

Supporting Information for

Heteronuclear Bimetallic Complexes with 3d and 4f Elements

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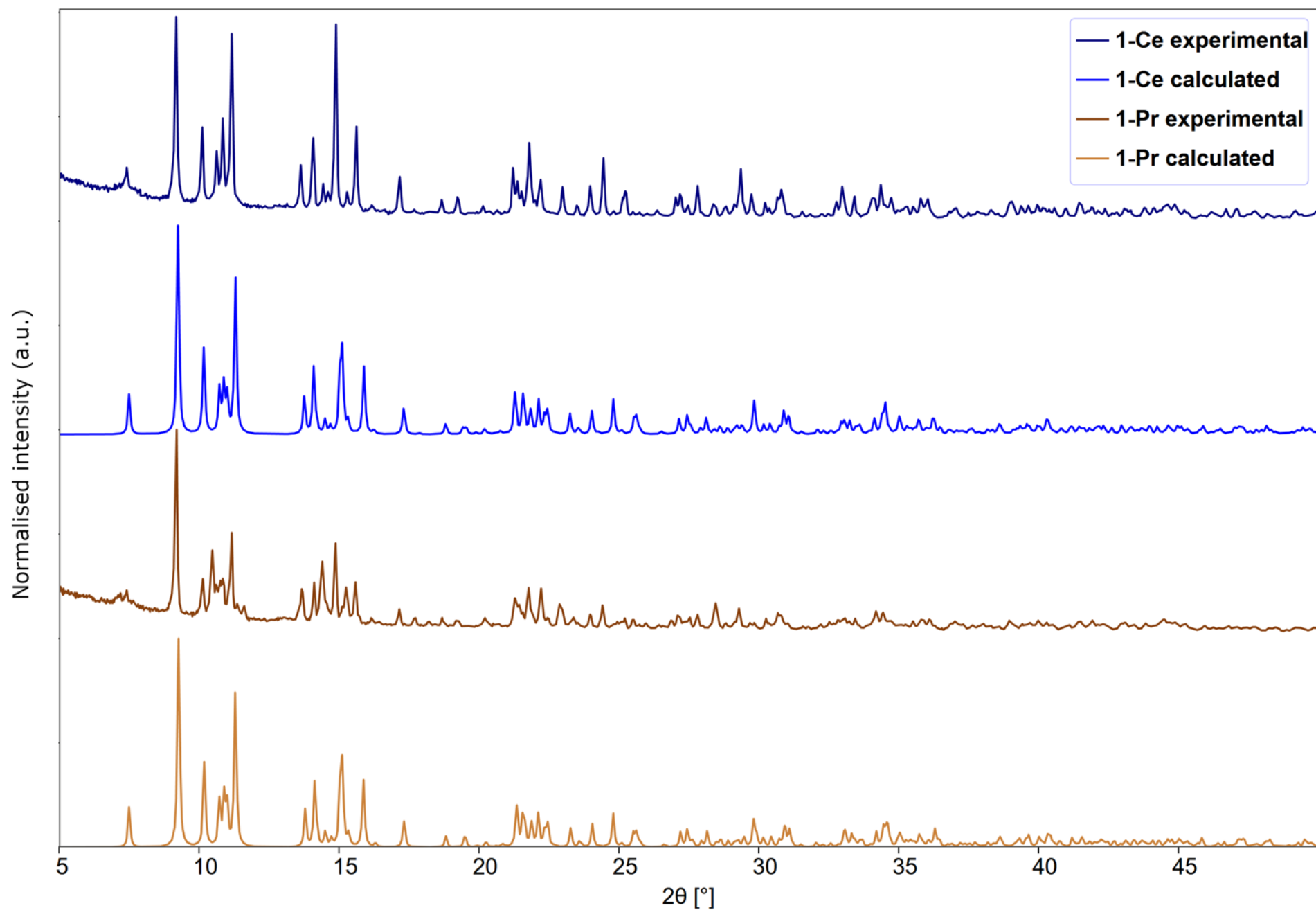


