

The conjugate base of methyl 3-oxobutanoate as antenna-ligand in visible-emitting photoluminescent lanthanide complexes

Electronic supplementary information (ESI)

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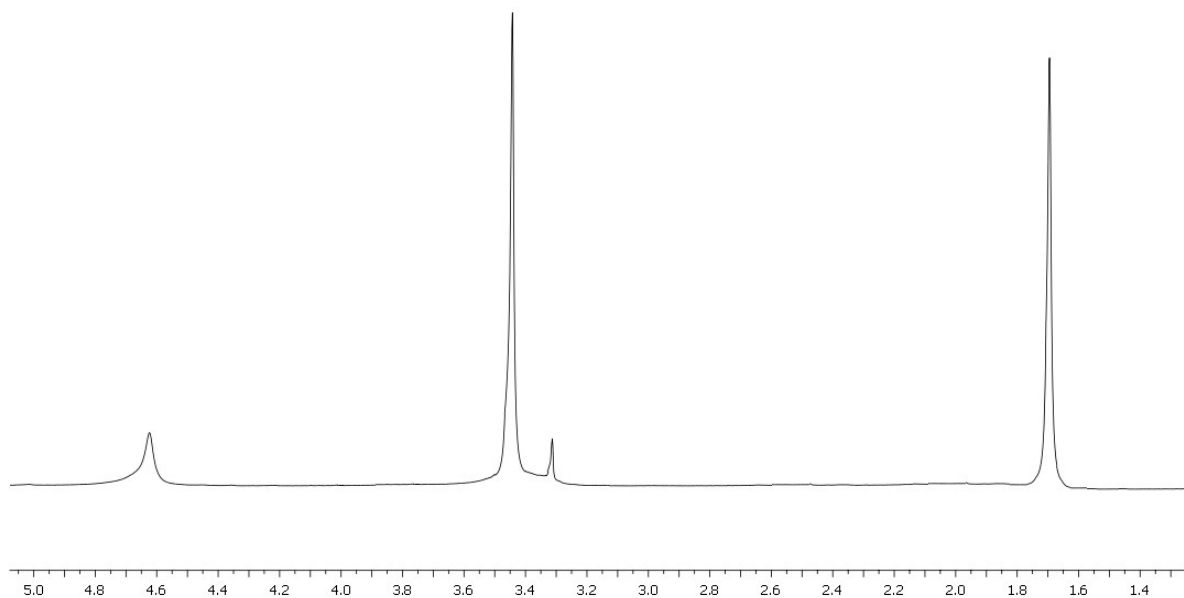
NMR spectra

Figure S1. ^1H NMR (DMSO-d_6 , 298 K) of **1^Y**.

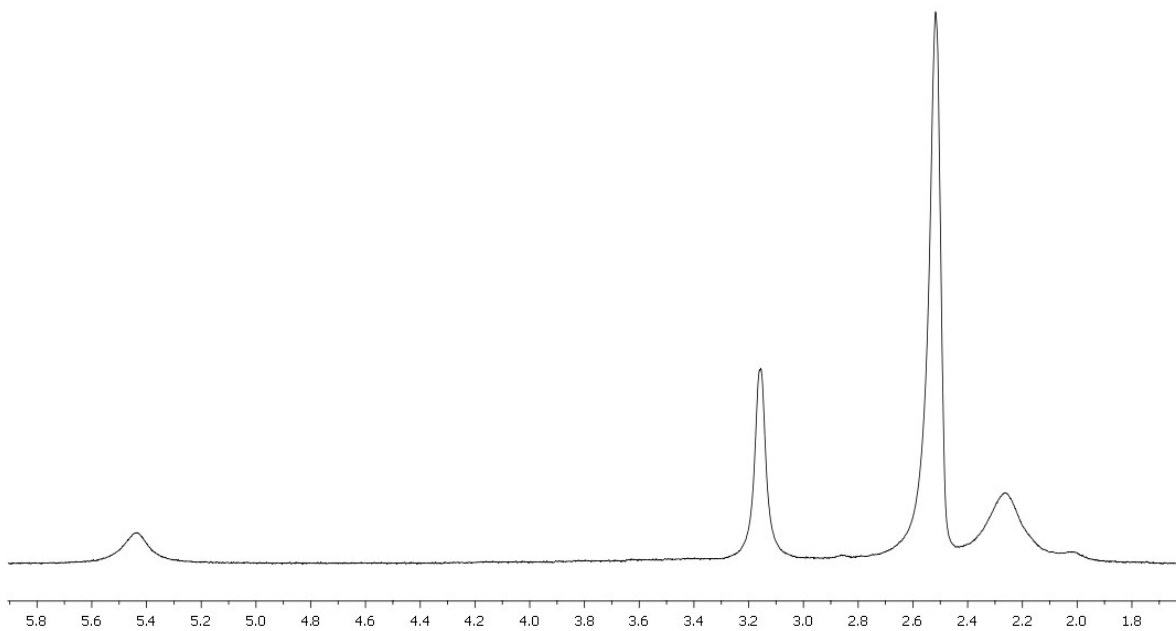


Figure S2. ^1H NMR (DMSO-d_6 , 315 K) of **1Sm**.

