1	6.170051	-1.736725	0.588278
1	5.651737	0.650155	0.055873
71	0.104334	0.065368	0.123302
7	1.915284	1.853364	-1.032654
1	3.967592	2.304998	-0.646340
1	2.914597	2.234182	0.771386
6	2.247307	1.454137	-2.417275
1	1.342426	1.443178	-3.027451
1	2.686992	0.453817	-2.426378
1	2.971021	2.146379	-2.872637
6	0.143755	3.367421	-0.090872
1	-0.319316	4.349094	-0.238555
1	0.429282	3.265898	0.962310
1	0.983096	3.438147	-2.045077
1	2.085094	3.978412	-0.782046
8	0.089197	-0.873947	-2.152986
1	-0.389534	-1.716654	-2.111667
1	0.990793	-1.112601	-2.417640

Output energies:

Zero-point correction= 0.458094 (Hartree/Particle)
Thermal correction to Energy= 0.488274
Thermal correction to Enthalpy= 0.489218
Thermal correction to Gibbs Free Energy= 0.397146
Sum of electronic and zero-point Energies= -1487.879358
Sum of electronic and thermal Energies= -1487.849178
Sum of electronic and thermal Enthalpies= -1487.848234
Sum of electronic and thermal Free Energies= -1487.940306

(8) Lu-OxyMepa, N1^{S}N2^{R}($\lambda\lambda$), enantiomer of N1^{R}N2^{S}($\delta\delta$)

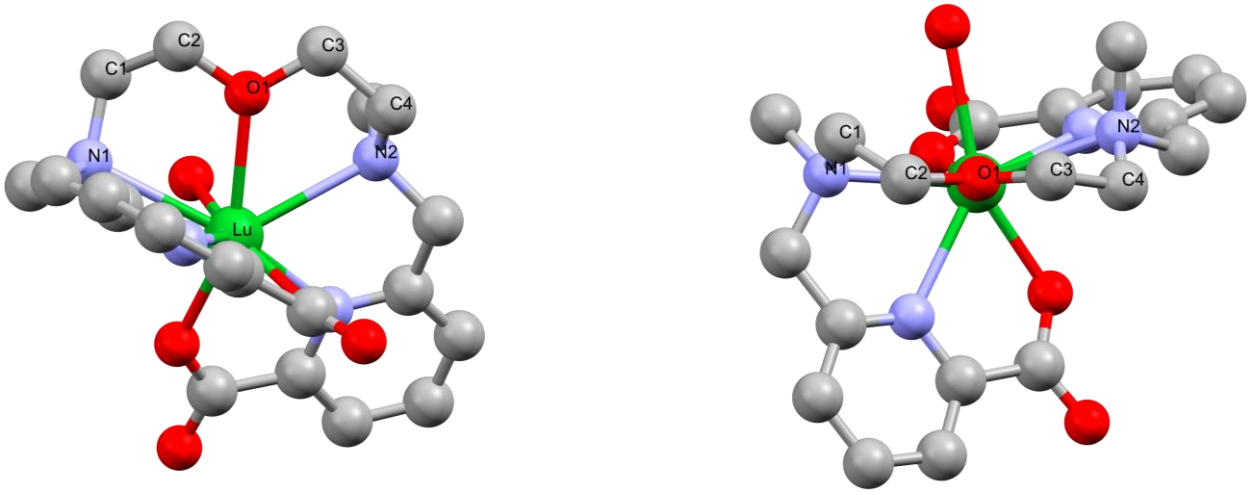

Figure S97. Side view (left) and top view (right) of optimized Lu-OxyMepa complex in N1^{S}N2^{R}($\lambda\lambda$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.190278	1.642952	0.106385
6	3.547904	0.176810	-0.000203
6	4.869625	-0.265601	-0.115633
6	5.127009	-1.634812	-0.117980
6	4.063002	-2.531332	-0.008672
6	2.774913	-2.014779	0.098426
6	1.558124	-2.905050	0.257105
8	1.697874	-4.137645	0.225523
6	1.287748	3.156762	0.068596
8	-0.888258	2.171286	-0.262733
6	-2.294146	2.310830	-0.540900
6	-2.809428	0.995371	-1.089601
7	-2.560178	-0.161118	-0.195156
6	-3.444888	-0.132157	0.991909
6	-2.836552	0.517971	2.209076
6	-3.643196	1.074891	3.209254
6	-3.045053	1.570717	4.362818
6	-1.656395	1.503809	4.492400
6	-0.922499	0.948053	3.450816
6	0.586811	0.855505	3.493527
8	1.194229	1.249951	4.501163
6	-2.810219	-1.409918	-0.952492
8	1.139134	0.351694	2.438948
7	-1.502863	0.461838	2.335213

8	0.434860	-2.285358	0.425189
7	2.531264	-0.692375	0.096172
1	-2.170730	-1.439976	-1.835204
1	-2.582977	-2.273349	-0.323251
1	-3.857601	-1.481806	-1.280632
1	-4.408920	0.337270	0.756519
1	-3.666966	-1.168428	1.270317
1	-2.301322	0.794855	-2.036191
1	-3.884409	1.098835	-1.303305
1	-2.440398	3.086561	-1.299870
1	-2.812885	2.623950	0.372637
1	-1.143778	1.879127	5.369568
1	-3.650707	2.008817	5.149814
1	-4.718724	1.112355	3.072323
1	4.216662	-3.603519	-0.000024
1	6.145690	-1.999751	-0.203384
1	5.675214	0.456377	-0.197318
71	0.113618	-0.006899	0.419693
7	1.878042	1.928532	-0.502656
1	3.986566	2.259680	-0.333436
1	3.140183	1.896236	1.170898
6	2.017963	2.014360	-1.967598
1	1.040752	2.052796	-2.452183
1	2.551912	1.133701	-2.333702
1	2.591143	2.906215	-2.263121
6	-0.135286	3.390529	-0.410984
1	-0.170812	3.696678	-1.462593
1	-0.590250	4.183974	0.192719
1	1.882503	4.050343	-0.179300
1	1.289077	3.047408	1.157036
8	0.127184	-0.658742	-2.143688
1	0.198195	-1.617819	-2.019708
1	0.943951	-0.410227	-2.599918

Output energies:

Zero-point correction= 0.458919 (Hartree/Particle)
Thermal correction to Energy= 0.489824
Thermal correction to Enthalpy= 0.490768
Thermal correction to Gibbs Free Energy= 0.397774
Sum of electronic and zero-point Energies= -1487.884930
Sum of electronic and thermal Energies= -1487.854025
Sum of electronic and thermal Enthalpies= -1487.853081
Sum of electronic and thermal Free Energies= -1487.946075

(9a) La-OxyMepa, N1^{S}N2^{S}($\delta\delta$), enantiomer of N1^{R}N2^{R}($\lambda\lambda$), q = 1

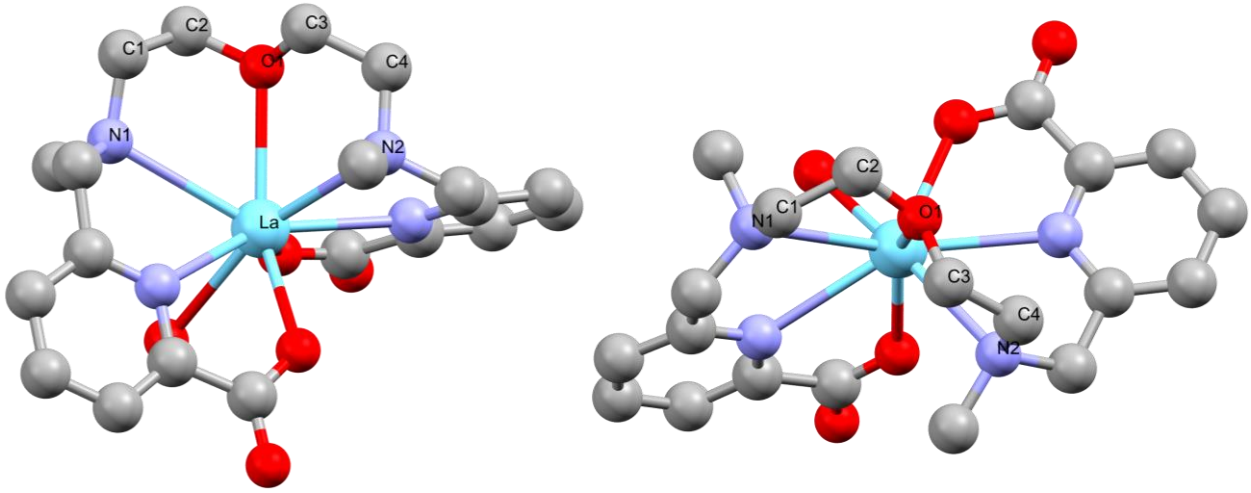

Figure S98. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{S}($\delta\delta$) conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.821267	-0.636037	2.833111
6	-3.044348	-0.082457	2.137118
6	-4.292351	-0.030043	2.765652
6	-5.365600	0.546018	2.089804
6	-5.170007	1.049571	0.804299
6	-3.900313	0.952315	0.239446
6	-3.620324	1.471960	-1.159290
8	-4.530061	2.055438	-1.773663
6	-1.553490	-2.669722	1.539965
8	-1.100607	-2.436614	-0.806281
6	-0.649795	-2.979230	-2.064379
6	0.862498	-2.894968	-2.219396
7	1.358152	-1.503544	-2.157775
6	2.768620	-1.459548	-1.738728
6	3.201697	-0.114012	-1.197092
6	4.497774	0.362528	-1.424393
6	4.902258	1.547540	-0.816034
6	4.004517	2.227114	0.005556
6	2.725529	1.699306	0.173364
6	1.711885	2.399768	1.066192
8	2.055594	3.441657	1.653221
6	1.197183	-0.824830	-3.457891
8	0.550575	1.848070	1.155408
7	2.332783	0.554996	-0.420068

8	-2.430683	1.261903	-1.612254
7	-2.863600	0.400852	0.897300
1	1.146999	-3.381800	-3.165842
1	1.335921	-3.465230	-1.416144
1	-0.975252	-4.022566	-2.149396
1	-1.164633	-2.397260	-2.832891
1	4.273820	3.148371	0.507023
1	5.903145	1.935193	-0.978469
1	5.171471	-0.195767	-2.065753
1	-5.974617	1.503290	0.238798
1	-6.344061	0.596472	2.556957
1	-4.412030	-0.437813	3.763666
57	-0.458812	0.182603	-0.412444
7	-0.932650	-1.375528	1.911247
1	-1.249035	0.204322	3.243119
1	-2.126937	-1.263084	3.683121
6	0.384934	-1.571991	2.545897
1	1.053055	-2.109472	1.869164
1	0.830356	-0.597998	2.763557
1	0.306293	-2.143091	3.483190
6	-0.926420	-3.316410	0.320248
1	0.137029	-3.527105	0.476443
1	-1.436704	-4.266028	0.118026
1	-1.497647	-3.380156	2.379323
1	-2.612485	-2.493157	1.332317
8	0.036851	2.292802	-2.127072
1	0.320767	3.022786	-1.556201
1	-0.929805	2.399862	-2.211378
1	1.747496	-1.347333	-4.256432
1	1.573779	0.198295	-3.393435
1	0.141405	-0.781086	-3.737332
1	2.907678	-2.189039	-0.932419
1	3.443243	-1.757921	-2.555189

Output energies:

Zero-point correction= 0.455640 (Hartree/Particle)
Thermal correction to Energy= 0.485047
Thermal correction to Enthalpy= 0.485991
Thermal correction to Gibbs Free Energy= 0.393968
Sum of electronic and zero-point Energies= -1479.552134
Sum of electronic and thermal Energies= -1479.522727
Sum of electronic and thermal Enthalpies= -1479.521783
Sum of electronic and thermal Free Energies= -1479.613806

(9b) La-OxyMepa, $N1^{S}N2^{S}(\delta\delta)$, enantiomer of $N1^{R}N2^{R}(\lambda\lambda)$, q = 2

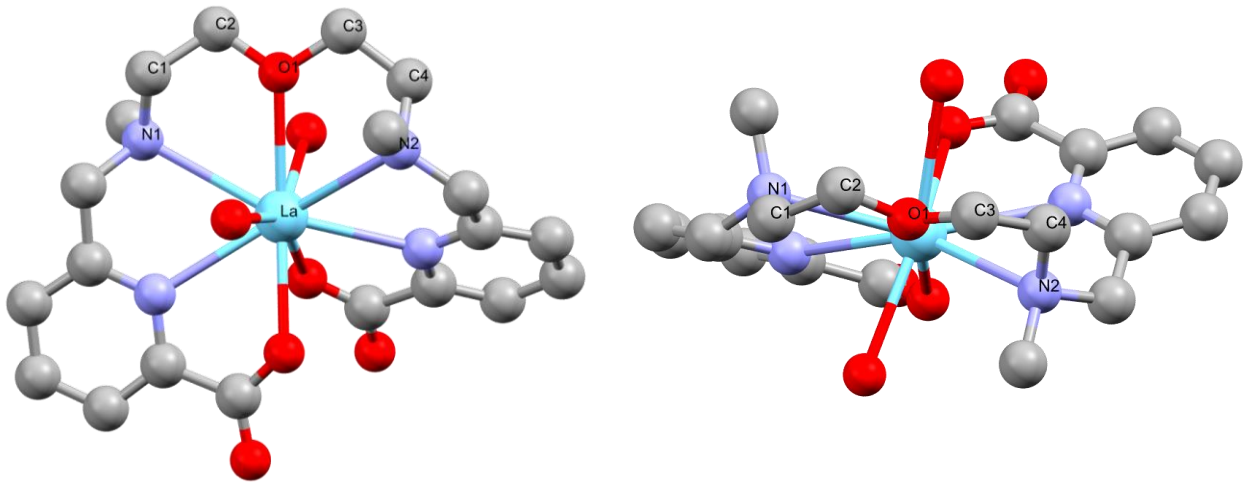

Figure S99. Side view (left) and top view (right) of optimized La-OxyMepa complex in $N1^{S}N2^{S}(\delta\delta)$ conformation (q = 2). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.435159	0.552024	9.238560
8	2.956010	-2.085362	8.833279
8	4.916065	0.180610	7.921239
8	0.444277	-0.565922	10.731628
8	1.110439	2.657093	9.839232
8	3.886044	2.601800	8.505168
8	1.326464	4.746307	10.657084
8	4.123891	4.489368	7.305927
7	3.999996	-0.871578	11.291348
7	0.958427	-0.958255	7.228597
7	2.697985	1.653518	11.745689
7	2.045483	1.661641	6.724646
6	3.705713	-2.312713	11.117443
1	2.671912	-2.480157	11.434968
1	4.353313	-2.930651	11.760532
6	3.848346	-2.815786	9.690700
1	4.872720	-2.726534	9.309799
1	3.576412	-3.878427	9.678008
6	2.715672	-2.727379	7.571766
1	2.098117	-3.617478	7.741723
1	3.664676	-3.055199	7.130361
6	2.047888	-1.750400	6.608869
1	2.794714	-1.048844	6.227051
1	1.672737	-2.330183	5.750253

6	5.439127	-0.586252	11.135217
6	-0.102707	-1.844657	7.746133
6	3.559817	-0.434769	12.632550
1	4.251133	-0.785348	13.412560
1	2.586966	-0.895538	12.838449
6	3.379050	1.062929	12.741523
6	3.806338	1.787926	13.857712
1	4.357919	1.290096	14.647948
6	3.508191	3.147861	13.934201
1	3.834012	3.731633	14.789490
6	2.780953	3.747140	12.906351
1	2.516020	4.797148	12.930367
6	2.388112	2.959402	11.825467
6	1.547747	3.520991	10.686724
6	0.360978	-0.050749	6.228093
1	-0.546892	0.373524	6.673560
1	0.042744	-0.607263	5.333792
6	1.238908	1.106152	5.805125
6	1.137227	1.628290	4.510393
1	0.493764	1.143844	3.783785
6	1.862134	2.769153	4.180395
1	1.794975	3.193113	3.183392
6	2.676537	3.357649	5.147066
1	3.253924	4.250383	4.940761
6	2.753568	2.763952	6.405051
6	3.655726	3.350996	7.479449
1	-0.525804	-2.477151	6.950740
1	-0.907989	-1.241597	8.170816
1	0.290553	-2.494366	8.529132
1	0.511461	-1.529274	10.649005
1	4.664610	-0.043675	7.012921
1	5.789950	-0.892326	10.150203
1	6.034947	-1.109024	11.899600
1	5.613822	0.488371	11.236886
1	4.859971	1.158574	7.956189
1	0.622146	-0.386743	11.667125

Output energies:

Zero-point correction= 0.481778 (Hartree/Particle)
Thermal correction to Energy= 0.514549
Thermal correction to Enthalpy= 0.515494
Thermal correction to Gibbs Free Energy= 0.418119
Sum of electronic and zero-point Energies= -1555.962532
Sum of electronic and thermal Energies= -1555.929760
Sum of electronic and thermal Enthalpies= -1555.928816
Sum of electronic and thermal Free Energies= -1556.026191

(10a) La-OxyMepa, $N1^{S}N2^{S}(\delta\lambda)$, enantiomer of $N1^{R}N2^{R}(\lambda\delta)$, q = 1

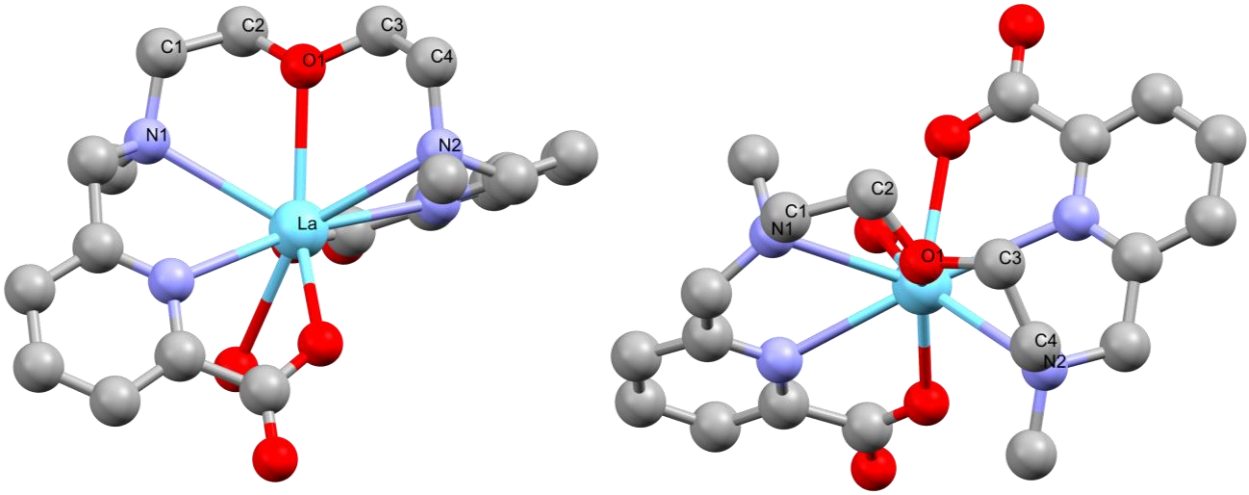

Figure S100. Side view (left) and top view (right) of optimized La-OxyMepa complex in $N1^{S}N2^{S}(\delta\lambda)$ conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-2.112946	-0.773760	2.909099
6	-3.161956	-0.370492	1.899219
6	-4.525904	-0.479608	2.188219
6	-5.453647	-0.012984	1.260382
6	-4.997795	0.539441	0.064664
6	-3.623088	0.597570	-0.159733
6	-3.070124	1.156995	-1.458622
8	-3.859255	1.673107	-2.269999
6	-1.206516	-2.843964	1.933631
8	-0.589688	-2.505545	-0.346373
6	-0.698321	-2.831764	-1.746258
6	0.683592	-2.675209	-2.355635
7	1.214005	-1.289684	-2.248145
6	2.692139	-1.305087	-2.186253
6	3.294455	-0.048254	-1.597825
6	4.494744	0.481056	-2.083203
6	5.064716	1.572683	-1.432104
6	4.423347	2.112430	-0.317748
6	3.221428	1.542430	0.097134
6	2.455141	2.098039	1.288987
8	2.928140	3.076039	1.895650
6	0.766793	-0.483855	-3.404544
8	1.351488	1.500266	1.585796
7	2.676829	0.483768	-0.530092

8	-1.797809	1.043944	-1.630511
7	-2.727035	0.159806	0.744107
1	0.653261	-3.005979	-3.403729
1	1.358908	-3.346846	-1.819615
1	-1.024395	-3.872231	-1.856930
1	-1.444118	-2.180854	-2.220196
1	4.828324	2.960973	0.219605
1	5.996064	1.999818	-1.790519
1	4.968456	0.039055	-2.953184
1	-5.679225	0.912557	-0.689997
1	-6.517480	-0.084596	1.464119
1	-4.844913	-0.923506	3.125137
57	-0.017027	0.131732	-0.006680
7	-0.927847	-1.435981	2.324958
1	-1.766335	0.142564	3.401708
1	-2.571913	-1.399373	3.688273
6	0.174156	-1.400586	3.309971
1	1.078534	-1.822133	2.863991
1	0.378527	-0.366433	3.596710
1	-0.064175	-1.972445	4.219643
6	-1.642317	-3.023819	0.488357
1	-0.284270	-3.414976	2.070572
1	-1.964666	-3.290418	2.592810
8	0.310304	2.690971	-1.140614
1	0.193773	3.303262	-0.399143
1	-0.585466	2.552045	-1.503626
1	1.177385	-0.877763	-4.346480
1	1.095288	0.552602	-3.290124
1	-0.322921	-0.494593	-3.468076
1	2.993767	-2.134836	-1.537064
1	3.130237	-1.499359	-3.175626
1	-1.769388	-4.094618	0.288471
1	-2.586252	-2.516699	0.260785

Output energies:

