Supporting Information for

Spectrally Undiscerned Isomers Might Lead to Erroneous Determination of Water Exchange Rates of paraCEST Eu(III) Agents

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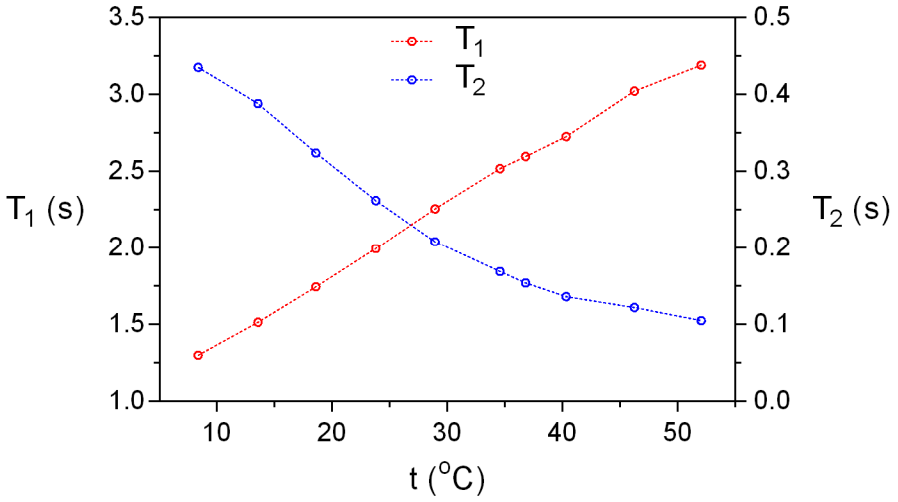

Figure S1. Development of T_1 and T_2 relaxation times for **EuL^1** (15 mM) in H_2O:D_2O (9:1, v/v) at pH 7 and 7 T magnetic field strength as a function of temperature.

Table S1. Exchange rate values (in Hz) obtained for **EuL^1** (15 mM) and **EuL^3** (10 mM) using different qCEST methods: BM equation with three or four exchanging pools, Omega plots or QUESP.

	t (°C)	BM 4-pool		BM 3-pool	Omega plots	QUESP
		Isomer A	*Isomer B*			
EuL^1	10	1197 ± 590	4715 ± 340	5163 ± 320	3540 ± 641	3993 ± 896
	15	1813 ± 427	6511 ± 417	5717 ± 254	3823 ± 680	4188 ± 954
	20	3287 ± 418	9541 ± 1063	6630 ± 237	4840 ± 536	5129 ± 683
	25	4983 ± 421	14449 ± 1909	8604 ± 229	6209 ± 488	6277 ± 594
	30	7781 ± 463	27190 ± 4678	11437 ± 279	8273 ± 623	8031 ± 694
	35	11437 ± 744	41403 ± 7044	15430 ± 326	11027 ± 800	9538 ± 977
	37	13010 ± 979	42653 ± 7605	17555 ± 372	12808 ± 1008	10238 ± 444
	40	16975 ± 1455	59939 ± 13429	21195 ± 421	14412 ± 1999	11286 ± 1167
	45	22214 ± 3938	51018 ± 14958	29325 ± 592	17439 ± 1664	11774 ± 1031
	50	16562 ± 11701	44590 ± 4175	40466 ± 1061	22484 ± 3014	10939 ± 843
EuL^3	10	-	-	2245 ± 194	1894 ± 233	1920 ± 324
	15	-	-	3038 ± 127	2712 ± 155	2702 ± 168
	20	-	-	4427 ± 116	4069 ± 126	4056 ± 168
	25	-	-	6953 ± 119	6172 ± 67	5956 ± 81
	30	-	-	10774 ± 167	9740 ± 397	8604 ± 290
	35	-	-	16586 ± 248	13810 ± 1595	10986 ± 679
	37	-	-	19438 ± 284	16694 ± 3138	11661 ± 610
	40	-	-	25284 ± 388	21410 ± 3408	12972 ± 319
	45	-	-	37808 ± 871	32542 ± 23405	13002 ± 883
	50	-	-	55497 ± 2341	38639 ± 33031	12618 ± 1480

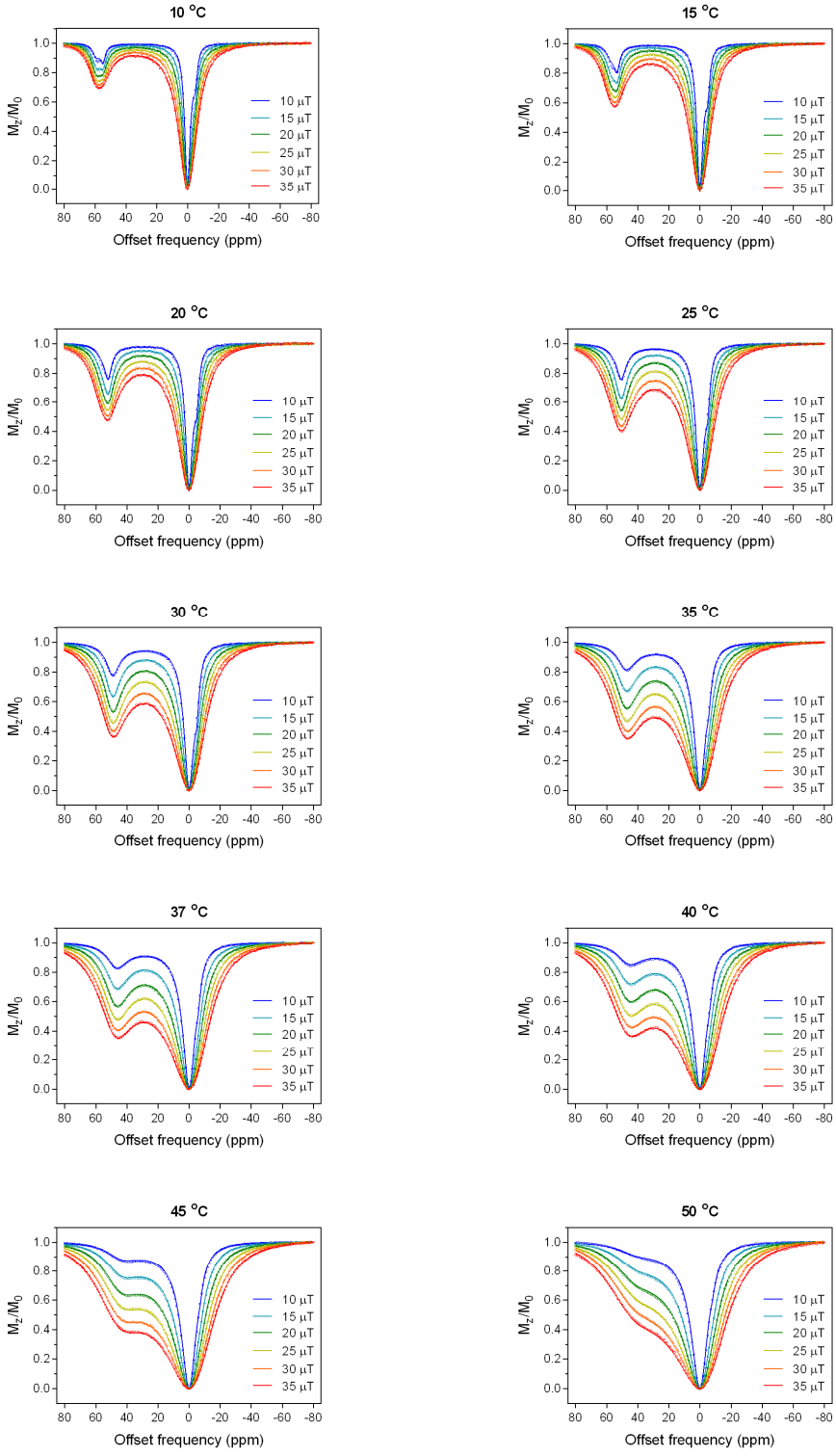

Figure S2. Z-spectra of **EuL**[1] (15 mM) at variable temperatures, B_1 fields and irradiation time of 10 s. The points represent obtained experimental values while lines represent values obtained from fits according to the BM equation with four exchanging pools.