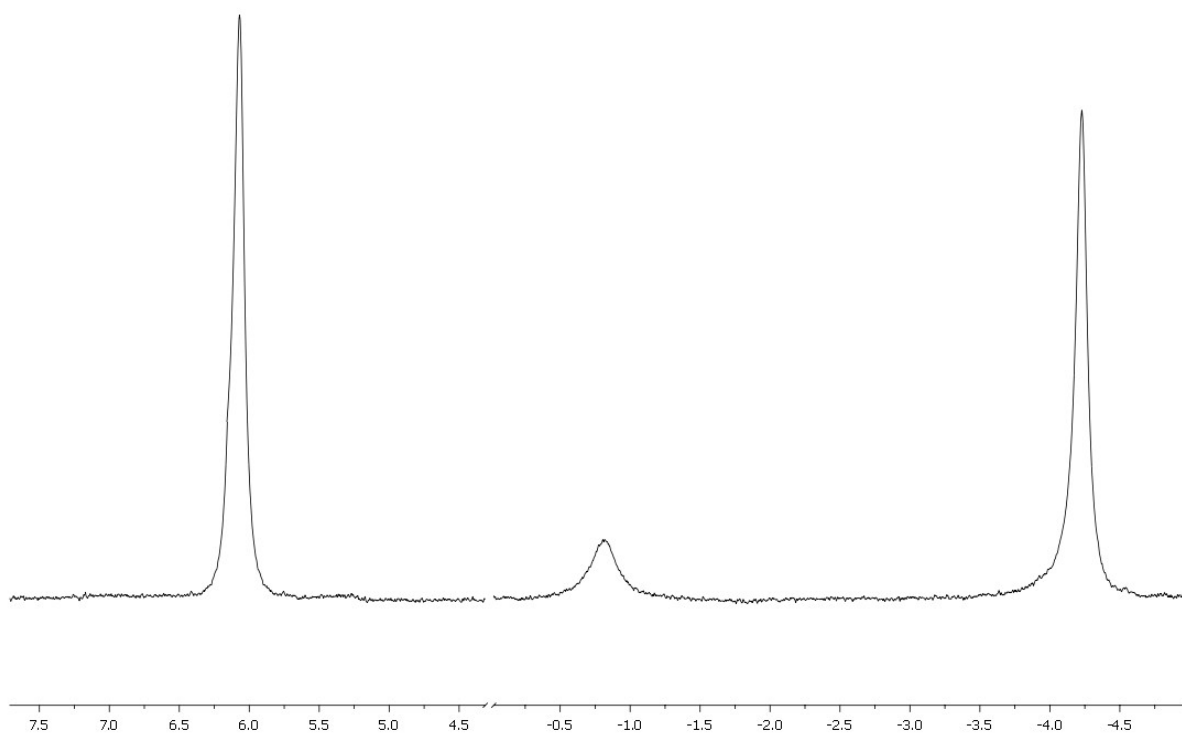


Figure S3. ^1H NMR (DMSO- d_6 , 295 K) of **1**^{Eu}.

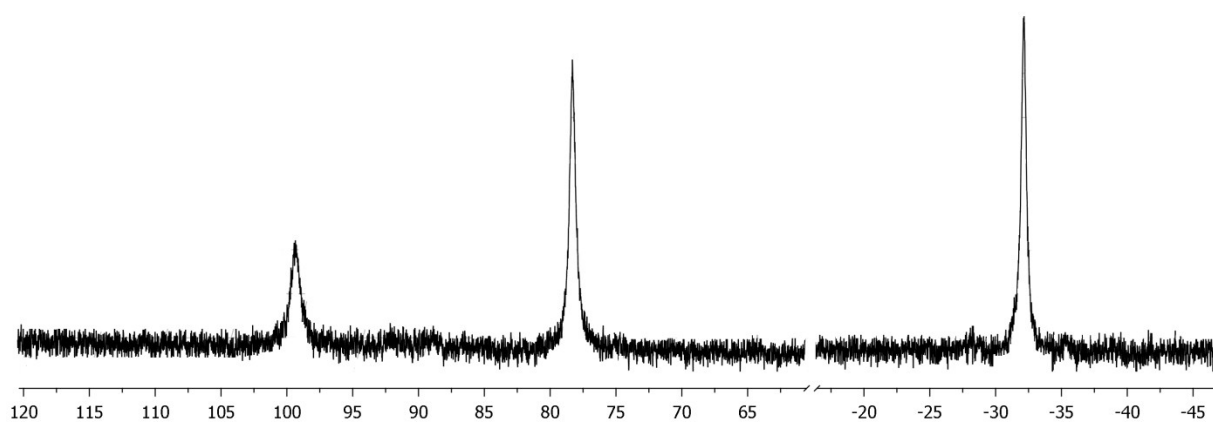


Figure S4. ^1H NMR (DMSO- d_6 , 295 K) of **1**^{Tb}.

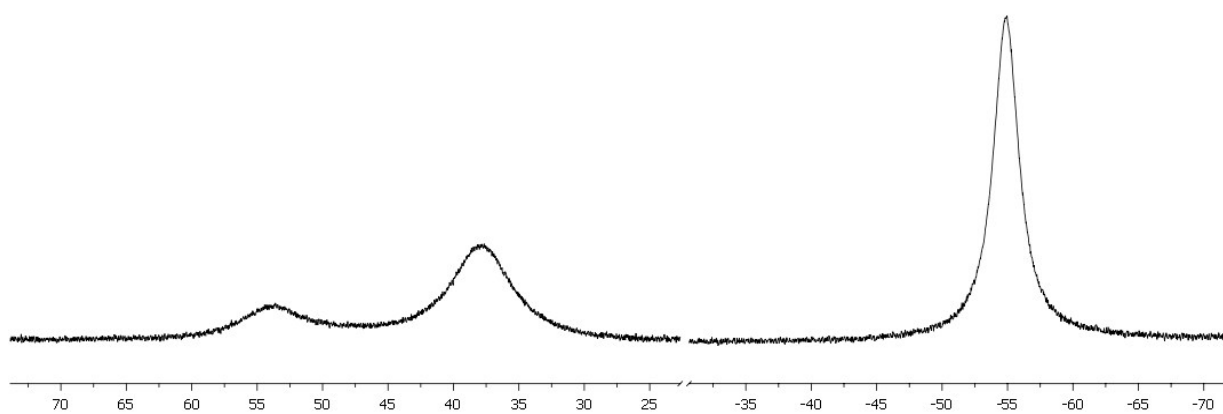


Figure S5. ^1H NMR (DMSO- d_6 , 295 K) of **1**^{Py}.