Zero-point correction= 0.456009 (Hartree/Particle)
Thermal correction to Energy= 0.485270
Thermal correction to Enthalpy= 0.486214
Thermal correction to Gibbs Free Energy= 0.396161
Sum of electronic and zero-point Energies= -1479.547950
Sum of electronic and thermal Energies= -1479.518688
Sum of electronic and thermal Enthalpies= -1479.517744
Sum of electronic and thermal Free Energies= -1479.607798

(10b) La-OxyMepa, N1^{S}N2^{S}($\delta\lambda$), enantiomer of N1^{R}N2^{R}($\lambda\delta$), q = 2

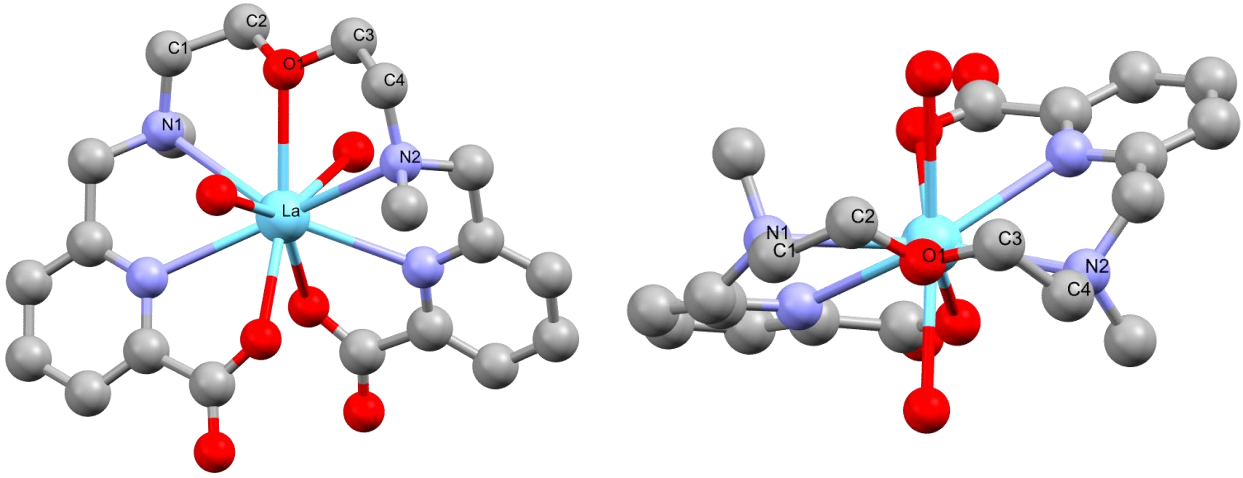

Figure S101. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{S}($\delta\lambda$) conformation (q = 2). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.490293	0.395485	9.249762
8	2.808268	-2.316936	9.073092
8	4.870445	0.045624	7.563491
8	0.507843	-0.761119	10.731985
8	0.886498	2.197435	9.979600
8	3.760404	2.580280	8.671780
8	0.671339	4.214170	10.958994
8	3.601672	4.633360	7.756916
7	4.319119	-0.865661	11.146335
7	0.894987	-0.955555	7.251601
7	2.719977	1.424551	11.779389
7	2.228066	1.518514	6.738161
6	4.275961	-2.339058	10.981682
1	3.436712	-2.721556	11.569266
1	5.191855	-2.807879	11.373169
6	4.083602	-2.791891	9.544227
1	4.878859	-2.433134	8.880610
1	4.089121	-3.888582	9.521230
6	2.421734	-2.878695	7.805953
1	2.424468	-3.973219	7.881907
1	3.150484	-2.592295	7.036725
6	1.012886	-2.417335	7.470974
1	0.661539	-2.976703	6.590419
1	0.355370	-2.684396	8.303635

6	5.645680	-0.327700	10.783702
6	-0.508736	-0.525093	7.413099
6	4.002230	-0.493643	12.540974
1	4.844677	-0.709647	13.213798
1	3.159695	-1.110445	12.873467
6	3.578994	0.950291	12.696056
6	3.972190	1.725604	13.791119
1	4.674276	1.324652	14.514343
6	3.444068	3.007506	13.935099
1	3.737778	3.628715	14.775522
6	2.528391	3.479924	12.995234
1	2.080845	4.462681	13.078073
6	2.190319	2.652419	11.925956
6	1.170108	3.076598	10.878074
6	1.364795	-0.591989	5.897493
1	0.660350	-0.947753	5.131658
1	2.318870	-1.098550	5.713877
6	1.602011	0.892886	5.728980
6	1.268862	1.568407	4.550750
1	0.758742	1.042743	3.750722
6	1.607565	2.914693	4.426642
1	1.356532	3.460424	3.522392
6	2.279331	3.550020	5.470855
1	2.576468	4.589892	5.410938
6	2.578407	2.810597	6.613834
6	3.367974	3.410439	7.768302
1	5.908246	-0.621401	9.767457
1	6.425641	-0.692748	11.469287
1	5.627336	0.765130	10.826043
1	4.494094	-0.070330	6.678411
1	0.116743	-1.532270	10.296049
1	-1.172729	-1.029732	6.694995
1	-0.586035	0.553261	7.253526
1	-0.852761	-0.748036	8.424569
1	-0.200791	-0.100014	10.755302
1	4.951184	1.010324	7.663554

Output energies:

Zero-point correction= 0.479600 (Hartree/Particle)
Thermal correction to Energy= 0.510650
Thermal correction to Enthalpy= 0.511594
Thermal correction to Gibbs Free Energy= 0.418911
Sum of electronic and zero-point Energies= -1555.967112
Sum of electronic and thermal Energies= -1555.936062
Sum of electronic and thermal Enthalpies= -1555.935118
Sum of electronic and thermal Free Energies= -1556.027801

(11a) La-OxyMepa, N1^{S}N2^S($\lambda\delta$), enantiomer of N1^{R}N2^R($\delta\lambda$), q = 1

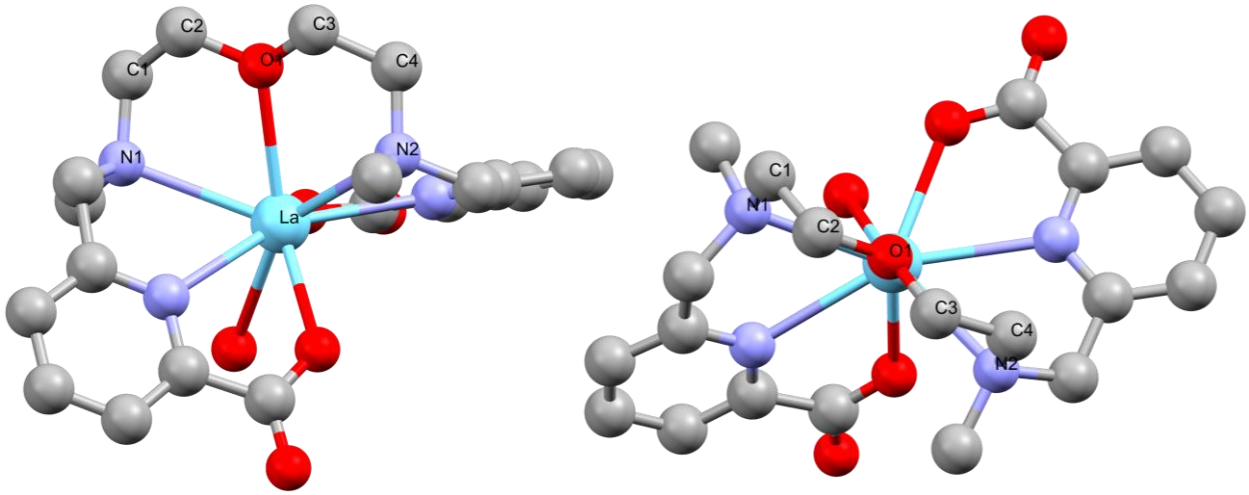

Figure S102. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^S($\lambda\delta$) conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.906492	-0.497566	2.854411
6	-3.092775	0.005054	2.061352
6	-4.353095	0.156652	2.649331
6	-5.395630	0.677406	1.886986
6	-5.162919	1.012302	0.553072
6	-3.885351	0.819552	0.032936
6	-3.574272	1.126480	-1.422299
8	-4.464902	1.629516	-2.129603
6	-1.557773	-2.603282	1.703533
8	-0.582807	-2.635779	-0.506522
6	0.156771	-3.353872	-1.508216
6	0.368472	-2.466253	-2.720441
7	1.073963	-1.196002	-2.427504
6	2.485322	-1.427806	-2.051673
6	3.113048	-0.231568	-1.371424
6	4.451230	0.118601	-1.576537
6	4.985993	1.186468	-0.858669
6	4.175991	1.880818	0.040129
6	2.850072	1.477773	0.184812
6	1.901177	2.183330	1.141877
8	2.326912	3.152333	1.796744
6	1.008226	-0.317086	-3.613142
8	0.705014	1.709619	1.204287
7	2.339805	0.442913	-0.505771

8	-2.384435	0.828515	-1.823869
7	-2.872724	0.340155	0.780370
1	-0.607153	-2.203260	-3.141449
1	0.905581	-3.051247	-3.483402
1	1.103196	-3.700471	-1.076138
1	-0.411279	-4.240601	-1.816758
1	4.549471	2.718518	0.616272
1	6.022127	1.476917	-1.001646
1	5.054175	-0.437629	-2.286306
1	-5.946149	1.406805	-0.082530
1	-6.381251	0.808730	2.322494
1	-4.505097	-0.131891	3.683895
57	-0.391136	0.091885	-0.378533
7	-0.957945	-1.292248	2.044488
1	-1.362403	0.371660	3.241712
1	-2.260798	-1.067306	3.725872
6	0.305975	-1.454167	2.790363
1	1.045517	-1.972739	2.176683
1	0.705740	-0.469274	3.041435
1	0.161149	-2.025475	3.719645
6	-0.753035	-3.403261	0.697342
1	0.232334	-3.685119	1.087194
1	-1.299772	-4.326151	0.466714
1	-1.677426	-3.220078	2.608369
1	-2.556180	-2.424611	1.295254
8	-0.205670	2.484065	-1.727839
1	-0.218060	3.178484	-1.051930
1	-1.138482	2.358445	-1.986679
1	1.454062	-0.799532	-4.495882
1	1.548285	0.612048	-3.419208
1	-0.034399	-0.076412	-3.836816
1	2.526347	-2.260770	-1.342542
1	3.083277	-1.721915	-2.926082

Output energies:

Zero-point correction= 0.455454 (Hartree/Particle)
Thermal correction to Energy= 0.484974
Thermal correction to Enthalpy= 0.485918
Thermal correction to Gibbs Free Energy= 0.395074
Sum of electronic and zero-point Energies= -1479.553394
Sum of electronic and thermal Energies= -1479.523875
Sum of electronic and thermal Enthalpies= -1479.522931
Sum of electronic and thermal Free Energies= -1479.613774

(11b) La-OxyMepa, N1^{S}N2^{S}($\lambda\delta$), enantiomer of N1^{R}N2^{R}($\delta\lambda$), q = 2

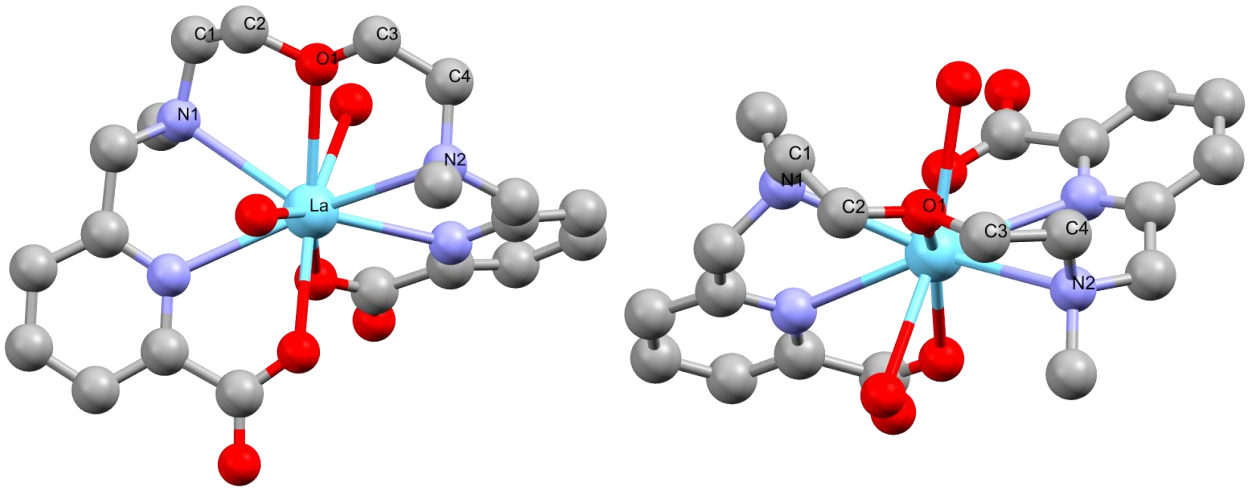

Figure S103. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{S}($\lambda\delta$) conformation (q = 2). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.412930	0.608941	9.167204
8	3.001647	-1.995892	8.801227
8	4.690026	0.062843	7.471903
8	0.647868	-0.683313	10.908664
8	0.852337	2.433822	10.038480
8	3.603258	2.786072	8.592146
8	0.503164	4.257664	11.313311
8	4.358904	4.370833	7.185068
7	4.512011	-0.478226	10.821890
7	0.753638	-0.817007	7.276545
7	2.656335	1.464078	11.772238
7	2.107904	1.667644	6.633689
6	4.801120	-1.871217	10.388973
1	5.304340	-2.432202	11.190666
1	5.495453	-1.820212	9.547267
6	3.576211	-2.656204	9.941835
1	3.896111	-3.665325	9.655393
1	2.822009	-2.748908	10.733391
6	2.123027	-2.809507	8.011494
1	1.327066	-3.220020	8.643297
1	2.688856	-3.652813	7.595974
6	1.574228	-1.981603	6.858193
1	2.411434	-1.607761	6.259241
1	0.984785	-2.653486	6.213893

6	5.720557	0.357669	10.670102
6	-0.502549	-1.264342	7.916047
6	4.071393	-0.460172	12.233563
1	4.902707	-0.720980	12.904580
1	3.301355	-1.229084	12.365106
6	3.476396	0.866461	12.651913
6	3.705637	1.413280	13.918356
1	4.377002	0.915238	14.609598
6	3.058090	2.596191	14.269391
1	3.222382	3.040361	15.246233
6	2.194443	3.200261	13.355629
1	1.663728	4.114649	13.590989
6	2.015001	2.596739	12.112494
6	1.048102	3.162002	11.081329
6	0.401210	0.004317	6.095094
1	-0.493226	0.581776	6.355356
1	0.124422	-0.631403	5.242551
6	1.446107	1.009474	5.667105
6	1.628299	1.320160	4.314756
1	1.095741	0.757862	3.555189
6	2.488706	2.358637	3.969070
1	2.642359	2.619962	2.926693
6	3.151590	3.055862	4.978065
1	3.826957	3.873169	4.757515
6	2.948689	2.666446	6.300522
6	3.699006	3.344805	7.438214
1	6.022523	0.382342	9.621738
1	6.557647	-0.029683	11.270596
1	5.509203	1.379567	10.994136
1	-1.129085	-1.840135	7.217993
1	-1.067264	-0.391180	8.252397
1	-0.292351	-1.889312	8.783454
1	-0.238598	-0.361501	10.684888
1	4.275345	-0.188907	6.633540
1	0.850271	-0.264171	11.758904
1	5.168400	0.880270	7.270818

Output energies:

Zero-point correction= 0.480044 (Hartree/Particle)
Thermal correction to Energy= 0.512726
Thermal correction to Enthalpy= 0.513670
Thermal correction to Gibbs Free Energy= 0.417145
Sum of electronic and zero-point Energies= -1555.963561
Sum of electronic and thermal Energies= -1555.930880
Sum of electronic and thermal Enthalpies= -1555.929936
Sum of electronic and thermal Free Energies= -1556.026461

(12) La-OxyMepa, N1^{S}N2^S($\lambda\lambda$), enantiomer of N1^{R}N2^R($\delta\delta$), q = 1

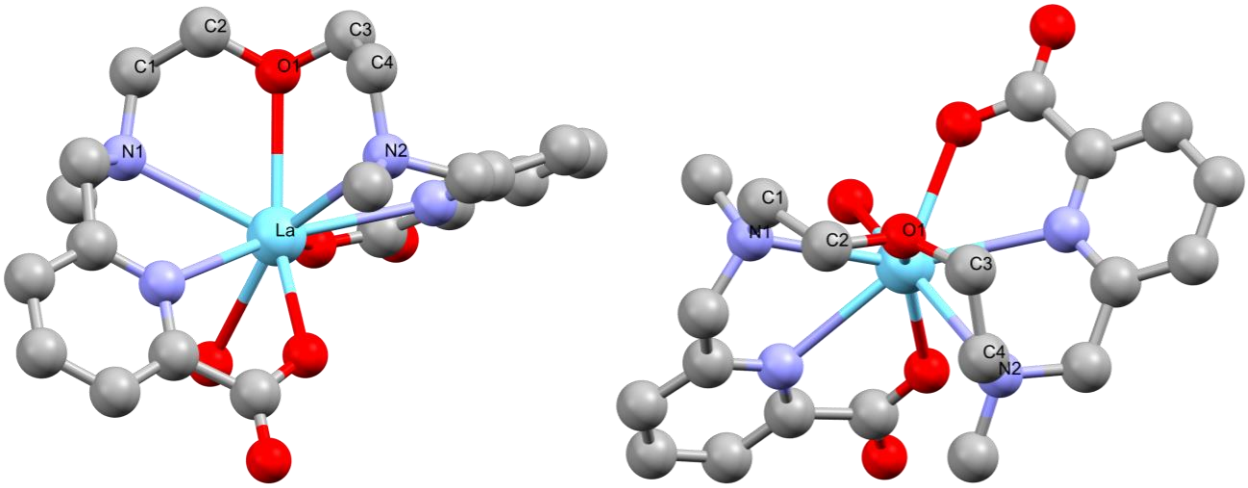

Figure S104. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^S($\lambda\lambda$) conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	-1.876168	-0.591077	2.863384
6	-3.111353	-0.276784	2.050840
6	-4.394597	-0.446988	2.580940
6	-5.496564	-0.072911	1.815650
6	-5.293563	0.442908	0.536074
6	-3.986126	0.566427	0.069332
6	-3.699659	1.072425	-1.335476
8	-4.651995	1.477809	-2.026558
6	-0.962353	-2.621243	1.797109
8	-1.127708	-2.351794	-0.645876
6	-0.159527	-3.225020	-1.261462
6	0.353846	-2.564521	-2.526727
7	1.091993	-1.301104	-2.286037
6	2.453931	-1.576706	-1.780582
6	3.111960	-0.361897	-1.164953
6	4.479137	-0.108650	-1.315866
6	5.039384	0.984336	-0.658191
6	4.225930	1.797678	0.130461
6	2.870621	1.487841	0.225180
6	1.923488	2.328047	1.069180
8	2.384756	3.307729	1.682533
6	1.178404	-0.533079	-3.545821
8	0.690623	1.952370	1.086745
7	2.333642	0.431103	-0.411575

8	-2.469903	1.027869	-1.718286
7	-2.922834	0.230631	0.822253
1	0.176522	-0.248232	-3.877481
1	1.657056	-1.121762	-4.342878
1	1.765469	0.374419	-3.389549
1	3.092339	-1.982687	-2.578473
1	2.388104	-2.346301	-1.004027
1	-0.503432	-2.330026	-3.164921
1	0.979605	-3.287511	-3.072164
1	-0.649312	-4.169141	-1.528590
1	0.647177	-3.449273	-0.554080
1	4.619415	2.656393	0.660316
1	6.097955	1.201348	-0.761907
1	5.084723	-0.758571	-1.938394
1	-6.119869	0.734613	-0.100394
1	-6.501791	-0.192548	2.207614
1	-4.518269	-0.867157	3.573346
57	-0.420898	0.283202	-0.421789
7	-0.757998	-1.177735	2.091475
1	-1.517397	0.355770	3.284220
1	-2.146949	-1.233558	3.713659
6	0.487245	-1.013755	2.872941
1	1.327901	-1.431580	2.314789
1	0.677152	0.047324	3.047349
1	0.432434	-1.525081	3.846071
6	-1.759062	-2.903839	0.529655
1	-1.866976	-3.987698	0.408222
1	-2.759635	-2.470807	0.566563
1	0.025861	-3.076381	1.688337
1	-1.455673	-3.126737	2.641526
8	0.018449	2.474793	-1.938932
1	0.242530	3.181881	-1.314939
1	-0.910589	2.632128	-2.176733

Output energies:

Zero-point correction= 0.454317 (Hartree/Particle)
Thermal correction to Energy= 0.481950
Thermal correction to Enthalpy= 0.482894
Thermal correction to Gibbs Free Energy= 0.395871
Sum of electronic and zero-point Energies= -1479.548876
Sum of electronic and thermal Energies= -1479.521243
Sum of electronic and thermal Enthalpies= -1479.520299
Sum of electronic and thermal Free Energies= -1479.607322

(13a) La-OxyMepa, N1^{S}N2^{R}($\delta\delta$), enantiomer of N1^{R}N2^{S}($\lambda\lambda$), q = 1