Figure S1: Experimental and Calculated PXRD patterns for **1-Ce** and **1-Pr**

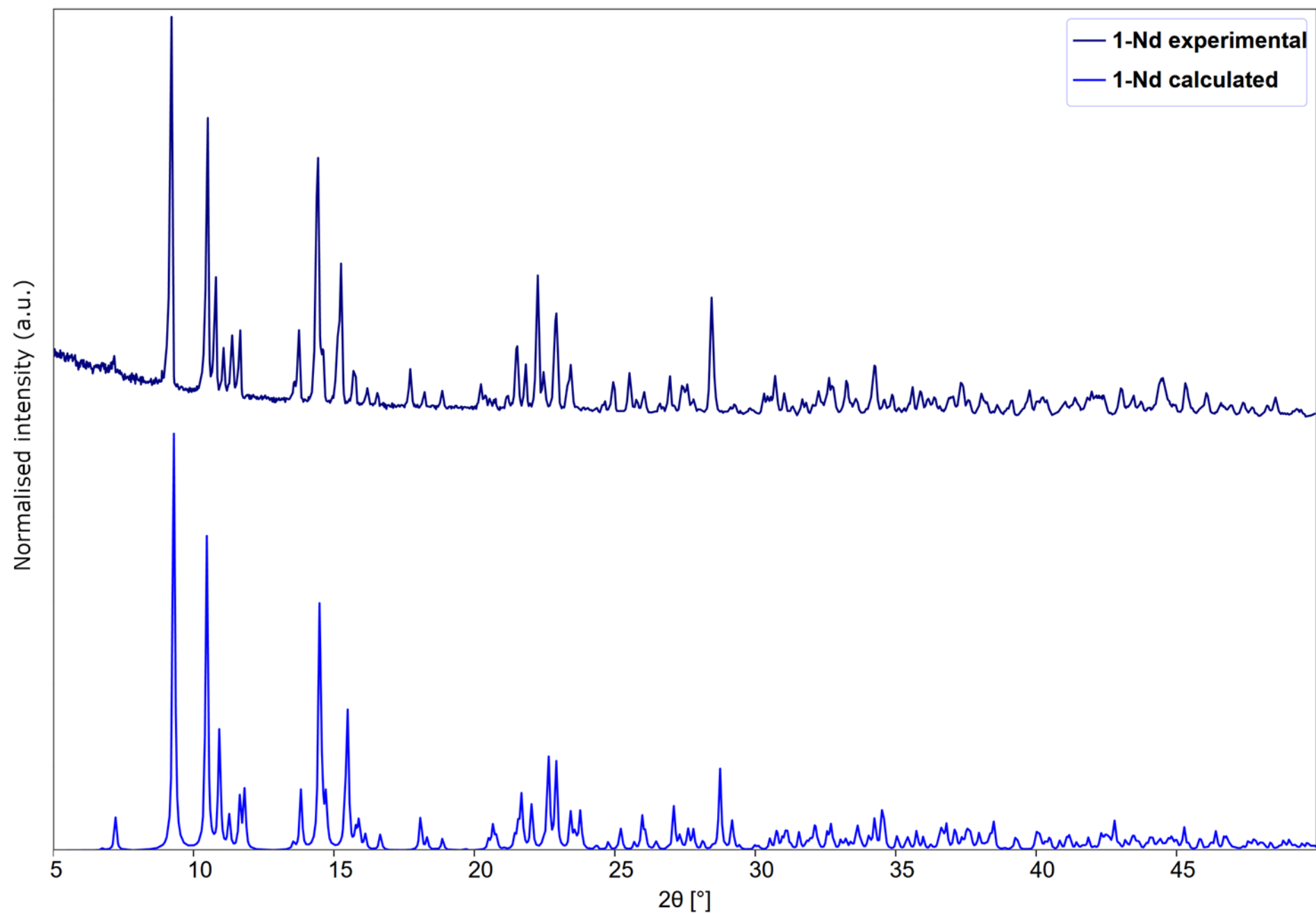


Figure S2: Experimental and Calculated PXRD patterns for **1-Nd**

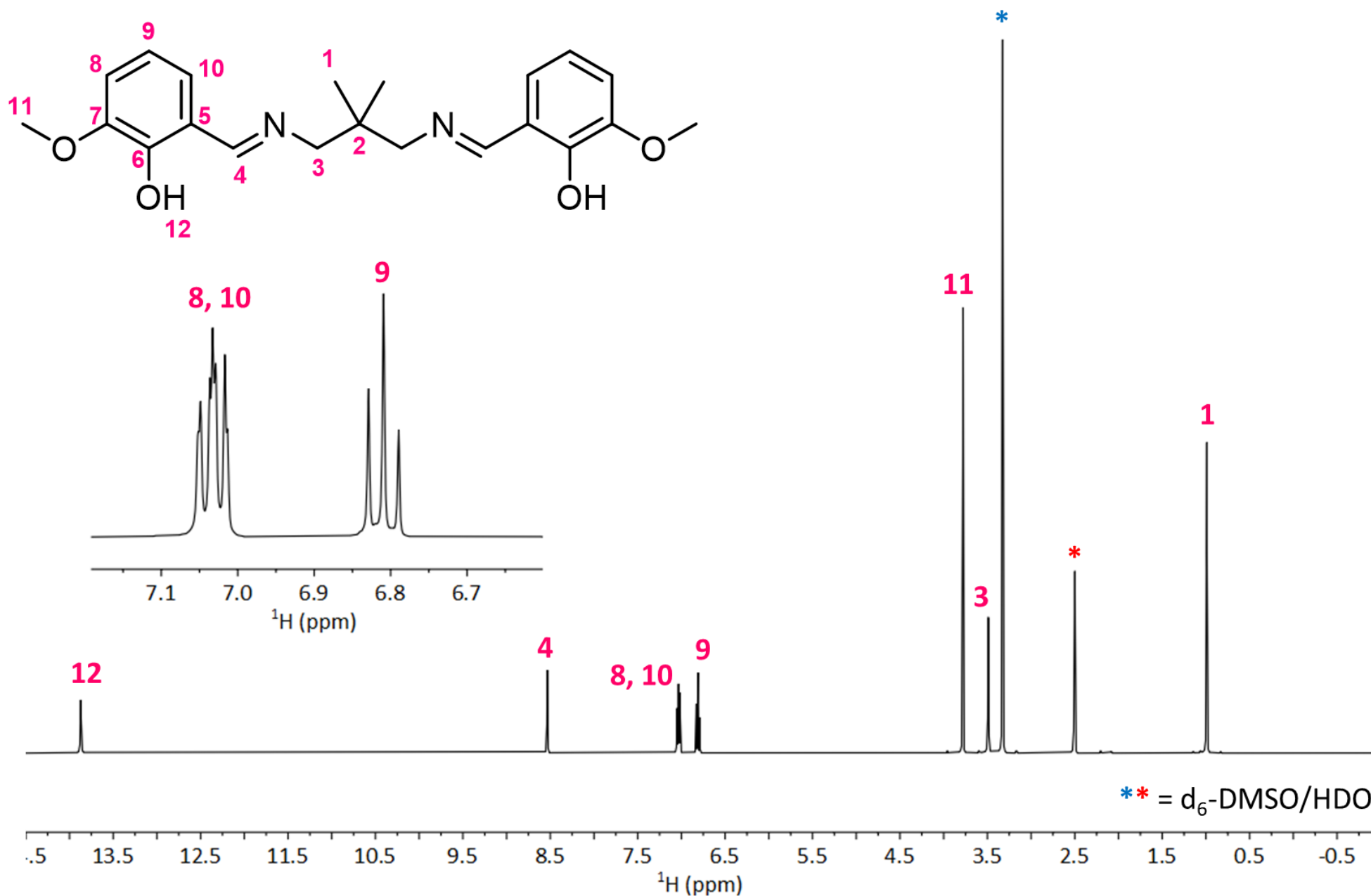


Figure S3: ¹H NMR spectrum of H₂L acquired at 400.3 MHz in d₆-DMSO

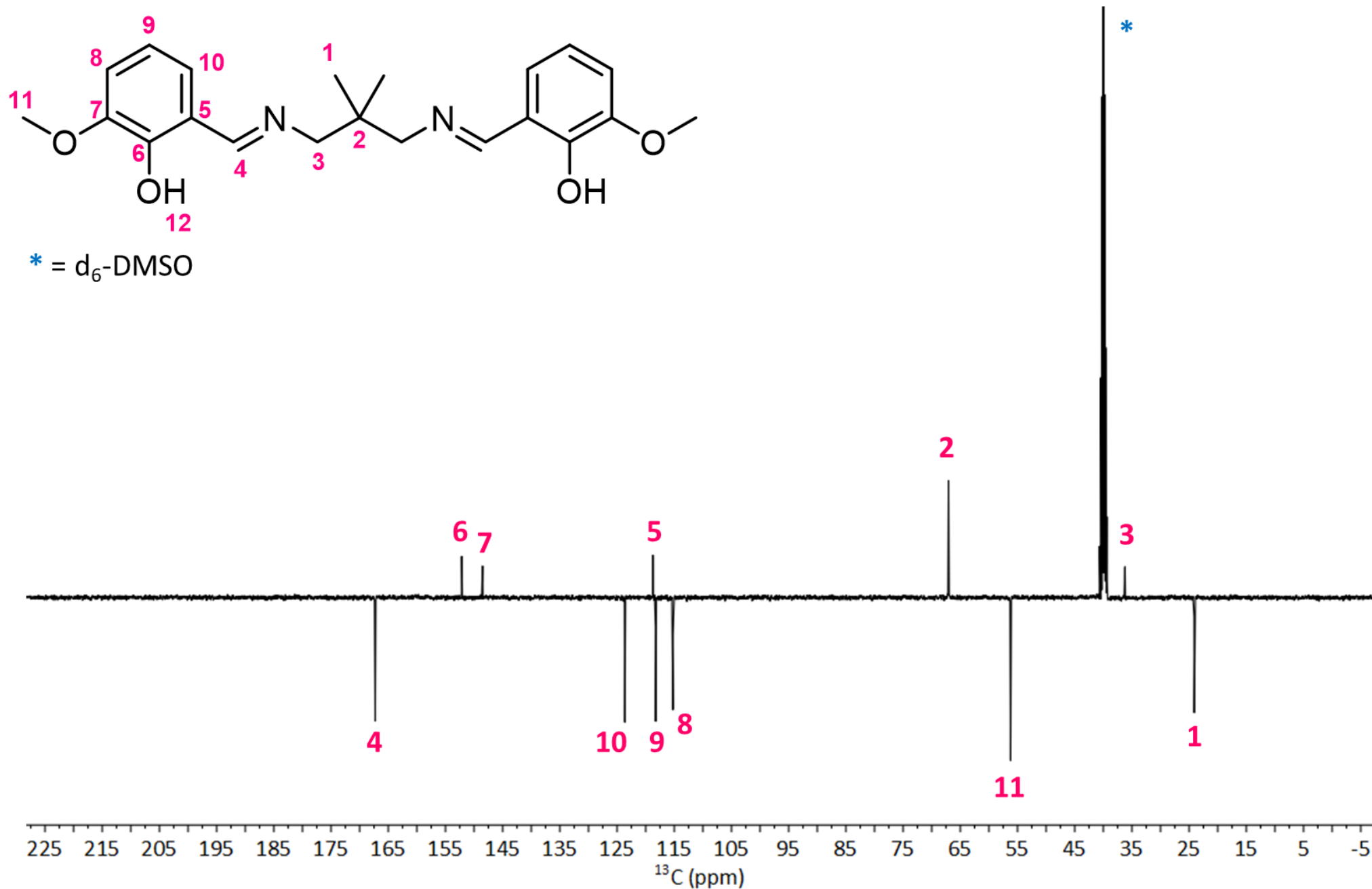


Figure S4: ^{13}C DEPTQ NMR spectrum of H_2L acquired at 100.6 MHz in d_6 -DMSO

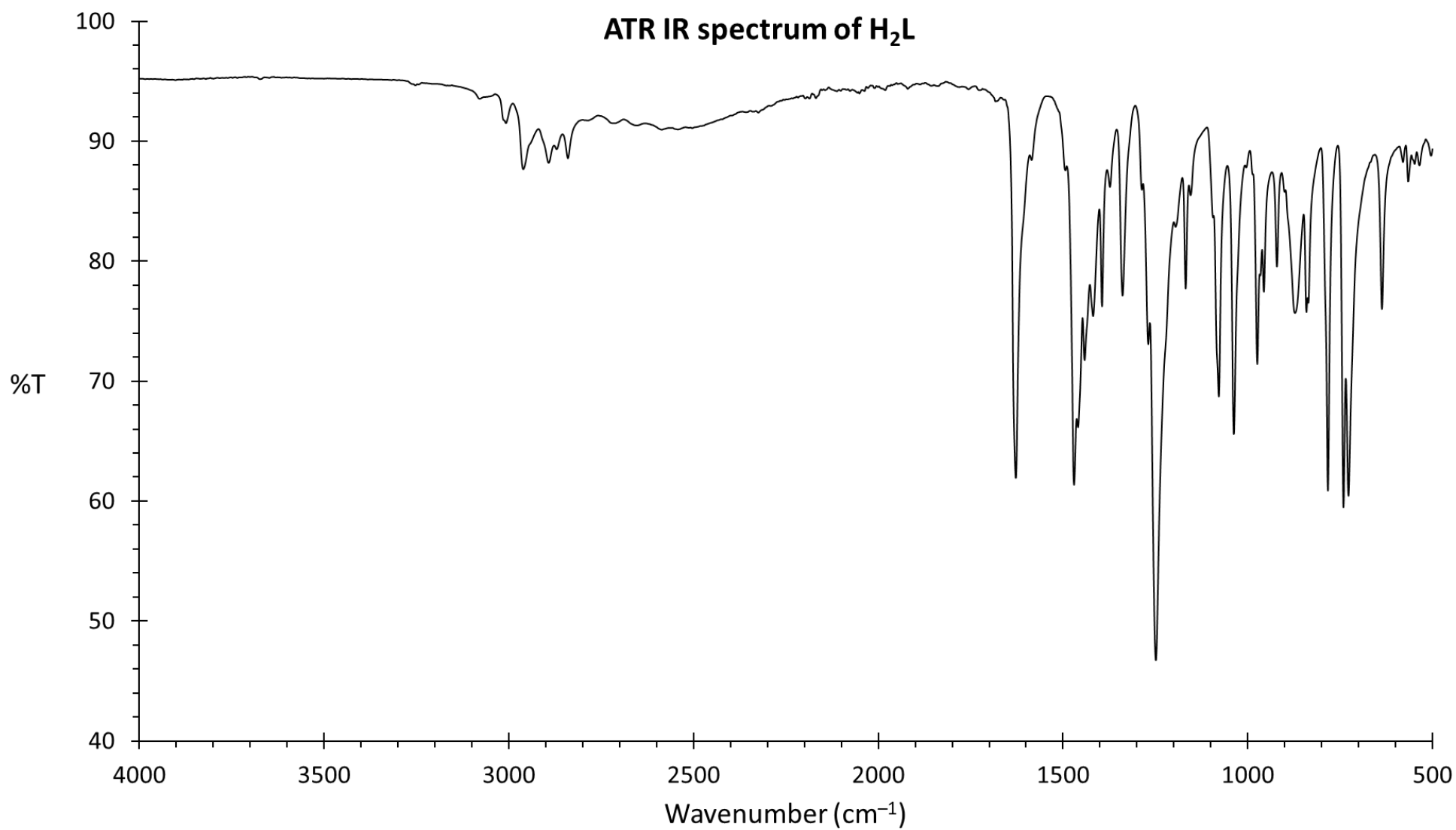


Figure S5: ATR FTIR spectrum of H₂L

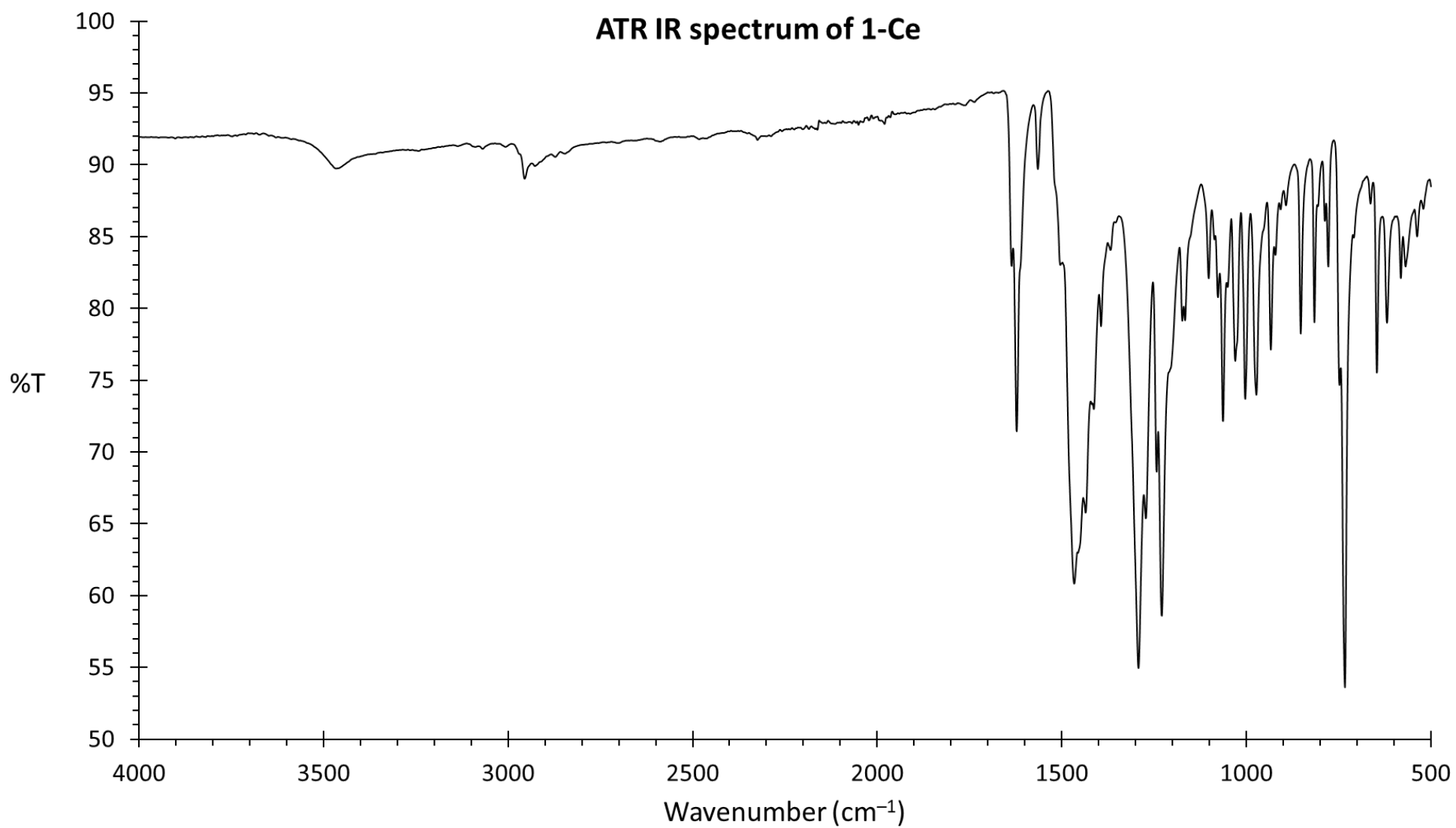


Figure S6: ATR FTIR spectrum of **1-Ce**

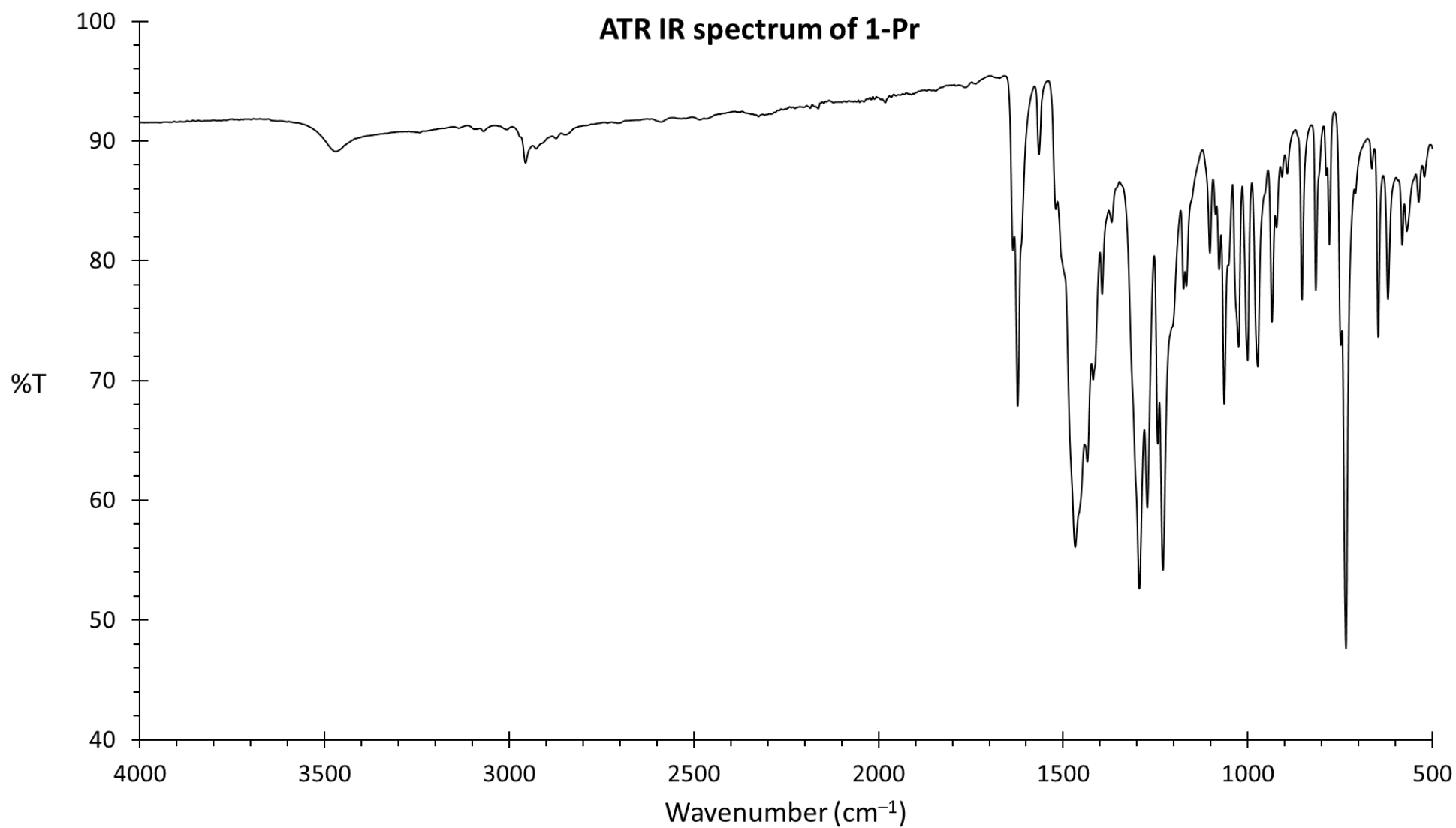