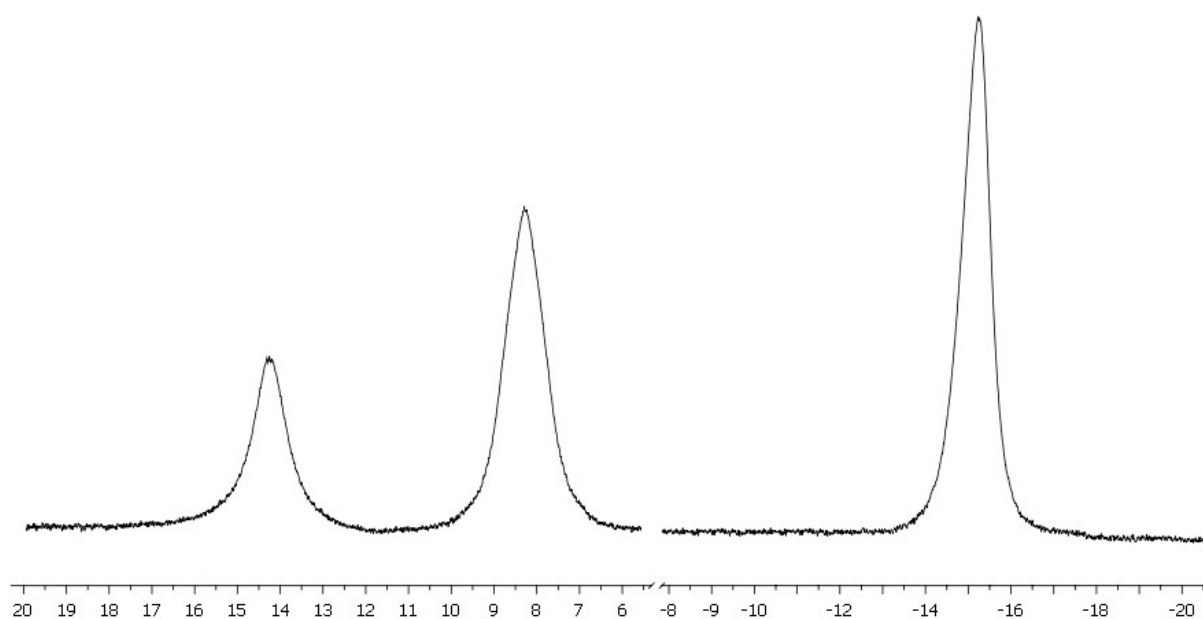


Figure S6. ^1H NMR (DMSO-d_6 , 319 K) of **1^{Yb}**.

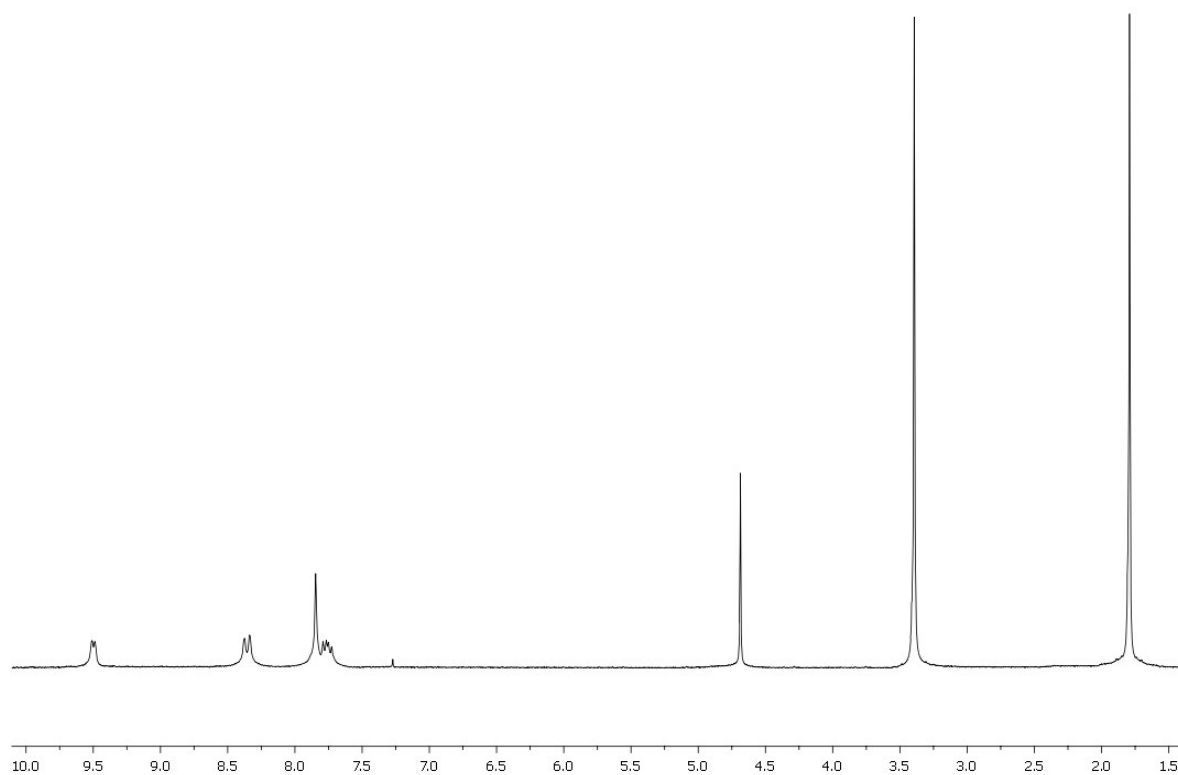


Figure S7. ^1H NMR (CDCl_3 , 298 K) of **2^Y**.

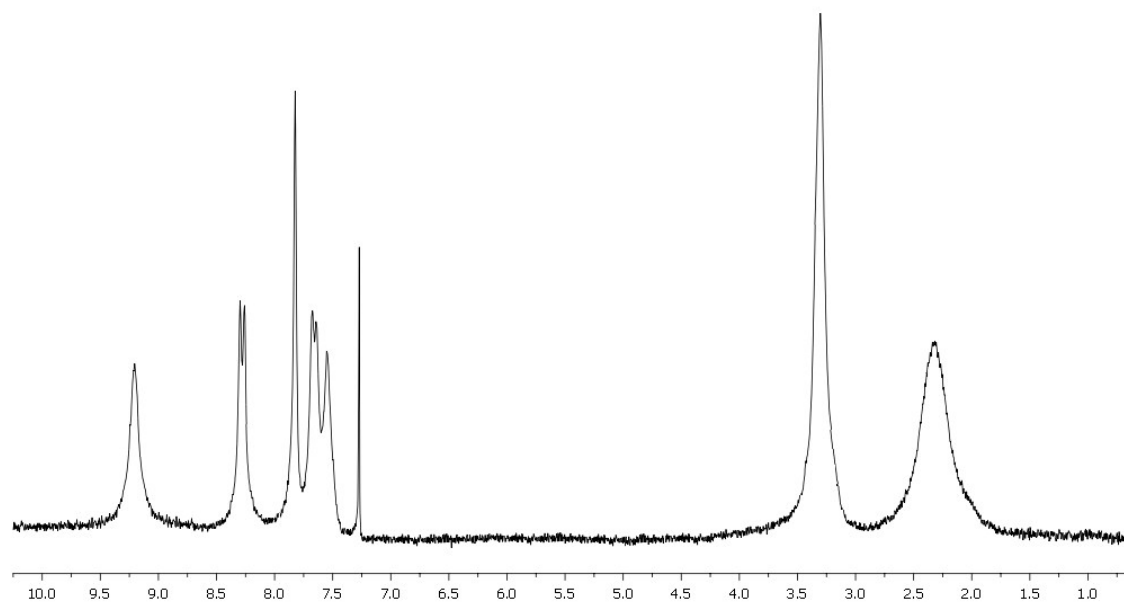


Figure S8. ^1H NMR (CDCl_3 , 298 K) of 2^{Sm} .