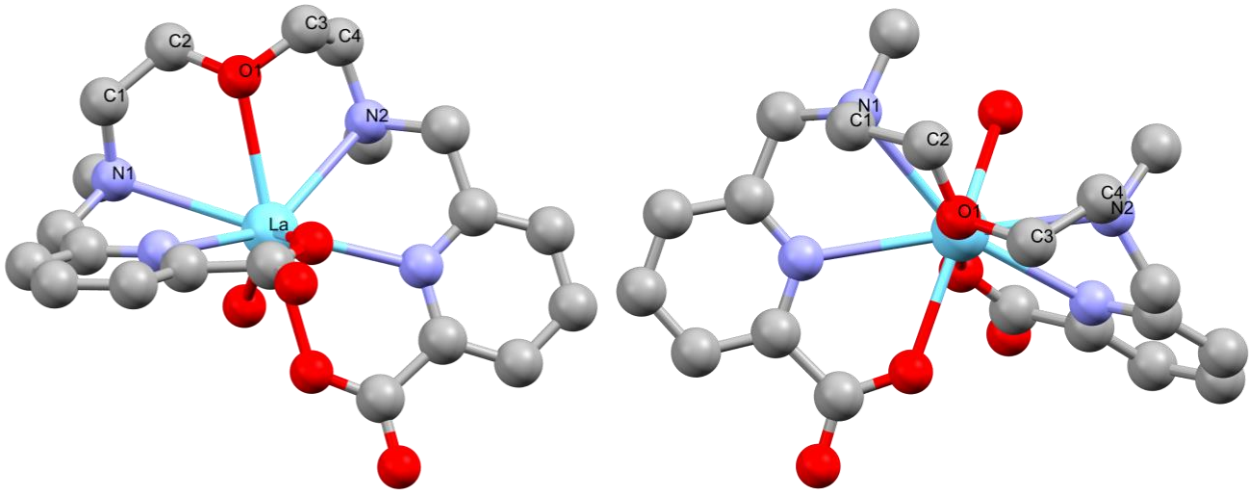

Figure S105. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}($\delta\delta$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.144344	1.731592	-0.736248
6	3.692747	0.400441	-0.274476
6	5.052959	0.093535	-0.383140
6	5.510912	-1.126415	0.108252
6	4.601729	-2.015363	0.681166
6	3.259575	-1.645814	0.743196
6	2.212510	-2.577457	1.335217
8	2.589430	-3.661793	1.816144
6	1.237017	2.987637	-1.551530
8	-0.515390	2.790253	0.153957
6	-1.741312	3.053641	-0.554995
6	-2.839995	2.182729	0.022448
7	-2.600024	0.728332	-0.141759
6	-3.483789	-0.033369	0.766806
6	-3.108323	0.126903	2.224979
6	-4.072364	0.110878	3.238468
6	-3.658730	0.214423	4.564634
6	-2.299878	0.353158	4.848543
6	-1.399955	0.377812	3.785586
6	0.091758	0.570769	4.009169
8	0.518384	0.618066	5.176835
6	-2.842441	0.311396	-1.534748
8	0.813215	0.681759	2.945734
7	-1.802756	0.253899	2.508233

8	0.991274	-2.169518	1.281891
7	2.824308	-0.458579	0.281894
1	-2.141074	0.813580	-2.205387
1	-2.690939	-0.765739	-1.627378
1	-3.866586	0.551018	-1.860084
1	-4.539412	0.243785	0.627003
1	-3.397898	-1.094008	0.501746
1	-2.926896	2.401053	1.089720
1	-3.792818	2.470926	-0.449011
1	-2.014127	4.107178	-0.417296
1	-1.604269	2.877121	-1.626902
1	-1.934809	0.449899	5.863709
1	-4.388562	0.200295	5.368123
1	-5.123162	0.021361	2.984367
1	4.911470	-2.977803	1.069216
1	6.562770	-1.385131	0.037682
1	5.731551	0.801733	-0.846367
57	0.152415	0.149956	0.569828
7	1.792116	1.629631	-1.329178
1	3.847757	2.191192	-1.446340
1	3.089816	2.396450	0.133347
6	1.862794	0.903482	-2.614073
1	0.857588	0.786561	-3.027079
1	2.294741	-0.088820	-2.464854
1	2.482426	1.439029	-3.349388
6	0.604516	3.576369	-0.299638
1	0.278048	4.604538	-0.493927
1	1.308712	3.596235	0.536468
1	0.479799	2.914296	-2.336747
1	2.012560	3.675698	-1.921433
8	-0.163593	-1.826335	-1.323626
1	0.302035	-2.452554	-0.741243
1	0.463179	-1.640907	-2.039728

Output energies:

Zero-point correction= 0.455678 (Hartree/Particle)
Thermal correction to Energy= 0.484167
Thermal correction to Enthalpy= 0.485111
Thermal correction to Gibbs Free Energy= 0.397747
Sum of electronic and zero-point Energies= -1479.551913
Sum of electronic and thermal Energies= -1479.523424
Sum of electronic and thermal Enthalpies= -1479.522480
Sum of electronic and thermal Free Energies= -1479.609844

(13b) La-OxyMepa, N1^{S}N2^{R}($\delta\delta$), enantiomer of N1^{R}N2^{S}($\lambda\lambda$), q = 2

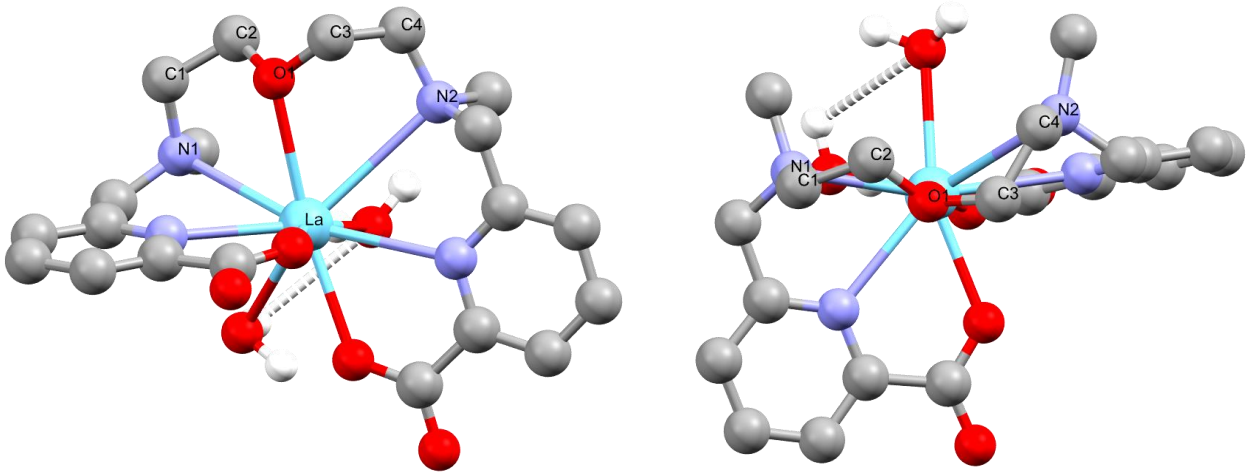

Figure S106. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}($\delta\delta$) conformation (q = 2). Hydrogen atoms on inner-sphere waters are shown to present the hydrogen bonding interaction. Other hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.250474	1.821166	-0.439971
6	3.792661	0.427431	-0.215705
6	5.163314	0.165612	-0.316075
6	5.631518	-1.118464	-0.049598
6	4.717574	-2.110478	0.298693
6	3.366277	-1.773839	0.379607
6	2.335575	-2.820811	0.766228
8	2.699179	-4.006039	0.874512
6	1.440975	3.190334	-1.287297
8	-0.518103	2.563851	0.083587
6	-1.630564	2.874146	-0.774823
6	-2.846146	2.136836	-0.247342
7	-2.692114	0.663932	-0.294828
6	-3.582237	0.019511	0.690658
6	-3.113345	0.203093	2.117692
6	-4.026663	0.295715	3.173849
6	-3.547216	0.413689	4.475463
6	-2.170094	0.458122	4.691891
6	-1.321525	0.373770	3.590708
6	0.187756	0.455775	3.750521
8	0.663308	0.528701	4.898515
6	-3.000667	0.153180	-1.643571
8	0.871658	0.452784	2.658859

7	-1.787882	0.234968	2.334940
8	1.136775	-2.393090	0.964735
7	2.915720	-0.530201	0.130882
1	-4.617141	0.380556	0.595344
1	-3.600171	-1.053257	0.471019
1	-3.005956	2.438471	0.791090
1	-3.732960	2.452070	-0.818514
1	-1.822716	3.953510	-0.745635
1	-1.402180	2.594453	-1.809829
1	-1.750294	0.564427	5.684636
1	-4.238068	0.483407	5.309897
1	-5.091737	0.278789	2.968417
1	5.028865	-3.126218	0.508670
1	6.691384	-1.342787	-0.118906
1	5.843312	0.961909	-0.599315
57	0.057040	-0.134035	0.335689
7	2.059618	1.850536	-1.305341
1	4.051570	2.458148	-0.848347
1	2.981424	2.236434	0.537081
6	2.423817	1.475607	-2.679267
6	0.607679	3.450866	-0.039650
1	0.251004	4.488103	-0.050407
1	1.190911	3.304013	0.872932
1	0.800607	3.275150	-2.170099
1	2.199653	3.986767	-1.371508
8	-1.402571	-2.457629	0.231615
8	0.162211	-1.174822	-2.177868
1	3.154003	2.173055	-3.122321
1	1.530844	1.473409	-3.311375
1	2.861553	0.474114	-2.693920
1	-0.707155	-1.407546	-2.535309
1	-1.579542	-2.659023	-0.699207
1	-2.347927	0.621434	-2.383438
1	-4.044419	0.358335	-1.928356
1	-2.841832	-0.927738	-1.673235
1	-0.559502	-2.913309	0.438514
1	0.558560	-0.588369	-2.838795

Output energies:

Zero-point correction= 0.480530 (Hartree/Particle)
Thermal correction to Energy= 0.511357
Thermal correction to Enthalpy= 0.512301
Thermal correction to Gibbs Free Energy= 0.417797
Sum of electronic and zero-point Energies= -1555.968043
Sum of electronic and thermal Energies= -1555.937216
Sum of electronic and thermal Enthalpies= -1555.936272
Sum of electronic and thermal Free Energies= -1556.030777

(14) La-OxyMepa, N1^{S}N2^{R}($\delta\lambda$), enantiomer of N1^{R}N2^{S}($\lambda\delta$), q = 1

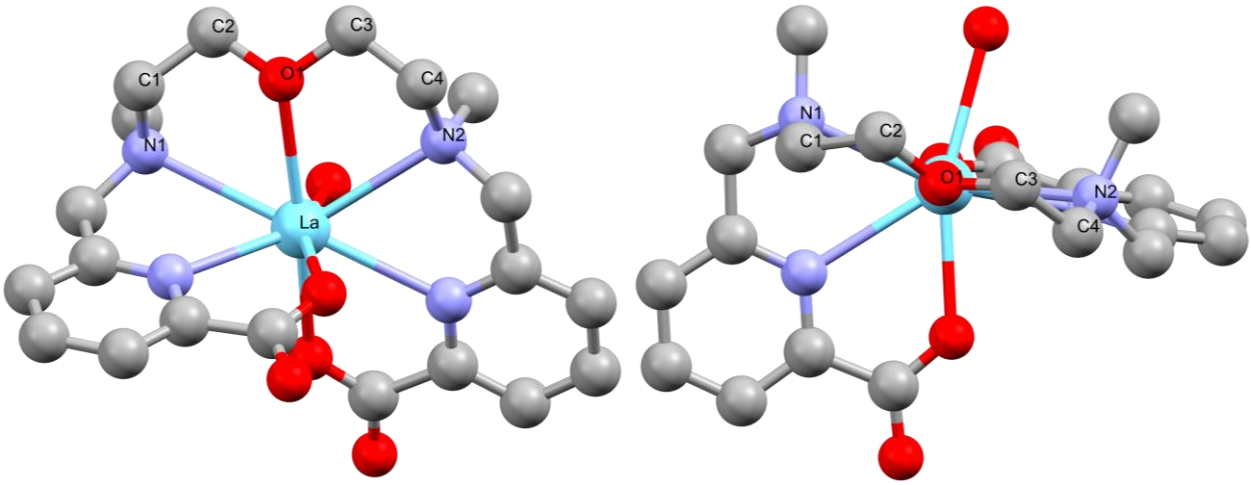

Figure S107. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}($\delta\lambda$) conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.345583	1.632739	-0.196063
6	3.732441	0.183695	0.007039
6	5.057813	-0.252116	-0.085623
6	5.345951	-1.592546	0.164748
6	4.308173	-2.465869	0.489850
6	3.011757	-1.958459	0.559056
6	1.824531	-2.847519	0.897272
8	2.024015	-4.063003	1.077323
6	1.563433	3.169420	-0.762690
8	-0.762300	2.536650	-0.597192
6	-2.105443	2.652946	-1.097413
6	-3.051185	1.890647	-0.188752
7	-2.767781	0.438299	-0.101986
6	-3.500065	-0.149360	1.039074
6	-2.951732	0.273034	2.384547
6	-3.787593	0.396917	3.499879
6	-3.229716	0.740275	4.728329
6	-1.857217	0.975851	4.811341
6	-1.091794	0.851983	3.654594
6	0.399533	1.144511	3.655457
8	0.962119	1.378634	4.740734
6	-3.170984	-0.249479	-1.342085
8	0.973721	1.140652	2.502766
7	-1.630160	0.491225	2.474317

8	0.680211	-2.259891	0.970488
7	2.741369	-0.662517	0.327330
1	-2.622540	0.155482	-2.194540
1	-2.940619	-1.314689	-1.260625
1	-4.248819	-0.137844	-1.537621
1	-4.573144	0.089134	0.990994
1	-3.416574	-1.239845	0.959318
1	-2.978968	2.316022	0.815698
1	-4.079813	2.062641	-0.543949
1	-2.400817	3.709623	-1.097986
1	-2.138136	2.292622	-2.132865
1	-1.381727	1.258740	5.742354
1	-3.858404	0.836412	5.607972
1	-4.854216	0.228242	3.396083
1	4.485322	-3.516889	0.682520
1	6.367148	-1.954435	0.097282
1	5.841450	0.448708	-0.352692
57	0.094156	0.122870	0.355291
7	2.052991	1.777924	-0.901723
1	4.149894	2.161923	-0.727272
1	3.248653	2.101271	0.789923
6	2.216591	1.407433	-2.321619
6	0.161486	3.383692	-1.302131
1	0.096268	3.179098	-2.377490
1	-0.116158	4.433307	-1.143062
1	2.233139	3.875556	-1.279076
1	1.575222	3.421603	0.302353
8	0.086902	-1.287862	-1.976986
1	0.451059	-2.149524	-1.721686
1	0.711905	-0.936445	-2.628463
1	2.664301	0.413940	-2.395385
1	1.249922	1.384257	-2.828530
1	2.870472	2.119623	-2.847409

Output energies:

Zero-point correction= 0.455847 (Hartree/Particle)
Thermal correction to Energy= 0.484518
Thermal correction to Enthalpy= 0.485462
Thermal correction to Gibbs Free Energy= 0.397583
Sum of electronic and zero-point Energies= -1479.553458
Sum of electronic and thermal Energies= -1479.524787
Sum of electronic and thermal Enthalpies= -1479.523843
Sum of electronic and thermal Free Energies= -1479.611722

(15a) La-OxyMepa, N1^{S}N2^{R}($\lambda\delta$), enantiomer of N1^{R}N2^{S}($\delta\lambda$), q = 1

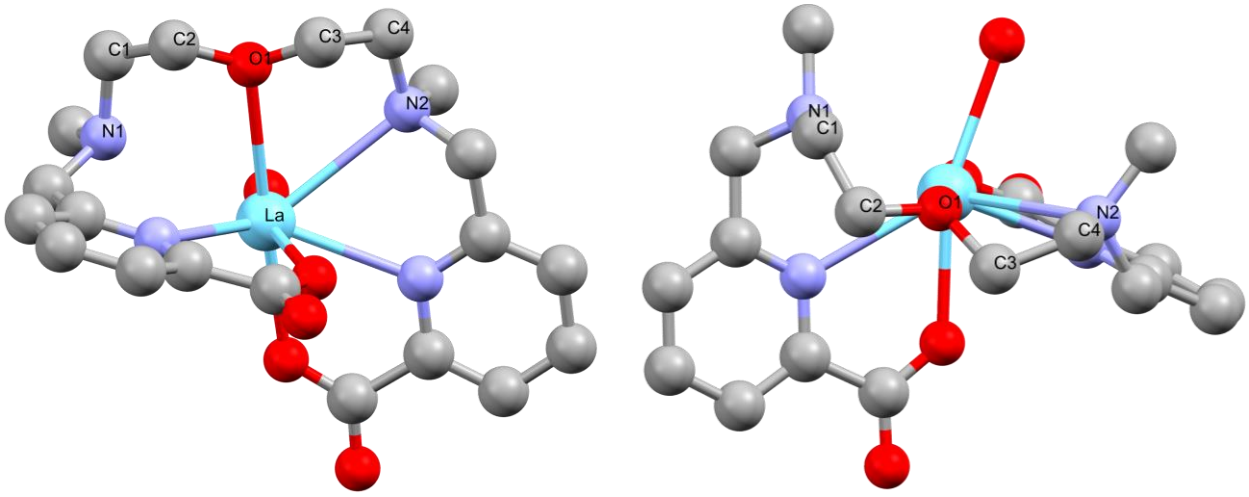

Figure S108. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}($\lambda\delta$) conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.086838	1.717693	-0.191559
6	3.646931	0.333886	0.055156
6	5.024098	0.113711	0.163846
6	5.483089	-1.166721	0.463443
6	4.560033	-2.195961	0.645849
6	3.204055	-1.902322	0.513176
6	2.141126	-2.968720	0.727126
8	2.504821	-4.129568	0.987168
6	1.288757	3.067559	-1.113673
8	-0.850007	2.310541	-0.402552
6	-2.167917	2.646762	0.057029
6	-3.150026	1.700942	-0.621101
7	-2.918019	0.255806	-0.368018
6	-3.631509	-0.222607	0.833054
6	-3.053666	0.268421	2.139203
6	-3.885754	0.683575	3.184070
6	-3.314922	1.077138	4.391734
6	-1.927696	1.059696	4.519910
6	-1.163242	0.643711	3.431349
6	0.353029	0.641397	3.503551
8	0.899990	0.950058	4.578772
6	-3.384842	-0.528665	-1.528831
8	0.970532	0.321164	2.422031
7	-1.715744	0.244358	2.270302

8	0.915606	-2.578117	0.627768
7	2.766303	-0.665711	0.216338
1	-2.847979	-0.214616	-2.426496
1	-3.189218	-1.590971	-1.359357
1	-4.463904	-0.401092	-1.708725
1	-4.699687	0.038574	0.787848
1	-3.572458	-1.317786	0.834651
1	-3.058861	1.863183	-1.698554
1	-4.173048	1.991272	-0.336977
1	-2.409978	3.671976	-0.250784
1	-2.210748	2.602293	1.150344
1	-1.432393	1.366605	5.432764
1	-3.941399	1.402509	5.216361
1	-4.960808	0.698538	3.041352
1	4.869062	-3.205931	0.885730
1	6.547604	-1.360000	0.552195
1	5.715790	0.936024	0.014974
57	0.036167	-0.287212	0.159355
7	1.903747	1.713766	-1.074317
1	3.879582	2.363146	-0.599626
1	2.789327	2.145624	0.773092
6	2.293389	1.305835	-2.438639
1	1.405634	1.260155	-3.074746
1	2.760681	0.318955	-2.418808
1	3.006659	2.013460	-2.888863
6	0.180406	3.264082	-0.093857
1	-0.215637	4.282269	-0.186783
1	0.527886	3.117902	0.937764
1	0.849332	3.208743	-2.104778
1	2.049202	3.850782	-0.984440
8	0.009405	-1.365655	-2.338453
1	0.238888	-2.302253	-2.236817
1	0.719930	-0.996861	-2.884599

Output energies:

Zero-point correction= 0.455544 (Hartree/Particle)
Thermal correction to Energy= 0.485231
Thermal correction to Enthalpy= 0.486175
Thermal correction to Gibbs Free Energy= 0.394640
Sum of electronic and zero-point Energies= -1479.547252
Sum of electronic and thermal Energies= -1479.517565
Sum of electronic and thermal Enthalpies= -1479.516621
Sum of electronic and thermal Free Energies= -1479.608157

(15b) La-OxyMepa, N1^{S}N2^{R}($\lambda\delta$), enantiomer of N1^{R}N2^{S}($\delta\lambda$), q = 2

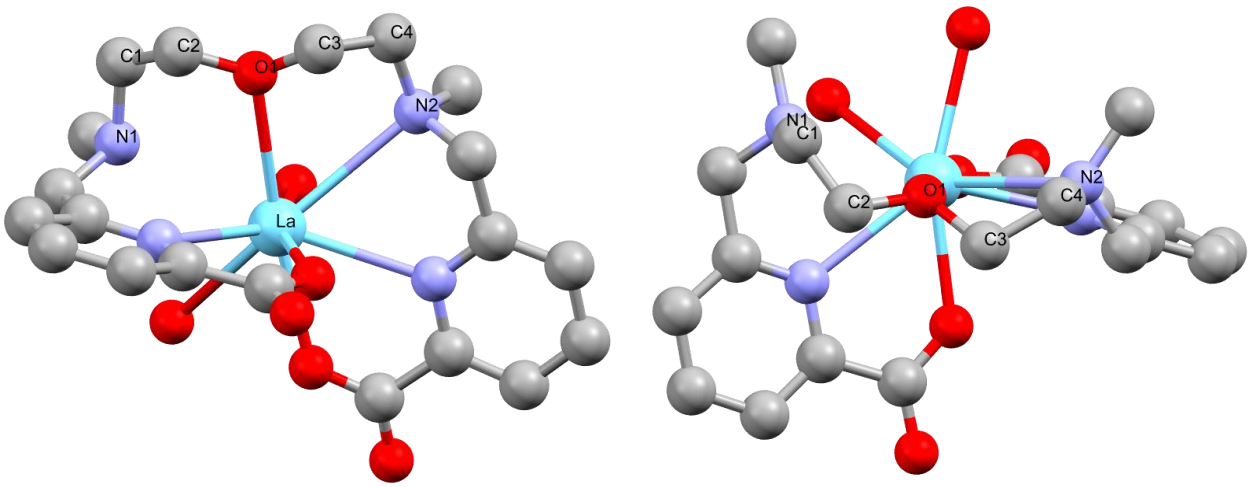

Figure S109. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}($\lambda\delta$) conformation (q = 2). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.219749	1.762574	-0.113761
6	3.788333	0.375264	0.082561
6	5.164379	0.167520	0.228091
6	5.636044	-1.123272	0.454421
6	4.723989	-2.175042	0.526853
6	3.368282	-1.888269	0.379654
6	2.321218	-2.979528	0.491278
8	2.684343	-4.167916	0.507693
6	1.513288	3.154301	-1.119228
8	-0.642303	2.385067	-0.465884
6	-1.972009	2.770369	-0.090014
6	-2.948689	1.874765	-0.836186
7	-2.795091	0.418787	-0.590997
6	-3.565339	-0.030628	0.585792
6	-3.003624	0.411713	1.916306
6	-3.856285	0.825517	2.945728
6	-3.313944	1.177128	4.178484
6	-1.931978	1.121850	4.347088
6	-1.145699	0.707788	3.273691
6	0.366730	0.664790	3.395196
8	0.885764	0.952747	4.489847
6	-3.288932	-0.317638	-1.772009
8	1.011753	0.334479	2.332701
7	-1.671555	0.346307	2.087587