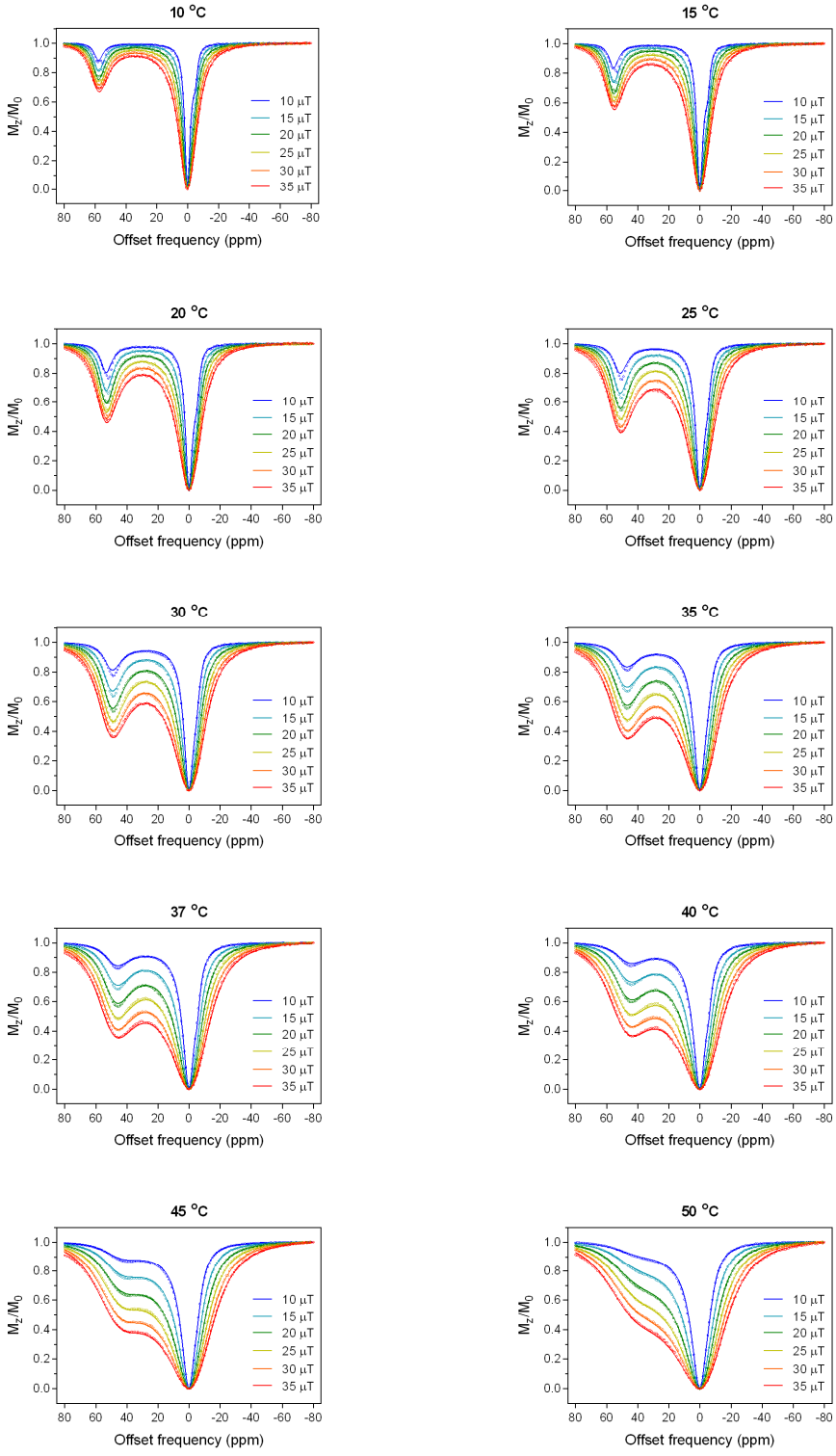

Figure S3. Z-spectra of **EuL**[1] (15 mM) at variable temperatures, B_1 fields and irradiation time of 10 s. The points represent obtained experimental values while lines represent values obtained from fits according to the BM equation with three exchanging pools.

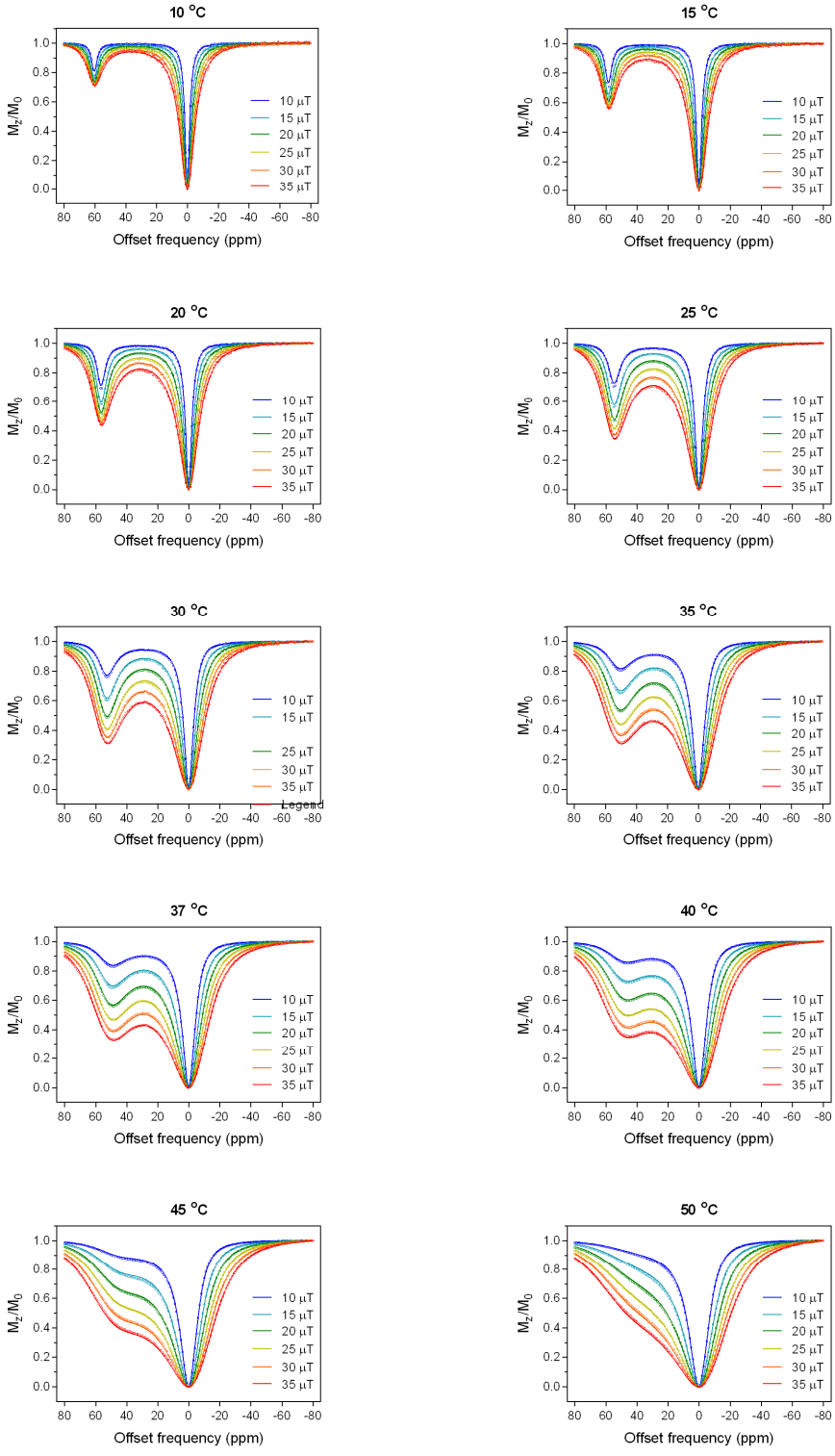

Figure S4. Z-spectra of **EuL^3** (10 mM) at variable temperatures, B_1 fields and irradiation time of 10 s. The points represent obtained experimental values while lines represent values obtained from fits according to the BM equation with three exchanging pools.