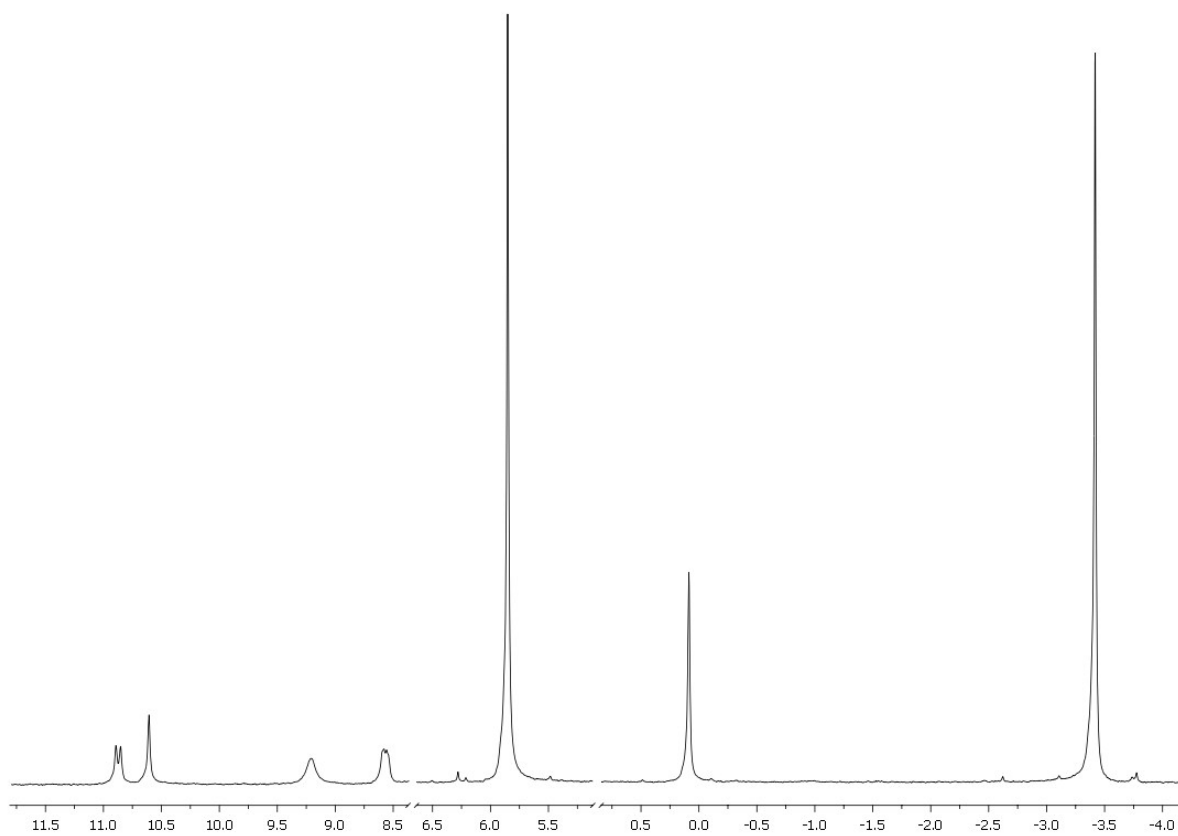


Figure S9. ^1H NMR (CDCl_3 , 298 K) of 2^{Eu} .

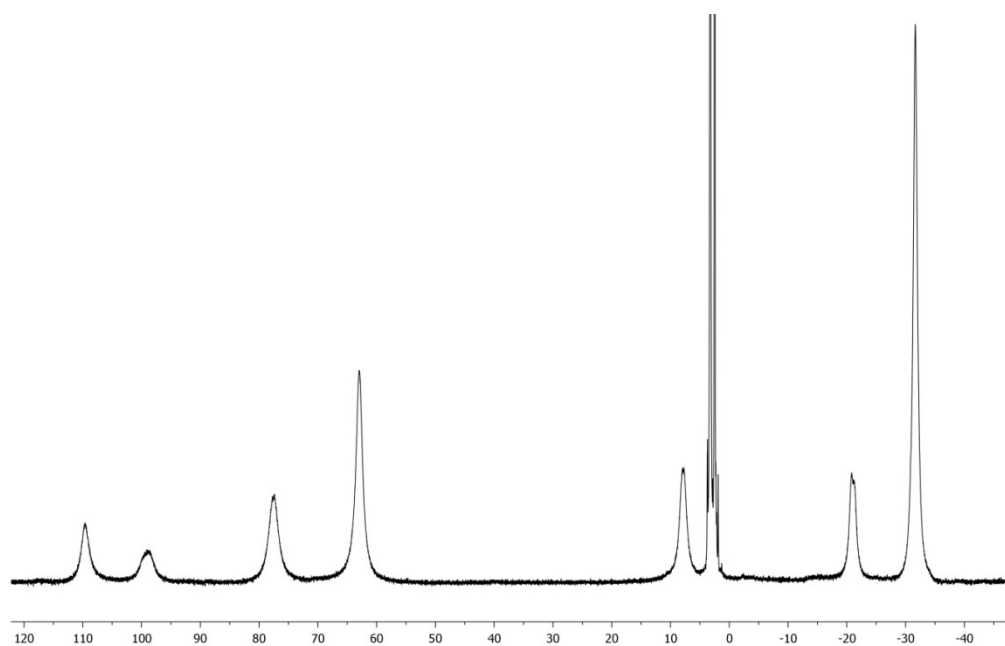


Figure S10. ^1H NMR (DMSO-d_6 , 298 K) of **2^{Tb}**.

