Electronic Supplementary Information for

Models of the putative antimony(V)-diolate motifs in antileishmanial pentavalent antimonial drugs

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Table S1. Refinement Details for the Crystal Structures of $Sb(tol)_3$ and $[(tol)_3Sb(\mu\text{-}C_4H_8O_2)]_2O$.

	$Sb(tol)_3$	**$[(tol)_3Sb(\mu\text{-}C_4H_8O_2)]_2O$**
Formula	$C_{21}H_{21}Sb$	$C_{36}H_{44}O_5Sb_2$
FW	395.13	800.21
T (K)	101.1(6)	102(2)
λ (Å)	1.54184	1.54184
Crystal System	Trigonal	Orthorhombic
Space group	$R\bar{3}$	$P2_12_12_1$
a (Å)	12.6758(3)	12.17550(10)
b (Å)		13.5809(2)
c (Å)	19.8058(4)	20.6690(3)
Volume (Å^3)	2755.96(14)	3417.71(8)
Z	6	4
ρ_{calc} (Mg/m^3)	1.428	1.555
Size (mm^3)	0.21×0.14×0.04	0.12×0.06×0.05
θ range (°)	4.605-67.036	3.895-67.684
Total data	6111	51012
Unique data	1099	7095
Parameters	68	397
Completeness	100.0%	100.0%
R_{int}	4.87%	5.45%
R_1 (I > 2σ)	2.11%	3.25%
R_1 (all data)	2.16%	3.39%
wR_2 (I > 2σ)	5.41%	8.52%
wR_2 (all data)	5.43%	8.64%
S	1.098	1.078
Flack *x*	—	-0.015(9)

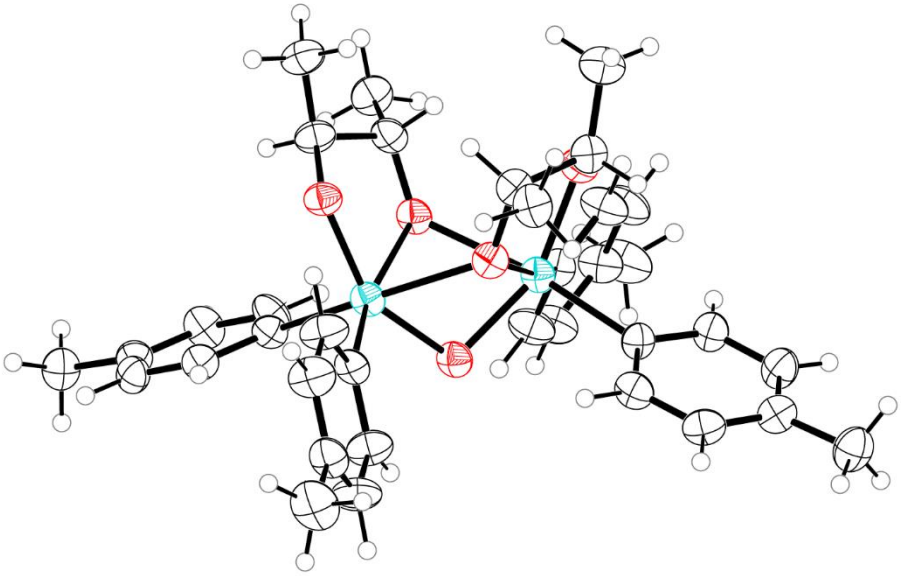


Figure S1. Thermal ellipsoid plot (50% probability, H atoms as spheres of arbitrary radius) of a hydrolysis decomposition product observed to form during the synthesis of butanediolate complexes**.** Color code: Sb teal, O red, C black, H white.

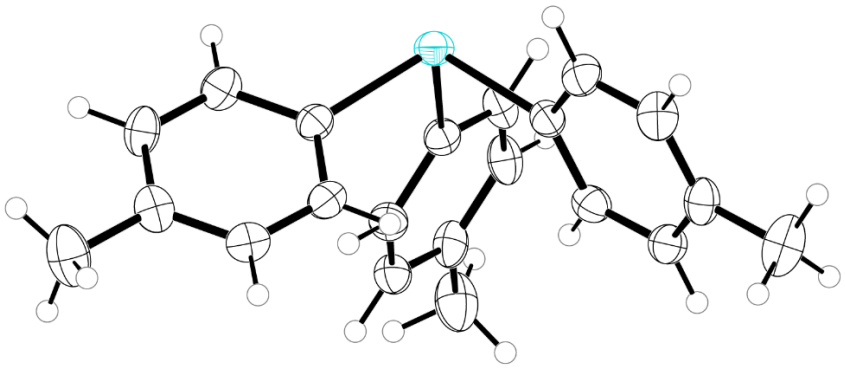


Figure S2. Thermal ellipsoid plot (50% probability, H atoms as spheres of arbitrary radius) of $Sb(tol)_3$**.** Color code: Sb teal, C black, H white.