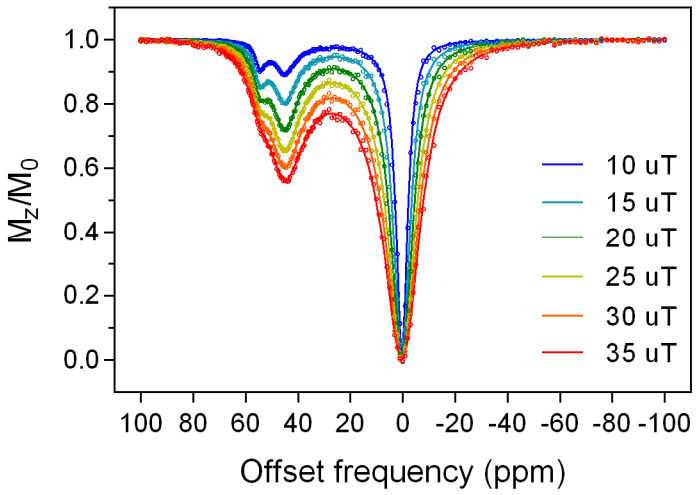

Figure S5. Z-spectra of **EuL^2** (15 mM) at variable B_1 fields and irradiation time of 10 s in solution of H_2O:D_2O:CH_3CN (4:1:5, v/v/v) at 25 ^oC. The points represent obtained experimental values while lines represent values obtained from fits according to the BM equation with three exchanging pools.

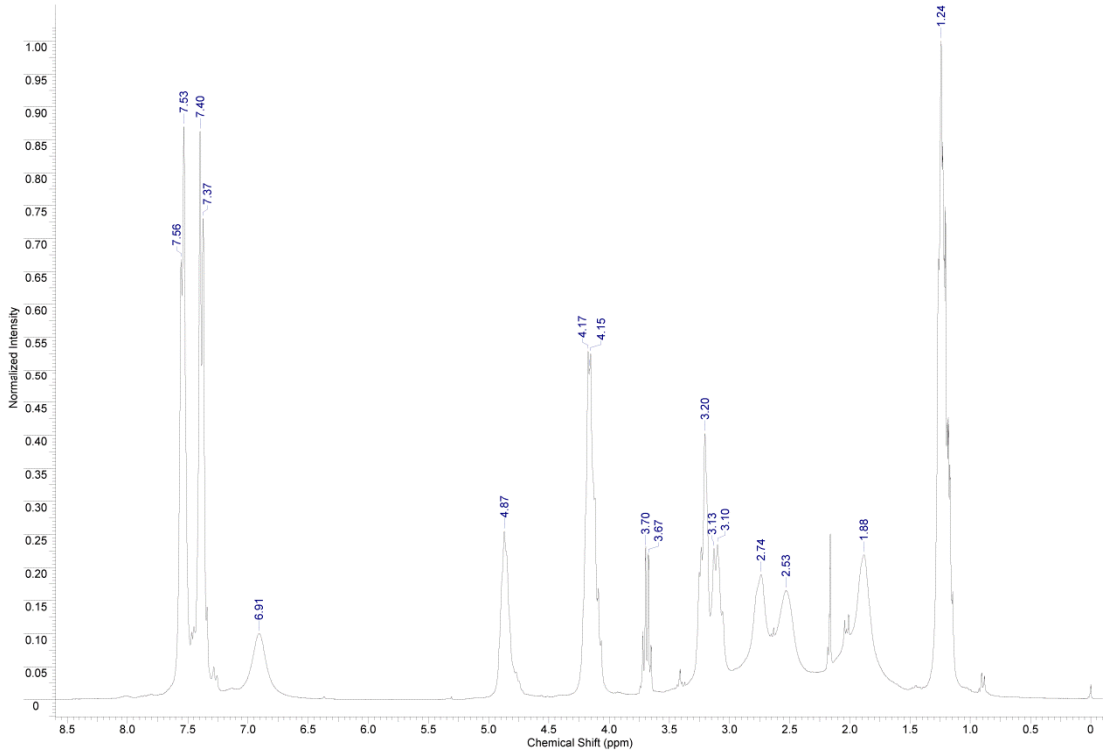

Figure S6. ^{1}H NMR spectrum of **3** recorded at 25 ºC in $CDCl_3$.

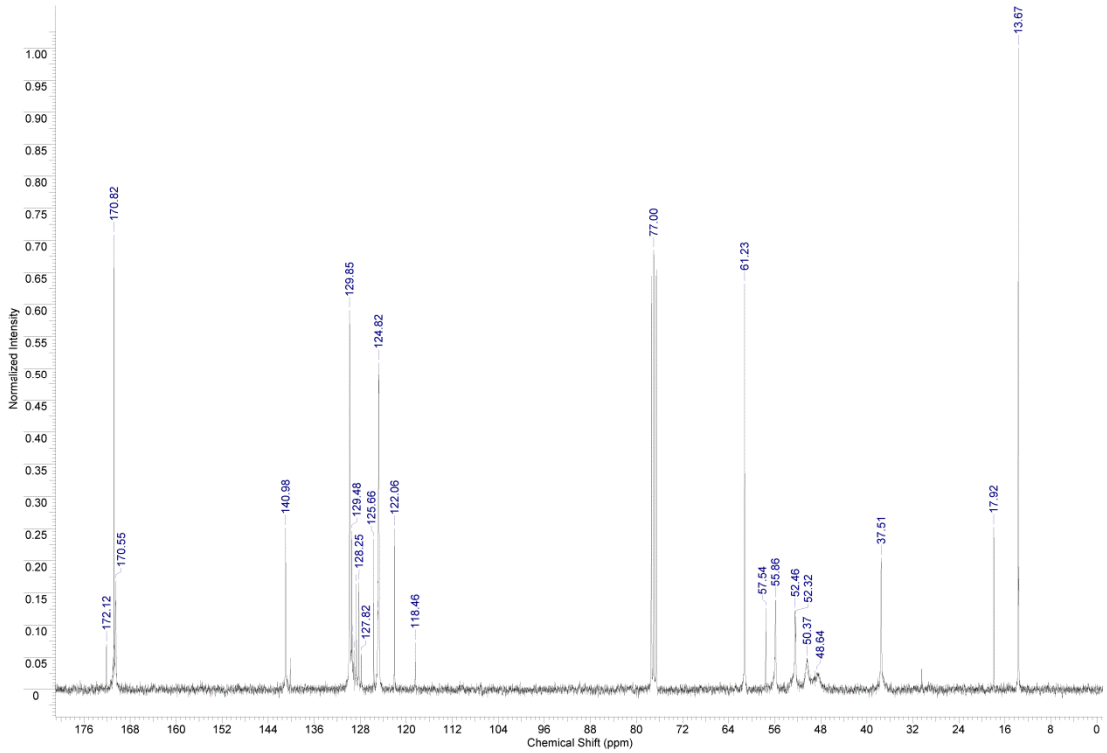

Figure S7. ^{13}C NMR spectrum of **3** recorded at 25 ºC in $CDCl_3$.