8	1.101061	-2.569362	0.579175
7	2.915132	-0.641802	0.155682
1	-4.615057	0.293049	0.514638
1	-3.570833	-1.126341	0.576941
1	-3.974084	2.205874	-0.609383
1	-2.785287	2.043530	-1.904394
1	-2.088250	2.725714	0.997690
1	-2.152042	3.805640	-0.406707
1	-1.456930	1.397229	5.280498
1	-3.957376	1.500296	4.990819
1	-4.925647	0.872676	2.770328
1	5.040027	-3.196799	0.698689
1	6.699792	-1.306868	0.569008
1	5.846326	1.008503	0.161291
57	0.144869	-0.259021	0.045716
7	2.126327	1.802833	-1.106866
1	4.031945	2.449778	-0.397033
1	2.825636	2.113666	0.846703
6	2.670763	1.504952	-2.447152
6	0.388840	3.323693	-0.114339
1	-0.000525	4.345858	-0.186738
1	0.712862	3.148728	0.919956
1	1.089402	3.321264	-2.113324
1	2.271272	3.935336	-0.955901
8	-1.403158	-2.720531	-0.250816
8	0.180911	-1.050721	-2.528197
1	3.425522	2.245835	-2.754219
1	1.863307	1.512874	-3.183932
1	3.138607	0.518280	-2.456244
1	-0.710396	-1.260576	-2.845393
1	0.523708	-0.398454	-3.157131
1	-1.440400	-2.823225	-1.212714
1	-2.704319	-0.040445	-2.653138
1	-4.348048	-0.099170	-1.982210
1	-3.190016	-1.392163	-1.609396
1	-0.523674	-3.072386	0.005135

Output energies:

Zero-point correction= 0.481506 (Hartree/Particle)
Thermal correction to Energy= 0.512545
Thermal correction to Enthalpy= 0.513489
Thermal correction to Gibbs Free Energy= 0.420694
Sum of electronic and zero-point Energies= -1555.963764
Sum of electronic and thermal Energies= -1555.932725
Sum of electronic and thermal Enthalpies= -1555.931781
Sum of electronic and thermal Free Energies= - 1556.024576

(16a) La-OxyMepa, N1^{S}N2^{R}($\lambda\lambda$), enantiomer of N1^{R}N2^{S}($\delta\delta$), q = 1

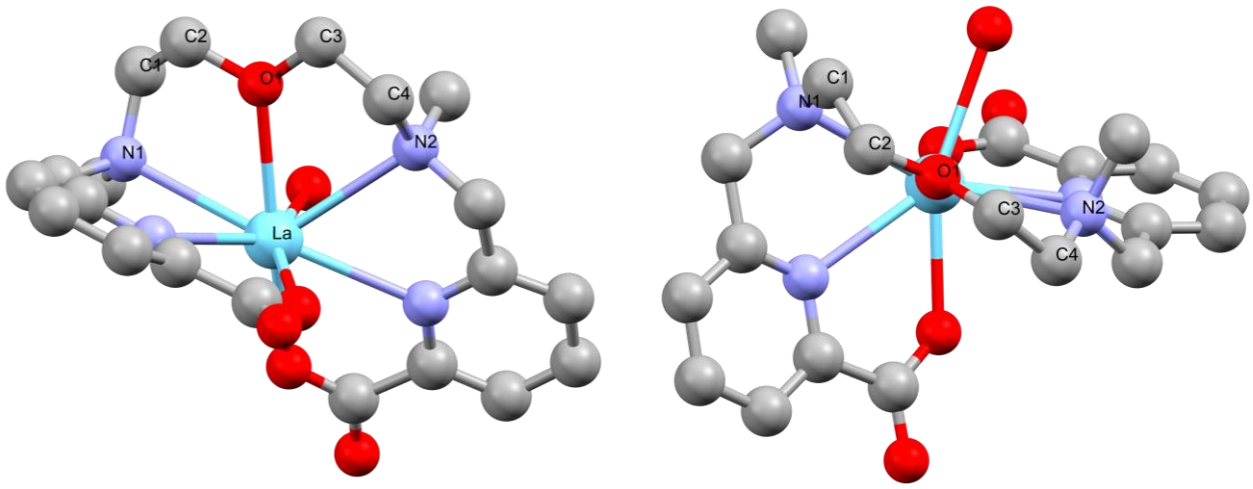

Figure S110. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}($\lambda\lambda$) conformation (q = 1). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.232707	1.559467	0.197891
6	3.704415	0.138867	-0.025920
6	5.033321	-0.164657	-0.335768
6	5.404560	-1.500913	-0.475720
6	4.444178	-2.497968	-0.307818
6	3.137537	-2.116725	-0.004184
6	2.033559	-3.144926	0.196257
8	2.310153	-4.349622	0.046413
6	1.310424	3.033005	0.165879
8	-0.867880	2.125029	-0.346309
6	-2.277925	2.350064	-0.513433
6	-2.923624	1.078635	-1.031425
7	-2.749790	-0.106324	-0.157060
6	-3.620604	-0.047512	1.039841
6	-3.019074	0.641323	2.243544
6	-3.830598	1.318999	3.161852
6	-3.255667	1.843888	4.315232
6	-1.884368	1.691975	4.520328
6	-1.139667	1.019983	3.554689
6	0.363186	0.853903	3.702460
8	0.914906	1.306698	4.721998
6	-3.079505	-1.323194	-0.932539
8	0.965182	0.250896	2.736612
7	-1.700396	0.497528	2.446115

8	0.874225	-2.680713	0.514882
7	2.785885	-0.827267	0.132395
1	-2.446869	-1.375868	-1.820395
1	-2.895523	-2.210372	-0.320715
1	-4.131687	-1.333449	-1.254506
1	-4.591705	0.406397	0.798802
1	-3.828279	-1.079473	1.345220
1	-2.471086	0.840202	-1.998363
1	-3.992238	1.279459	-1.206937
1	-2.437516	3.140343	-1.256264
1	-2.708884	2.685861	0.437680
1	-1.389011	2.087584	5.398452
1	-3.866089	2.369771	5.042698
1	-4.892557	1.424723	2.967077
1	4.687882	-3.548252	-0.410875
1	6.430142	-1.760579	-0.719021
1	5.754555	0.634919	-0.467544
57	0.073923	-0.278231	0.451269
7	1.908170	1.806642	-0.406366
1	3.983784	2.267206	-0.182118
1	3.149075	1.726742	1.277767
6	2.030185	1.890738	-1.873996
1	1.043568	1.916345	-2.341609
1	2.563236	1.012829	-2.247444
1	2.588693	2.787452	-2.183660
6	-0.081138	3.327460	-0.374985
1	-0.054060	3.706355	-1.403349
1	-0.544756	4.093839	0.257262
1	1.940630	3.916456	-0.025143
1	1.252589	2.890464	1.249799
8	0.197200	-1.056920	-2.170812
1	0.633682	-1.922433	-2.179550
1	0.780937	-0.480272	-2.685981

Output energies:

Zero-point correction= 0.456021 (Hartree/Particle)
Thermal correction to Energy= 0.485428
Thermal correction to Enthalpy= 0.486372
Thermal correction to Gibbs Free Energy= 0.396016
Sum of electronic and zero-point Energies= -1479.548345
Sum of electronic and thermal Energies= -1479.518938
Sum of electronic and thermal Enthalpies= -1479.517993
Sum of electronic and thermal Free Energies= -1479.608349

(16b) La-OxyMepa, N1^{S}N2^{R}(λλ), enantiomer of N1^{R}N2^{S}(δδ), q = 1

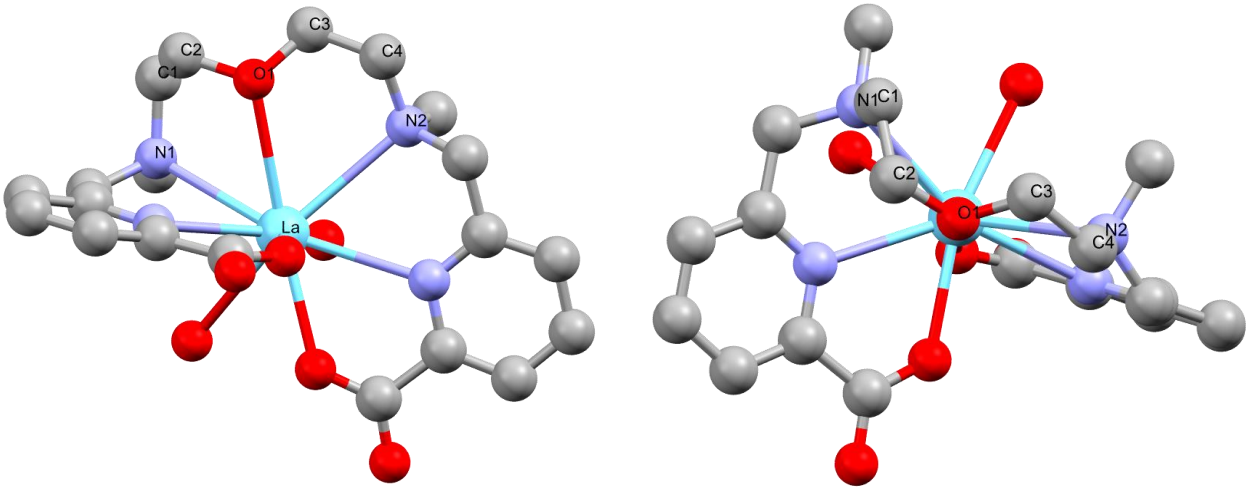

Figure S111. Side view (left) and top view (right) of optimized La-OxyMepa complex in N1^{S}N2^{R}(λλ) conformation (q = 2). Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.432964	1.734878	-0.175870
6	3.921266	0.306297	-0.116394
6	5.269645	-0.007111	-0.319635
6	5.686201	-1.328546	-0.182310
6	4.746352	-2.303572	0.147756
6	3.420685	-1.913991	0.331765
6	2.357351	-2.930268	0.704638
8	2.656840	-4.136589	0.728009
6	1.614877	3.252228	-0.615790
8	-0.597662	2.676779	0.111660
6	-2.020733	2.866104	0.043170
6	-2.686441	1.910101	-0.934666
7	-2.537797	0.468047	-0.607155
6	-3.474503	0.048691	0.461657
6	-3.055422	0.414484	1.868076
6	-4.015160	0.741654	2.833638
6	-3.602842	1.018319	4.133597
6	-2.241886	0.982378	4.435383
6	-1.343724	0.659331	3.421084
6	0.154364	0.651425	3.678227
8	0.562220	0.883662	4.830525
6	-2.858994	-0.306547	-1.827093
8	0.902754	0.409648	2.657830
7	-1.747596	0.362725	2.170340

8	1.194932	-2.446810	0.986125
7	3.019162	-0.635916	0.201686
1	-4.483701	0.443195	0.271875
1	-3.550173	-1.042870	0.420567
1	-3.752934	2.175369	-1.014027
1	-2.245680	2.066649	-1.923651
1	-2.398136	2.744004	1.059293
1	-2.240456	3.894742	-0.267529
1	-1.869575	1.206688	5.427232
1	-4.330348	1.272056	4.898128
1	-5.063523	0.781365	2.557940
1	5.019333	-3.345322	0.262945
1	6.727480	-1.594854	-0.334370
1	5.971621	0.777827	-0.580017
57	0.206687	-0.167947	0.306452
7	2.114018	1.873834	-0.822470
1	4.189475	2.359572	-0.674599
1	3.342627	2.100776	0.853740
6	2.231416	1.578290	-2.263416
6	0.131959	3.415187	-0.880730
1	-0.144071	3.079459	-1.887602
1	-0.123801	4.479410	-0.799661
1	2.162519	3.963818	-1.254515
1	1.805886	3.533680	0.424142
8	-1.348030	-2.584179	0.374865
8	0.329952	-1.262121	-2.192767
1	-2.157809	-0.048161	-2.623663
1	-3.879402	-0.099305	-2.184333
1	-2.782781	-1.376697	-1.623292
1	-1.484572	-2.865766	-0.541199
1	-0.504560	-1.718326	-2.378842
1	2.916197	2.281461	-2.763237
1	1.255161	1.647102	-2.748977
1	2.611814	0.565048	-2.409724
1	0.402830	-0.588939	-2.885740
1	-0.460107	-2.933276	0.612524

Output energies:

Zero-point correction= 0.480256 (Hartree/Particle)
Thermal correction to Energy= 0.510233
Thermal correction to Enthalpy= 0.511177
Thermal correction to Gibbs Free Energy= 0.419201
Sum of electronic and zero-point Energies= -1555.966361
Sum of electronic and thermal Energies= -1555.936384
Sum of electronic and thermal Enthalpies= -1555.935440
Sum of electronic and thermal Free Energies= -1556.027417

(17) Lu-Oxyaapa, $N1^{S}N2^{S}(\delta\delta)$, enantiomer of $N1^{R}N2^{R}(\lambda\lambda)$

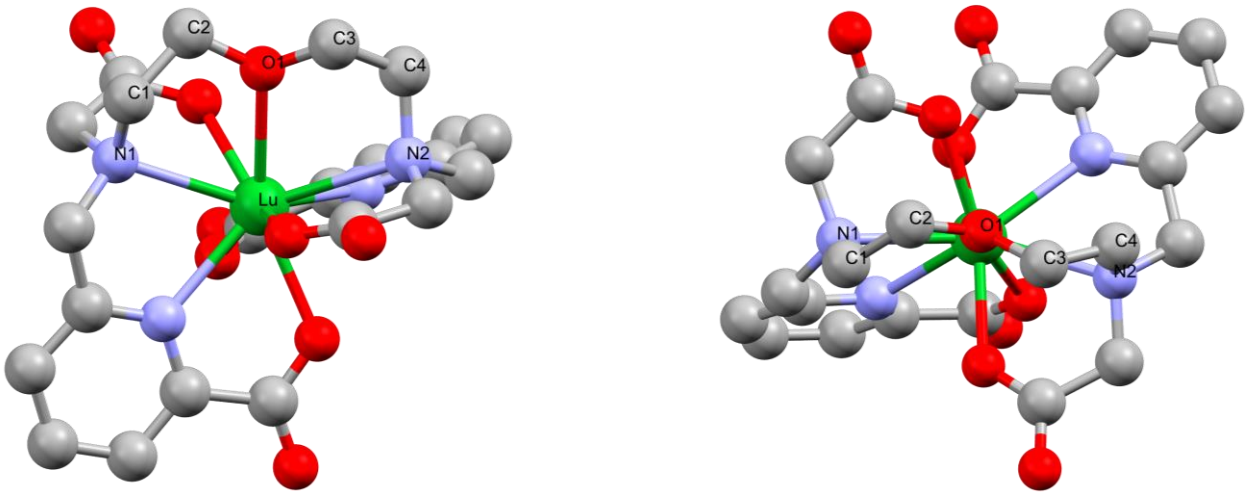

Figure S112. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in $N1^{S}N2^{S}(\delta\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
71	2.549861	0.443147	9.193226
8	3.131246	-2.002320	8.603340
8	4.733740	0.192764	8.309299
8	0.953575	-0.868033	10.325063
8	0.809539	2.084666	9.594801
8	3.626788	2.667408	8.947688
8	6.953973	-0.069717	8.531115
8	-0.831924	-2.224134	10.451525
8	0.270884	4.015343	10.621176
8	4.817195	3.957060	7.534550
7	4.282797	-0.693265	10.915067
7	0.756942	-0.747238	7.540673
7	2.585949	1.461881	11.500155
7	2.266496	1.552320	6.920937
6	4.164613	-2.170863	10.788695
1	3.224213	-2.461454	11.262935
1	4.983277	-2.673278	11.326991
6	4.145900	-2.682436	9.357841
1	5.106373	-2.541189	8.851381
1	3.938732	-3.756785	9.382086
6	2.154523	-2.812149	7.945759
1	1.473181	-3.262886	8.678410
1	2.647293	-3.623625	7.397487
6	1.435257	-1.928773	6.943604

1	2.171632	-1.559969	6.223651
1	0.707194	-2.542656	6.392503
6	5.616241	-0.202635	10.505851
1	6.416226	-0.842157	10.901791
1	5.756668	0.795959	10.935332
6	5.796059	-0.032705	8.993377
6	-0.403626	-1.157261	8.358951
1	-0.929661	-2.013610	7.918279
1	-1.115738	-0.326452	8.395870
6	-0.067661	-1.468372	9.822041
6	4.022880	-0.314004	12.322622
1	4.927044	-0.405123	12.938022
1	3.293345	-1.018381	12.736989
6	3.421791	1.062576	12.470344
6	3.628273	1.831729	13.620138
1	4.319359	1.486802	14.381841
6	2.929530	3.026960	13.766776
1	3.073862	3.641825	14.649627
6	2.034453	3.418120	12.770621
1	1.454738	4.329613	12.847743
6	1.892757	2.607254	11.648039
6	0.912684	2.950032	10.538434
6	0.341286	0.154370	6.441777
1	-0.463866	0.795641	6.815403
1	-0.068073	-0.407593	5.591816
6	1.442739	1.078565	5.974528
6	1.520986	1.525001	4.651632
1	0.851416	1.116485	3.902257
6	2.457874	2.502997	4.325434
1	2.540104	2.863397	3.304717
6	3.274864	3.027367	5.327437
1	3.995688	3.810299	5.126234
6	3.146751	2.526105	6.620518
6	3.945796	3.098607	7.783347

Output energies:

Zero-point correction= 0.439464 (Hartree/Particle)
Thermal correction to Energy= 0.471591
Thermal correction to Enthalpy= 0.472535
Thermal correction to Gibbs Free Energy= 0.376007
Sum of electronic and zero-point Energies= -1787.704099
Sum of electronic and thermal Energies= -1787.671972
Sum of electronic and thermal Enthalpies= -1787.671028
Sum of electronic and thermal Free Energies= -1787.767556

(18) Lu-Oxyaapa, $N1^{S}N2^{S}(\delta\lambda)$, enantiomer of $N1^{R}N2^{R}(\lambda\delta)$

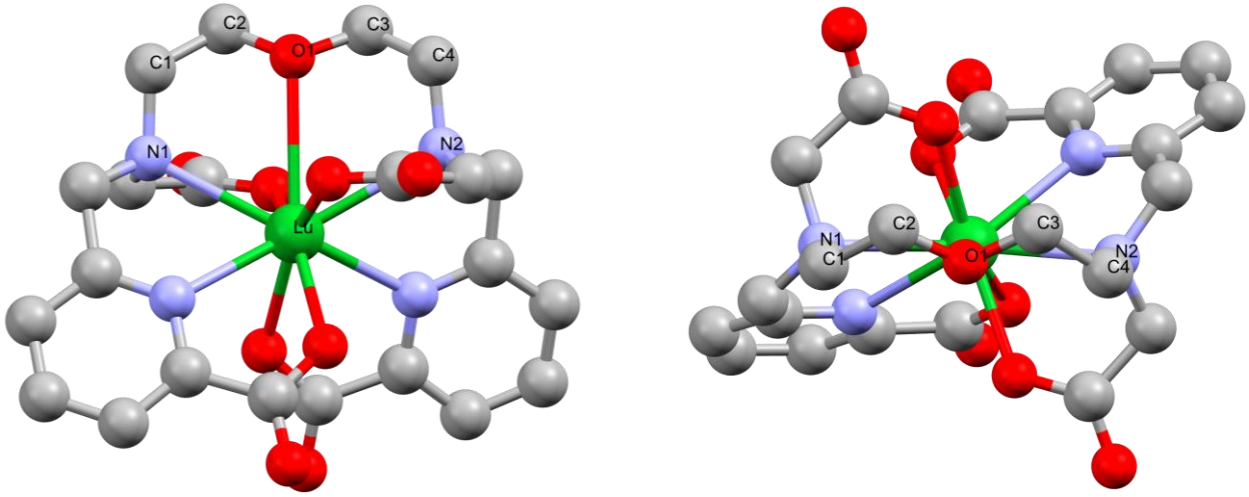

Figure S113. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in $N1^{S}N2^{S}(\delta\lambda)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
71	2.449122	0.420307	9.259597
8	2.789708	-2.502074	9.090892
8	4.485161	-0.183644	8.226888
8	0.468502	-0.607891	10.015263
8	0.961299	2.218291	9.694717
8	3.688355	2.451298	8.959569
8	6.726998	-0.315280	8.304924
8	-1.758064	-0.795807	9.762567
8	0.469801	4.123510	10.787053
8	3.872384	4.465632	7.973810
7	4.288475	-0.784317	10.948792
7	0.928938	-0.997313	7.359272
7	2.689550	1.463804	11.593752
7	2.206489	1.493040	6.938131
6	4.270707	-2.274840	10.933041
1	3.442305	-2.597390	11.569466
1	5.198727	-2.672495	11.371164
6	4.065242	-2.911480	9.570840
1	4.851939	-2.652322	8.853945
1	4.085902	-4.003664	9.698996
6	2.492715	-2.923129	7.761013
1	2.544162	-4.019076	7.691089
1	3.227452	-2.505396	7.058924
6	1.079562	-2.473610	7.438517