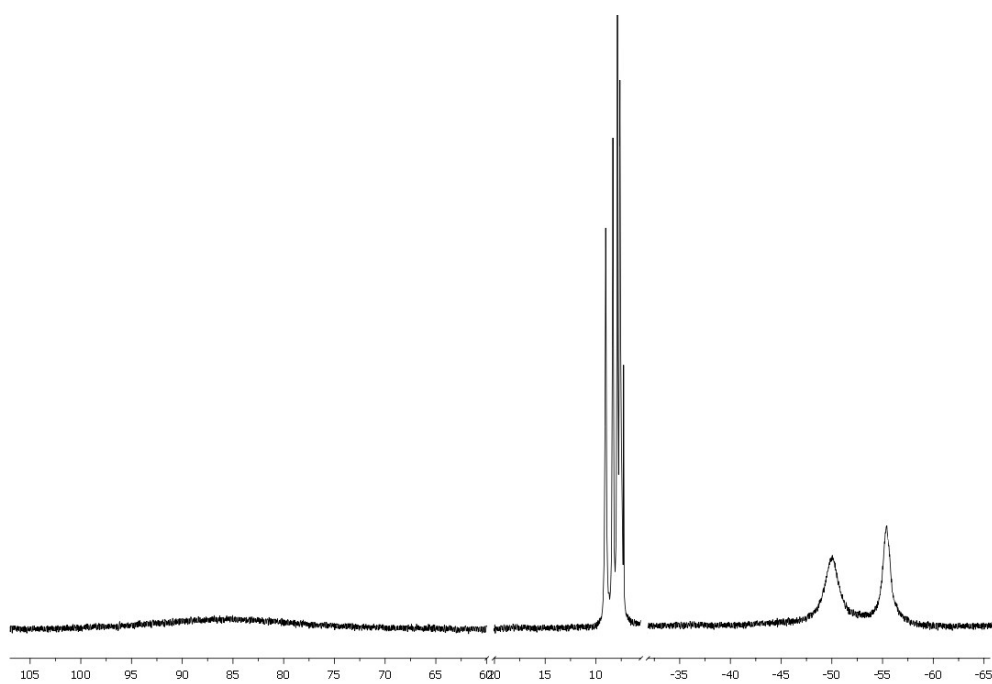


Figure S11. ^1H NMR (CDCl_3 , 311 K) of **2^{Dy}**.

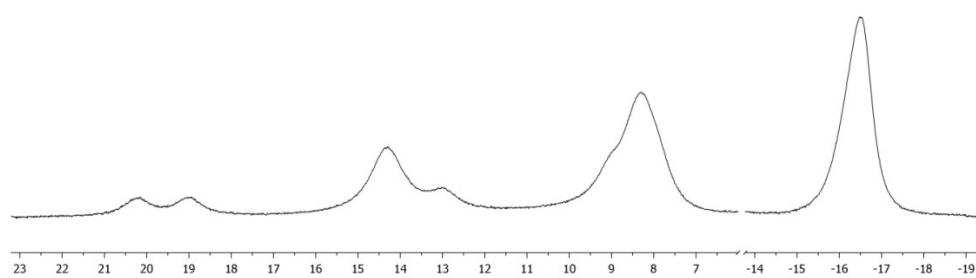


Figure S12. ^1H NMR (DMSO-d_6 , 315 K) of **2^{Yb}**.

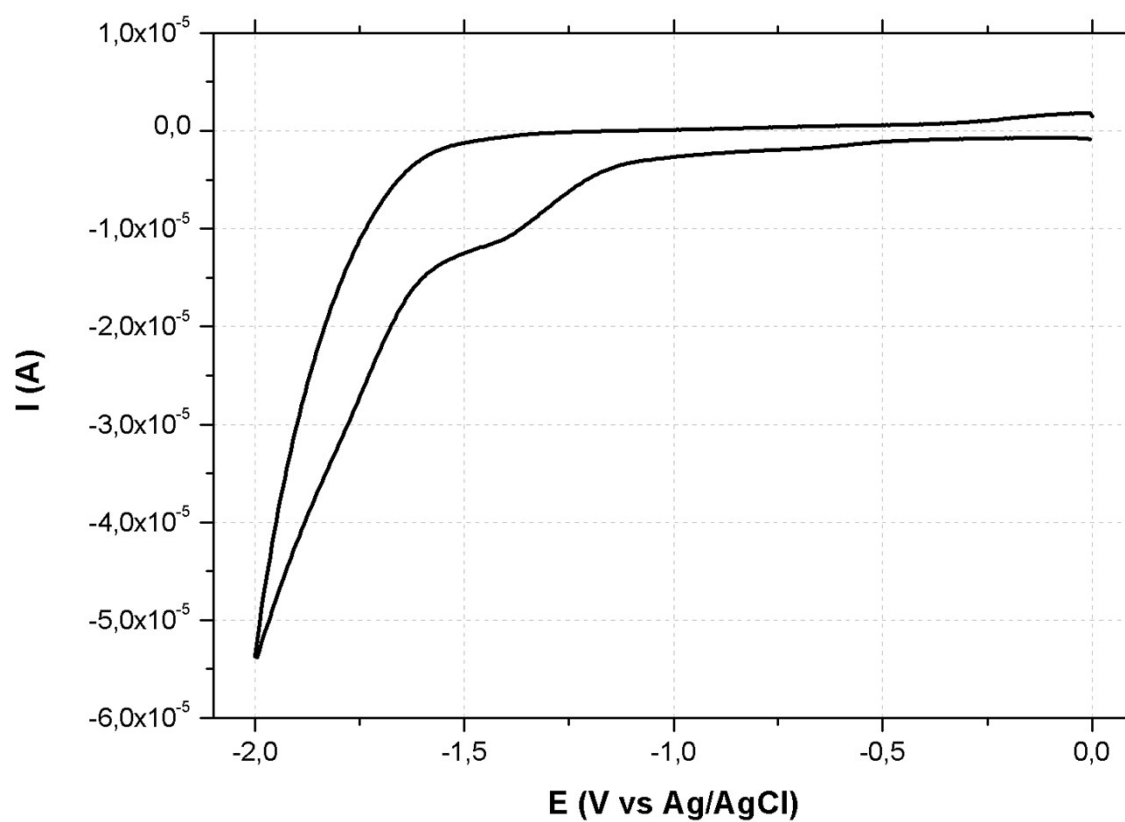
Electrochemistry

Figure S13. Cyclic voltammogram recorded for **1^{Eu}** (1 mM CH₂Cl₂ solution). 0.1 M [NEt₃Bz]Cl as supporting electrolyte. Scan rate = 100 mV s⁻¹.