Figure S7: ATR FTIR spectrum of **1-Pr**

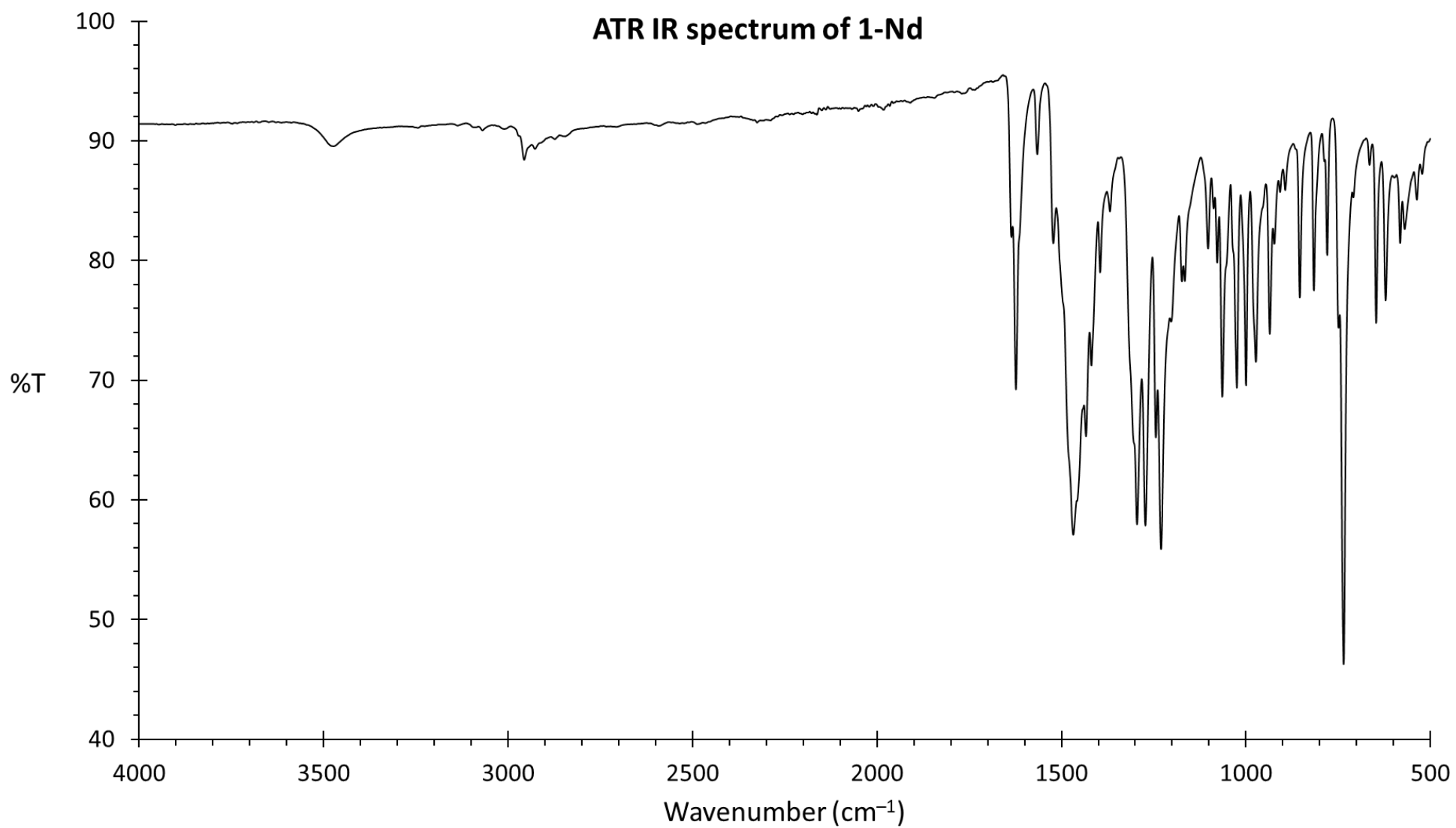


Figure S8: ATR FTIR spectrum of **1-Nd**

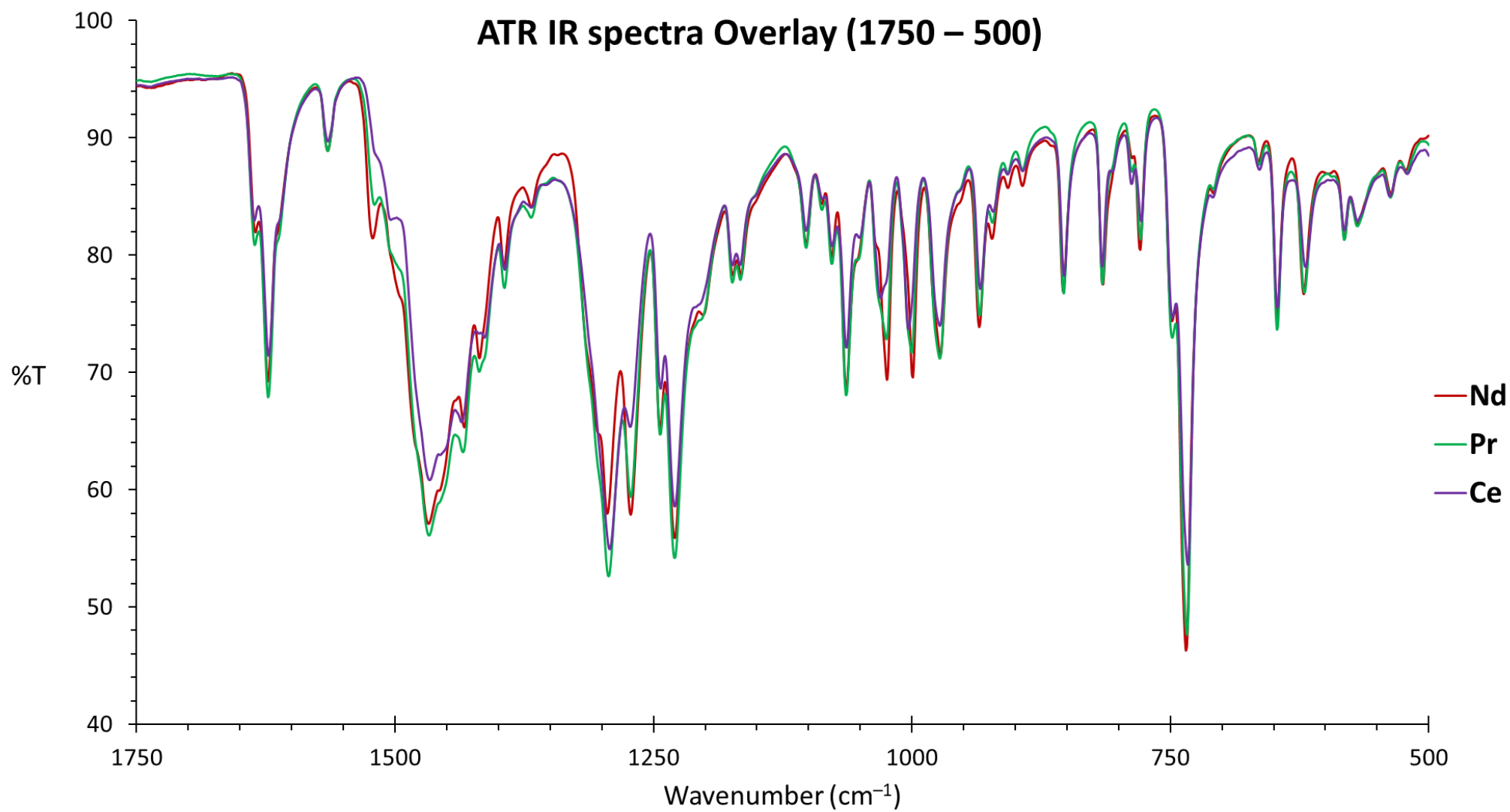


Figure S9: Overlay of ATR FTIR spectra of **1-Ce**, **1-Pr**, and **1-Nd**

C:\Xcalibur\data\BAC_01_Ce

BAC_01_Ce #1-296 RT: 0.00-1.00 AV: 296 NL: 9.69E6

T: FTMS + p ESI Full ms [80.00-1600.00]

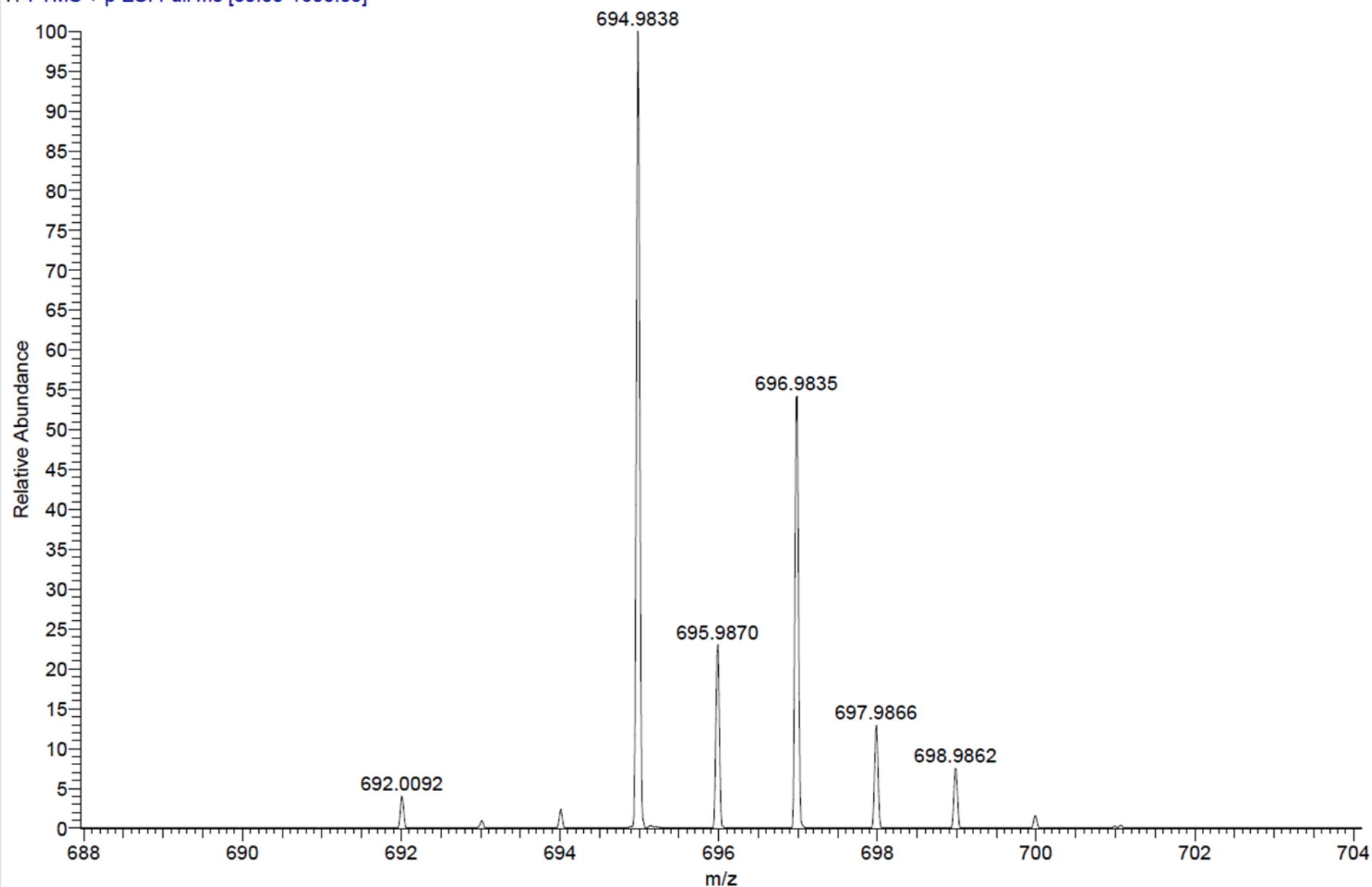


Figure S10: HRMS spectrum of **1-Ce** showing the characteristic isotope pattern

C:\Xcalibur\Data\BAC_03_Pr

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T: FTMS + p ESI Full ms [80.00-1600.00]