1	0.750913	-2.946439	6.502023
1	0.420998	-2.846293	8.227403
6	5.552119	-0.265014	10.383866
1	6.419953	-0.811151	10.778066
1	5.661265	0.782125	10.688881
6	5.607697	-0.271782	8.850352
6	-0.427273	-0.605389	7.782401
1	-1.206089	-1.205019	7.291324
1	-0.597930	0.439470	7.497835
6	-0.605248	-0.690029	9.305320
6	4.144511	-0.338839	12.353857
1	5.092346	-0.422149	12.902772
1	3.438426	-1.014763	12.848729
6	3.583891	1.054696	12.505551
6	3.910566	1.844376	13.613658
1	4.645897	1.490785	14.328575
6	3.275703	3.071507	13.780269
1	3.510640	3.699819	14.633730
6	2.335767	3.484174	12.835427
1	1.814660	4.429469	12.922357
6	2.078407	2.654411	11.748157
6	1.087931	3.047919	10.666522
6	1.215877	-0.529674	5.992665
1	0.392262	-0.764866	5.302885
1	2.093684	-1.076082	5.628244
6	1.549442	0.942193	5.905560
6	1.275796	1.671301	4.742521
1	0.731787	1.202309	3.929614
6	1.720889	2.986367	4.646229
1	1.521864	3.569839	3.752711
6	2.434495	3.540359	5.708845
1	2.818126	4.552684	5.676241
6	2.655786	2.760081	6.840039
6	3.463985	3.287804	8.013809

Output energies:

Zero-point correction= 0.439050 (Hartree/Particle)
Thermal correction to Energy= 0.471123
Thermal correction to Enthalpy= 0.472067
Thermal correction to Gibbs Free Energy= 0.375558
Sum of electronic and zero-point Energies= -1787.704166
Sum of electronic and thermal Energies= -1787.672093
Sum of electronic and thermal Enthalpies= -1787.671149
Sum of electronic and thermal Free Energies= -1787.767657

(19) Lu-Oxyaapa, $N1^{S}N2^{S}(\lambda\delta)$, enantiomer of $N1^{R}N2^{R}(\delta\lambda)$

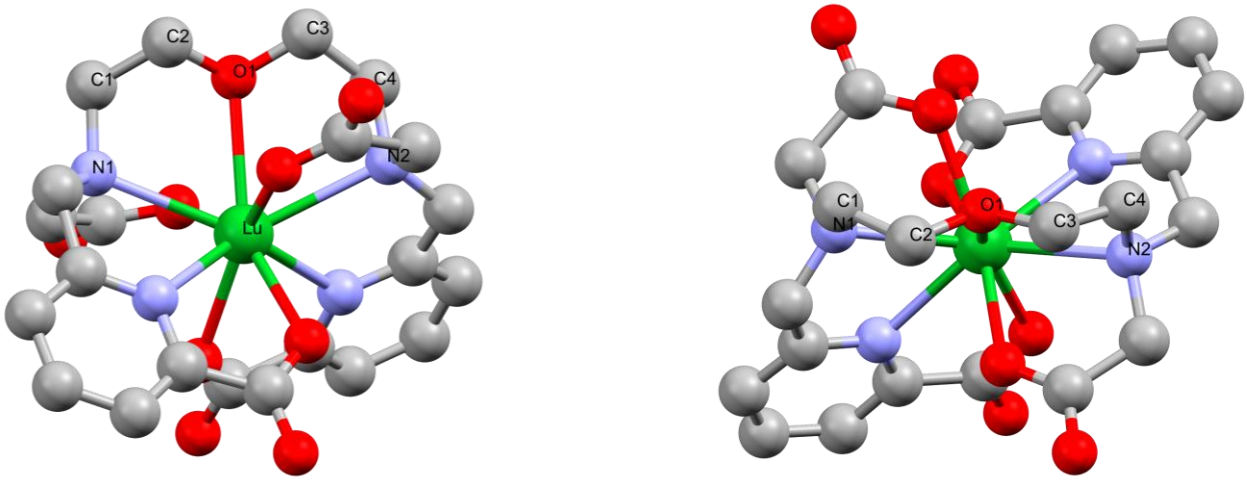

Figure S114. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in $N1^{S}N2^{S}(\lambda\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
71	2.572132	0.470596	9.120721
8	3.086581	-2.093709	8.765570
8	4.720272	0.208159	8.118946
8	0.971775	-0.776715	10.303361
8	0.889571	2.124963	9.583237
8	3.649927	2.667388	8.857854
8	6.875022	0.825044	8.315051
8	-0.864548	-2.054312	10.503268
8	0.177513	3.881086	10.799535
8	4.726492	4.040831	7.434157
7	4.526521	-0.519540	10.711023
7	0.768308	-0.751344	7.532210
7	2.642495	1.406984	11.469406
7	2.236931	1.561926	6.858396
6	4.813490	-1.948820	10.405717
1	5.260386	-2.449847	11.275004
1	5.553662	-1.987483	9.603435
6	3.588187	-2.720665	9.955750
1	3.875020	-3.756488	9.734962
1	2.803019	-2.733022	10.721722
6	2.063138	-2.840039	8.102454
1	1.311559	-3.182174	8.823567
1	2.501629	-3.731840	7.636034
6	1.459197	-1.966512	7.019804

1	2.255224	-1.639835	6.343384
1	0.756880	-2.578975	6.434404
6	5.678649	0.315114	10.320255
1	6.624540	-0.075418	10.719552
1	5.543586	1.321339	10.731829
6	5.784793	0.457679	8.794766
6	-0.402042	-1.112016	8.359156
1	-0.935644	-1.981539	7.954452
1	-1.104686	-0.272556	8.355399
6	-0.074455	-1.359498	9.835552
6	4.196468	-0.345256	12.136549
1	5.090495	-0.423977	12.771101
1	3.526869	-1.162413	12.429640
6	3.476557	0.953572	12.418340
6	3.608103	1.609104	13.647147
1	4.301255	1.228456	14.389710
6	2.837333	2.741591	13.894989
1	2.924040	3.268002	14.840330
6	1.947679	3.186449	12.917207
1	1.314532	4.051578	13.070647
6	1.879698	2.489236	11.714028
6	0.901465	2.882730	10.620468
6	0.365507	0.085833	6.378435
1	-0.484129	0.704282	6.686555
1	0.016856	-0.527620	5.537214
6	1.438669	1.043728	5.913703
6	1.512110	1.470662	4.583587
1	0.863986	1.025343	3.836246
6	2.415832	2.475422	4.247927
1	2.491353	2.823700	3.222511
6	3.213483	3.037515	5.245399
1	3.914192	3.835983	5.034712
6	3.097590	2.549546	6.544194
6	3.904654	3.137839	7.693194

Output energies:

Zero-point correction= 0.439235 (Hartree/Particle)
Thermal correction to Energy= 0.471140
Thermal correction to Enthalpy= 0.472084
Thermal correction to Gibbs Free Energy= 0.376889
Sum of electronic and zero-point Energies= -1787.707970
Sum of electronic and thermal Energies= -1787.676065
Sum of electronic and thermal Enthalpies= -1787.675121
Sum of electronic and thermal Free Energies= -1787.770315

(20) Lu-Oxyaapa, $N1^{S}N2^{S}(\lambda\lambda)$, enantiomer of $N1^{R}N2^{R}(\delta\delta)$

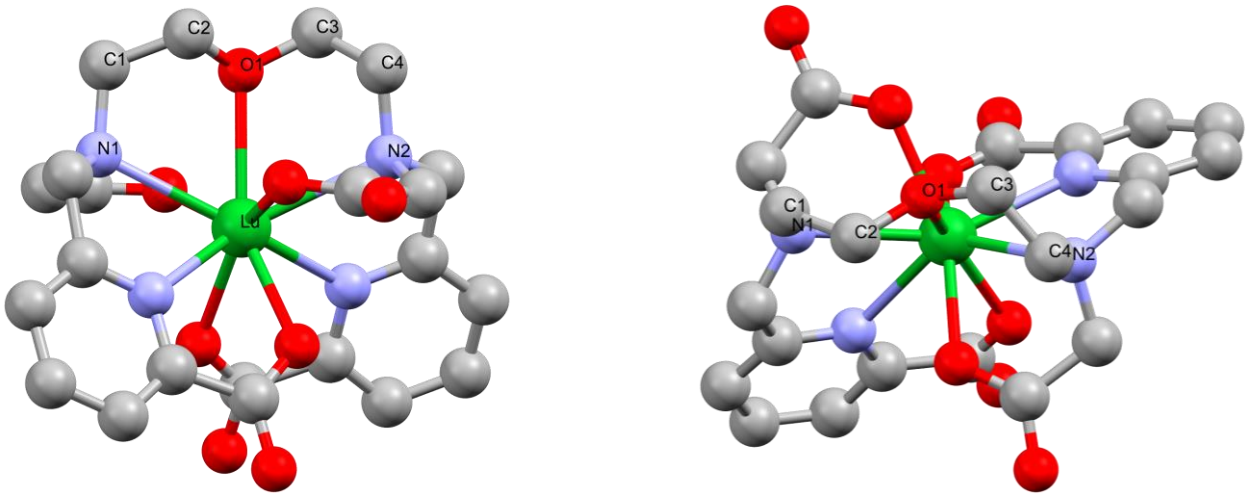

Figure S115. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in $N1^{S}N2^{S}(\lambda\lambda)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
71	2.809278	0.383142	9.012425
8	3.260969	-2.178542	8.610059
8	5.071457	0.008102	8.305940
8	0.943819	-0.624615	10.163770
8	1.251888	2.199149	9.353756
8	3.942740	2.467096	8.669563
8	7.261436	0.168013	8.800458
8	-1.302281	-0.554819	10.297266
8	0.818564	4.155335	10.381918
8	4.269715	4.359610	7.498823
7	4.440527	-0.806417	10.828183
7	0.938487	-0.877636	7.486521
7	2.775271	1.359481	11.369412
7	2.325239	1.464344	6.768597
6	4.591363	-2.266288	10.564304
1	4.788807	-2.811362	11.496532
1	5.460607	-2.413585	9.918697
6	3.383476	-2.864177	9.865604
1	3.558950	-3.932005	9.688659
1	2.467965	-2.750778	10.456977
6	2.492528	-2.819594	7.583006
1	2.540677	-3.908127	7.698454
1	2.980487	-2.559940	6.638467
6	1.048373	-2.355889	7.604548

1	0.487009	-2.855277	6.801127
1	0.595774	-2.661614	8.549377
6	5.724819	-0.113954	10.609352
1	6.552347	-0.610965	11.133056
1	5.651848	0.902137	11.013417
6	6.065067	0.020069	9.120576
6	-0.313763	-0.431829	8.123016
1	-1.183156	-0.996484	7.757971
1	-0.485439	0.622294	7.881953
6	-0.235795	-0.553714	9.652301
6	3.959551	-0.585377	12.204968
1	4.744133	-0.797618	12.944999
1	3.144145	-1.293369	12.393531
6	3.413111	0.806597	12.411307
6	3.490059	1.454253	13.648459
1	4.023868	0.987689	14.469502
6	2.871503	2.692579	13.801212
1	2.921976	3.217745	14.749887
6	2.176050	3.242912	12.724393
1	1.660124	4.192182	12.800981
6	2.146373	2.538943	11.523401
6	1.346485	3.025453	10.328577
6	1.008395	-0.470368	6.070549
1	0.050518	-0.631738	5.556951
1	1.741787	-1.110774	5.568077
6	1.458100	0.959189	5.876579
6	1.034699	1.699621	4.767220
1	0.322176	1.267824	4.072374
6	1.540050	2.981777	4.577119
1	1.228019	3.573350	3.722035
6	2.444619	3.499085	5.504244
1	2.859696	4.494088	5.402920
6	2.804561	2.712959	6.595032
6	3.750685	3.236432	7.663174

Output energies:

Zero-point correction= 0.439449 (Hartree/Particle)
Thermal correction to Energy= 0.471353
Thermal correction to Enthalpy= 0.472297
Thermal correction to Gibbs Free Energy= 0.376354
Sum of electronic and zero-point Energies= -1787.700581
Sum of electronic and thermal Energies= -1787.668678
Sum of electronic and thermal Enthalpies= -1787.667733
Sum of electronic and thermal Free Energies= -1787.763677

(21) Lu-Oxyaapa, $N1^{S}N2^{R}(\delta\delta)$, enantiomer of $N1^{R}N2^{S}(\lambda\lambda)$

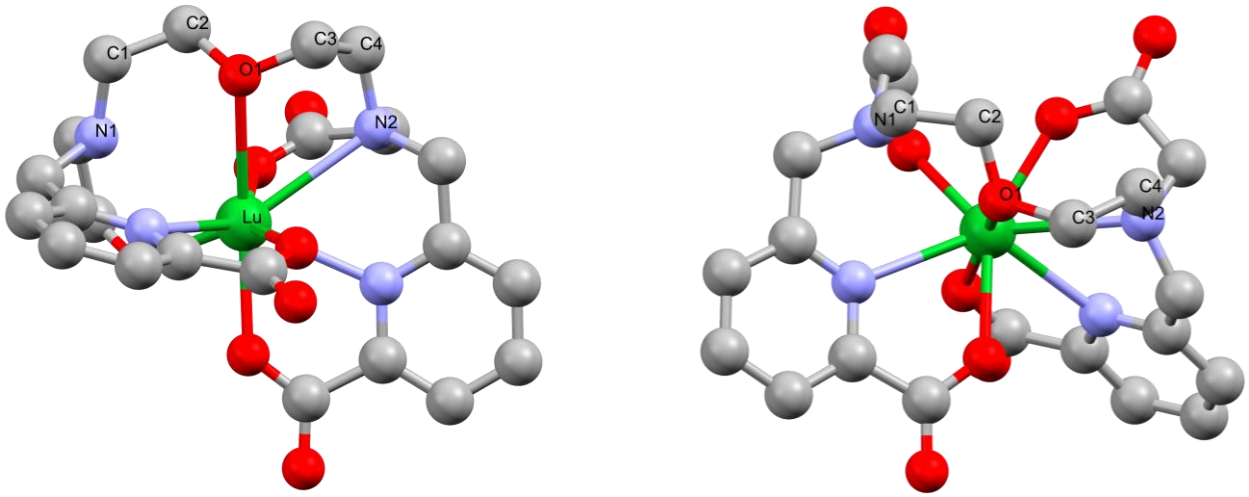

Figure S116. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in $N1^{S}N2^{R}(\delta\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.227598	1.800000	-0.447547
6	3.729165	0.428838	-0.050046
6	5.094762	0.179182	0.129508
6	5.502710	-1.078791	0.564513
6	4.538092	-2.052856	0.819932
6	3.199272	-1.727314	0.615506
6	2.088863	-2.706414	0.934994
8	2.384985	-3.860479	1.295621
6	1.331508	3.042780	-1.350768
8	-0.650809	2.536964	0.040144
6	-1.737710	2.722005	-0.880209
6	-2.951429	1.983993	-0.338854
7	-2.741398	0.527752	-0.246762
6	-3.526315	-0.069827	0.840730
6	-2.882958	0.132363	2.193073
6	-3.652586	0.284620	3.352724
6	-3.009985	0.439775	4.577832
6	-1.616038	0.473474	4.610533
6	-0.922935	0.337087	3.409403
6	0.583582	0.481167	3.345536
8	1.229687	0.539003	4.410029
6	-2.980109	-0.178276	-1.503224
8	1.086468	0.564962	2.165848
7	-1.543099	0.141062	2.233086

8	0.890570	-2.248666	0.820569
7	2.808008	-0.519984	0.172821
1	-4.559092	0.310010	0.861865
1	-3.599174	-1.147888	0.662758
1	-3.157786	2.364953	0.665718
1	-3.826579	2.231701	-0.960431
1	-1.971755	3.792073	-0.958216
1	-1.463018	2.361149	-1.878618
1	-1.069056	0.623483	5.533400
1	-3.586373	0.556566	5.490361
1	-4.735470	0.288237	3.283096
1	4.801827	-3.042017	1.173862
1	6.556762	-1.295707	0.707398
1	5.816549	0.963805	-0.071737
71	0.168845	-0.153297	0.088300
7	1.986144	1.722732	-1.226227
1	4.020633	2.340861	-0.987196
1	3.029508	2.368018	0.468896
6	2.233481	1.152322	-2.556795
6	0.467076	3.414155	-0.153744
1	0.107437	4.444274	-0.278751
1	1.038280	3.367572	0.777295
1	0.706131	3.026853	-2.247774
1	2.075974	3.840341	-1.506642
6	-2.307243	-1.557707	-1.517362
1	-2.547823	0.396160	-2.328199
1	-4.050945	-0.304336	-1.728117
8	-1.373615	-1.763526	-0.653057
8	-2.685908	-2.388483	-2.366086
6	1.010097	0.423425	-3.109592
1	3.029251	0.402641	-2.490069
1	2.572984	1.906677	-3.279306
8	0.886411	0.304141	-4.343249
8	0.201415	-0.076662	-2.241134

Output energies:

Zero-point correction= 0.438008 (Hartree/Particle)
Thermal correction to Energy= 0.469730
Thermal correction to Enthalpy= 0.470674
Thermal correction to Gibbs Free Energy= 0.374984
Sum of electronic and zero-point Energies= -1787.698875
Sum of electronic and thermal Energies= -1787.667153
Sum of electronic and thermal Enthalpies= -1787.666209
Sum of electronic and thermal Free Energies= -1787.761900

(22) Lu-Oxyaapa, N1^{S}N2^{R}($\delta\lambda$), enantiomer of N1^{R}N2^{S}($\lambda\delta$)

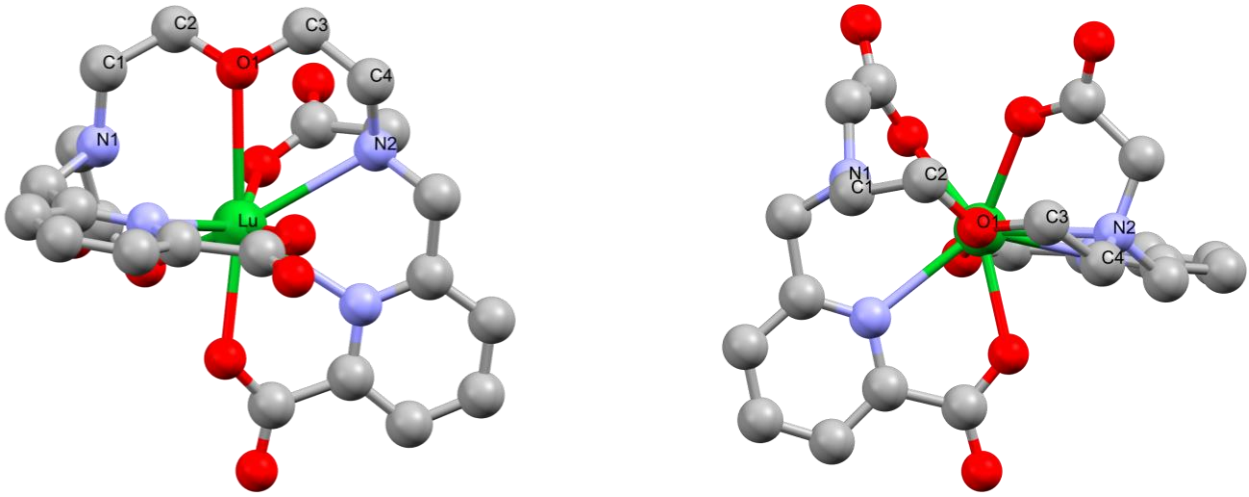

Figure S117. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in N1^{S}N2^{R}($\delta\lambda$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.364765	1.666799	-0.139155
6	3.720628	0.208599	0.035365
6	5.040553	-0.250297	-0.022775
6	5.303383	-1.591672	0.249083
6	4.249404	-2.435380	0.599180
6	2.963538	-1.901547	0.643050
6	1.771217	-2.705722	1.125291
8	1.911433	-3.923035	1.346837
6	1.558626	3.208106	-0.588473
8	-0.777744	2.614584	-0.574746
6	-2.036385	2.640254	-1.253815
6	-3.047758	1.816431	-0.477018
7	-2.675607	0.394300	-0.338581
6	-3.391742	-0.223665	0.786536
6	-2.818240	0.194517	2.118786
6	-3.619974	0.320746	3.258523
6	-3.027987	0.677213	4.466950
6	-1.655383	0.923835	4.503011
6	-0.928871	0.793485	3.322418
6	0.550668	1.106465	3.254385
8	1.164200	1.368443	4.306484
6	-2.902354	-0.372085	-1.566364
8	1.063162	1.095623	2.075693
7	-1.496769	0.419744	2.161640

8	0.690644	-2.030655	1.303983
7	2.708251	-0.618108	0.335956
1	-4.469425	-0.001331	0.758833
1	-3.293248	-1.311124	0.699044
1	-3.136568	2.243463	0.526108
1	-4.032152	1.929417	-0.959095
1	-2.404415	3.673945	-1.315669
1	-1.905990	2.273840	-2.280840
1	-1.151731	1.221782	5.414431
1	-3.629855	0.776940	5.364805
1	-4.688212	0.145026	3.186869
1	4.408654	-3.478238	0.845157
1	6.319073	-1.971617	0.199719
1	5.840851	0.437183	-0.274916
71	0.185596	0.001544	0.162394
7	2.072052	1.839795	-0.828078
1	4.177686	2.195870	-0.656250
1	3.280064	2.107548	0.859699
6	2.234274	1.565321	-2.269428
6	0.190545	3.467273	-1.189732
1	0.190058	3.308920	-2.275793
1	-0.075049	4.519028	-1.013245
1	2.250970	3.960446	-0.999767
1	1.509236	3.362259	0.493257
6	-2.083112	-1.667952	-1.621851
1	-2.595387	0.227336	-2.428335
1	-3.964542	-0.619147	-1.717310
8	-1.111357	-1.792426	-0.789758
8	-2.395800	-2.511235	-2.487176
6	1.010475	0.924912	-2.925642
1	3.044679	0.839179	-2.398607
1	2.526821	2.466335	-2.823692
8	0.811161	1.123525	-4.139984
8	0.295495	0.155626	-2.181804