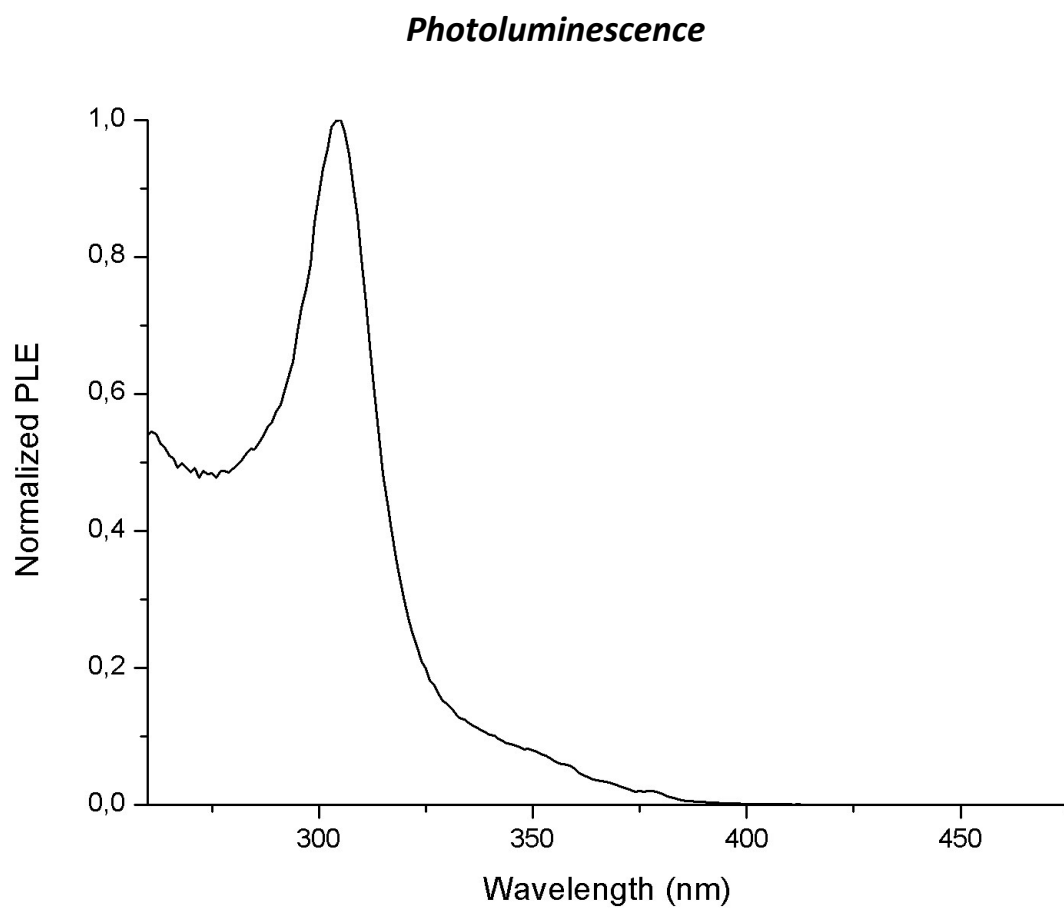


Figure S14. Excitation spectrum of **1^{Tb}** (solid sample, 298 K, $\lambda_{\text{excitation}} = 546 \text{ nm}$).

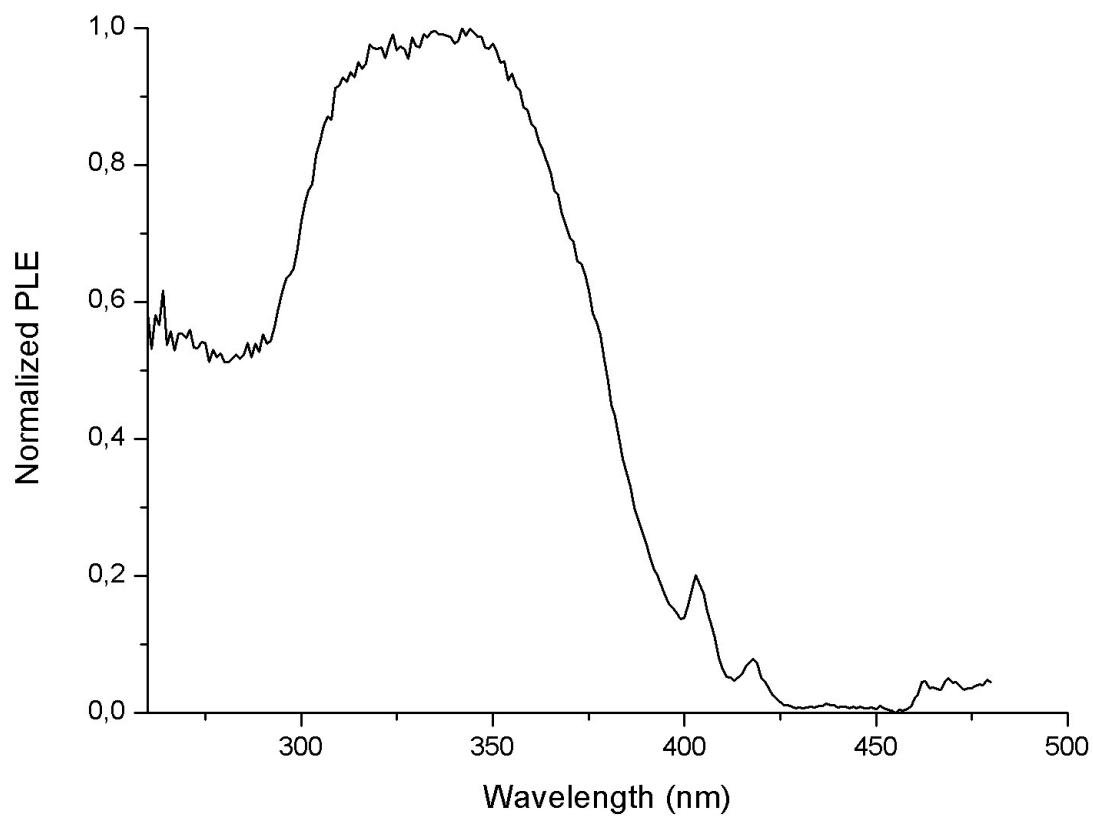


Figure S15. Excitation spectrum of **2Sm** (solid sample, 298 K, $\lambda_{\text{excitation}} = 646 \text{ nm}$).