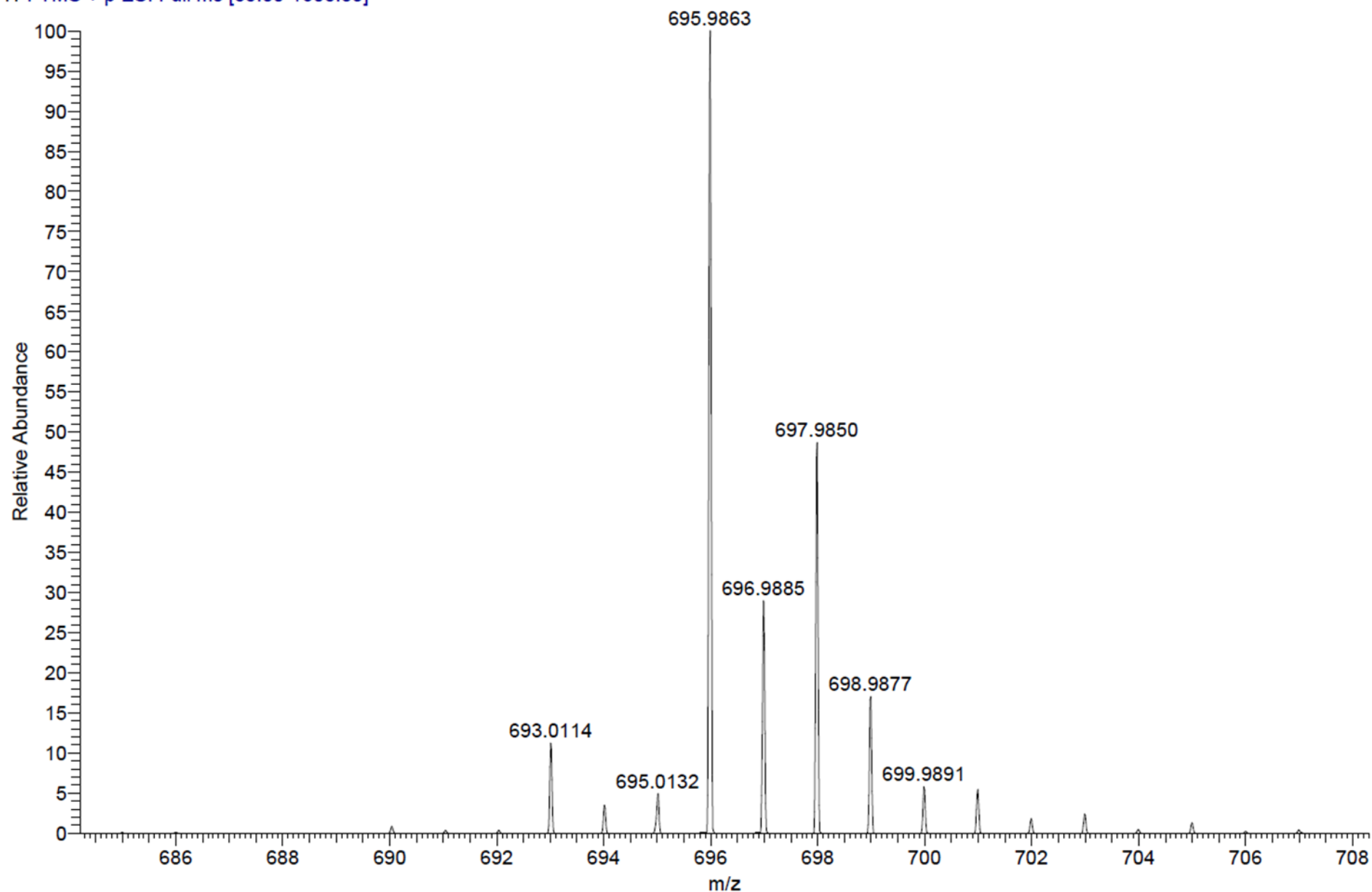


Figure S11: HRMS spectrum of **1-Pr** showing the characteristic isotope pattern

C:\Xcalibur\data\BAC_02_Nd

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T: FTMS + p ESI Full ms [80.00-1600.00]

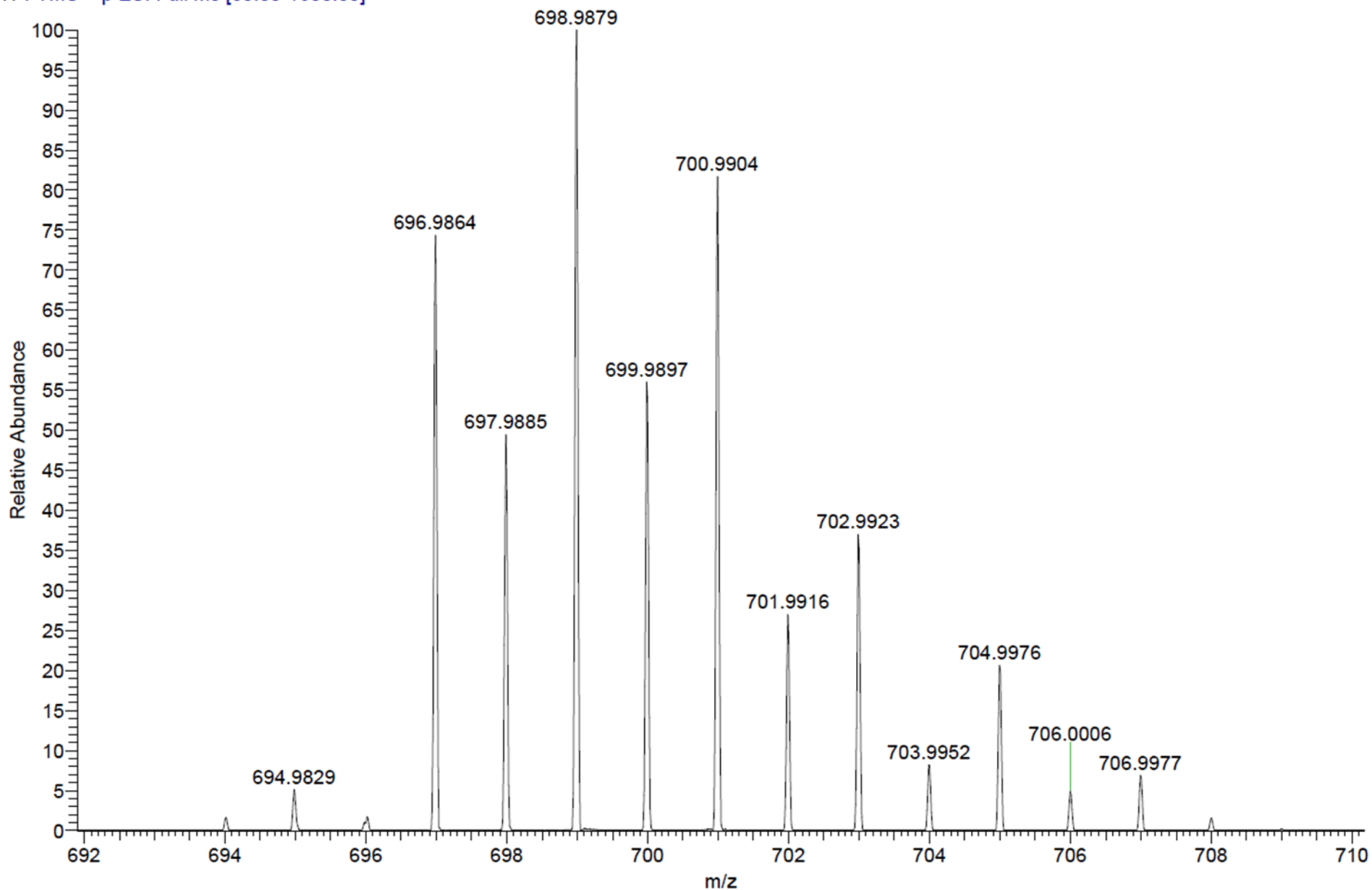
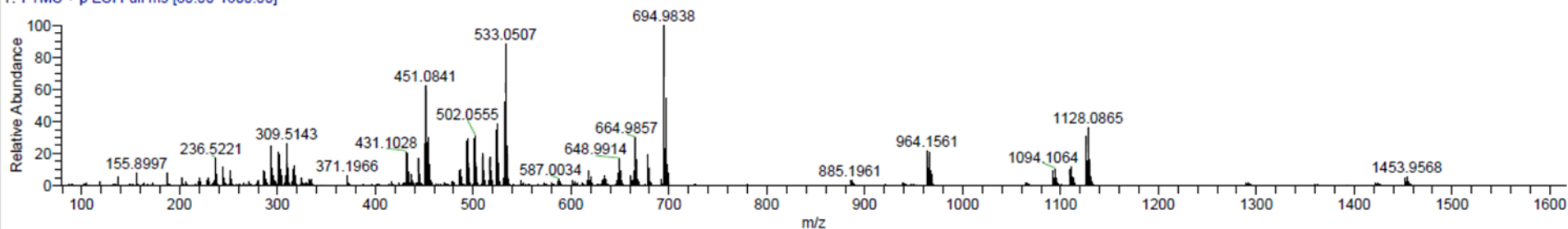


Figure S12: HRMS spectrum of **1-Nd** showing the characteristic isotope pattern

C:\Xcalibur\Data\BAC_01_Ce

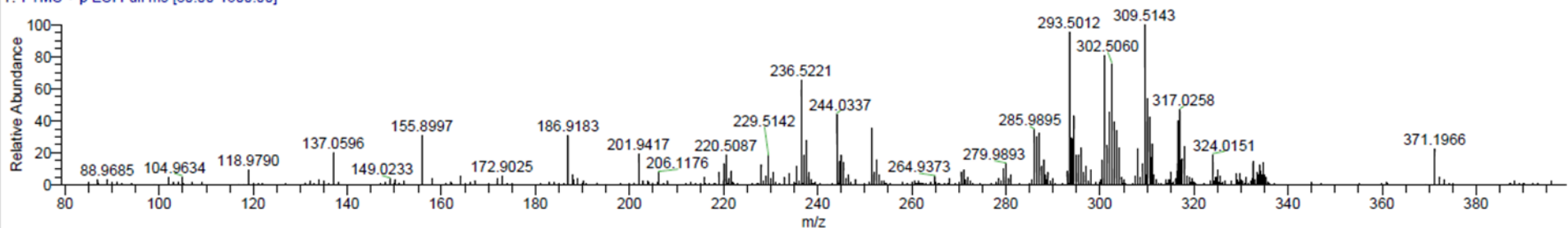
BAC_01_Ce #1-296 RT: 0.00-1.00 AV: 296 NL: 9.69E6

T: FTMS + p ESI Full ms [80.00-1600.00]



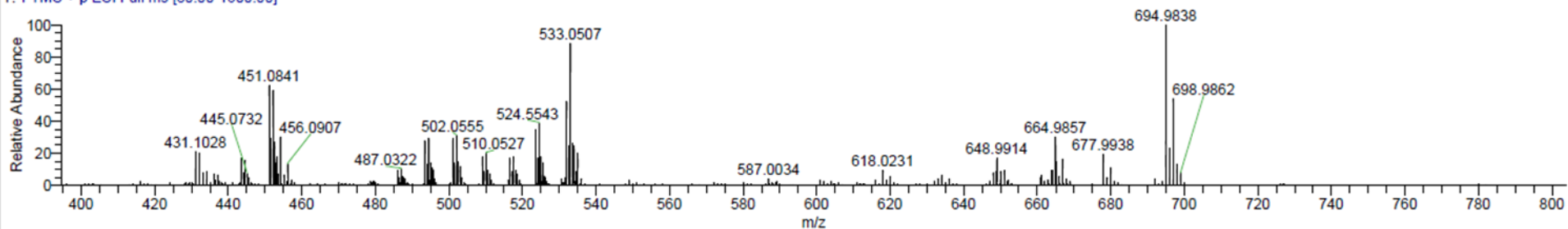
BAC_01_Ce #1-296 RT: 0.00-1.00 AV: 296 NL: 2.52E6

T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_01_Ce #1-296 RT: 0.00-1.00 AV: 296 NL: 9.69E6

T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_01_Ce #1-296 RT: 0.00-1.00 AV: 296 NL: 3.47E6

T: FTMS + p ESI Full ms [80.00-1600.00]

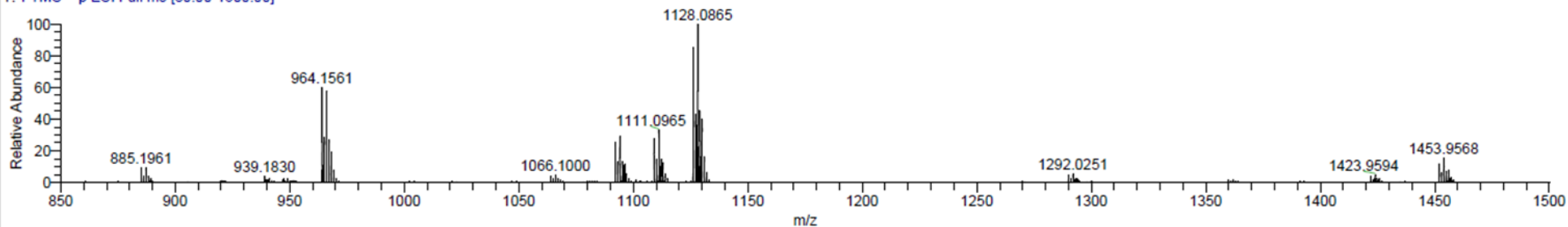
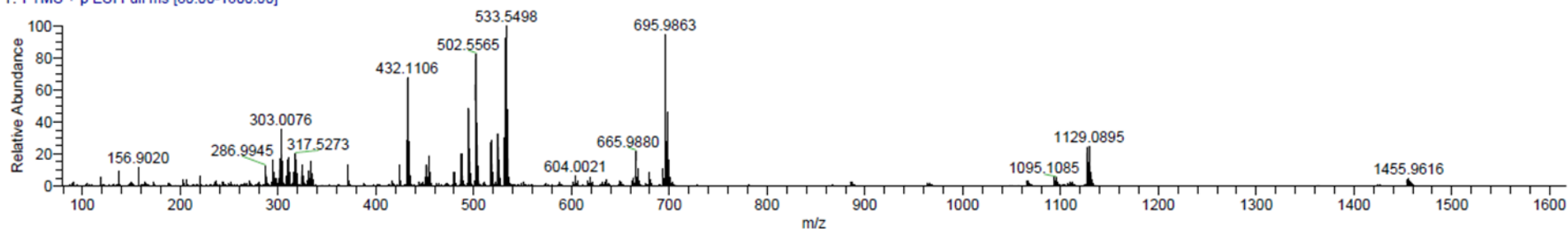