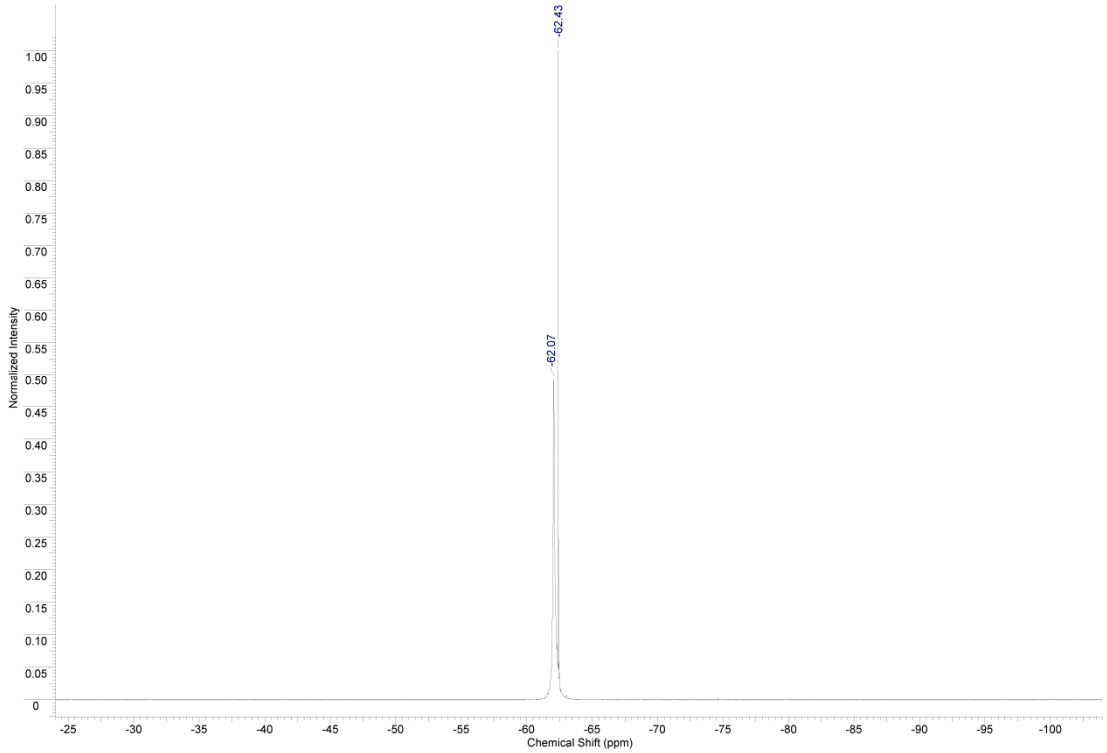

Figure S8. ^{19}F NMR spectrum of **3** recorded at 25 ºC in $CDCl_3$.

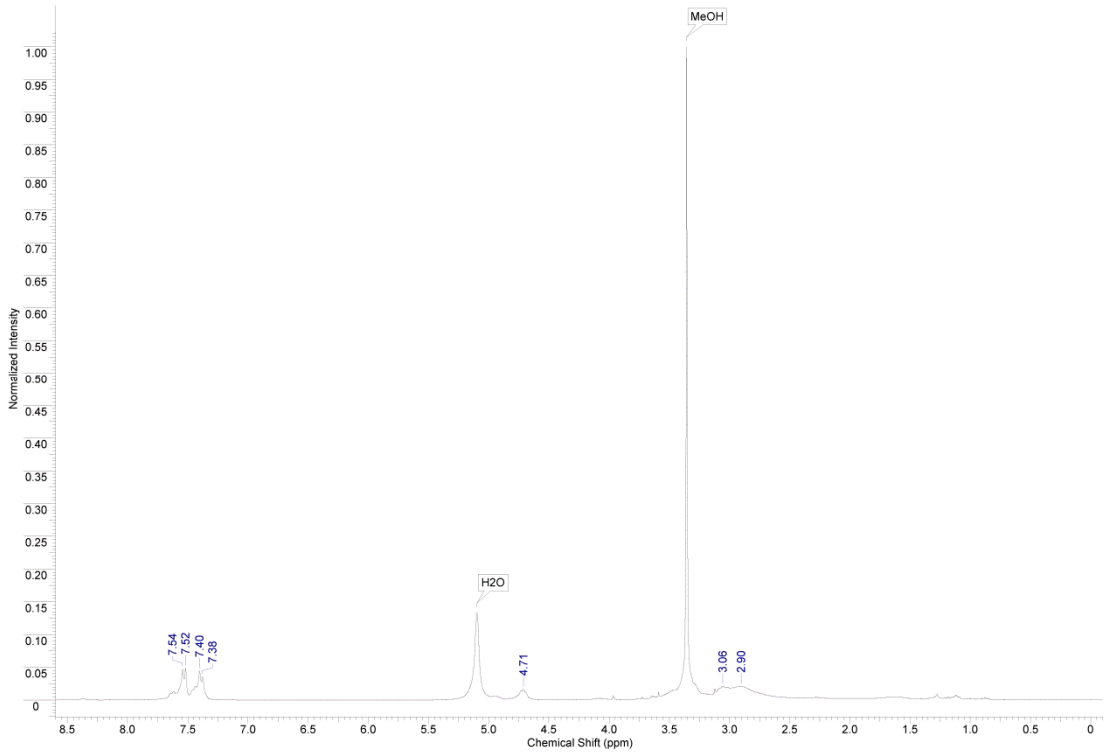

Figure S9. ^{1}H NMR spectrum of $\mathbf{L^2}$ recorded at 25 ºC in D_2O.

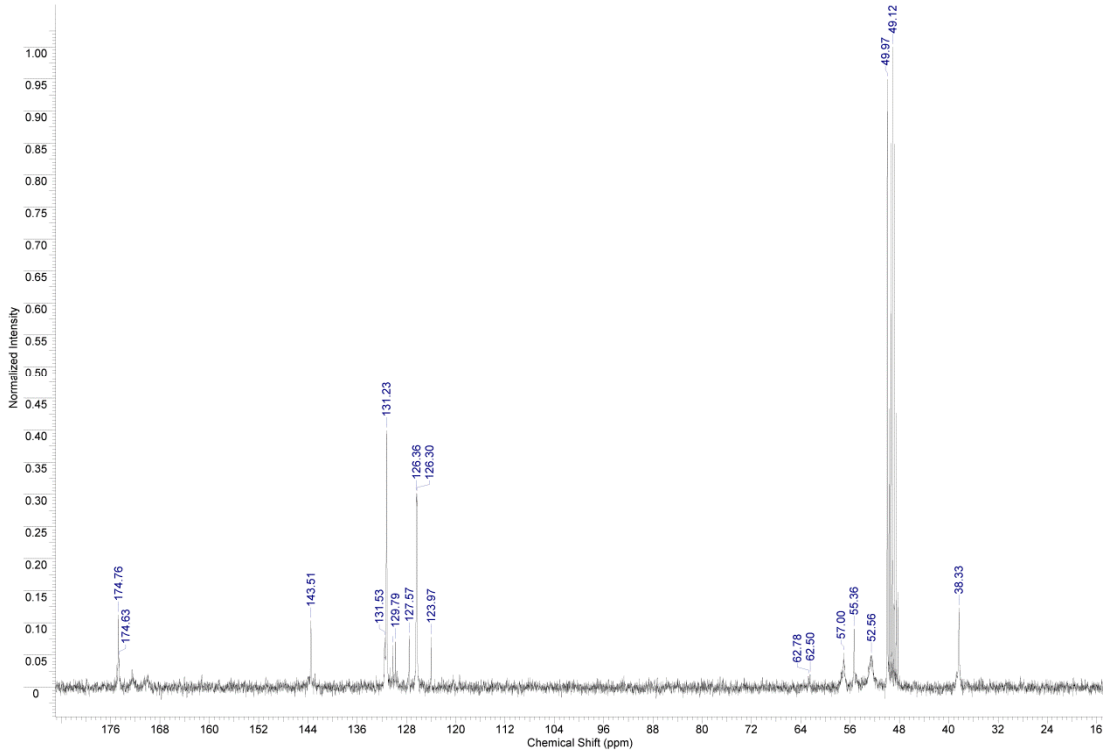

Figure S10. ^{13}C NMR spectrum of $\mathbf{L^2}$ recorded at 25 ºC in D_2O.