Output energies:

Zero-point correction= 0.438476 (Hartree/Particle)
Thermal correction to Energy= 0.470079
Thermal correction to Enthalpy= 0.471023
Thermal correction to Gibbs Free Energy= 0.375714
Sum of electronic and zero-point Energies= -1787.704099
Sum of electronic and thermal Energies= -1787.672496
Sum of electronic and thermal Enthalpies= -1787.671552
Sum of electronic and thermal Free Energies= -1787.766861

(23) Lu-Oxyaapa, N1^{S}N2^{R}($\lambda\delta$), enantiomer of N1^{R}N2^{S}($\delta\lambda$)

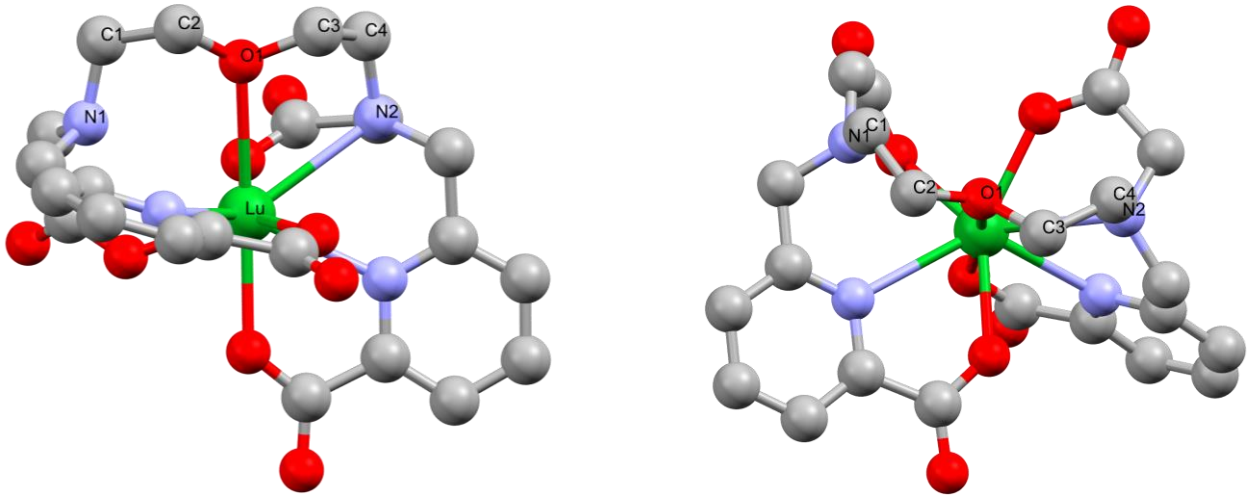

Figure S118. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in N1^{S}N2^{R}($\lambda\delta$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.260478	1.781734	-0.326330
6	3.767159	0.408566	0.046871
6	5.125998	0.170828	0.281540
6	5.531207	-1.097212	0.689410
6	4.568947	-2.090659	0.866506
6	3.236409	-1.773384	0.614065
6	2.119001	-2.761977	0.864619
8	2.401186	-3.924850	1.208539
6	1.421006	3.032653	-1.312556
8	-0.676787	2.323399	-0.438622
6	-1.990711	2.742758	-0.044264
6	-3.007762	1.879139	-0.781987
7	-2.826190	0.441472	-0.549467
6	-3.574256	-0.071205	0.599547
6	-2.946867	0.243104	1.939669
6	-3.750435	0.498985	3.058067
6	-3.148212	0.750241	4.287011
6	-1.756361	0.771065	4.361539
6	-1.027538	0.525444	3.199353
6	0.481558	0.641408	3.186989
8	1.087602	0.793395	4.264737
6	-3.024502	-0.401965	-1.721022
8	1.034153	0.603894	2.026895
7	-1.607651	0.237545	2.020394

8	0.928888	-2.296399	0.713880
7	2.848476	-0.557974	0.192006
1	-4.615658	0.289227	0.599644
1	-3.627451	-1.162315	0.514993
1	-4.018885	2.218905	-0.503858
1	-2.889557	2.072183	-1.852055
1	-2.097601	2.680947	1.044084
1	-2.142283	3.788351	-0.340737
1	-1.235890	0.992476	5.285267
1	-3.752214	0.949381	5.166868
1	-4.830241	0.507340	2.951515
1	4.828909	-3.087997	1.199746
1	6.580667	-1.306168	0.872216
1	5.844588	0.971674	0.142375
71	0.242059	-0.180429	-0.034718
7	2.068533	1.705069	-1.182232
1	4.068184	2.360748	-0.799321
1	2.988596	2.311074	0.594374
6	2.409850	1.171674	-2.511484
6	0.364227	3.294904	-0.255317
1	-0.039205	4.304003	-0.400812
1	0.766431	3.229106	0.763591
1	0.927067	3.077266	-2.287252
1	2.168881	3.838998	-1.292806
6	-2.267324	-1.732634	-1.608812
1	-2.626727	0.111010	-2.602516
1	-4.082761	-0.624211	-1.932454
8	-1.306605	-1.797989	-0.756491
8	-2.610991	-2.665336	-2.363062
6	1.246388	0.425884	-3.166089
1	3.218163	0.439420	-2.411083
1	2.775690	1.953031	-3.189944
8	1.200226	0.359437	-4.408605
8	0.409559	-0.146512	-2.370166

Output energies:

Zero-point correction= 0.437933 (Hartree/Particle)
Thermal correction to Energy= 0.470715
Thermal correction to Enthalpy= 0.471660
Thermal correction to Gibbs Free Energy= 0.371737
Sum of electronic and zero-point Energies= -1787.695364
Sum of electronic and thermal Energies= -1787.662581
Sum of electronic and thermal Enthalpies= -1787.661637
Sum of electronic and thermal Free Energies= -1787.761560

(24) Lu-Oxyaapa, $N1^{S}N2^{R}(\lambda\lambda)$, enantiomer of $N1^{R}N2^{S}(\delta\delta)$

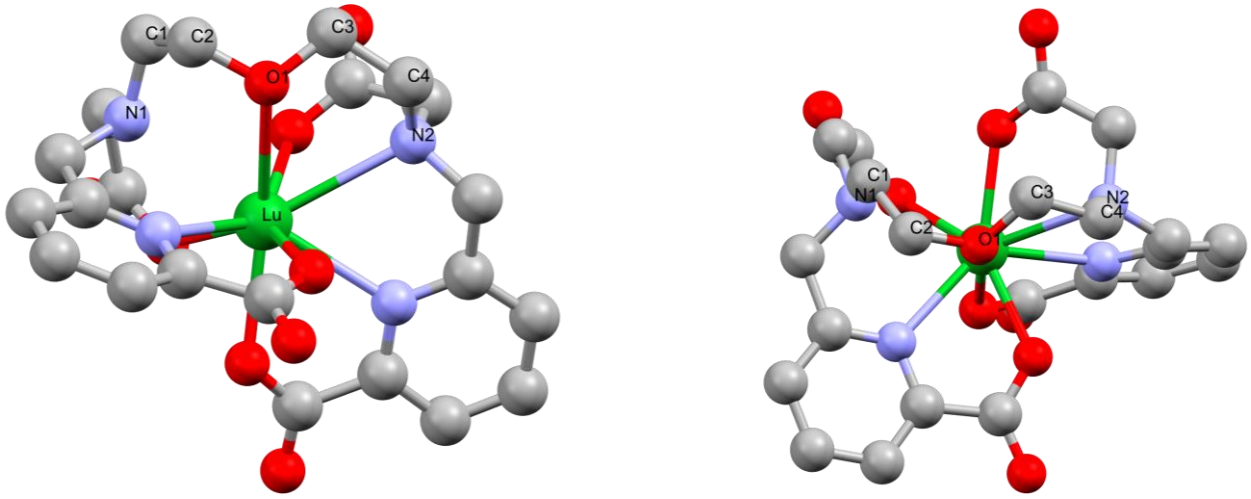

Figure S119. Side view (left) and top view (right) of optimized Lu-Oxyaapa complex in $N1^{S}N2^{R}(\lambda\lambda)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.373544	1.661772	-0.255214
6	3.768002	0.213318	-0.073326
6	5.097310	-0.208587	-0.178533
6	5.413416	-1.530168	0.129935
6	4.402512	-2.388166	0.561305
6	3.101601	-1.893804	0.640072
6	1.963459	-2.724713	1.208186
8	2.175785	-3.924429	1.476517
6	1.513701	3.167641	-0.636116
8	-0.717095	2.601592	0.060227
6	-2.141859	2.728034	-0.077623
6	-2.743410	1.677529	-1.003935
7	-2.516922	0.282266	-0.568743
6	-3.377824	-0.117936	0.560667
6	-2.849752	0.273379	1.919212
6	-3.723167	0.522499	2.985143
6	-3.197471	0.849639	4.230646
6	-1.813449	0.953018	4.374743
6	-1.012134	0.708868	3.263990
6	0.486953	0.916907	3.307499
8	1.037639	1.145481	4.400689
6	-2.722364	-0.659108	-1.679692
8	1.078483	0.868250	2.167870
7	-1.519420	0.344451	2.069714

8	0.860803	-2.098001	1.405951
7	2.793949	-0.631172	0.296934
1	-4.398921	0.273130	0.439506
1	-3.463005	-1.210453	0.549984
1	-3.819611	1.891799	-1.112174
1	-2.292433	1.789760	-1.993767
1	-2.555589	2.662804	0.930608
1	-2.387105	3.722652	-0.469554
1	-1.354563	1.237712	5.313706
1	-3.855968	1.045279	5.071166
1	-4.794680	0.467936	2.824052
1	4.605734	-3.413904	0.843646
1	6.437041	-1.882618	0.049526
1	5.863341	0.493027	-0.491187
71	0.210581	-0.083795	0.196032
7	2.048539	1.808995	-0.884974
1	4.155375	2.197253	-0.812837
1	3.329058	2.112564	0.742244
6	2.147248	1.524683	-2.329085
6	0.032164	3.325256	-0.927343
1	-0.226033	2.988398	-1.938783
1	-0.221176	4.391608	-0.860087
1	2.060064	3.914210	-1.234109
1	1.676619	3.409691	0.417792
6	-1.960144	-1.972978	-1.482414
1	-2.335898	-0.214601	-2.600127
1	-3.785079	-0.881349	-1.851731
8	-0.995760	-1.969324	-0.631951
8	-2.293280	-2.951909	-2.180154
6	0.923465	0.828046	-2.918134
1	2.977705	0.828635	-2.494408
1	2.373008	2.430542	-2.906213
8	0.663452	0.992403	-4.125401
8	0.275788	0.044473	-2.128697

Output energies:

Zero-point correction= 0.438861 (Hartree/Particle)
Thermal correction to Energy= 0.470317
Thermal correction to Enthalpy= 0.471261
Thermal correction to Gibbs Free Energy= 0.376726
Sum of electronic and zero-point Energies= -1787.700233
Sum of electronic and thermal Energies= -1787.668777
Sum of electronic and thermal Enthalpies= -1787.667833
Sum of electronic and thermal Free Energies= -1787.762368

(25) La-Oxyaapa, $N1^{S}N2^{S}(\delta\delta)$, enantiomer of $N1^{R}N2^{R}(\lambda\lambda)$

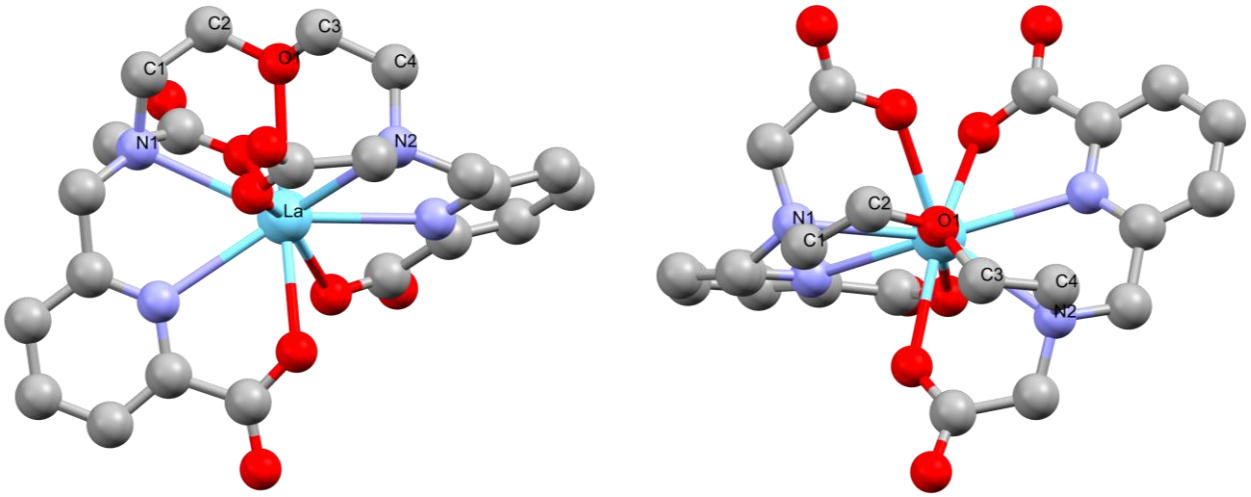

Figure S120. Side view (left) and top view (right) of optimized La-Oxyaapa complex in $N1^{S}N2^{S}(\delta\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.582813	0.804195	9.141903
8	3.370004	-1.757579	8.372866
8	5.102772	0.642603	8.779131
8	0.901719	-0.748587	10.248395
8	1.029960	2.661554	9.991620
8	3.518323	3.103687	8.246338
8	7.232255	0.134510	9.289627
8	-0.667553	-2.352264	10.352025
8	0.861182	4.563388	11.187378
8	4.677419	4.065811	6.569818
7	4.191396	-0.720313	11.078399
7	0.716258	-0.707603	7.434377
7	2.615881	1.539372	11.839221
7	2.064221	1.648915	6.508879
6	4.078100	-2.148569	10.696801
1	3.066859	-2.481889	10.945685
1	4.783243	-2.764592	11.279492
6	4.323992	-2.427258	9.221385
1	5.319692	-2.109788	8.902656
1	4.261764	-3.508425	9.059015
6	2.337872	-2.610909	7.857042
1	1.735987	-3.024168	8.675174
1	2.798287	-3.451919	7.323947
6	1.501813	-1.829203	6.861174

1	2.174908	-1.418475	6.102462
1	0.830290	-2.540317	6.354121
6	5.579363	-0.231970	10.971211
1	6.294799	-0.968479	11.362699
1	5.675326	0.667842	11.589903
6	6.015656	0.194050	9.563040
6	-0.390859	-1.210213	8.272213
1	-0.850234	-2.110383	7.842743
1	-1.169719	-0.440820	8.312907
6	-0.016983	-1.484159	9.735218
6	3.703248	-0.543733	12.462130
1	4.435701	-0.904072	13.198539
1	2.804520	-1.158235	12.581708
6	3.313958	0.882782	12.779727
6	3.579444	1.459140	14.025880
1	4.152518	0.909392	14.765028
6	3.093864	2.737408	14.295866
1	3.291326	3.206775	15.254723
6	2.346156	3.401277	13.324271
1	1.936512	4.389096	13.496071
6	2.125570	2.762806	12.104322
6	1.273449	3.399089	11.014996
6	0.187090	0.117794	6.326010
1	-0.577094	0.782829	6.742789
1	-0.305413	-0.500366	5.561637
6	1.235732	0.993438	5.679384
6	1.279617	1.186933	4.295661
1	0.600593	0.638877	3.651170
6	2.200482	2.091413	3.769844
1	2.255646	2.257475	2.698379
6	3.043175	2.784402	4.637051
1	3.765804	3.506044	4.276356
6	2.941073	2.536801	6.005970
6	3.794260	3.299817	7.011371

Output energies:

Zero-point correction= 0.436503 (Hartree/Particle)
Thermal correction to Energy= 0.468073
Thermal correction to Enthalpy= 0.469018
Thermal correction to Gibbs Free Energy= 0.371174
Sum of electronic and zero-point Energies= -1779.355698
Sum of electronic and thermal Energies= -1779.324127
Sum of electronic and thermal Enthalpies= -1779.323183
Sum of electronic and thermal Free Energies= -1779.421026

(26) La-Oxyaapa, N1^{S}N2^{S}($\delta\lambda$), enantiomer of N1^{R}N2^{R}($\lambda\delta$)

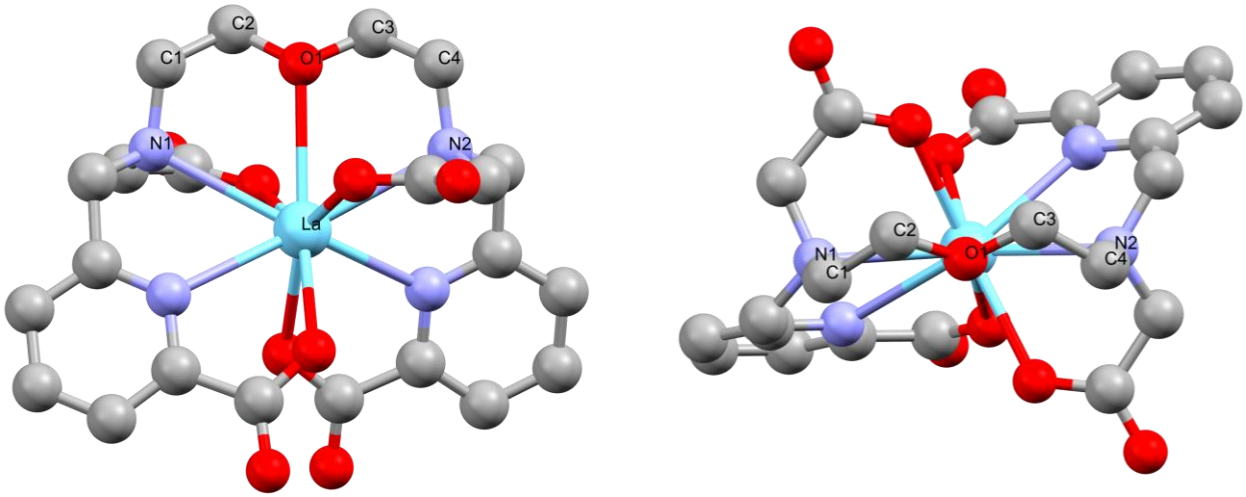

Figure S121. Side view (left) and top view (right) of optimized La-Oxyaapa complex in N1^{S}N2^{S}($\delta\lambda$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.398886	0.435492	9.245404
8	2.828611	-2.365639	9.052791
8	4.773577	-0.036947	8.430631
8	0.143755	-0.675791	9.847279
8	0.856982	2.322154	10.107021
8	3.515672	2.719409	8.715634
8	6.975312	-0.387494	8.709642
8	-2.031791	-0.853082	9.292796
8	0.735051	4.332796	11.114376
8	3.496707	4.704346	7.651807
7	4.288435	-0.839696	11.111307
7	0.942730	-0.999799	7.226332
7	2.749404	1.483220	11.823496
7	2.154472	1.541591	6.711397
6	4.197036	-2.318596	11.016937
1	3.317844	-2.632481	11.586719
1	5.076570	-2.792557	11.480349
6	4.048855	-2.865956	9.609115
1	4.895355	-2.612250	8.961285
1	3.997935	-3.961331	9.673644
6	2.547544	-2.869433	7.740753
1	2.615282	-3.965259	7.745312
1	3.291724	-2.486271	7.029149
6	1.131181	-2.467904	7.370803

1	0.841078	-2.987843	6.446189
1	0.465069	-2.824397	8.160074
6	5.612154	-0.353656	10.667862
1	6.420755	-0.956535	11.104368
1	5.740378	0.671125	11.035930
6	5.812124	-0.275291	9.147559
6	-0.459159	-0.641474	7.511874
1	-1.161514	-1.252670	6.927470
1	-0.620571	0.402283	7.217766
6	-0.823424	-0.745866	9.002252
6	4.068879	-0.438224	12.520335
1	4.950790	-0.650988	13.140638
1	3.249182	-1.046965	12.917716
6	3.662577	1.008313	12.686191
6	4.137320	1.783339	13.748942
1	4.881396	1.376336	14.425348
6	3.635089	3.071621	13.922225
1	3.988854	3.692329	14.739648
6	2.672096	3.551006	13.035954
1	2.247150	4.542093	13.136158
6	2.256722	2.723783	11.993175
6	1.199673	3.180279	10.996764
6	1.316644	-0.583144	5.858819
1	0.577279	-0.931425	5.123214
1	2.265894	-1.069459	5.607121
6	1.521021	0.907300	5.710729
6	1.138539	1.578450	4.544856
1	0.620649	1.041203	3.757511
6	1.436184	2.933018	4.417046
1	1.148166	3.475480	3.521838
6	2.110474	3.580990	5.450797
1	2.370566	4.630640	5.392944
6	2.452499	2.848625	6.586520
6	3.212910	3.491558	7.738848

Output energies:

Zero-point correction= 0.436474 (Hartree/Particle)
Thermal correction to Energy= 0.468022
Thermal correction to Enthalpy= 0.468966
Thermal correction to Gibbs Free Energy= 0.370480
Sum of electronic and zero-point Energies= -1779.359452
Sum of electronic and thermal Energies= -1779.327904
Sum of electronic and thermal Enthalpies= -1779.326960
Sum of electronic and thermal Free Energies= -1779.425446

(27) La-Oxyaapa, $N1^{S}N2^{S}(\delta\lambda)$, enantiomer of $N1^{R}N2^{R}(\lambda\delta)$