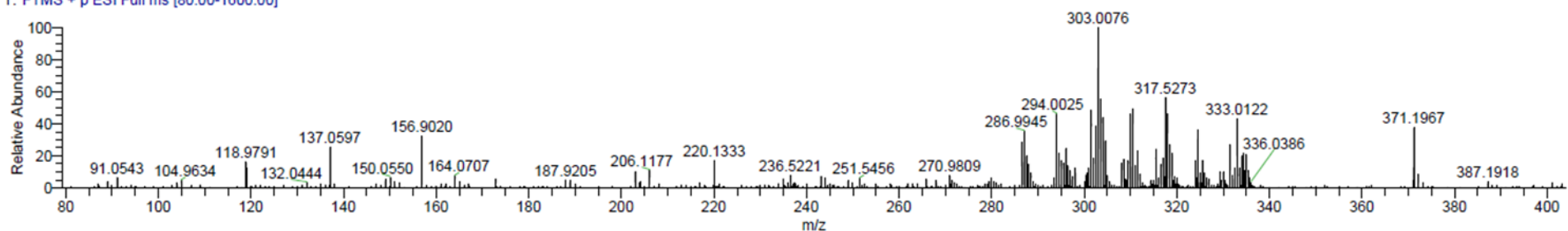
Figure S13: HRMS spectrum of 1-Ce

C:\Xcalibur\Data\BAC_03_Pr

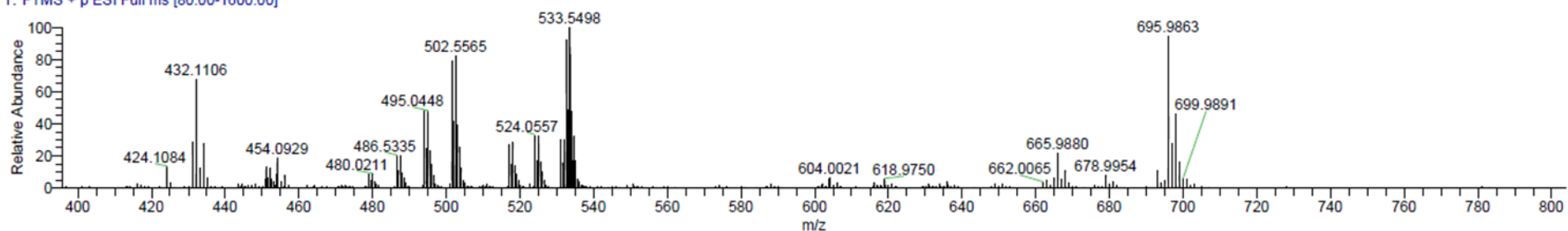
BAC_03_Pr #1-296 RT: 0.00-1.00 AV: 296 NL: 5.59E6
T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_03_Pr #1-296 RT: 0.00-1.00 AV: 296 NL: 1.99E6
T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_03_Pr #1-296 RT: 0.00-1.00 AV: 296 NL: 5.59E6
T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_03_Pr #1-296 RT: 0.00-1.00 AV: 296 NL: 1.39E6
T: FTMS + p ESI Full ms [80.00-1600.00]

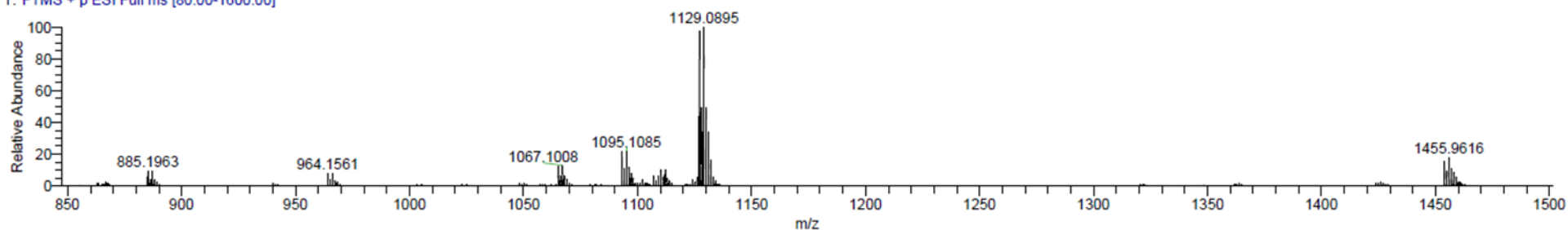
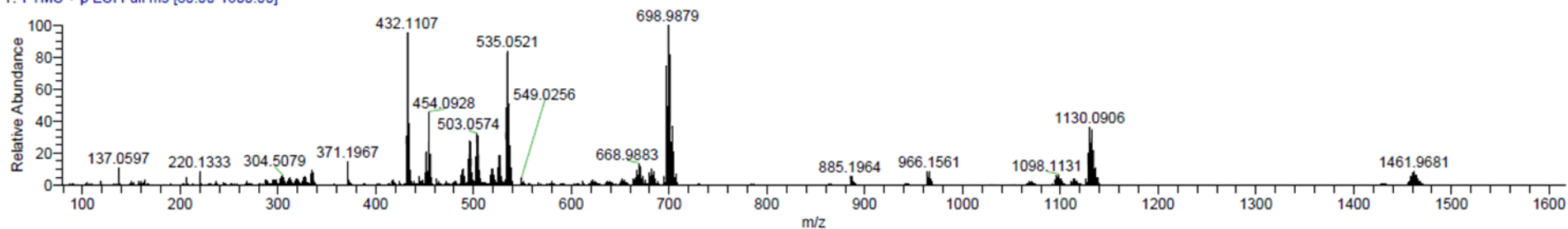


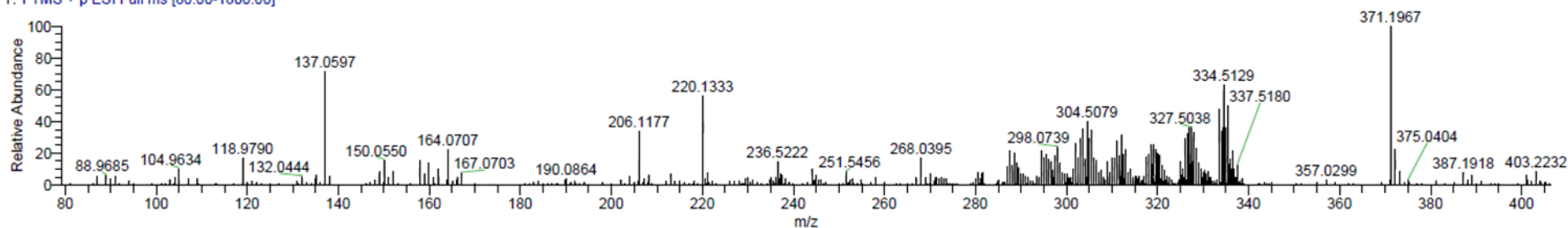
Figure S14: HRMS spectrum of **1-Pr**

C:\Xcalibur\Data\BAC_02_Nd

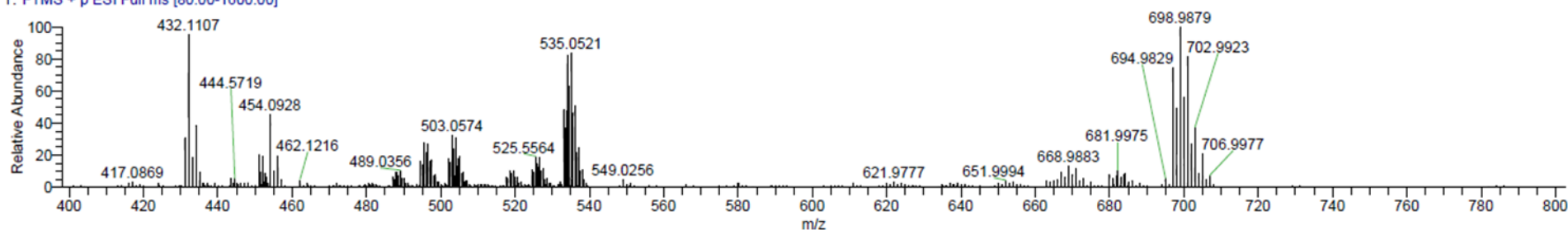
BAC_02_Nd #1-296 RT: 0.00-1.00 AV: 296 NL: 6.89E6
T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_02_Nd #1-296 RT: 0.00-1.00 AV: 296 NL: 1.02E6
T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_02_Nd #1-296 RT: 0.00-1.00 AV: 296 NL: 6.89E6
T: FTMS + p ESI Full ms [80.00-1600.00]



BAC_02_Nd #1-296 RT: 0.00-1.00 AV: 296 NL: 2.47E6
T: FTMS + p ESI Full ms [80.00-1600.00]

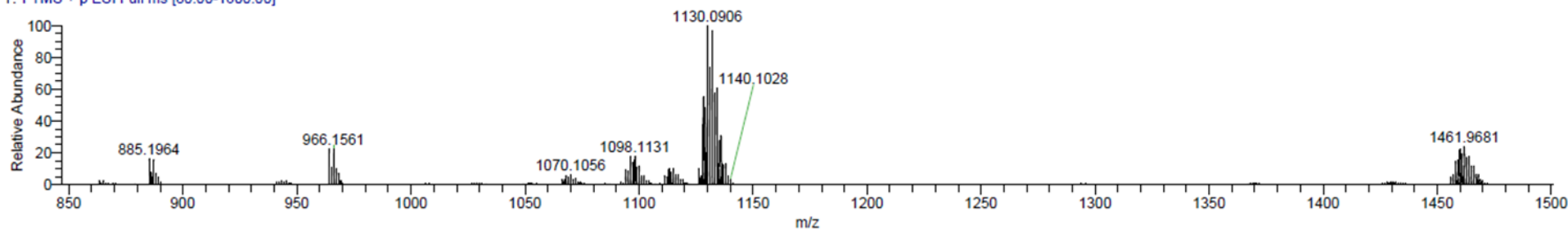


Figure S15: HRMS spectrum of 1-Nd

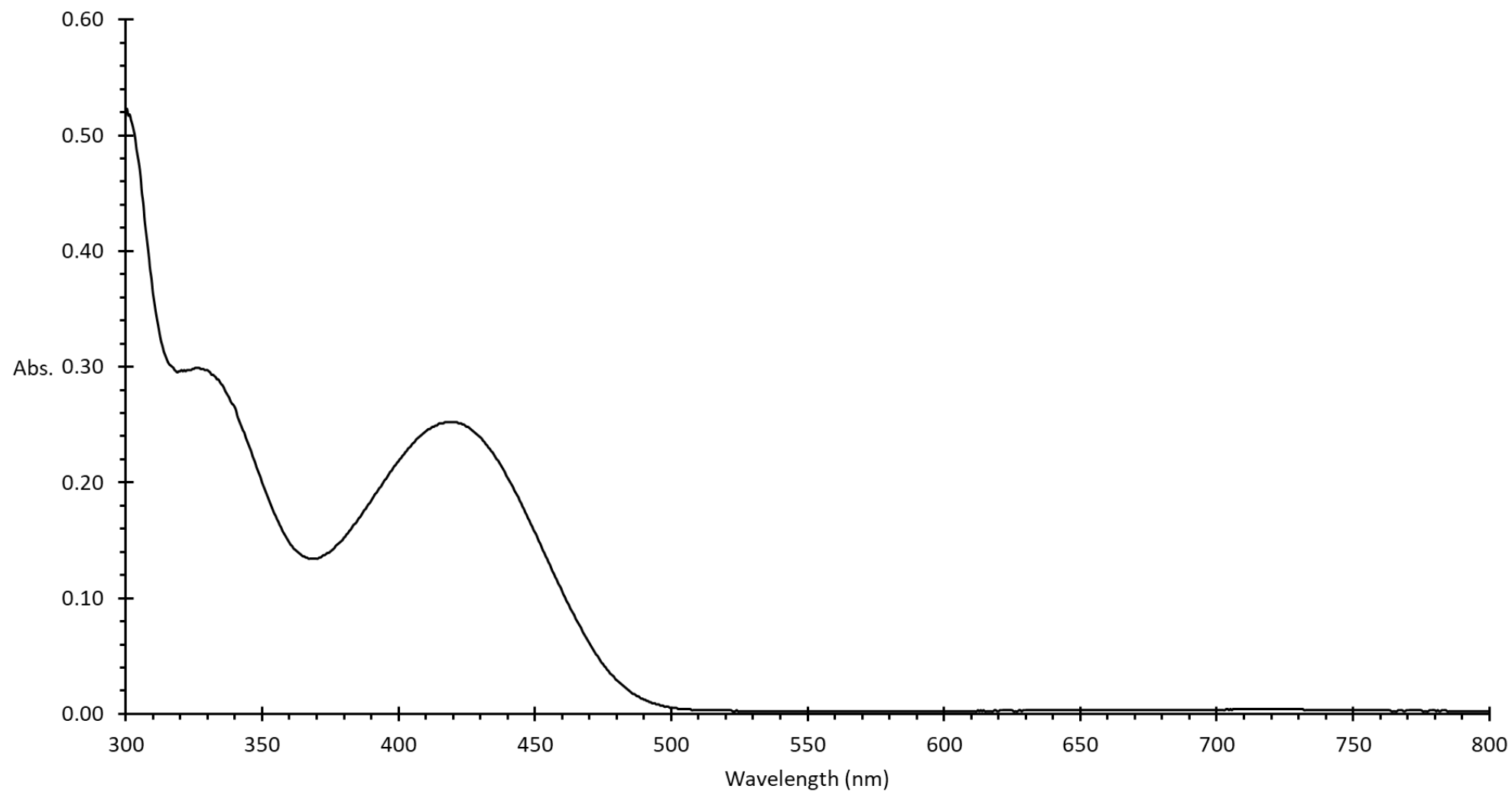


Figure S16: UV-vis spectrum of H_2L in methanol ($c = 86 \mu\text{mol}$)

