Supplementary Material

Biological Evaluation and Synthesis of Calcitroic Acid

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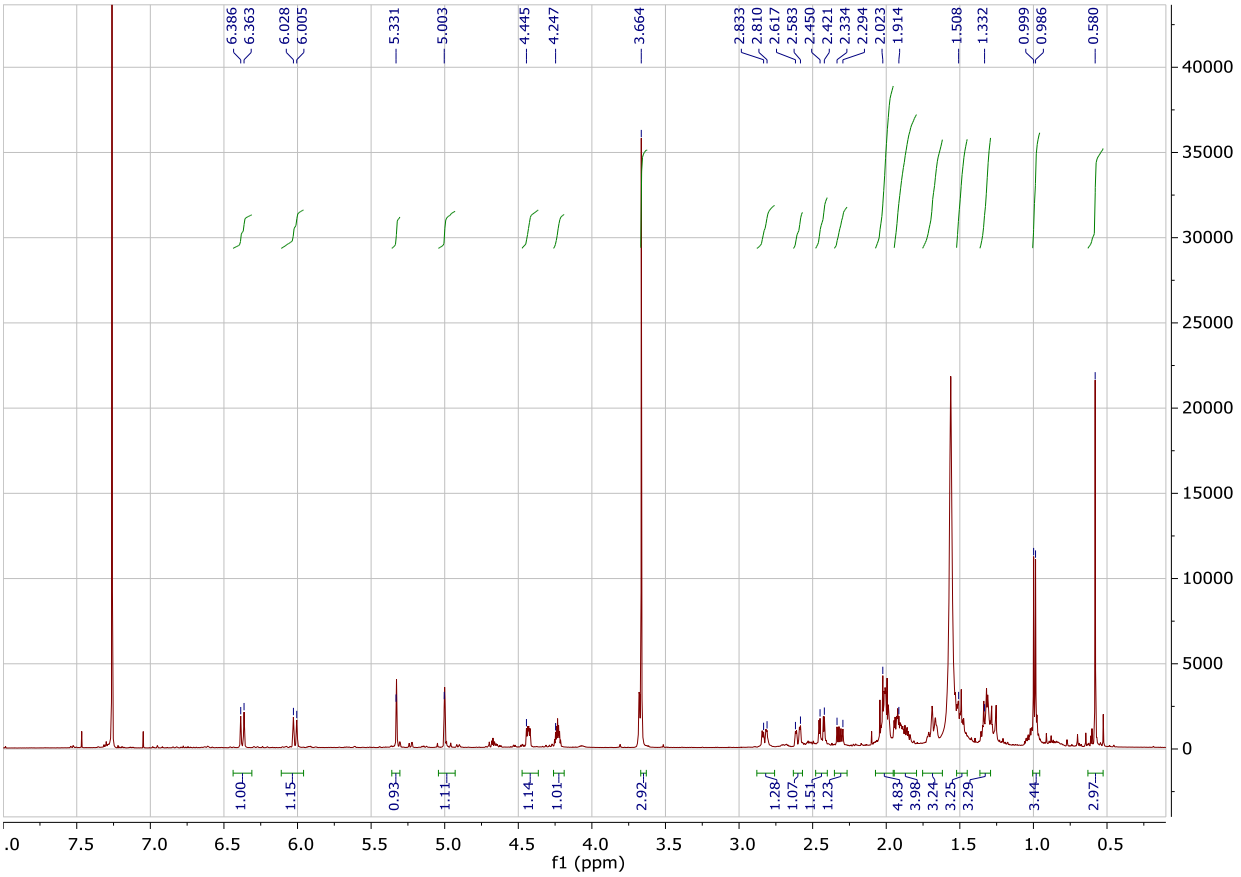
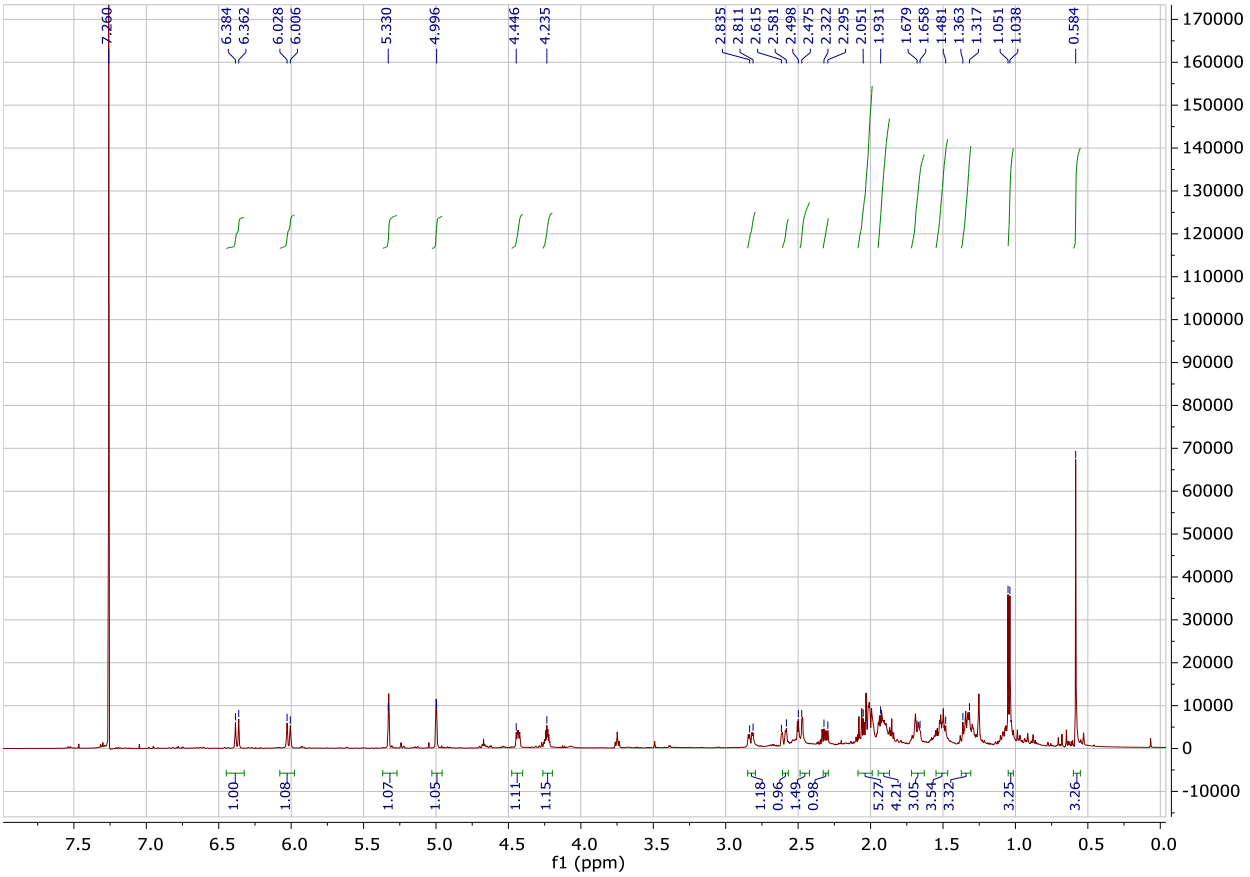
Contents