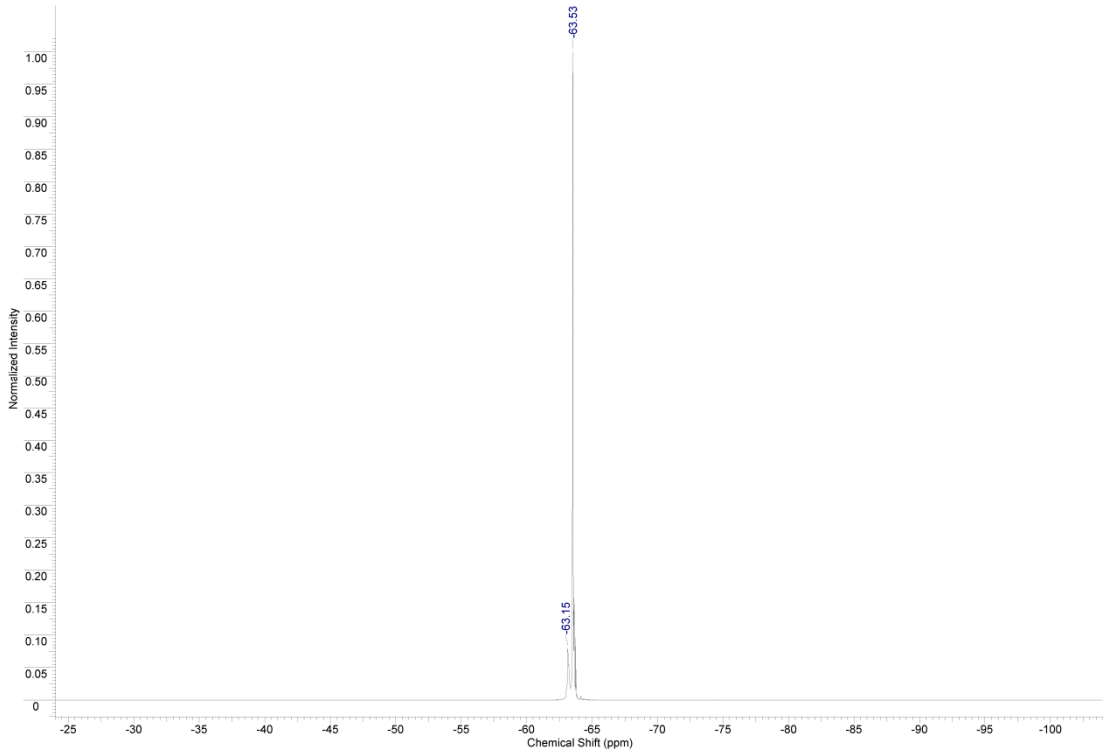

Figure S11. ^{19}F NMR spectrum of $\mathbf{L^2}$ recorded at 25 ºC in D_2O.

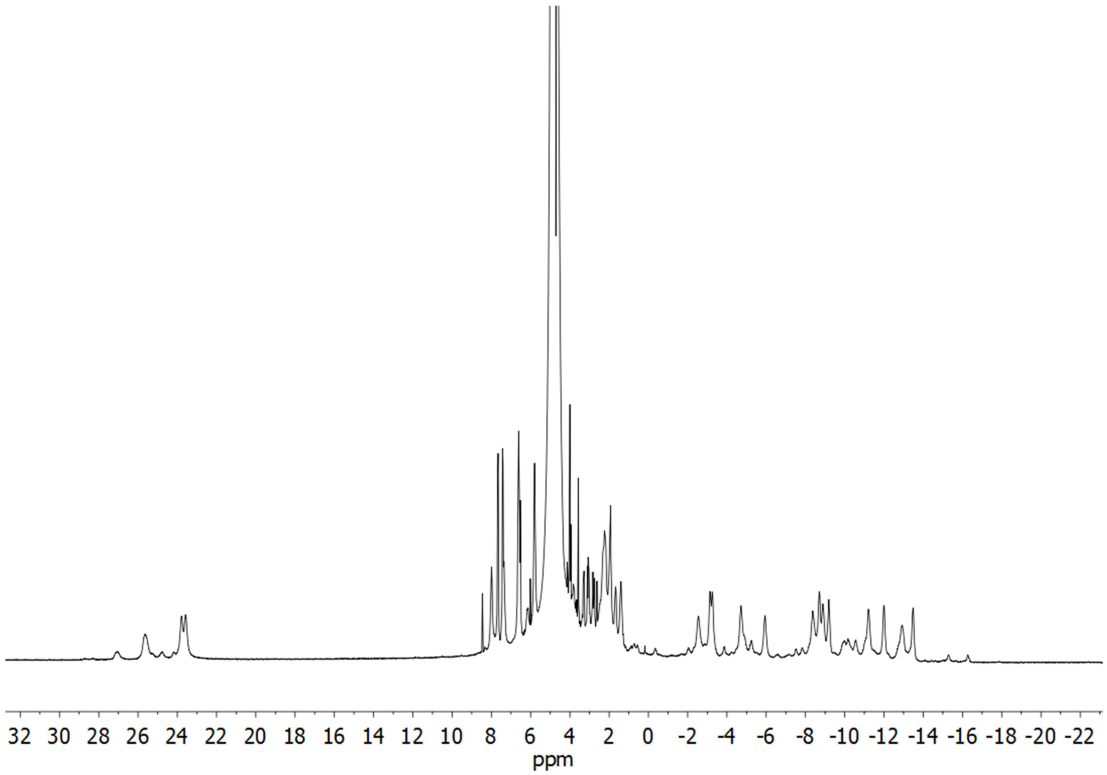

Figure S12. ^{1}H NMR spectrum of $\mathbf{EuL^1}$ (15 mM) recorded at 25 ºC in H_2O:D_2O (9:1, v/v).

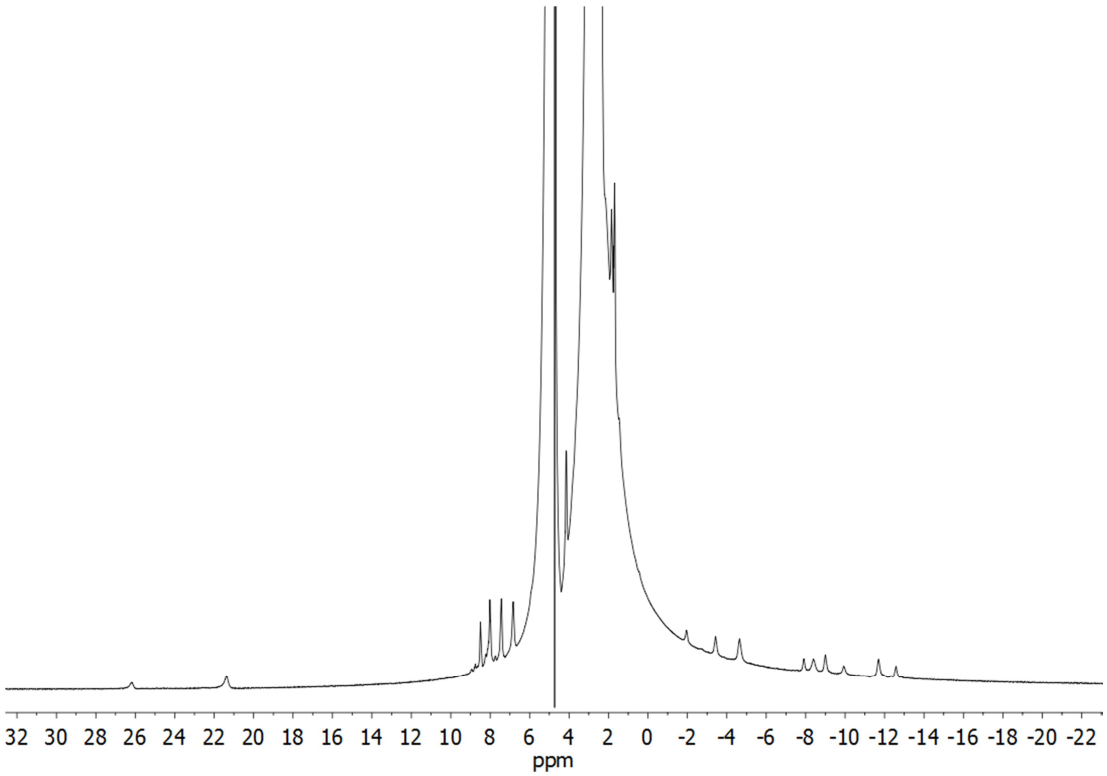

Figure S13. ^{1}H NMR spectrum of **EuL^{2}** (15 mM) recorded at 25 ºC in H_2O:D_2O:CH_3CN (4:1:5).