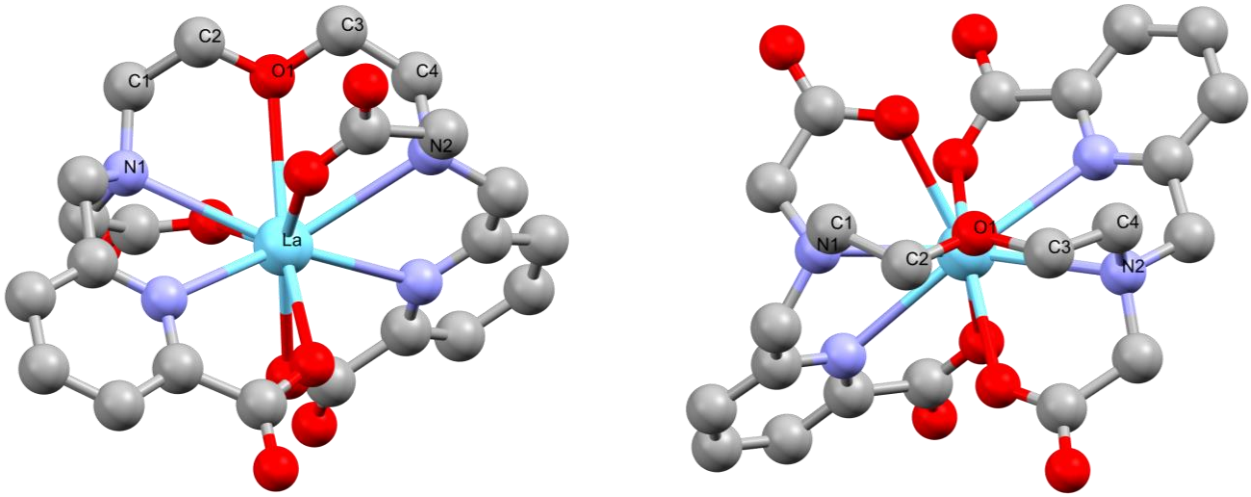

Figure S122. Side view (left) and top view (right) of optimized La-Oxyaapa complex in $N1^{S}N2^{S}(\lambda\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.599025	0.823649	9.094671
8	3.092633	-1.951510	8.718078
8	5.075759	0.576357	8.365841
8	0.775226	-0.561221	10.247395
8	1.068451	2.665300	10.015248
8	3.514772	3.125380	8.222628
8	7.210697	1.012577	8.929809
8	-0.865001	-2.092303	10.363531
8	0.487605	4.252474	11.501842
8	4.670326	4.122222	6.564265
7	4.519445	-0.485888	10.833483
7	0.700382	-0.662341	7.419685
7	2.681345	1.463353	11.811901
7	2.105871	1.653428	6.462733
6	4.812319	-1.871397	10.383025
1	5.283007	-2.450586	11.191050
1	5.534784	-1.822885	9.565010
6	3.593026	-2.621770	9.883686
1	3.890460	-3.645347	9.620908
1	2.800041	-2.681051	10.640628
6	2.080410	-2.697674	8.034744
1	1.327133	-3.053328	8.748026
1	2.532962	-3.583591	7.569383
6	1.466974	-1.842930	6.941183

1	2.267019	-1.484028	6.285472
1	0.815296	-2.493957	6.336655
6	5.721353	0.352414	10.675138
1	6.603245	-0.101271	11.149683
1	5.549216	1.313969	11.172938
6	6.044858	0.662648	9.205299
6	-0.455855	-1.078783	8.240463
1	-0.933732	-1.983430	7.841776
1	-1.204594	-0.279723	8.210364
6	-0.150917	-1.285539	9.732349
6	4.073449	-0.496780	12.239875
1	4.899284	-0.763663	12.915790
1	3.313849	-1.279849	12.346978
6	3.450202	0.804413	12.693489
6	3.605869	1.255490	14.008778
1	4.244326	0.709205	14.694998
6	2.929296	2.403049	14.413770
1	3.034769	2.772211	15.429226
6	2.112795	3.068405	13.500016
1	1.558773	3.958024	13.772840
6	2.016215	2.566176	12.203300
6	1.117852	3.229162	11.167797
6	0.242886	0.106416	6.240543
1	-0.553128	0.782862	6.569931
1	-0.195432	-0.552247	5.477110
6	1.317013	0.968821	5.618309
6	1.410029	1.133053	4.232914
1	0.764160	0.560166	3.575995
6	2.333527	2.042750	3.721726
1	2.424638	2.187952	2.649690
6	3.131898	2.768833	4.603953
1	3.854027	3.496285	4.254294
6	2.987477	2.544423	5.972657
6	3.802404	3.331691	6.990896

Output energies:

Zero-point correction= 0.437640 (Hartree/Particle)
Thermal correction to Energy= 0.469289
Thermal correction to Enthalpy= 0.470233
Thermal correction to Gibbs Free Energy= 0.374784
Sum of electronic and zero-point Energies= -1779.358868
Sum of electronic and thermal Energies= -1779.327219
Sum of electronic and thermal Enthalpies= -1779.326275
Sum of electronic and thermal Free Energies= -1779.421723

(28) La-Oxyaapa, N1^{S}N2^S($\lambda\lambda$), enantiomer of N1^{R}N2^R($\delta\delta$)

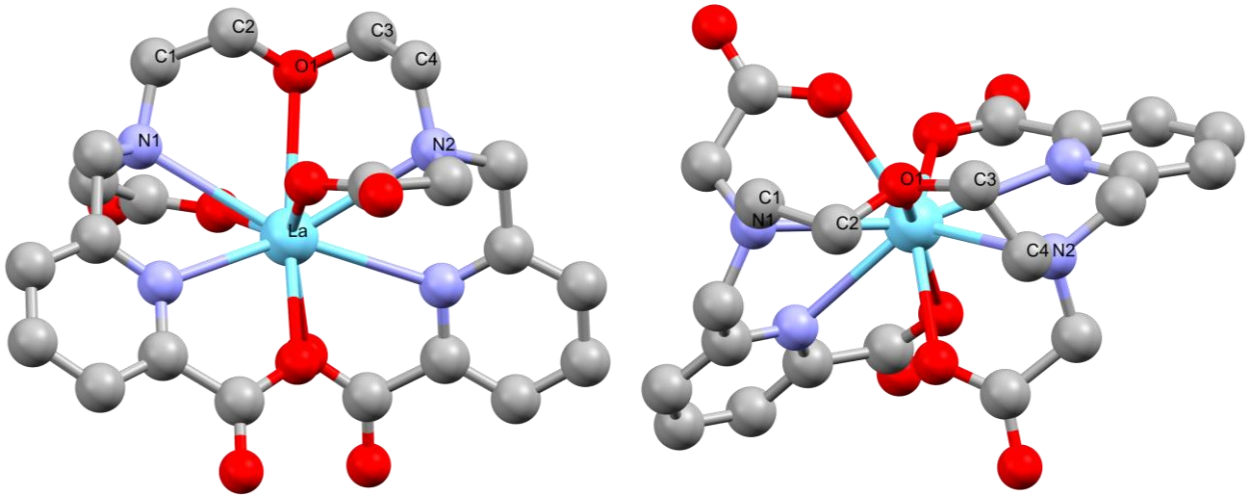

Figure S123. Side view (left) and top view (right) of optimized La-Oxyaapa complex in N1^{S}N2^S($\lambda\lambda$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
57	2.973271	0.660511	8.953254
8	3.407037	-2.123476	8.551524
8	5.509406	0.286933	8.709580
8	0.837421	-0.324047	10.045655
8	1.649014	2.748361	9.662628
8	4.057078	2.720574	7.870667
8	7.607882	0.232065	9.515263
8	-1.408571	-0.186263	10.034771
8	1.429603	4.582801	10.949490
8	3.943921	4.600555	6.638029
7	4.502267	-0.855883	11.006607
7	0.959577	-0.845222	7.357669
7	2.895208	1.415421	11.646704
7	2.219974	1.499010	6.321726
6	4.631895	-2.278175	10.602244
1	4.791706	-2.919048	11.481838
1	5.519814	-2.377554	9.972289
6	3.445338	-2.807740	9.816386
1	3.587406	-3.881843	9.643422
1	2.500457	-2.667142	10.355978
6	2.583596	-2.740982	7.547875
1	2.636220	-3.831667	7.647821
1	3.035613	-2.473060	6.588564
6	1.130401	-2.294841	7.618743

1	0.539764	-2.893721	6.907108
1	0.742554	-2.512555	8.615982
6	5.826821	-0.215922	11.043084
1	6.564343	-0.825854	11.583644
1	5.746425	0.735761	11.580418
6	6.372259	0.112350	9.645489
6	-0.311876	-0.368936	7.926947
1	-1.162542	-0.988101	7.605114
1	-0.501942	0.645922	7.558267
6	-0.305019	-0.296429	9.461183
6	3.824320	-0.748069	12.309081
1	4.453903	-1.137014	13.123805
1	2.928020	-1.378989	12.277150
6	3.382343	0.659868	12.645220
6	3.407819	1.120762	13.966260
1	3.815463	0.490353	14.749402
6	2.901925	2.386121	14.252075
1	2.911953	2.764232	15.269631
6	2.378745	3.156578	13.214996
1	1.963975	4.141801	13.388985
6	2.389020	2.631474	11.923565
6	1.777787	3.399614	10.761041
6	1.006687	-0.576638	5.908315
1	0.075420	-0.889056	5.412995
1	1.808594	-1.182295	5.473164
6	1.302865	0.867013	5.571055
6	0.696178	1.488388	4.474149
1	-0.047788	0.953146	3.893666
6	1.060846	2.791804	4.147089
1	0.603132	3.295011	3.301017
6	2.016633	3.442048	4.925470
1	2.332129	4.456478	4.715386
6	2.568595	2.761629	6.009966
6	3.604849	3.428534	6.902131

Output energies:

Zero-point correction= 0.435613 (Hartree/Particle)
Thermal correction to Energy= 0.465714
Thermal correction to Enthalpy= 0.466659
Thermal correction to Gibbs Free Energy= 0.373885
Sum of electronic and zero-point Energies= -1779.359470
Sum of electronic and thermal Energies= -1779.329369
Sum of electronic and thermal Enthalpies= -1779.328425
Sum of electronic and thermal Free Energies= -1779.421199

(29) La-Oxyaapa, $N1^{S}N2^{R}(\delta\delta)$, enantiomer of $N1^{R}N2^{S}(\lambda\lambda)$

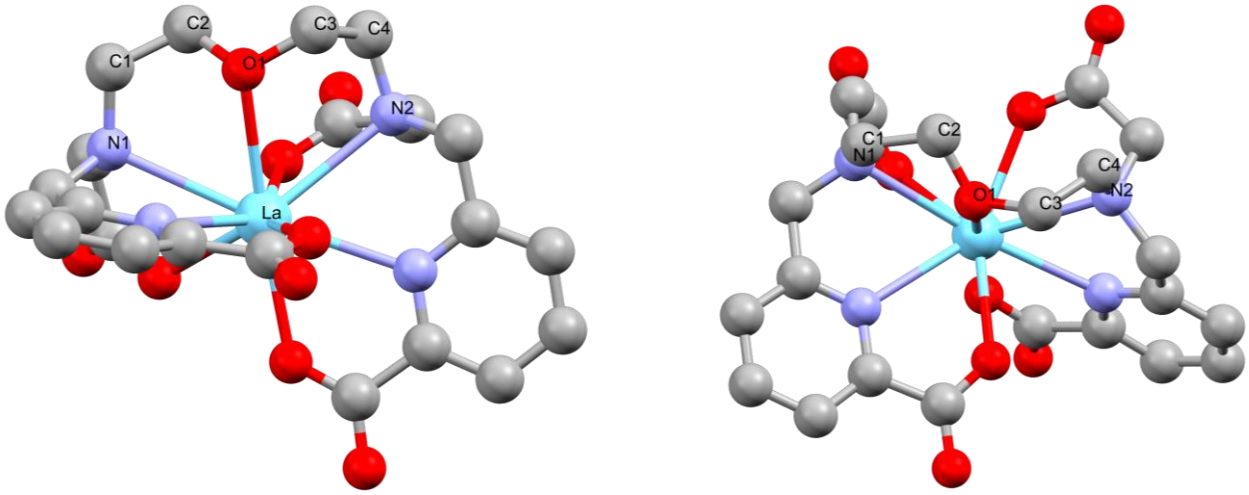

Figure S124. Side view (left) and top view (right) of optimized La-Oxyaapa complex in $N1^{S}N2^{R}(\delta\delta)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.248596	1.767711	-0.432011
6	3.796115	0.404270	-0.063649
6	5.172763	0.188833	0.066635
6	5.625088	-1.065327	0.468561
6	4.695756	-2.071056	0.731407
6	3.341276	-1.782403	0.573671
6	2.275453	-2.824945	0.875807
8	2.644377	-3.957230	1.245662
6	1.365072	3.019642	-1.345093
8	-0.628987	2.469370	-0.005100
6	-1.743112	2.685951	-0.894665
6	-2.940424	1.945546	-0.321696
7	-2.724665	0.481867	-0.229462
6	-3.510984	-0.098081	0.875233
6	-2.925284	0.194382	2.237044
6	-3.747561	0.379510	3.354138
6	-3.159818	0.576998	4.600547
6	-1.769092	0.606991	4.696492
6	-1.017391	0.438405	3.534414
6	0.500352	0.520730	3.562098
8	1.069861	0.587791	4.670539
6	-3.059634	-0.205202	-1.485760
8	1.086362	0.527752	2.420503
7	-1.586773	0.221692	2.334776

8	1.054249	-2.451142	0.730574
7	2.908066	-0.572591	0.176092
1	-4.558595	0.235702	0.841828
1	-3.524270	-1.185505	0.744063
1	-3.124428	2.329880	0.685378
1	-3.830597	2.181473	-0.923786
1	-1.967674	3.758334	-0.940309
1	-1.493234	2.340000	-1.904492
1	-1.266168	0.769616	5.641766
1	-3.776717	0.717989	5.482646
1	-4.826181	0.367996	3.237188
1	4.998467	-3.060193	1.052549
1	6.688331	-1.257136	0.575016
1	5.868633	0.993294	-0.146904
57	0.137765	-0.157272	0.107140
7	2.006231	1.687138	-1.222112
1	4.024620	2.342866	-0.959375
1	3.032005	2.310564	0.495520
6	2.279154	1.148506	-2.567247
6	0.478537	3.375649	-0.161612
1	0.100533	4.398268	-0.280283
1	1.029666	3.324232	0.781418
1	0.756572	3.021140	-2.253838
1	2.121384	3.809581	-1.473378
6	-2.476561	-1.625805	-1.572793
1	-2.637029	0.360238	-2.322205
1	-4.146237	-0.256650	-1.651296
8	-1.512524	-1.922385	-0.774254
8	-2.954421	-2.389257	-2.436539
6	1.025715	0.571252	-3.236498
1	2.993008	0.322454	-2.483926
1	2.734114	1.902913	-3.223187
8	0.921279	0.658628	-4.477022
8	0.183828	-0.018031	-2.464573

Output energies:

Zero-point correction= 0.437072 (Hartree/Particle)
Thermal correction to Energy= 0.468331
Thermal correction to Enthalpy= 0.469275
Thermal correction to Gibbs Free Energy= 0.373373
Sum of electronic and zero-point Energies= -1779.360266
Sum of electronic and thermal Energies= -1779.329007
Sum of electronic and thermal Enthalpies= -1779.328063
Sum of electronic and thermal Free Energies= -1779.423965

(30) La-Oxyaapa, N1^{S}N2^{R}($\delta\lambda$), enantiomer of N1^{R}N2^{S}($\lambda\delta$)

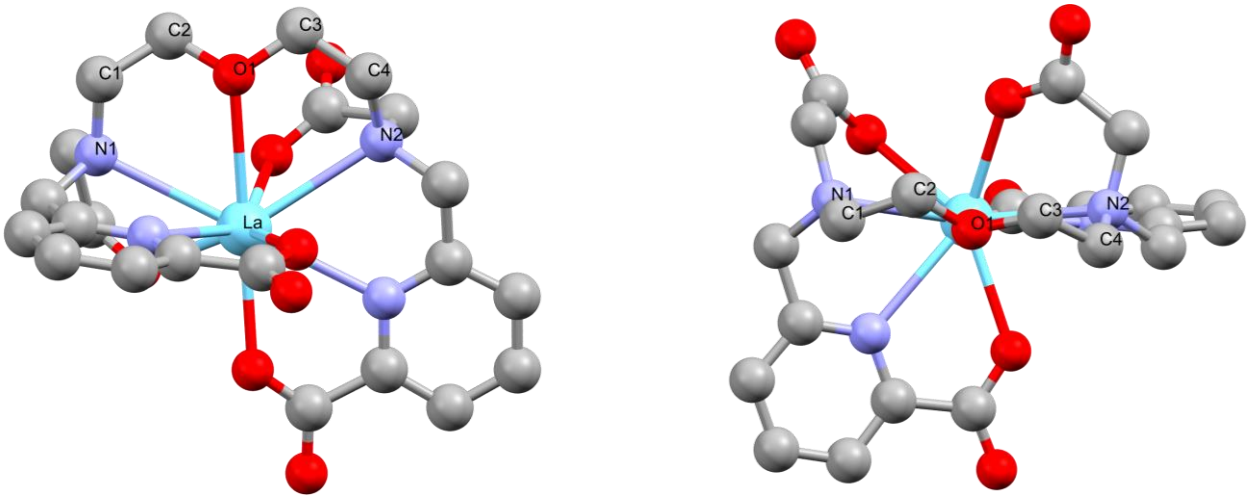

Figure S125. Side view (left) and top view (right) of optimized La-Oxyaapa complex in N1^{S}N2^{R}($\delta\lambda$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.408314	1.650516	-0.122306
6	3.843797	0.209207	0.024938
6	5.193898	-0.154206	-0.021625
6	5.545206	-1.480336	0.222249
6	4.544076	-2.405795	0.513272
6	3.220285	-1.968174	0.536309
6	2.082554	-2.911768	0.893327
8	2.348302	-4.115609	1.084030
6	1.584397	3.149547	-0.617174
8	-0.753923	2.517760	-0.589299
6	-2.030760	2.602858	-1.241824
6	-3.067129	1.841616	-0.438065
7	-2.767345	0.400494	-0.298957
6	-3.499719	-0.168989	0.847073
6	-2.946418	0.280305	2.180399
6	-3.783755	0.475867	3.284280
6	-3.220331	0.844772	4.502813
6	-1.840442	1.029174	4.584328
6	-1.074137	0.830621	3.437300
6	0.428368	1.059686	3.441164
8	0.986856	1.326700	4.524351
6	-3.095658	-0.348746	-1.520074
8	1.013832	0.968036	2.302835
7	-1.617713	0.450423	2.266467

8	0.916975	-2.380848	0.987632
7	2.882947	-0.692176	0.282544
1	-4.573596	0.066289	0.795204
1	-3.412767	-1.259820	0.792990
1	-3.113501	2.279553	0.562729
1	-4.053144	2.001312	-0.902438
1	-2.340107	3.654645	-1.300268
1	-1.937704	2.224329	-2.267990
1	-1.358464	1.329675	5.506461
1	-3.849390	0.999913	5.373853
1	-4.855324	0.342803	3.178643
1	4.768341	-3.444637	0.722316
1	6.586072	-1.786956	0.190057
1	5.948060	0.593903	-0.241683
57	0.128858	-0.087833	0.129242
7	2.135896	1.795843	-0.858022
1	4.213442	2.236015	-0.589406
1	3.263753	2.058089	0.884440
6	2.348752	1.542025	-2.298650
6	0.210244	3.378673	-1.215105
1	0.204950	3.211424	-2.299472
1	-0.073512	4.425272	-1.042665
1	2.255811	3.921870	-1.026335
1	1.528754	3.301399	0.465167
6	-2.424648	-1.729014	-1.590908
1	-2.738945	0.211692	-2.389868
1	-4.181408	-0.474321	-1.647311
8	-1.416397	-1.936623	-0.822728
8	-2.881794	-2.546421	-2.416608
6	1.154072	0.923976	-3.039642
1	3.160461	0.813722	-2.405252
1	2.669098	2.452461	-2.821778
8	1.019915	1.183073	-4.252117
8	0.404251	0.117153	-2.373255

Output energies:

Zero-point correction= 0.436360 (Hartree/Particle)
Thermal correction to Energy= 0.467973
Thermal correction to Enthalpy= 0.468917
Thermal correction to Gibbs Free Energy= 0.371572
Sum of electronic and zero-point Energies= -1779.364485
Sum of electronic and thermal Energies= -1779.332872
Sum of electronic and thermal Enthalpies= -1779.331927
Sum of electronic and thermal Free Energies= -1779.429272

(31) La-Oxyaapa, N1^{S}N2^{R}($\lambda\delta$), enantiomer of N1^{R}N2^{S}($\delta\lambda$)