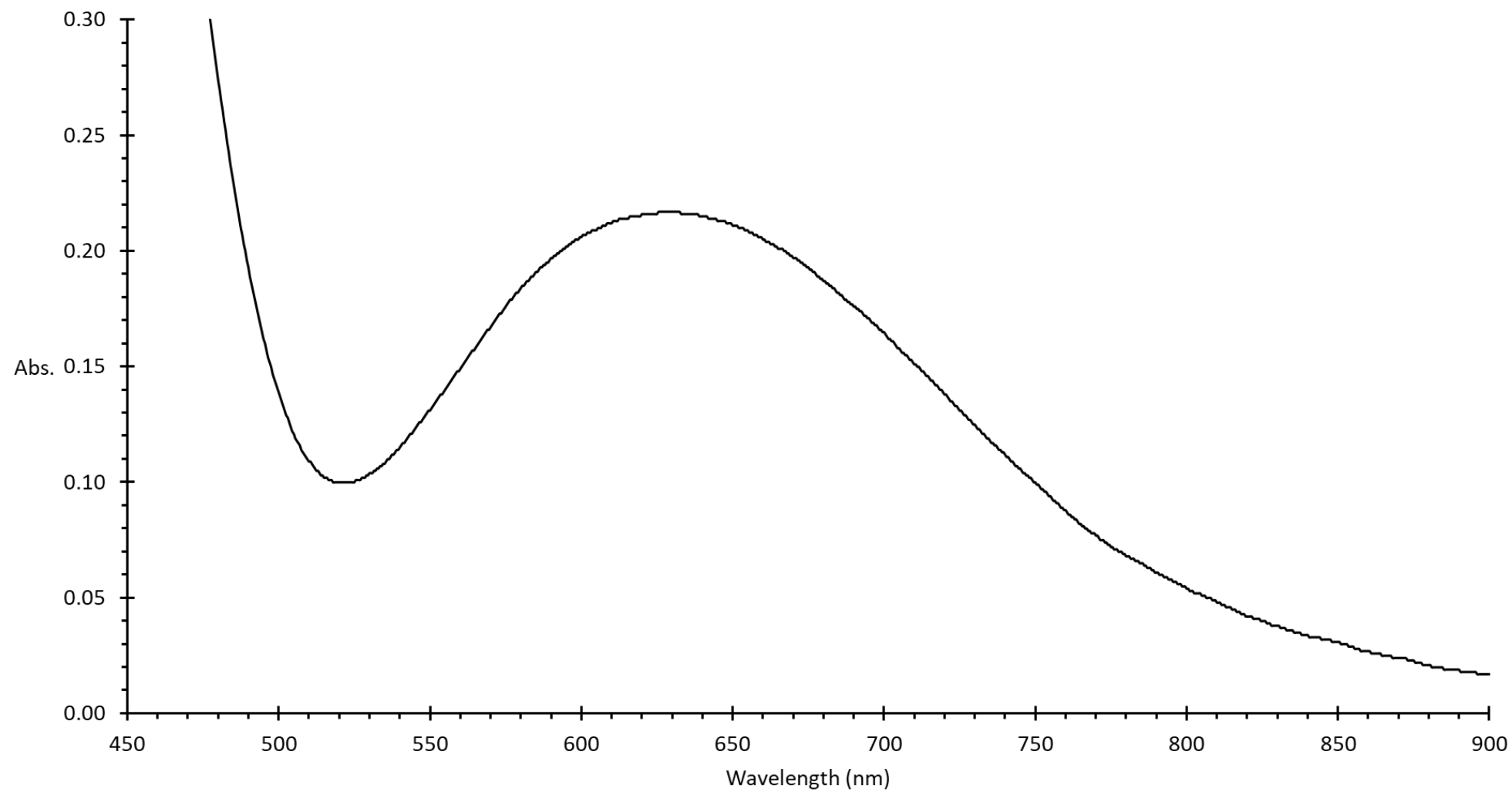


Figure S17: UV-vis spectrum of **1-Ce** in methanol ($c = 4.20$ mmol)

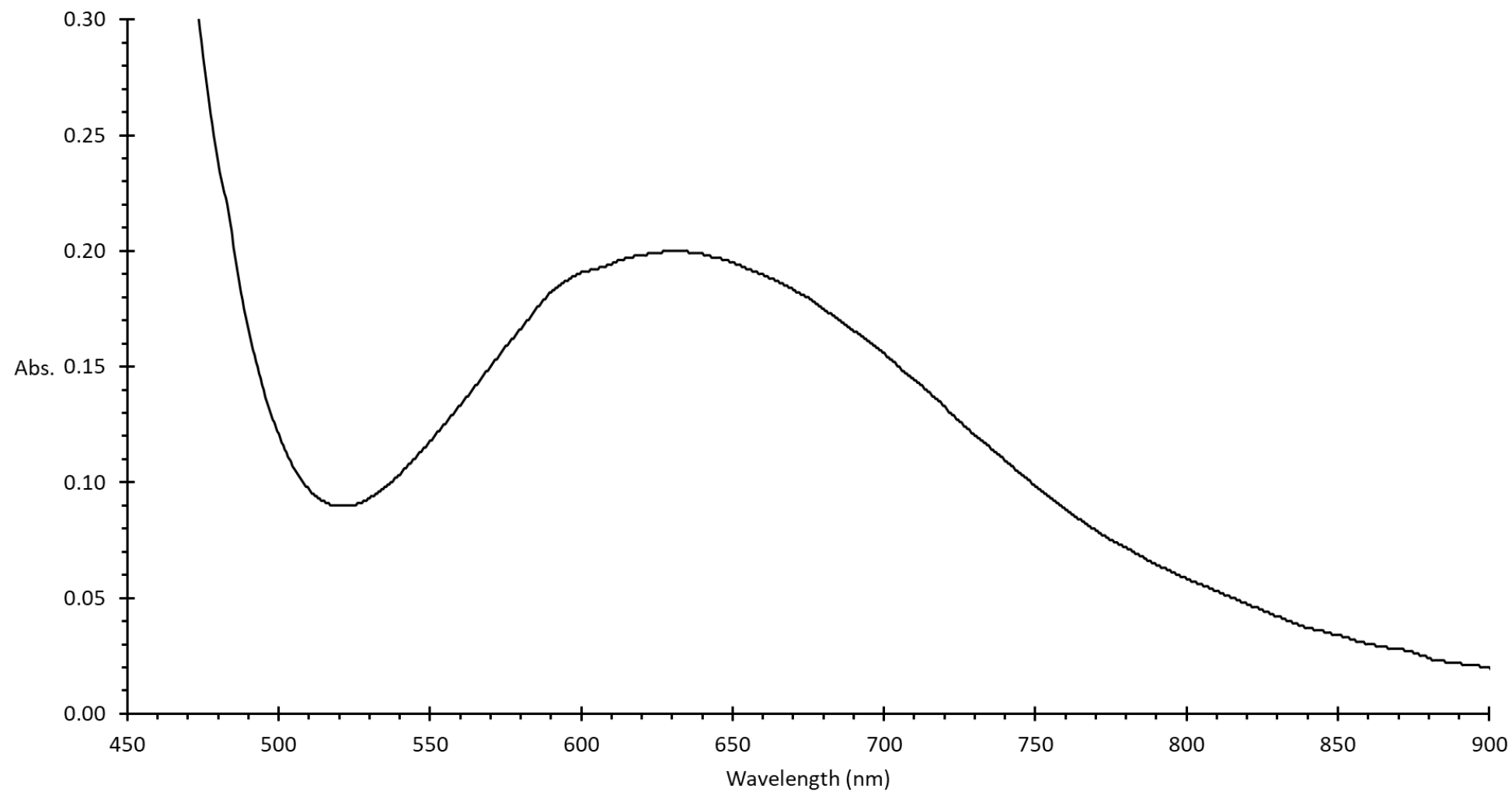


Figure S18: UV-vis spectrum of **1-Pr** in methanol ($c = 3.74$ mmol)

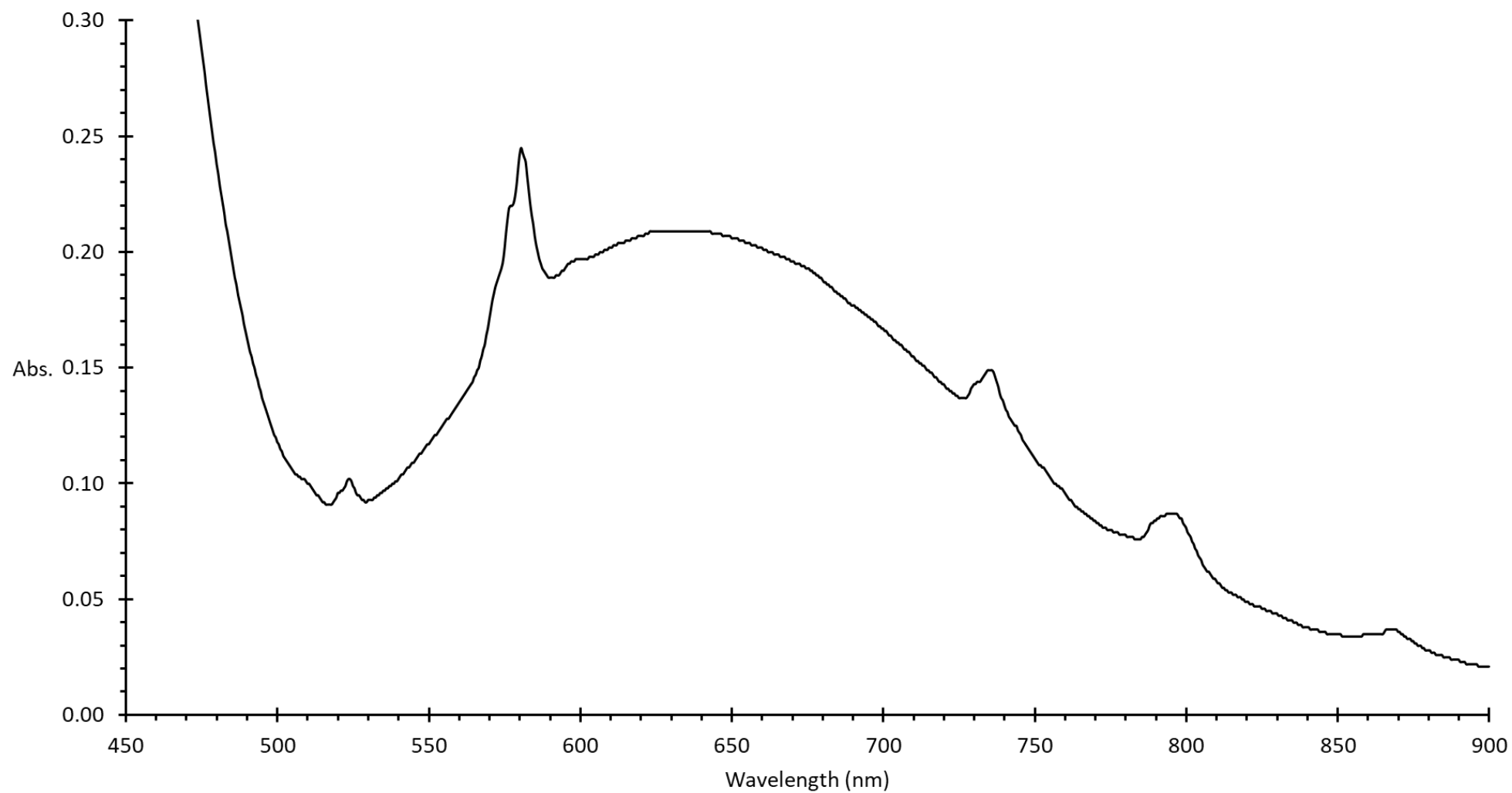


Figure S19: UV-vis spectrum of **1-Nd** in methanol ($c = 3.94$ mmol)

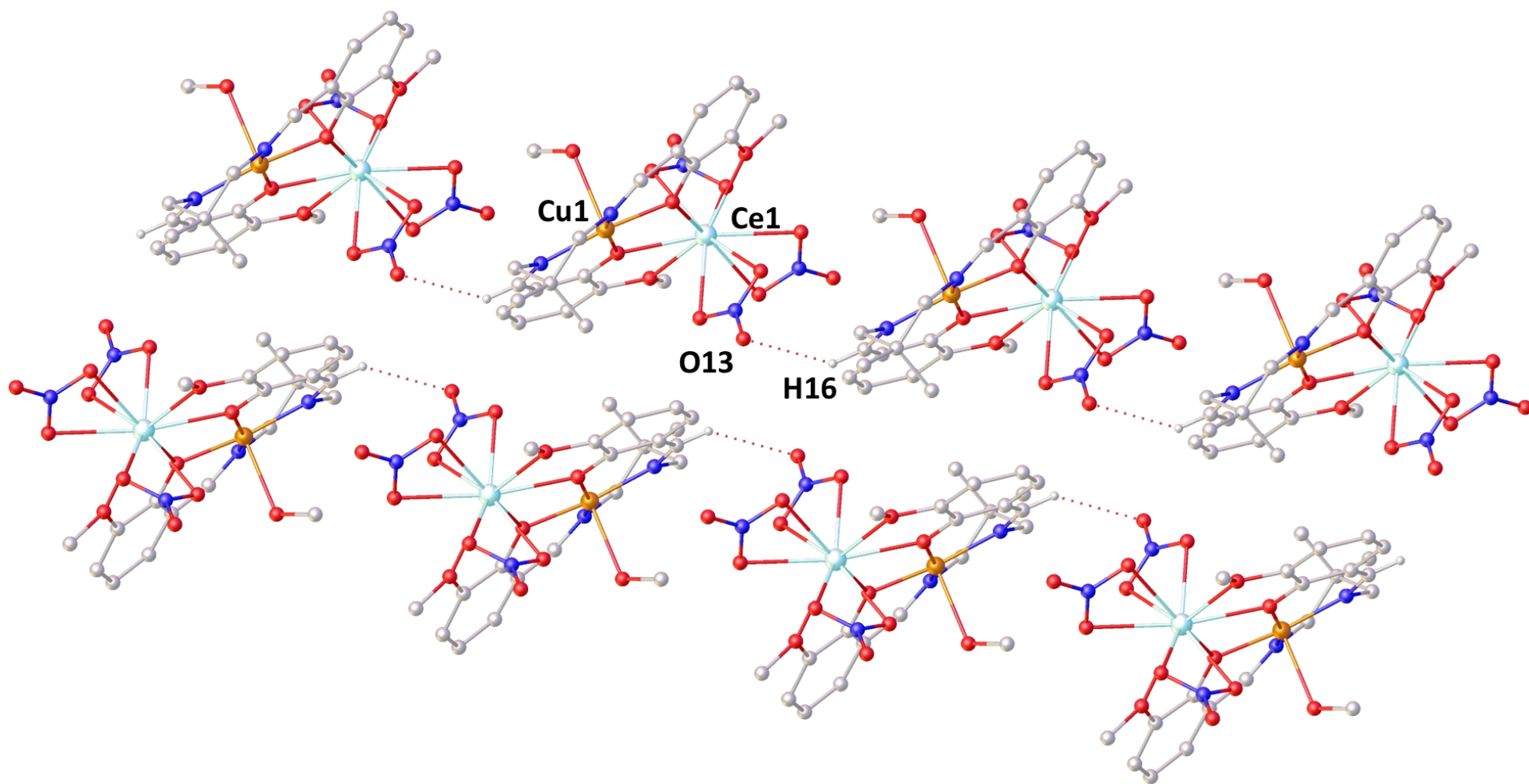


Figure S20: Weak CH...O interactions in **1-Ce** between O13 and H16 forming 1D chains