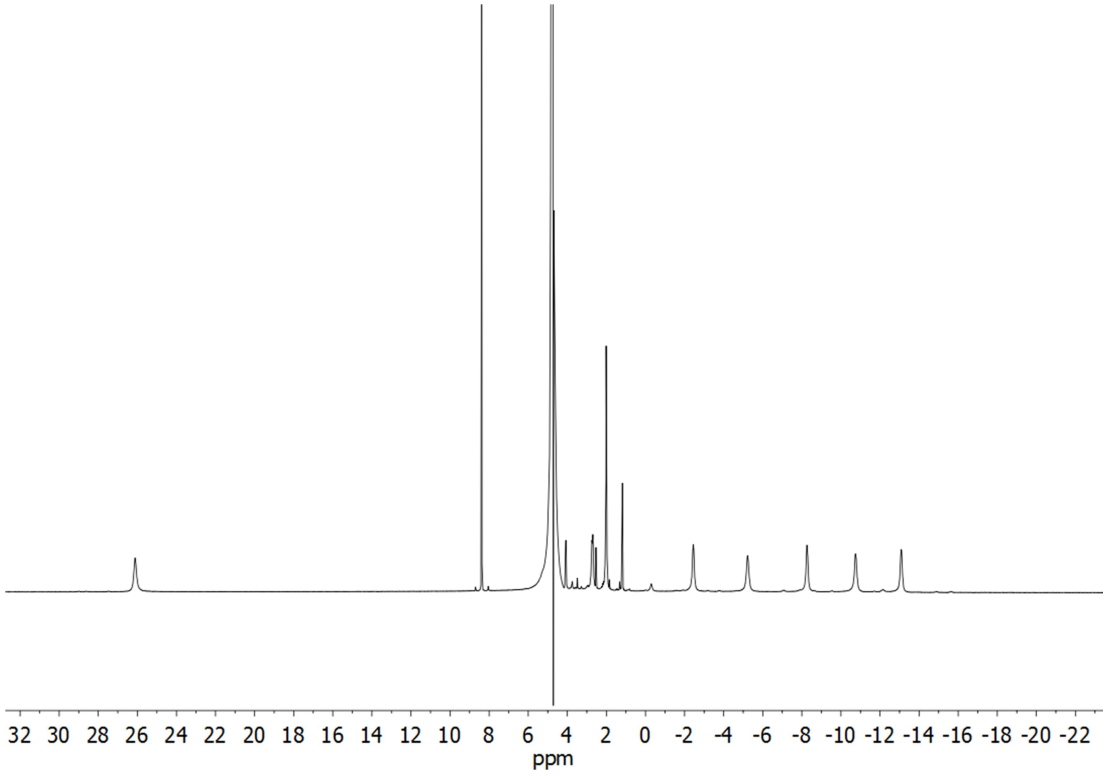

Figure S14. ^{1}H NMR spectrum of **EuL^{3}** (15 mM) recorded at 25 ºC in H_2O:D_2O (9:1, v/v).

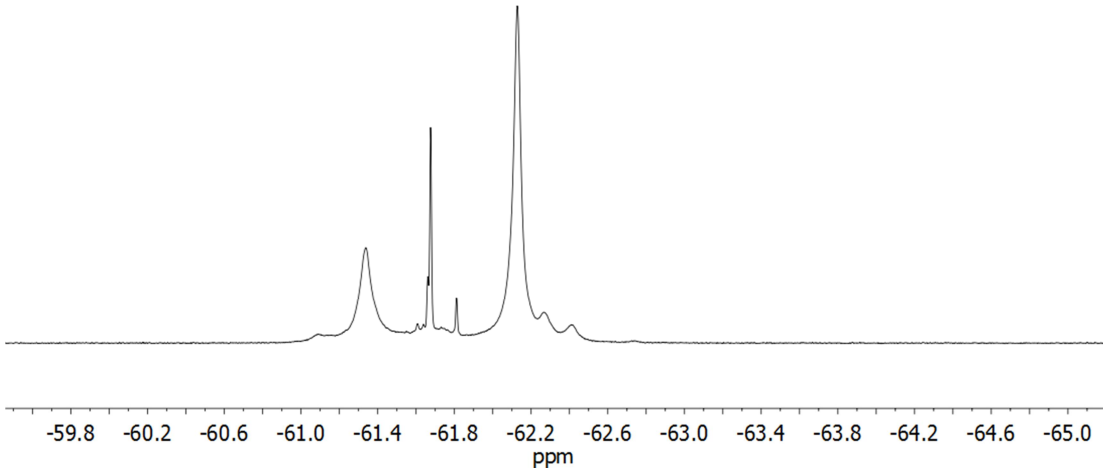

Figure S15. ^{19}F NMR spectrum of **EuL^{1}** (15 mM) recorded at 25 ºC in H_2O:D_2O (9:1, v/v).

Table S2. Optimized Cartesian coordinates (Å) of the *SS*-Δ(λλλλ) isomer of **EuL[1]** obtained with DFT calculations at the TPSSh/LCRECP/6-31G(d) level (0 imaginary frequencies).

N	-0.00785700	-2.16050800	-3.00780100
C	-1.36380300	-2.34515500	-3.61472400
C	-1.97775900	-1.03093400	-4.08668300
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C	-0.99823800	1.93248200	-4.10970900
N	0.01770800	2.12593800	-3.03536100
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C	1.98419700	0.97993700	-4.10573700
N	2.15280100	-0.02358100	-3.01148300
C	2.32628400	-1.38430200	-3.60484400
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Thermal correction to Enthalpy = 0.968097
Thermal correction to Gibbs Free Energy = 0.787311
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Sum of electronic and thermal Energies = -3603.139596
Sum of electronic and thermal Enthalpies = -3603.138652
Sum of electronic and thermal Free Energies = -3603.319439

Table S3. Optimized Cartesian coordinates (Å) of the *SS*-Λ(δδδδ) isomer of **EuL**[1] obtained with DFT calculations at the TPSSh/LCRECP/6-31G(d) level (0 imaginary frequencies).

N	-1.98437600	-3.23302600	0.36925000
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H	-2.37597300	0.67550500	3.89874000
C	2.54508100	0.77210300	-4.23543600
H	1.56264400	0.62312400	-4.69566000
H	2.47844500	1.63654300	-3.56629800
C	-3.54413800	-0.34581100	5.45868000
O	-4.50687300	-1.14969200	5.26781600
O	-3.33772800	0.43096800	6.41847400
C	3.63026200	1.01205400	-5.33405300
O	4.57726100	0.16745900	-5.34704800
O	3.44201000	2.00469000	-6.07264300
C	-4.14026000	0.76766200	-2.59760700