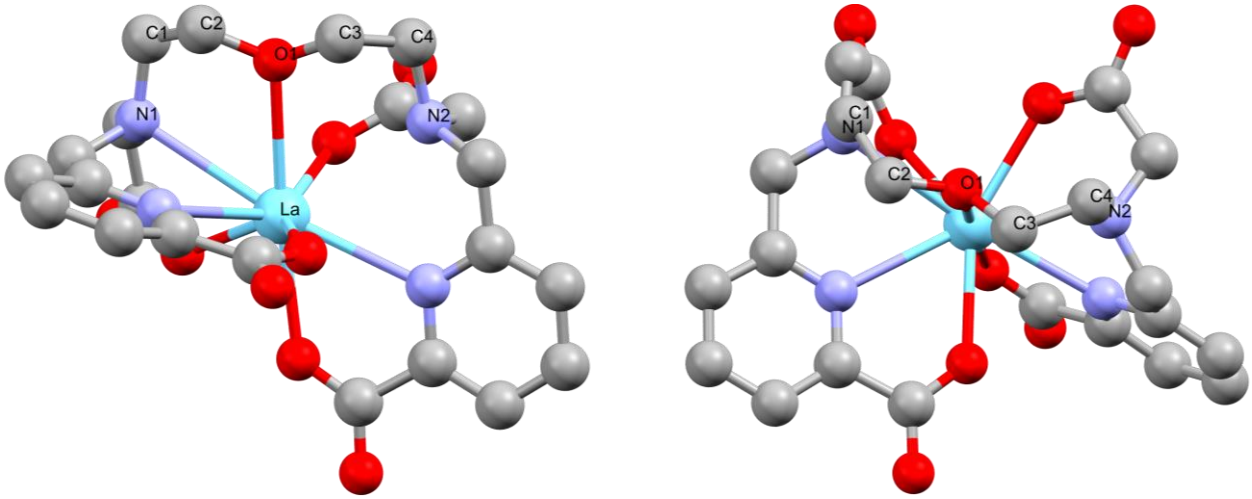

Figure S126. Side view (left) and top view (right) of optimized La-Oxyaapa complex in N1^{S}N2^{R}($\lambda\delta$) conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.274937	1.745524	-0.292643
6	3.819424	0.371887	0.037677
6	5.191206	0.175255	0.235551
6	5.647958	-1.087360	0.603735
6	4.726662	-2.120920	0.766216
6	3.376807	-1.849096	0.547932
6	2.321437	-2.926122	0.747499
8	2.698271	-4.070639	1.068472
6	1.467221	3.053117	-1.255352
8	-0.666073	2.342726	-0.488495
6	-1.985408	2.718528	-0.074044
6	-2.968412	1.798592	-0.787910
7	-2.755693	0.354646	-0.522562
6	-3.537309	-0.117648	0.635402
6	-2.982463	0.308111	1.973955
6	-3.835593	0.645567	3.030325
6	-3.285448	0.970554	4.267192
6	-1.899012	0.970527	4.409988
6	-1.114753	0.639136	3.306050
6	0.401867	0.673493	3.389136
8	0.930970	0.908237	4.494939
6	-3.078610	-0.471976	-1.696052
8	1.032218	0.465279	2.292206
7	-1.647450	0.297407	2.118099

8	1.098741	-2.567656	0.577846
7	2.939432	-0.631021	0.181679
1	-4.588307	0.198729	0.558104
1	-3.536150	-1.212903	0.617944
1	-3.992250	2.106463	-0.527799
1	-2.846236	1.966210	-1.861235
1	-2.071174	2.671633	1.016932
1	-2.187532	3.750937	-0.387255
1	-1.420277	1.229170	5.346459
1	-3.926824	1.231554	5.103311
1	-4.909075	0.653431	2.873784
1	5.030943	-3.119113	1.056466
1	6.707655	-1.263810	0.760421
1	5.880516	1.001900	0.099040
57	0.140911	-0.290930	-0.019669
7	2.089225	1.708209	-1.164781
1	4.079086	2.356734	-0.730906
1	2.985230	2.232857	0.646221
6	2.425991	1.209040	-2.508824
6	0.378086	3.291134	-0.223344
1	-0.008407	4.310963	-0.337696
1	0.742691	3.171479	0.805735
1	1.007819	3.152080	-2.243244
1	2.226753	3.844543	-1.174368
6	-2.475976	-1.885328	-1.639097
1	-2.654712	0.005975	-2.584935
1	-4.162233	-0.562164	-1.864242
8	-1.494319	-2.083411	-0.831582
8	-2.952353	-2.740766	-2.412525
6	1.221327	0.608861	-3.249995
1	3.158562	0.400294	-2.414570
1	2.884771	1.987442	-3.132997
8	1.158813	0.749219	-4.487460
8	0.375939	-0.058059	-2.542484

Output energies:

Zero-point correction= 0.436425 (Hartree/Particle)
Thermal correction to Energy= 0.468902
Thermal correction to Enthalpy= 0.469846
Thermal correction to Gibbs Free Energy= 0.369623
Sum of electronic and zero-point Energies= -1779.357695
Sum of electronic and thermal Energies= -1779.325218
Sum of electronic and thermal Enthalpies= -1779.324274
Sum of electronic and thermal Free Energies= -1779.424496

(32) La-Oxyaapa, $N1^{S}N2^{R}(\lambda\lambda)$, enantiomer of $N1^{R}N2^{S}(\delta\delta)$

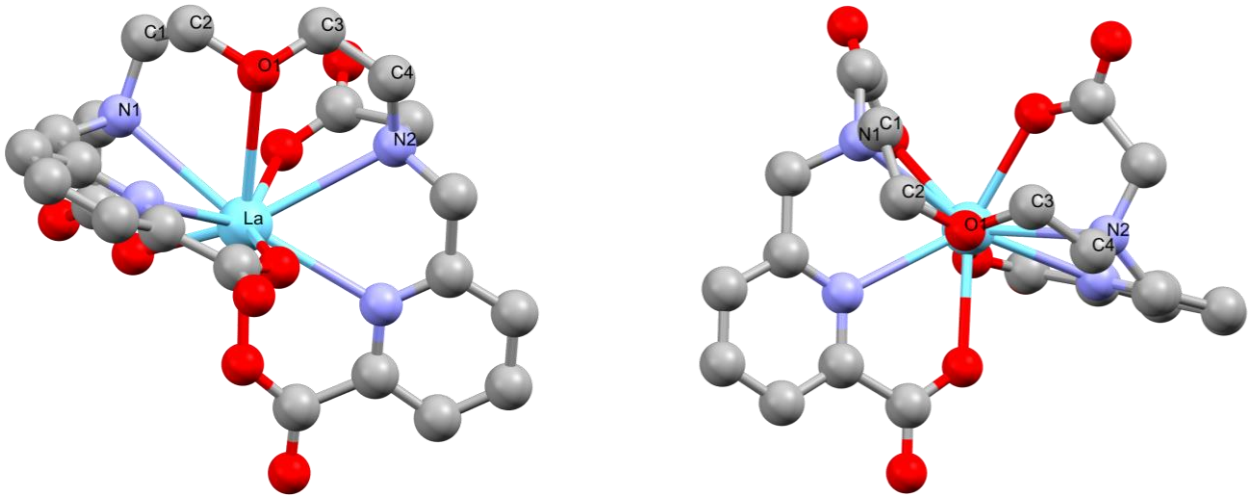

Figure S127. Side view (left) and top view (right) of optimized La-Oxyaapa complex in $N1^{S}N2^{R}(\lambda\lambda)$ conformation. Hydrogen atoms are omitted for clarity.

Optimized Cartesian coordinates in Å:

Atomic #	x	y	z
6	3.410950	1.662099	-0.191638
6	3.912538	0.240325	-0.075844
6	5.270228	-0.058089	-0.233446
6	5.704353	-1.365970	-0.032208
6	4.773089	-2.339721	0.323098
6	3.435904	-1.967047	0.456516
6	2.382813	-2.983371	0.871070
8	2.741703	-4.160998	1.071404
6	1.546122	3.120110	-0.645629
8	-0.692074	2.538988	0.003221
6	-2.113018	2.712060	-0.125583
6	-2.746909	1.653332	-1.016171
7	-2.601052	0.268309	-0.513952
6	-3.500817	-0.020361	0.621938
6	-3.009596	0.430014	1.980327
6	-3.926585	0.813153	2.967315
6	-3.457771	1.154388	4.231831
6	-2.084911	1.125003	4.474467
6	-1.232486	0.746989	3.439241
6	0.275438	0.746290	3.640332
8	0.719419	0.999028	4.778436
6	-2.879331	-0.692723	-1.595492
8	0.988493	0.493285	2.603198
7	-1.690339	0.388751	2.223369

8	1.184175	-2.540486	0.998073
7	3.015632	-0.704894	0.251880
1	-4.502655	0.397933	0.442675
1	-3.626553	-1.107334	0.678449
1	-3.809390	1.910615	-1.160890
1	-2.266494	1.699083	-1.997400
1	-2.524218	2.691817	0.885564
1	-2.327546	3.701338	-0.547258
1	-1.668384	1.395195	5.436867
1	-4.150291	1.450408	5.013668
1	-4.985946	0.842699	2.735274
1	5.059951	-3.369566	0.496475
1	6.752722	-1.621447	-0.151197
1	5.966028	0.727571	-0.508083
57	0.206988	-0.302413	0.268913
7	2.100453	1.764237	-0.863365
1	4.173055	2.279109	-0.690738
1	3.299466	2.058261	0.824423
6	2.236571	1.469417	-2.304061
6	0.071651	3.265105	-0.970107
1	-0.165354	2.924129	-1.985395
1	-0.188571	4.330214	-0.910341
1	2.101510	3.864855	-1.238157
1	1.680797	3.376696	0.409457
6	-2.305824	-2.091656	-1.333579
1	-2.403309	-0.333602	-2.512814
1	-3.954613	-0.783205	-1.807584
8	-1.363348	-2.191721	-0.464953
8	-2.757845	-3.035865	-2.013182
6	1.012822	0.810382	-2.952883
1	3.052697	0.750488	-2.438463
1	2.508247	2.368486	-2.873046
8	0.774941	1.061969	-4.151075
8	0.348707	-0.023178	-2.231698

Output energies:

Zero-point correction= 0.437543 (Hartree/Particle)
Thermal correction to Energy= 0.470301
Thermal correction to Enthalpy= 0.471245
Thermal correction to Gibbs Free Energy= 0.371178
Sum of electronic and zero-point Energies= -1779.359856
Sum of electronic and thermal Energies= -1779.327098
Sum of electronic and thermal Enthalpies= -1779.326154
Sum of electronic and thermal Free Energies= -1779.426220

11. ^{17}O NMR Measurements

(1) Theoretical background

In this study, Swift-Connick theory[1] was employed to deal with the $1/T_2$ data:

$$\frac{1}{P_\mathrm{m}}\left(\frac{1}{T_2}-\frac{1}{T_{2\mathrm{A}}}\right)=\frac{1}{T_{2\mathrm{r}}}=\frac{1}{\tau_\mathrm{m}}\cdot\frac{\frac{1}{T_{2\mathrm{m}}}\left(\frac{1}{\tau_\mathrm{m}}+\frac{1}{T_{2\mathrm{m}}}\right)+(\Delta\omega_\mathrm{m})^2}{\left(\frac{1}{\tau_\mathrm{m}}+\frac{1}{T_{2\mathrm{m}}}\right)^2+(\Delta\omega_\mathrm{m})^2}+\frac{1}{T_{2\mathrm{os}}}. \tag{S1}$$

In this equation, $1/T_2$ and $1/T_{2\mathrm{A}}$ are the transverse relaxation rates of the sample solution (Gd-OxyMepa) and reference solution (acidified water), P_m is the mole fraction of bound water, $1/T_{2\mathrm{r}}$ is the reduced transverse relaxation rate,$1/T_{2\mathrm{m}}$ is the relaxation rate of the bound water, τ_m is the mean lifetime (reciprocal of the exchange rate k_ex) of the bound water, and $\Delta\omega_\mathrm{m}$ is the chemical shift difference between bound water and bulk water. Since the outer-sphere contribution $1/T_{2\mathrm{os}}$ is negligible,[2,3] the above equation can be simplified to

$$\frac{1}{P_\mathrm{m}}\left(\frac{1}{T_2}-\frac{1}{T_{2\mathrm{A}}}\right)=\frac{1}{T_{2\mathrm{r}}}=\frac{1}{\tau_\mathrm{m}}\cdot\frac{\frac{1}{T_{2\mathrm{m}}}\left(\frac{1}{\tau_\mathrm{m}}+\frac{1}{T_{2\mathrm{m}}}\right)+(\Delta\omega_\mathrm{m})^2}{\left(\frac{1}{\tau_\mathrm{m}}+\frac{1}{T_{2\mathrm{m}}}\right)^2+(\Delta\omega_\mathrm{m})^2}. \tag{S2}$$

$\Delta\omega_\mathrm{m}$ is determined by the hyperfine interaction between the Gd^{3+} electron spin and the ^{17}O nucleus. It has the expression as below:[2–4]

$$\Delta\omega_\mathrm{m}=\frac{g_\mathrm{L}\mu_\mathrm{B}S(S+1)B}{3k_BT}\frac{A}{\hbar}, \tag{S3}$$

where g_L is the isotropic Landé g-factor (g_L = 2.0 for Gd^{3+}), μ_B is the Bohr magneton (μ_B = 9.274 × 10^{-24} J·T^{-1}), S is the electron spin (S = 7/2 for Gd^{3+}), B is the applied magnetic field (B = 14.1 T in this work), k_B is the Boltzmann constant (k_B = 1.381 × 10^{-23} J·K^{-1}), T is the temperature in K, and $A/\hbar$ is the hyperfine coupling constant.

The exchange rate k_ex obeys the Eyring Equation:

$$\frac{1}{\tau_\mathrm{m}}=k_\mathrm{ex}=\frac{k_\mathrm{B}T}{h}\exp\left(\frac{\Delta S^\ddagger}{R}-\frac{\Delta H^\ddagger}{RT}\right), \tag{S4}$$

where $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ are the enthalpy and entropy of activation for the water exchange process, h is the Planck constant ($h = 6.626 \times 10^{-34}$ J·s), R is the ideal gas constant ($R = 8.314$ J·K^{-1}·mol^{-1}). This equation can be used to derive the exchange rate at 298.15 K (25 °C), k_{ex}^{298}:

$$\frac{1}{\tau_{\mathrm{m}}} = k_{\mathrm{ex}} = \frac{k_{\mathrm{ex}}^{298} T}{298.15} \exp\left(\frac{\Delta H^{\ddagger}}{R}\left(\frac{1}{298.15} - \frac{1}{T}\right)\right). \tag{S5}$$

In regard to the transverse relaxation, the scalar contribution $1/T_{2\mathrm{sc}}$ is the dominant term,[2–5] and thus

$$\frac{1}{T_{2\mathrm{m}}} \approx \frac{1}{T_{2\mathrm{sc}}} = \frac{S(S+1)}{3}\left(\frac{A}{\hbar}\right)^2 \left(\tau_{\mathrm{S1}} + \frac{\tau_{\mathrm{S2}}}{{\omega_{\mathrm{S}}}^2 {\tau_{\mathrm{S2}}}^2 + 1}\right), \tag{S6}$$

where ω_{S} is the Larmor frequency of the spin S. In this expression, $\frac{1}{\tau_{\mathrm{S}j}}$ is the sum of the exchange rate ($\frac{1}{\tau_{\mathrm{m}}} = k_{\mathrm{ex}}$) and the reciprocal of the longitudinal ($\frac{1}{T_{1\mathrm{e}}}$) or transverse ($\frac{1}{T_{2\mathrm{e}}}$) electron spin relaxation time:

$$\frac{1}{\tau_{\mathrm{S}j}} = \frac{1}{\tau_{\mathrm{m}}} + \frac{1}{T_{j\mathrm{e}}} \qquad j = 1, 2. \tag{S7}$$

Since $\frac{\tau_{\mathrm{S2}}}{{\omega_{\mathrm{S}}}^2 {\tau_{\mathrm{S2}}}^2 + 1}$ term is typically small for Gd^{3+} complexes,[3] Equation (S6) can therefore be approximated by:

$$\frac{1}{T_{2\mathrm{m}}} \approx \frac{1}{T_{2\mathrm{sc}}} = \frac{S(S+1)}{3}\left(\frac{A}{\hbar}\right)^2 \tau_{\mathrm{S1}} = \frac{S(S+1)}{3}\left(\frac{A}{\hbar}\right)^2 \Big/ \left(\frac{1}{\tau_{\mathrm{m}}} + \frac{1}{T_{1\mathrm{e}}}\right), \tag{S8}$$

and $1/T_{1\mathrm{e}}$ is assumed to have a simple exponential temperature dependence:[5]

$$\frac{1}{T_{1\mathrm{e}}} = \frac{1}{T_{1\mathrm{e}}^{298}} \exp\left(\frac{\Delta E_{\mathrm{T1e}}}{R}\left(\frac{1}{T} - \frac{1}{298.15}\right)\right), \tag{S9}$$

where $1/T_{1\mathrm{e}}^{298}$ is the electronic relaxation rate at 298.15 K (25 °C), and ΔE_{T1e} is the activation energy for electronic relaxation. By globally fitting the experimental data using Equation (S2)–(S9), four parameters (k_{ex}^{298}, $\Delta H^{\ddagger}$, $1/T_{1\mathrm{e}}^{298}$, and ΔE_{T1e}) can be obtained.

During the optimization procedure, we employed the following loss function:

$$L\left(k_{\mathrm{ex}}^{298}, \Delta H^{\ddagger}, \frac{1}{T_{1\mathrm{e}}^{298}}, \Delta E_{\mathrm{T1e}}\right) = \left(\frac{1}{n}\sum_{i=1}^{n}\left[\frac{T_{2\mathrm{r}}\left(T_i \middle| k_{\mathrm{ex}}^{298}, \Delta H^{\ddagger}, \frac{1}{T_{1\mathrm{e}}^{298}}, \Delta E_{\mathrm{T1e}}\right) - T_{2\mathrm{r}}^{\mathrm{exp}}(T_i)}{T_{2\mathrm{r}}^{\mathrm{exp}}(T_i)}\right]^2\right)^{\frac{1}{2}}, \quad \text{(S10)}$$

where $T_{2\mathrm{r}}(T_i \mid k_{\mathrm{ex}}^{298}, \Delta H^{\ddagger}, 1/T_{1\mathrm{e}}^{298}, \Delta E_{\mathrm{T1e}})$ is the theoretically calculated $T_{2\mathrm{r}}$ from k_{ex}^{298}, $\Delta H^{\ddagger}$, $1/T_{1\mathrm{e}}^{298}$, ΔE_{T1e} based on Equations (S2)–(S9), and $T_{2\mathrm{r}}^{\mathrm{exp}}(T_i)$ is the experimentally measured $T_{2\mathrm{r}}$ value at temperature T_i. The loss function shown above was minimized during the optimization process by varying the listed four parameters (i.e. k_{ex}^{298}, $\Delta H^{\ddagger}$, $1/T_{1\mathrm{e}}^{298}$, ΔE_{T1e}).

When considering the "slow-exchange" and "fast-exchange" limits, it is beneficial to further simplify Equation (S2) by assuming a negligible $\Delta\omega_{\mathrm{m}}$:

$$\frac{1}{P_{\mathrm{m}}}\left(\frac{1}{T_2} - \frac{1}{T_{2\mathrm{A}}}\right) = \frac{1}{T_{2\mathrm{r}}} = \frac{1}{\tau_{\mathrm{m}} + T_{2\mathrm{m}}}. \quad \text{(S11)}$$

At low T, τ_{m} is dominant and Equation (S11) becomes

$$\frac{1}{T_{2\mathrm{r}}} = \frac{1}{\tau_{\mathrm{m}}} = k_{\mathrm{ex}}. \quad \text{(S12)}$$

Following Equation (S4), a plot of $\ln(1/T_{2\mathrm{r}})$ vs $1000/T$ will therefore have a negative slope at low T. Whereas at high T, the $T_{2\mathrm{m}}$ term dominates and Equation (S11) becomes

$$\frac{1}{T_{2\mathrm{r}}} = \frac{1}{T_{2\mathrm{m}}} = \frac{S(S+1)}{3}\left(\frac{A}{\hbar}\right)^2 / \left(k_{\mathrm{ex}} + \frac{1}{T_{1\mathrm{e}}}\right). \quad \text{(S13)}$$

Following Equations (S4) and (S9), a plot of $\ln(1/T_{2\mathrm{r}})$ vs $1000/T$ will now have a positive slope at high T. Hence, a change in the sign of the slope indicates a switchover between the "slow-exchange" and the "fast-exchange" limits.

(2) Raw data and refined parameters

Table S8. Raw data from the variable-temperature ^{17}O NMR measurement of 3.0 mM Gd-OxyMepa complex.

T (°C)	1000/T (K^{-1})	Sample T_2 (s)	Reference T_{2A} (s)	$1/T_{2r}$ (10^6 s^{-1})	ln($1/T_{2r}$)
6.13	3.580	0.002964	0.003920	0.846	13.65
10.86	3.520	0.003032	0.004649	1.179	13.98
15.58	3.463	0.002978	0.005427	1.556	14.26
20.30	3.407	0.002942	0.006221	1.842	14.43
25.03	3.353	0.002834	0.007117	2.182	14.60
29.75	3.301	0.002666	0.008133	2.591	14.77
34.48	3.250	0.002620	0.009119	2.795	14.84
39.20	3.201	0.002545	0.009842	2.994	14.91
43.92	3.153	0.002719	0.011057	2.851	14.86
48.65	3.107	0.002917	0.011858	2.657	14.79
53.37	3.062	0.003245	0.012729	2.360	14.67
58.10	3.018	0.003618	0.013983	2.106	14.56
62.82	2.976	0.004171	0.014785	1.769	14.39
67.55	2.935	0.004872	0.016086	1.471	14.20
72.27	2.895	0.005667	0.016947	1.207	14.00
76.99	2.856	0.006415	0.017234	1.006	13.82
81.72	2.818	0.007160	0.019496	0.908	13.72
86.44	2.781	0.007930	0.020111	0.785	13.57

Table S9. Parameters obtained by fitting the experimental data at different $A/\hbar$ values.

$A/\hbar$ (10^6 rad·s^{-1})	k_{ex}^{298} (10^6 s^{-1})	$\Delta H^{\ddagger}$ (kJ·mol^{-1})	$1/T_{1e}^{298}$ (10^7 s^{-1})	ΔE_{T1e} (kJ·mol^{-1})
-2.9	2.8 ± 0.1	39.1 ± 0.7	0.11 ± 0.01	-32.0 ± 5.5
-3.2	2.8 ± 0.1	39.6 ± 1.0	0.20 ± 0.02	-34.1 ± 4.6
-3.5	2.8 ± 0.1	39.7 ± 1.0	0.29 ± 0.03	-35.6 ± 3.7
-3.8	2.8 ± 0.1	39.8 ± 1.1	0.40 ± 0.03	-36.5 ± 3.0
-4.1	2.8 ± 0.1	39.9 ± 1.1	0.52 ± 0.04	-37.1 ± 2.6

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