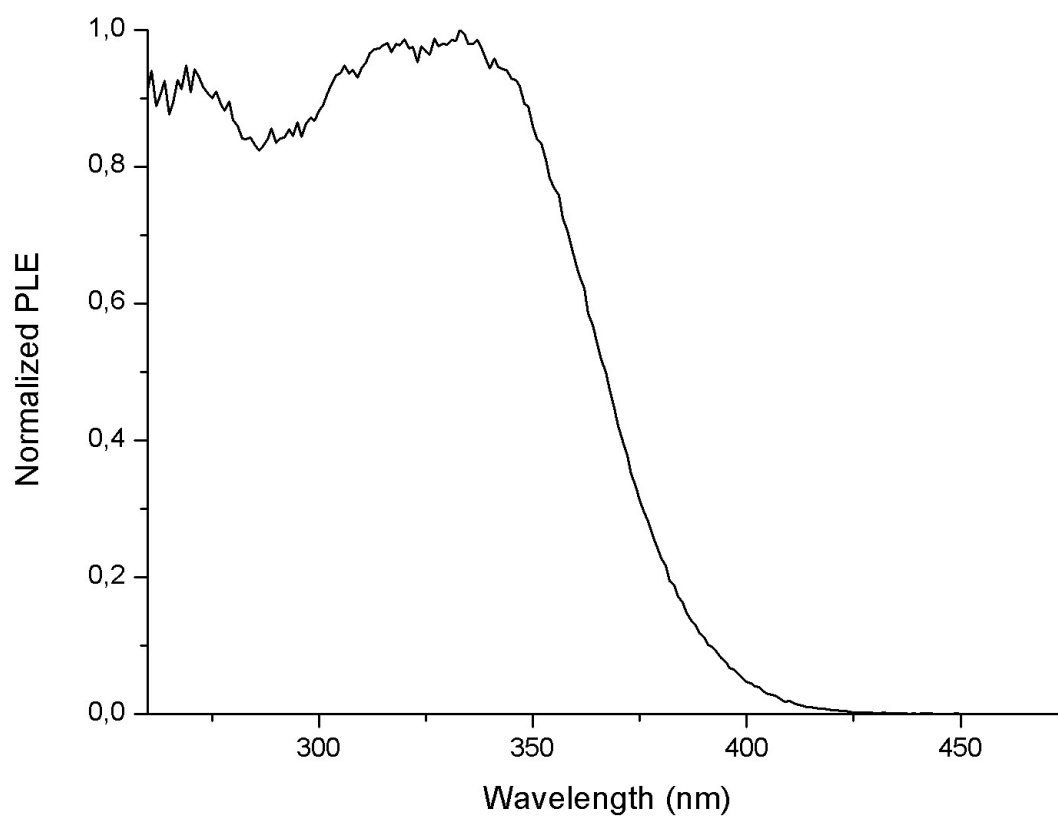


Figure S16. Excitation spectrum of **2Tb** (solid sample, 298 K, $\lambda_{\text{excitation}} = 548$ nm).

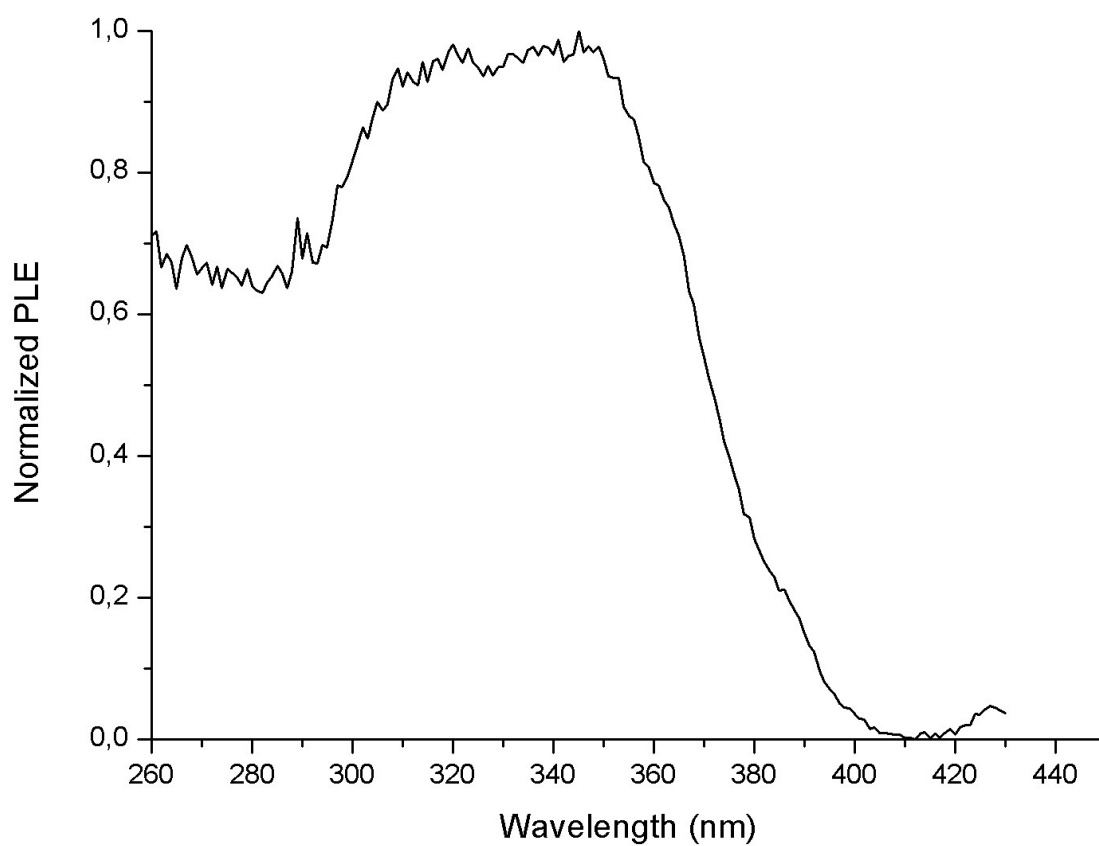


Figure S17. Excitation spectrum of **2Py** (solid sample, 298 K, $\lambda_{\text{excitation}} = 576$ nm).