C	4.14559800	0.08004600	2.73511600
C	4.82949500	0.32446800	4.12530800
O	5.40472400	1.42705300	4.26476600
O	4.74012700	-0.63966800	4.94654800
C	-4.74376600	1.41518000	-3.89266900
O	-4.63199000	0.71370100	-4.94486100
O	-5.28665700	2.53259800	-3.74371300
H	-3.49441000	1.48436300	-2.08140000
H	3.47569400	0.91119200	2.49343600
C	5.18941400	-0.08851500	1.59939400
H	5.91583500	-0.85090700	1.90212600
H	4.65859900	-0.47209800	0.72036300
C	5.89941400	1.18993300	1.21450300
C	7.24832500	1.39838800	1.53838500
C	5.22430700	2.18664900	0.49065000
C	7.90754800	2.56633500	1.15603500
H	7.78706400	0.63999200	2.09936700
C	5.87118800	3.36139900	0.10783400
H	4.18069900	2.04282600	0.22065100
C	7.21710500	3.55287300	0.44166000
H	8.95060300	2.71402000	1.41782800
H	5.33427800	4.12389500	-0.44720600
C	7.93880000	4.78476800	-0.01652400
F	8.90617700	5.16673800	0.85564300
F	7.10411400	5.84200300	-0.17663900
F	8.55932100	4.60217100	-1.21520500
C	-5.25074500	0.27679200	-1.63044400
H	-5.95687700	-0.34221600	-2.19502700
H	-4.77669500	-0.36960000	-0.88234200
C	-5.98345100	1.38872300	-0.91356900
C	-7.31752200	1.69664300	-1.21906500
C	-5.34741800	2.11216500	0.10880300
C	-7.99901800	2.70097300	-0.53178700
H	-7.82908600	1.14273600	-2.00128200
C	-6.01642200	3.12272400	0.79860000
H	-4.31963800	1.87753600	0.37589300
C	-7.34701100	3.41776000	0.47863700
H	-9.03397000	2.92105400	-0.77407700
H	-5.51308100	3.66792600	1.59050900
C	-8.06267900	4.53149000	1.18307800
F	-9.39180000	4.28681600	1.31154300
F	-7.57432800	4.75195600	2.42912900
F	-7.95687100	5.71404200	0.51613200

E(RTPSSh) = -3604.1002098 Hartree
Zero-point correction = 0.900104
Thermal correction to Energy = 0.966685
Thermal correction to Enthalpy = 0.967629
Thermal correction to Gibbs Free Energy = 0.785502
Sum of electronic and zero-point Energies = -3603.200106
Sum of electronic and thermal Energies = -3603.133525
Sum of electronic and thermal Enthalpies = -3603.132580

Sum of electronic and thermal Free Energies = -3603.314707

Table S4. Optimized Cartesian coordinates (Å) of the *SS*-Λ(λλλλ) isomer of **EuL^1** obtained with DFT calculations at the TPSSh/LCRECP/6-31G(d) level (0 imaginary frequencies).

N	1.76567000	-1.18337400	2.10155200
C	1.08891600	-1.93252400	3.19813500
C	-0.16132600	-2.66445700	2.72450400
N	-1.18056700	-1.74654100	2.13019200
C	-1.95261000	-1.06940600	3.20913400
C	-2.67177900	0.18202000	2.71947300
N	-1.74529200	1.19704100	2.13222700
C	-1.05285600	1.95191700	3.21385800
C	0.18885900	2.68185300	2.71562900
N	1.19849400	1.76303600	2.10539500
C	1.98429600	1.08339400	3.17327400
C	2.69957200	-0.16540600	2.67156800
C	2.54881800	-2.10938900	1.25269000
C	2.93738600	-1.41110500	-0.04364100
O	2.22291300	-0.44568900	-0.46338600
C	-2.08067500	-2.54240600	1.26401600
C	-1.31464100	-2.96301000	0.01575200
O	-0.36636700	-2.22663700	-0.40153700
C	-2.53909800	2.11495200	1.28415300
C	-2.93362900	1.39904100	-0.00228000
O	-2.22508100	0.42855900	-0.41188500
C	2.09155000	2.56307700	1.23544400
C	1.31796400	2.99542300	-0.00232000
O	0.37189200	2.25388200	-0.42290900
H	0.82773100	-1.21528400	3.97873900
H	1.77807600	-2.65778800	3.65278200
H	0.10245300	-3.40682500	1.96719800
H	-0.59533900	-3.21611400	3.56953200
H	-1.25253400	-0.81206900	4.00663300
H	-2.69005600	-1.75676900	3.64644400
H	-3.40273300	-0.08208300	1.95161500
H	-3.23438800	0.62169200	3.55452200
H	-0.77890200	1.23958500	3.99469700
H	-1.73452700	2.68010900	3.67507200
H	-0.08901400	3.42152600	1.96057200
H	0.63826400	3.23642700	3.55064300
H	1.29372500	0.82141300	3.97729300
H	2.72524200	1.77071300	3.60453300
H	3.41662100	0.09998800	1.89106900
H	3.27780900	-0.60261300	3.49718100
H	3.43293700	-2.49308500	1.77948000
H	1.92229300	-2.96537300	0.98399100
H	-2.49338600	-3.41115000	1.79447900
H	-2.91817000	-1.91418500	0.94607900

H	-3.42072800	2.49844000	1.81529400
H	-1.91902600	2.97216000	1.00446500
H	2.51229800	3.42625700	1.76853600
H	2.92444500	1.93562100	0.90384900
O	0.13858800	0.12434500	-2.07720000
H	1.06902000	-0.15525200	-2.19852800
H	0.15358900	1.09330000	-2.21325100
Eu	-0.00666600	0.00349300	0.45880100
N	1.67355500	4.11006700	-0.60106800
N	-3.98873400	1.84844000	-0.65528000
N	-1.68252800	-4.07026000	-0.59233900
N	3.98857500	-1.86777900	-0.69473100
H	2.42190500	4.73701500	-0.26006900
H	-4.48448000	2.71123200	-0.37657000
H	-2.43530700	-4.69215900	-0.25438800
H	4.48772800	-2.72606600	-0.40538500
C	1.11382900	4.67106400	-1.82517100
H	1.24180600	3.97579100	-2.66152800
H	0.04267100	4.86309500	-1.70374300
C	-1.13675800	-4.61801200	-1.82832700
H	-1.25428700	-3.90416400	-2.65037800
H	-0.06845400	-4.83066300	-1.71460600
C	1.88031300	6.00489100	-2.10221100
O	2.77845000	6.29439500	-1.25399400
O	1.52201200	6.63181100	-3.12429000
C	-1.92445300	-5.93388800	-2.12842200
O	-2.81986500	-6.23056500	-1.27981200
O	-1.58315600	-6.54347100	-3.16715200
C	4.39204000	-1.53209300	-2.06106700
C	-4.38549500	1.49813300	-2.01995000
H	3.49586500	-1.47514900	-2.68911900
H	-3.48457400	1.42882800	-2.63986000
C	5.27570500	-2.73212400	-2.55311800
O	5.47328500	-3.64887600	-1.70130000
O	5.69578100	-2.64225200	-3.73121100
C	5.13475200	-0.17965300	-2.18064200
H	4.44563800	0.63015300	-1.91887000
H	5.38299100	-0.08234200	-3.24263300
C	6.39273600	-0.07232200	-1.34525100
C	7.57981400	-0.71115500	-1.74498400
C	6.40568800	0.67622100	-0.15815200
C	8.73942900	-0.61477000	-0.97650000
H	7.58570100	-1.28629700	-2.66622900
C	7.56100200	0.78000100	0.61807400
H	5.50702400	1.20145700	0.15383800
C	8.73104400	0.13142500	0.20845700
H	9.65069700	-1.10631200	-1.30194200
H	7.55557200	1.37167500	1.52801900
C	9.96161600	0.20167800	1.06335300
F	10.05979900	1.38260300	1.72492400
F	11.09989300	0.05144700	0.34132600
F	9.98130100	-0.77064900	2.01638200