CTA-ME (5) ^{1}H NMR



CTA (6) ^{1}H NMR


7.260
6.384
6.362
6.028
6.006
5.330
4.996
4.446
4.235
2.835
2.811
2.615
2.581
2.498
2.475
2.322
2.295
2.051
1.931
1.679
1.658
1.481
1.363
1.317
1.051
1.038
0.584
1.00
1.08
1.07
1.05
1.11
1.15
1.18
0.96
1.49
0.98
5.27
4.21
3.05
3.54
3.32
3.25
3.26
f1 (ppm)

Supplementary Table: Data collection and refinement statistics for zVDR-LBD-CTA

	zVDR LBD **/ CTA**
Data Collection and processing statistics	
Beamline	Proxima 2A
Wavelength (Å)	0.98
Space group	$P6_522$
Unit cell parameters (Å, °)	a=b=65.74 c=264.82, α=β=90 γ=120
Resolution (Å)	28.47-2.39
Total reflections	352720
Unique reflections	14257
Multiplicity	24.7
I/σ(I)	12.26
Completness	99.22
Wilson B-factor	71.49
$CC_{1/2}$	0.999
Refinement	
Reflections used in refinement	14189
Reflections used for R-free	710
R_{work} / R_{free}	0.24 / 0.28
R.M.S.D. Bond lengths (Å)	0.004
R.M.S.D. Bond angles (°)	0.64
Ramachandran	
Outliers (%)	0
Favored (%)	95.85
Mean B factor ($Å^2$)	
Protein	88.08
Ligand	77.26