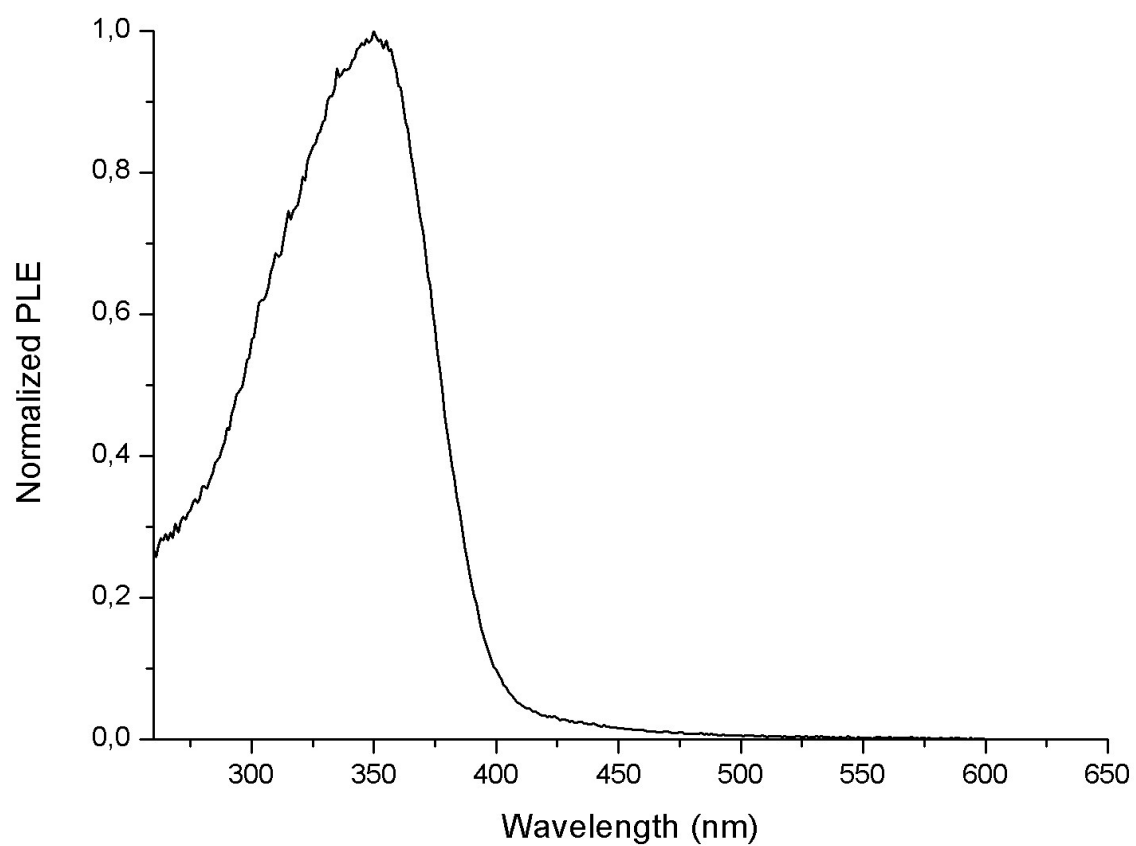


Figure S18. Excitation spectrum of **2^yb** (solid sample, 298 K, $\lambda_{\text{excitation}} = 1000$ nm).

DFT calculations**Cartesian coordinates (Å) of Lu(acac)₃**

C	-3.068245000	-0.259409000	-1.100167000
C	-3.556804000	-0.999526000	0.001092000
H	-4.599751000	-1.292550000	0.001397000
C	-2.753297000	-1.376480000	1.101689000
O	-1.836747000	0.148673000	-1.195430000
O	-1.489116000	-1.083742000	1.195298000
Lu	-0.000841000	-0.000694000	-0.000454000
C	2.569388000	-1.693019000	1.100684000
C	2.648824000	-2.574542000	-0.001638000
H	3.427128000	-3.328263000	-0.002330000
C	1.763431000	-2.522053000	-1.103061000
O	1.681121000	-0.747190000	1.195357000
O	0.790814000	-1.663232000	-1.196550000
C	0.187950000	3.068951000	1.103998000
C	0.913635000	3.577040000	0.002328000
H	1.184423000	4.625988000	0.004616000
C	1.304976000	2.785303000	-1.101857000
O	-0.192672000	1.828399000	1.196113000
O	1.041389000	1.514904000	-1.198142000
C	-3.984455000	0.100883000	-2.245814000
H	-5.004129000	-0.263480000	-2.095975000
H	-4.003248000	1.190608000	-2.367874000
H	-3.582987000	-0.318269000	-3.176351000
C	-3.346005000	-2.162350000	2.247399000
H	-4.409662000	-2.370939000	2.105331000
H	-2.803729000	-3.109274000	2.358677000

H	-3.207266000	-1.602754000	3.180129000
C	2.070237000	3.400708000	-2.249520000
H	2.263631000	4.466104000	-2.099177000
H	3.023380000	2.873309000	-2.376565000
H	1.502346000	3.263364000	-3.177563000
C	-0.190861000	3.973543000	2.252815000
H	0.152614000	5.001145000	2.107438000
H	-1.280716000	3.969396000	2.374353000
H	0.236435000	3.576791000	3.181751000
C	1.912615000	-3.493353000	-2.250403000
H	2.748673000	-4.183058000	-2.108342000
H	0.985084000	-4.067662000	-2.363245000
H	2.057778000	-2.933877000	-3.182278000
C	3.542371000	-1.816205000	2.249349000
H	4.266959000	-2.620980000	2.099383000
H	4.076336000	-0.866979000	2.377929000
H	2.985548000	-1.998795000	3.176396000

Cartesian coordinates (Å) of Lu(MAA)₃

C	-2.561995000	-1.805681000	1.251073000
C	-3.541477000	-1.290302000	0.382039000
H	-4.556102000	-1.647851000	0.488475000
C	-3.223801000	-0.323898000	-0.612997000
O	-1.307146000	-1.455988000	1.214188000
O	-2.059363000	0.166771000	-0.806973000
Lu	-0.055516000	-0.085236000	0.064697000
C	0.987847000	2.899082000	-0.690433000
C	0.731555000	3.496997000	0.574921000
H	0.963140000	4.539780000	0.740898000
C	0.182141000	2.762334000	1.641541000

O	0.766660000	1.672489000	-0.974661000
O	-0.145194000	1.503330000	1.559510000
C	1.687041000	-2.204936000	-1.701563000
C	2.746745000	-2.350065000	-0.786603000
H	3.568816000	-2.997329000	-1.058258000
C	2.753251000	-1.669573000	0.462457000
O	0.641190000	-1.459653000	-1.481829000
O	1.835588000	-0.875761000	0.865924000
C	-2.938932000	-2.825834000	2.299753000
H	-4.003989000	-3.072606000	2.281688000
H	-2.352902000	-3.739464000	2.144134000
H	-2.672631000	-2.439897000	3.290861000
C	1.720329000	-2.934991000	-3.023560000
H	2.615153000	-3.552630000	-3.139385000
H	0.828706000	-3.566779000	-3.112845000
H	1.677514000	-2.203125000	-3.838965000
C	-0.061279000	3.428350000	2.975525000
H	0.222257000	4.484364000	2.975142000
H	-1.121856000	3.337825000	3.238490000
H	0.508142000	2.900907000	3.750088000
O	-4.188705000	0.169596000	-1.461233000
C	-5.565212000	-0.296232000	-1.374834000
H	-6.003421000	-0.054167000	-0.399221000
H	-6.094126000	0.244022000	-2.160691000
H	-5.628830000	-1.375254000	-1.559088000
O	3.791785000	-1.822971000	1.353354000
C	4.920934000	-2.685932000	1.038154000
H	5.449633000	-2.332553000	0.144903000
H	5.577447000	-2.617867000	1.906292000
H	4.597770000	-3.724411000	0.898375000

O	1.519339000	3.628437000	-1.729551000
C	1.808317000	5.046414000	-1.572245000
H	2.570218000	5.210915000	-0.800861000
H	2.191613000	5.364152000	-2.542506000
H	0.899093000	5.609376000	-1.330227000