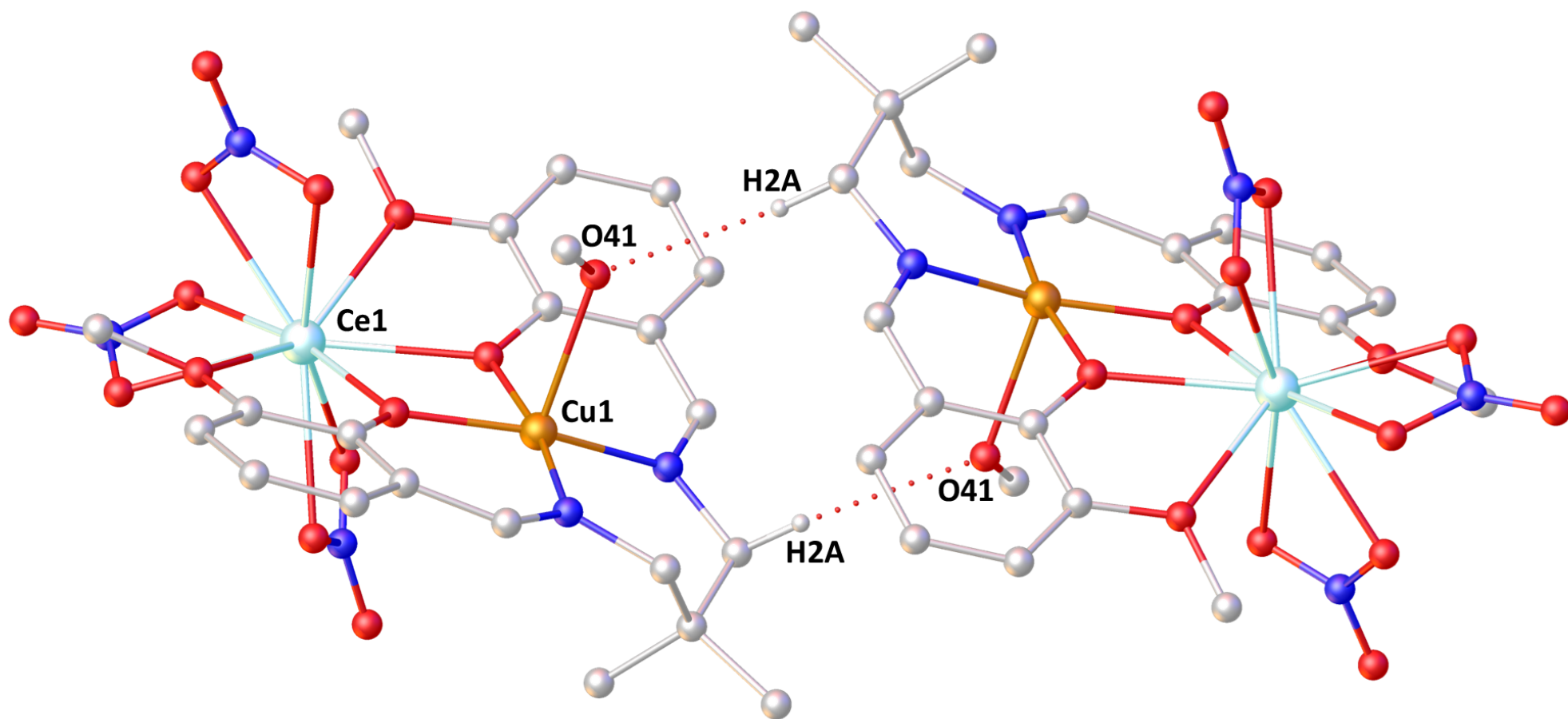


Figure S21: Weak CH...O interactions in **1-Ce** between O41 and H2A

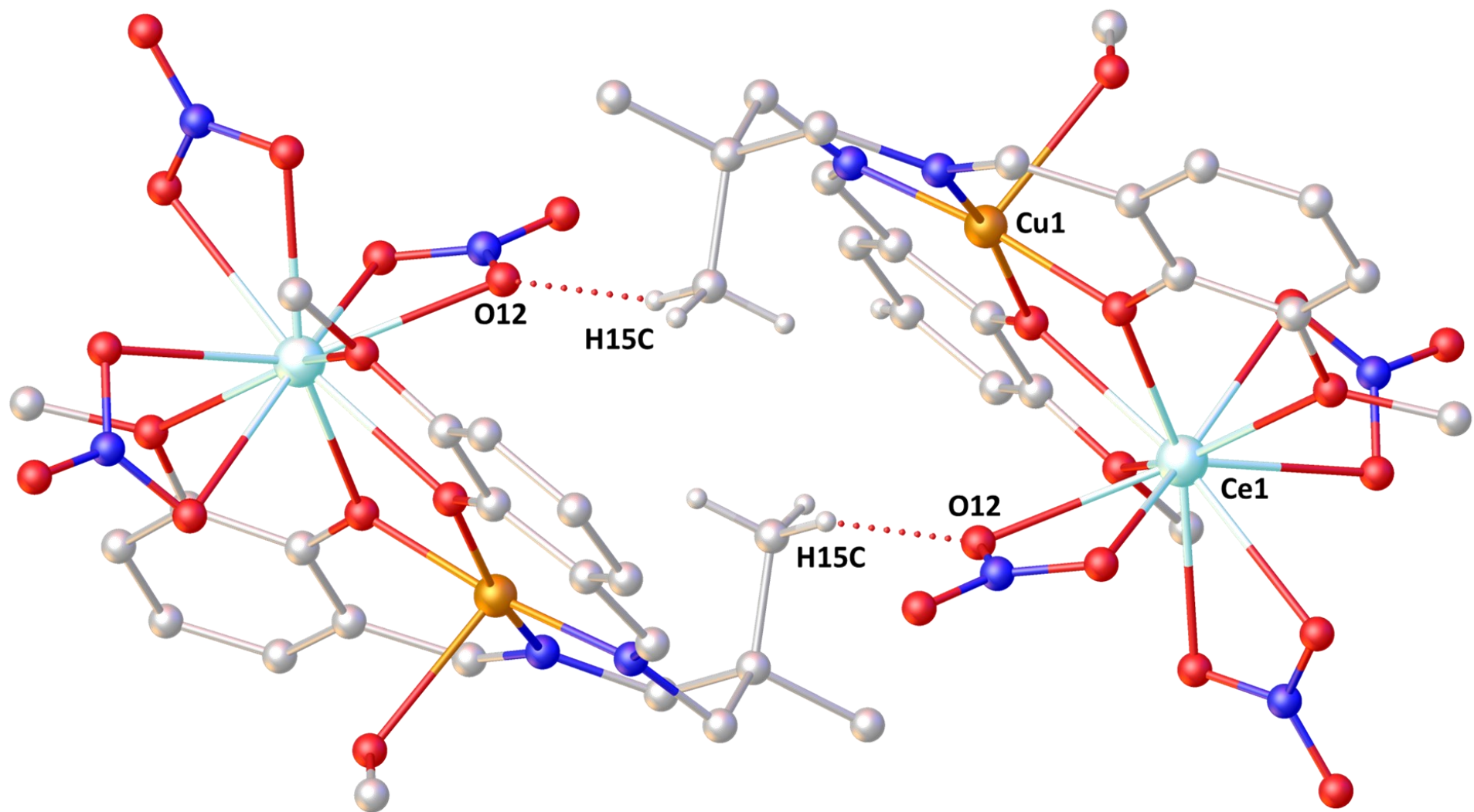


Figure S22: Weak CH...O interactions in **1-Ce** between O12 and H15C

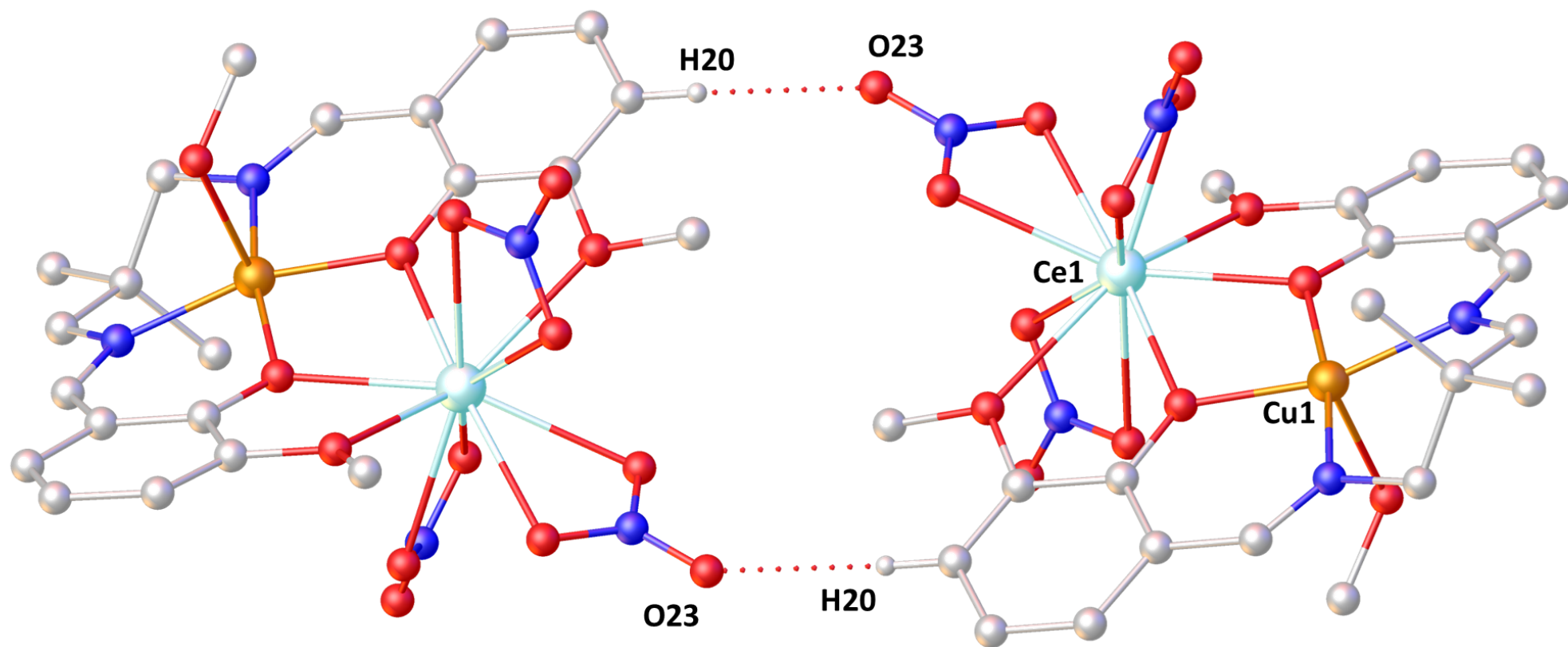


Figure S23: Weak CH...O interactions in **1-Ce** between O23 and H20

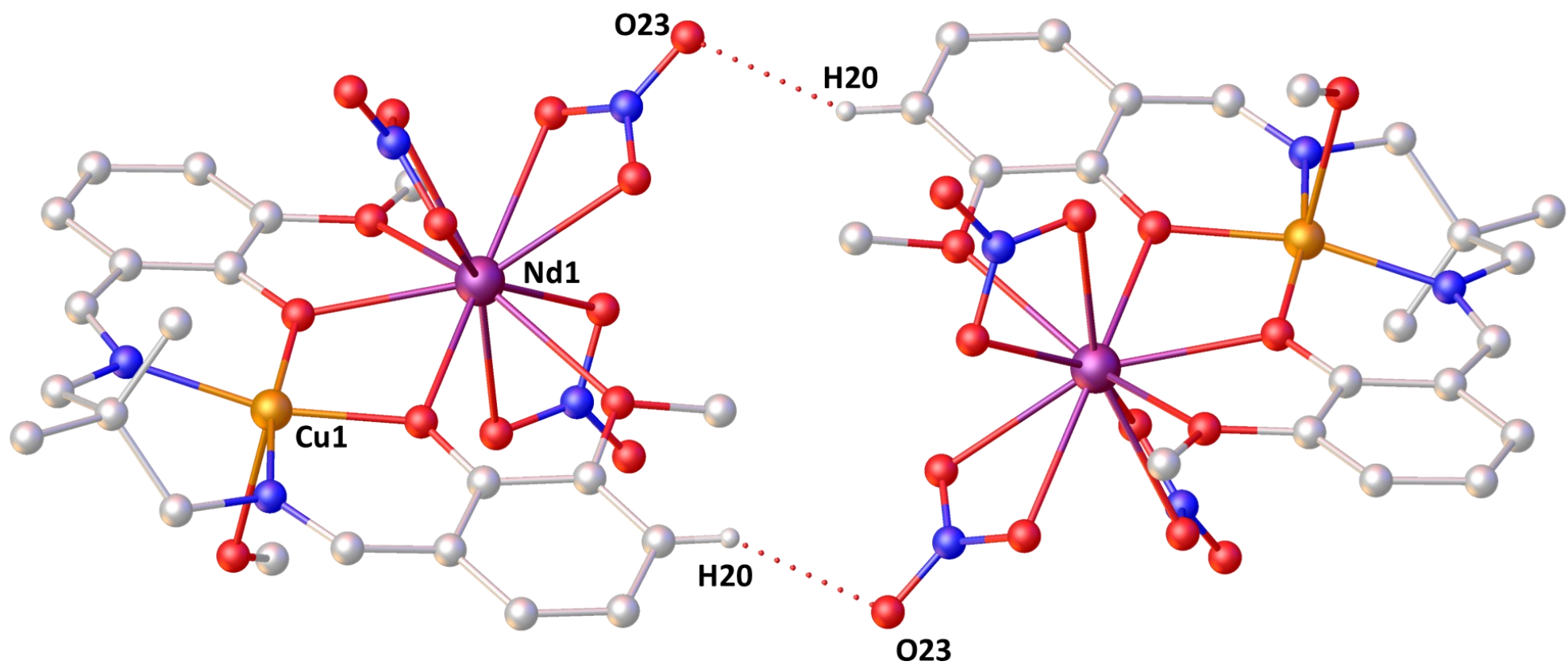


Figure S24: Weak CH \cdots O interactions in **1-Nd** between O23 and H20

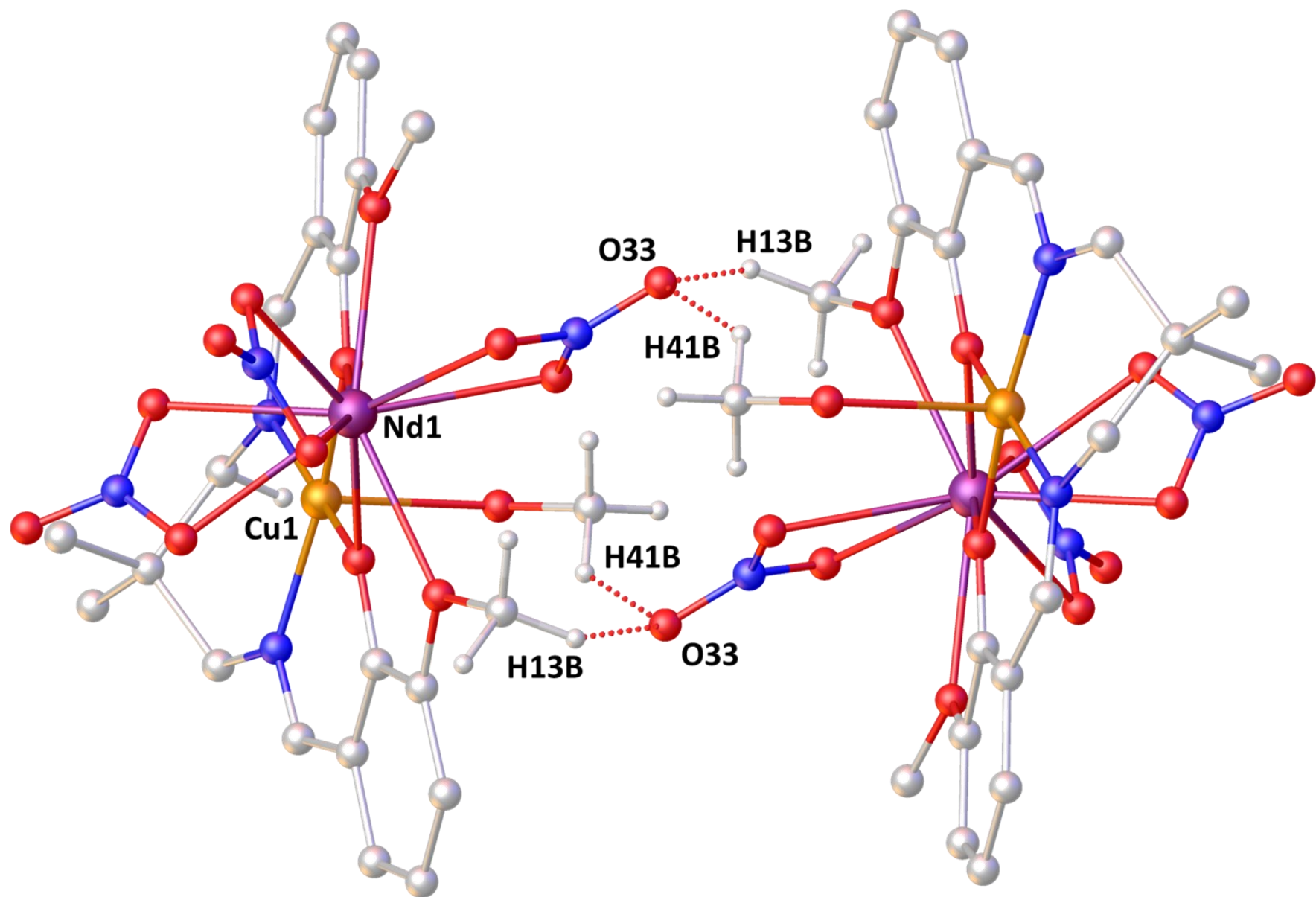


Figure S25: Weak CH...O interactions in **1-Nd** between O33 and H41B and H13B

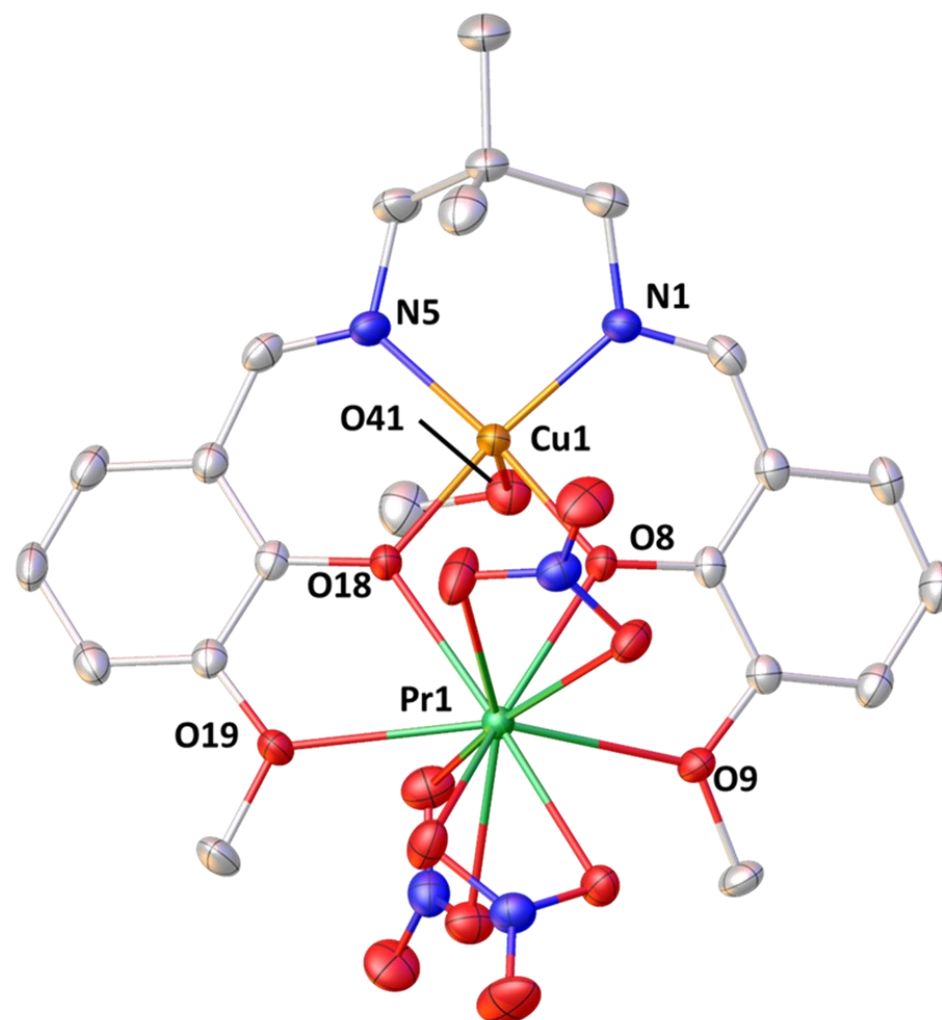
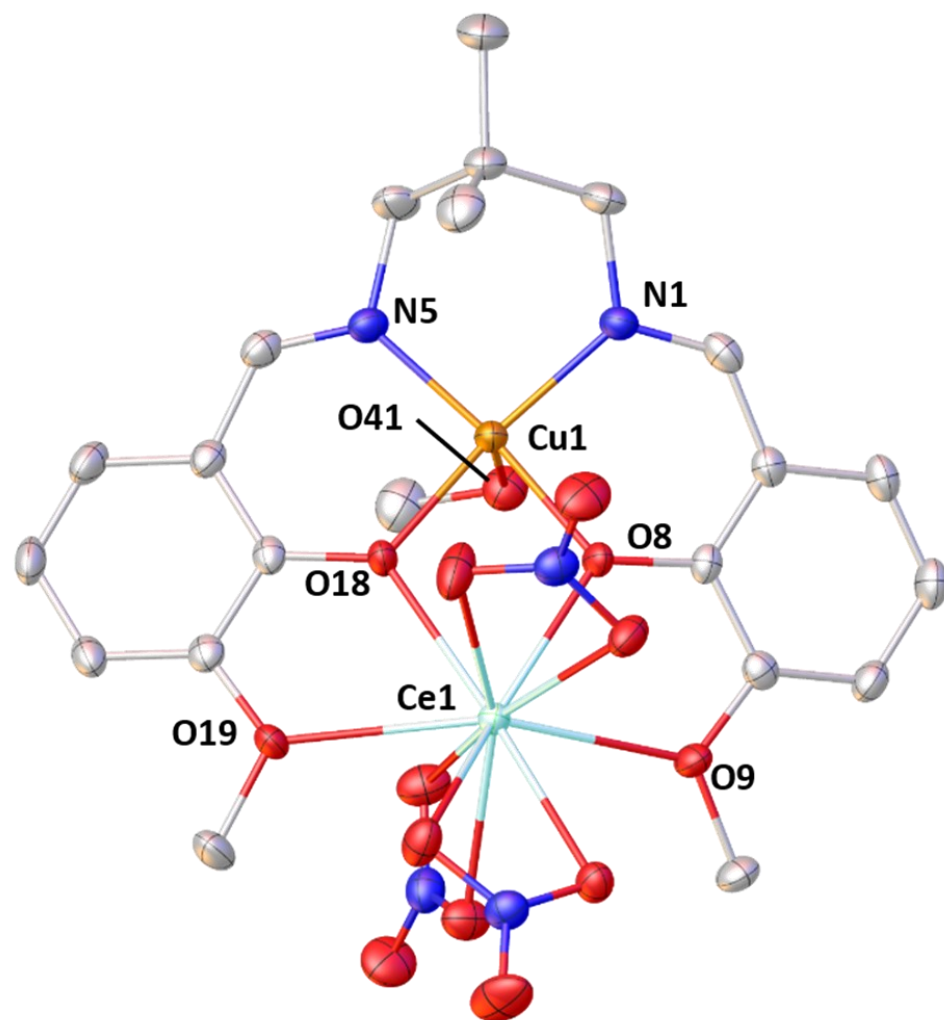


Figure S26: X-ray structures of **1-Ce** and **1-Pr**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 50% probability level

Table S1. Selected crystallographic data.

	1-Ce	1-Pr	1-Nd
formula	C ₂₂ H ₂₈ CeCuN ₅ O ₁₄	C ₂₂ H ₂₈ CuN ₅ O ₁₄ Pr	C ₂₂ H ₂₈ CuN ₅ NdO ₁₄
fw	790.15	790.94	794.27
crystal description	Green prism	Green prism	Green prism
crystal size [mm ³]	0.21×0.09×0.04	0.07×0.03×0.02	0.07×0.06×0.02