C	-5.13001900	0.14580500	-2.12911200
C	-5.26320200	2.69308600	-2.53258000
O	-5.67705900	2.58928800	-3.71219300
O	-5.46397700	3.62233500	-1.69500200
H	-5.37068500	0.03590000	-3.19163100
H	-4.44363500	-0.66130300	-1.85247400
C	-6.39444000	0.04853300	-1.30282600
C	-7.58044200	0.67649400	-1.72350700
C	-6.41338000	-0.67483000	-0.10061400
C	-8.74613200	0.58812900	-0.96381400
H	-7.57825800	1.24091900	-2.65142300
C	-7.57504300	-0.76987400	0.66776500
H	-5.51263800	-1.18323800	0.23253300
C	-8.74414400	-0.13498100	0.23588200
H	-9.65380100	1.07948400	-1.30012500
H	-7.57151700	-1.33298400	1.59551600
C	-10.01347600	-0.28312900	1.02098700
F	-9.78181800	-0.48069500	2.34305800
F	-10.75573700	-1.34425900	0.59992400
F	-10.81451200	0.80703700	0.91339000

E(RTPSSh) = -3604.1069362 Hartree
Zero-point correction = 0.900327
Thermal correction to Energy = 0.966638
Thermal correction to Enthalpy = 0.967582
Thermal correction to Gibbs Free Energy = 0.788011
Sum of electronic and zero-point Energies = -3603.206610
Sum of electronic and thermal Energies = -3603.140298
Sum of electronic and thermal Enthalpies = -3603.139354
Sum of electronic and thermal Free Energies = -3603.318926

Table S5. Optimized Cartesian coordinates (Å) of the *SS*-Δ(δδδδ) isomer of **EuL^1** obtained with DFT calculations at the TPSSh/LCRECP/6-31G(d) level (0 imaginary frequencies).

N	-2.03302300	-0.07772700	-3.22425900
C	-2.00784500	-1.21029000	-4.18892200
C	-1.51113000	-2.50681300	-3.56037500
N	-0.13348600	-2.39618400	-2.99537200
C	0.87480200	-2.44949400	-4.08885500
C	2.24013600	-1.94018700	-3.64425900
N	2.19250100	-0.52311900	-3.16397000
C	2.18378300	0.41771700	-4.31419800
C	1.68156200	1.80499100	-3.93267200
N	0.29796000	1.79718500	-3.36895200
C	-0.70148500	1.65398000	-4.46432000
C	-2.07241100	1.23038600	-3.95113100
C	-3.22956100	-0.15993800	-2.35323900
C	-3.06324300	0.87608700	-1.25400800
O	-1.91875500	1.02350000	-0.73158200
C	0.07540200	-3.51826900	-2.04898600

C	-0.73152500	-3.26419200	-0.78776200
O	-1.00922800	-2.06492400	-0.45673700
C	3.36849700	-0.28920300	-2.29306600
C	3.16692300	-1.11908700	-1.03475100
O	2.00973900	-1.18555800	-0.52885100
C	0.08719500	3.07162500	-2.64031000
C	0.87649500	3.03109000	-1.34302200
O	1.11696000	1.90975700	-0.79292100
H	-1.36396100	-0.91877900	-5.02173400
H	-3.00883900	-1.37942000	-4.61091800
H	-2.17886500	-2.80555300	-2.74766900
H	-1.54876900	-3.30772700	-4.31257400
H	0.49377500	-1.85056800	-4.91925600
H	0.98174400	-3.47758600	-4.46396400
H	2.62564300	-2.56684500	-2.83115100
H	2.94531500	-2.02632700	-4.48337700
H	1.54675800	-0.01751600	-5.08739000
H	3.18958400	0.50835800	-4.74859400
H	2.34246500	2.24510300	-3.18082500
H	1.72598300	2.45854300	-4.81564700
H	-0.31269800	0.92038600	-5.17497400
H	-0.80477000	2.60031100	-5.01441900
H	-2.46693800	1.99189200	-3.26712000
H	-2.76717900	1.16457000	-4.80081500
H	-4.15579500	-0.00834200	-2.92469700
H	-3.27077800	-1.15018700	-1.88860500
H	-0.20294600	-4.47966700	-2.50452800
H	1.13634800	-3.58050300	-1.76249500
H	4.30759000	-0.53977000	-2.80596900
H	3.40545200	0.76734100	-2.00885400
H	0.38595100	3.93320900	-3.25472800
H	-0.97752700	3.19448500	-2.38951400
O	-0.13818600	-0.00856300	1.02002000
H	-0.54174300	-0.89184700	1.15483200
H	-0.88254400	0.61777900	1.11772400
Eu	0.07297500	-0.14286800	-1.52062400
N	1.26502200	4.17563300	-0.81765700
N	4.21339700	-1.73600600	-0.50097600
N	-1.09460700	-4.29834500	-0.05903500
N	-4.11725100	1.58110000	-0.86686700
H	1.10483200	5.09288800	-1.26161000
H	5.07560000	-1.72991100	-1.03614700
H	-0.90699300	-5.27908500	-0.32020400
H	-4.96639300	1.48029600	-1.41335100
C	1.96634400	4.36776800	0.44506400
H	1.36881500	3.98566200	1.27983100
H	2.92042900	3.82982600	0.43979400
C	-1.80620200	-4.26923600	1.21282600
H	-1.22543300	-3.72767700	1.96743600
H	-2.77085900	-3.76307600	1.10072700
C	2.20972800	5.90210700	0.60866300
O	1.76581700	6.62338300	-0.33566400

O	2.81405200	6.24512600	1.65070600
C	-2.01834700	-5.75274100	1.65508000
O	-1.54638400	-6.62431700	0.86370500
O	-2.62818900	-5.91069200	2.73733600
C	-3.99812900	2.77151800	-0.02504500
C	4.07416000	-2.75749200	0.53572500
H	-3.27788500	2.53180400	0.76289800
H	3.28511500	-2.40953700	1.20919800
C	-5.35281000	3.12656300	0.61162600
H	-5.18938500	4.07962600	1.12292600
H	-6.09142300	3.30814900	-0.18001700
C	-3.39682700	3.99007300	-0.83616200
O	-2.96770000	3.74950100	-2.00028600
O	-3.39480900	5.07132700	-0.20252200
C	-5.87182700	2.07995400	1.57303200
C	-6.95578100	1.25666900	1.23237400
C	-5.26511700	1.89972200	2.82810400
C	-7.42429500	0.28026500	2.11345100
H	-7.44405400	1.38208200	0.26920600
C	-5.72434800	0.92826700	3.71582800
H	-4.42607800	2.52862700	3.11567700
C	-6.80656600	0.11432000	3.35720100
H	-8.26189100	-0.35018800	1.83255000
H	-5.24450200	0.80142700	4.68094200
C	-7.34120600	-0.89374400	4.33091600
F	-6.37850000	-1.36637500	5.16151500
F	-7.89540200	-1.96433900	3.70855700
F	-8.31239700	-0.37108000	5.12915400
C	3.57135600	-4.12721400	-0.07566600
O	3.13123700	-4.09597800	-1.26035400
O	3.63486700	-5.09773500	0.71516400
C	5.38469000	-2.91718400	1.32527800
H	6.19672200	-3.18528100	0.63693100
H	5.22414000	-3.77684800	1.98235400
C	5.76517300	-1.68931600	2.12328800
C	6.82534600	-0.86159500	1.72341100
C	5.04495800	-1.33916700	3.27857300
C	7.16028200	0.28298400	2.44939400
H	7.40003800	-1.11589100	0.83642400
C	5.36969500	-0.19861400	4.01092600
H	4.22142600	-1.96681500	3.61036900
C	6.42987000	0.61685100	3.59447000
H	7.98088000	0.91391000	2.12302200
H	4.80179900	0.05894100	4.89918500
C	6.81898700	1.81485100	4.40888400
F	5.76231400	2.35301600	5.06756500
F	7.74676700	1.51100100	5.35815500
F	7.36111400	2.79888500	3.64836100

E(RTPSSh) = -3604.1066012 Hartree
Zero-point correction = 0.900797
Thermal correction to Energy = 0.967198

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Thermal correction to Enthalpy = 0.968143
Thermal correction to Gibbs Free Energy = 0.787703
Sum of electronic and zero-point Energies = -3603.205805
Sum of electronic and thermal Energies = -3603.139403
Sum of electronic and thermal Enthalpies = -3603.138459
Sum of electronic and thermal Free Energies = -3603.318898
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