space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> [Å]	9.4469(4)	9.4412(3)	8.6415(7)
<i>b</i> [Å]	12.6653(9)	12.6685(5)	12.9533(11)
<i>c</i> [Å]	13.3774(6)	13.3569(4)	13.4632(16)
α [°]	73.950(9)	74.017(4)	79.830(9)
β [°]	71.912(9)	71.828(5)	77.505(8)
γ [°]	71.554(9)	71.364(4)	71.963(7)
vol [Å ³]	1414.83(18)	1410.65(10)	1389.2(2)
<i>Z</i>	2	2	2
ρ (calc) [g/cm ³]	1.855	1.862	1.899
μ [mm ⁻¹]	2.418	2.538	2.693
<i>F</i> (000)	788	790	792
2 θ range for data collection [°]	3.268 to 50.762	3.460 to 50.772	4.286 to 50.810
index range	-11 ≤ <i>h</i> ≤ 11 -15 ≤ <i>k</i> ≤ 15 -16 ≤ <i>l</i> ≤ 16	-11 ≤ <i>h</i> ≤ 11 -15 ≤ <i>k</i> ≤ 15 -16 ≤ <i>l</i> ≤ 16	-10 ≤ <i>h</i> ≤ 10 -15 ≤ <i>k</i> ≤ 15 -16 ≤ <i>l</i> ≤ 16
reflections collected	17512	23264	17030
independent reflections (<i>R</i> _{int})	5132 (0.0268)	5130 (0.0274)	5062 (0.0403)
parameters, restraints	394, 0	394, 0	394, 0
GoF on <i>F</i> ²	1.039	1.043	0.971
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.0200	0.0171	0.0229
<i>wR</i> ₂ (all data)	0.0439	0.0411	0.0570
largest diff. peak/hole [e/Å ³]	0.364, -0.437	0.604, -0.236	0.731, -0.471