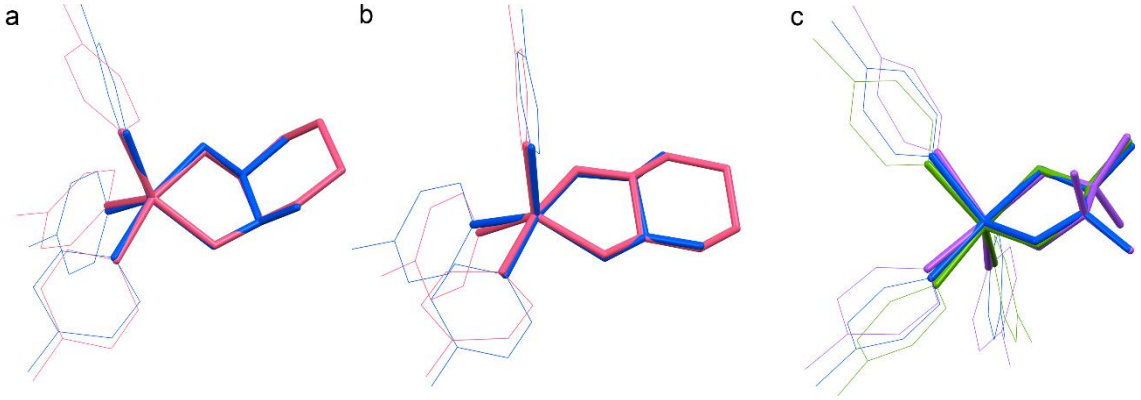


Figure S3. Overlays of: a) **2** (blue) and **3** (pink). b) **4** (blue) and **5** (pink). c) **1** (purple), **4** (blue), and **6** (green).

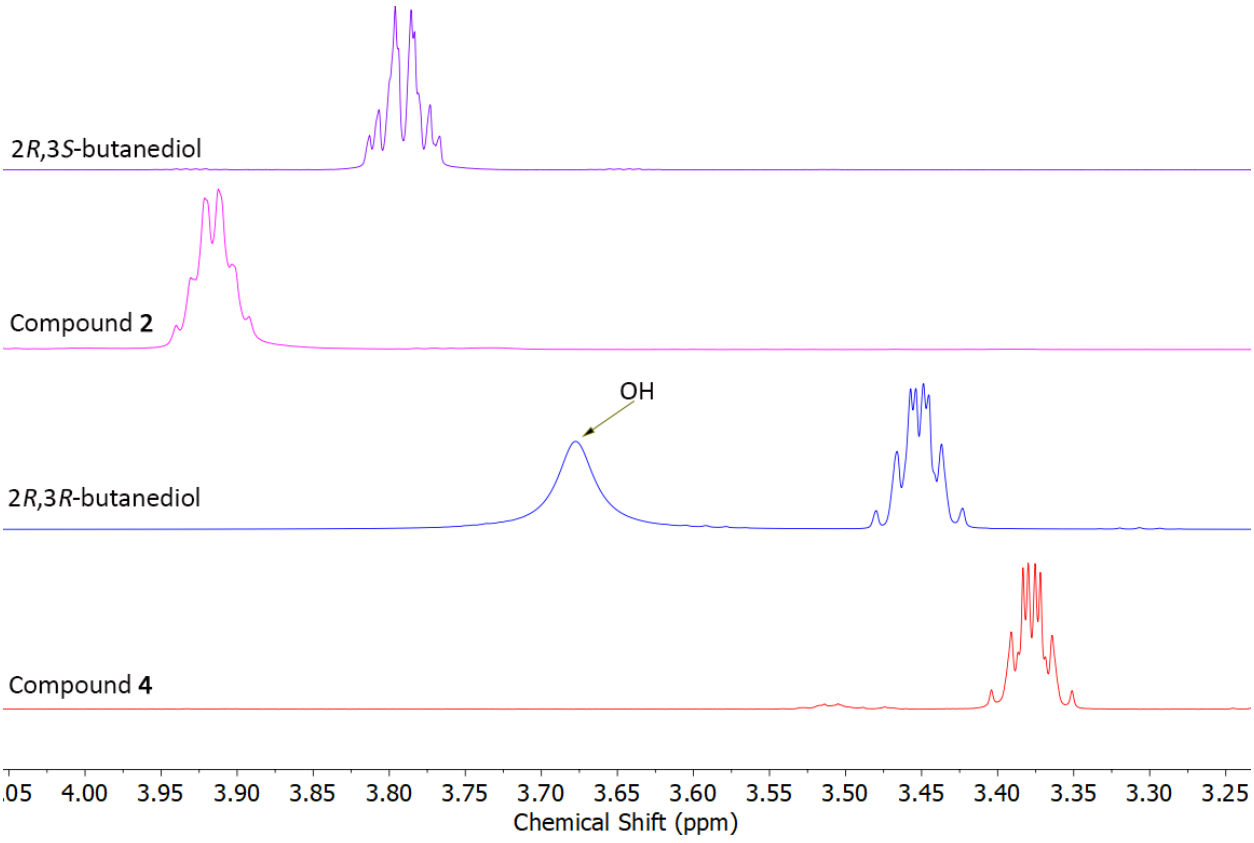


Figure S4. Stacked ^{1}H NMR spectra showing shift in backbone CH resonances. Color code: unbound 2*R*,3*S*-butanediol purple, compound **2** pink, unbound 2*R*,3*R*-butanediol blue, compound **4** red.

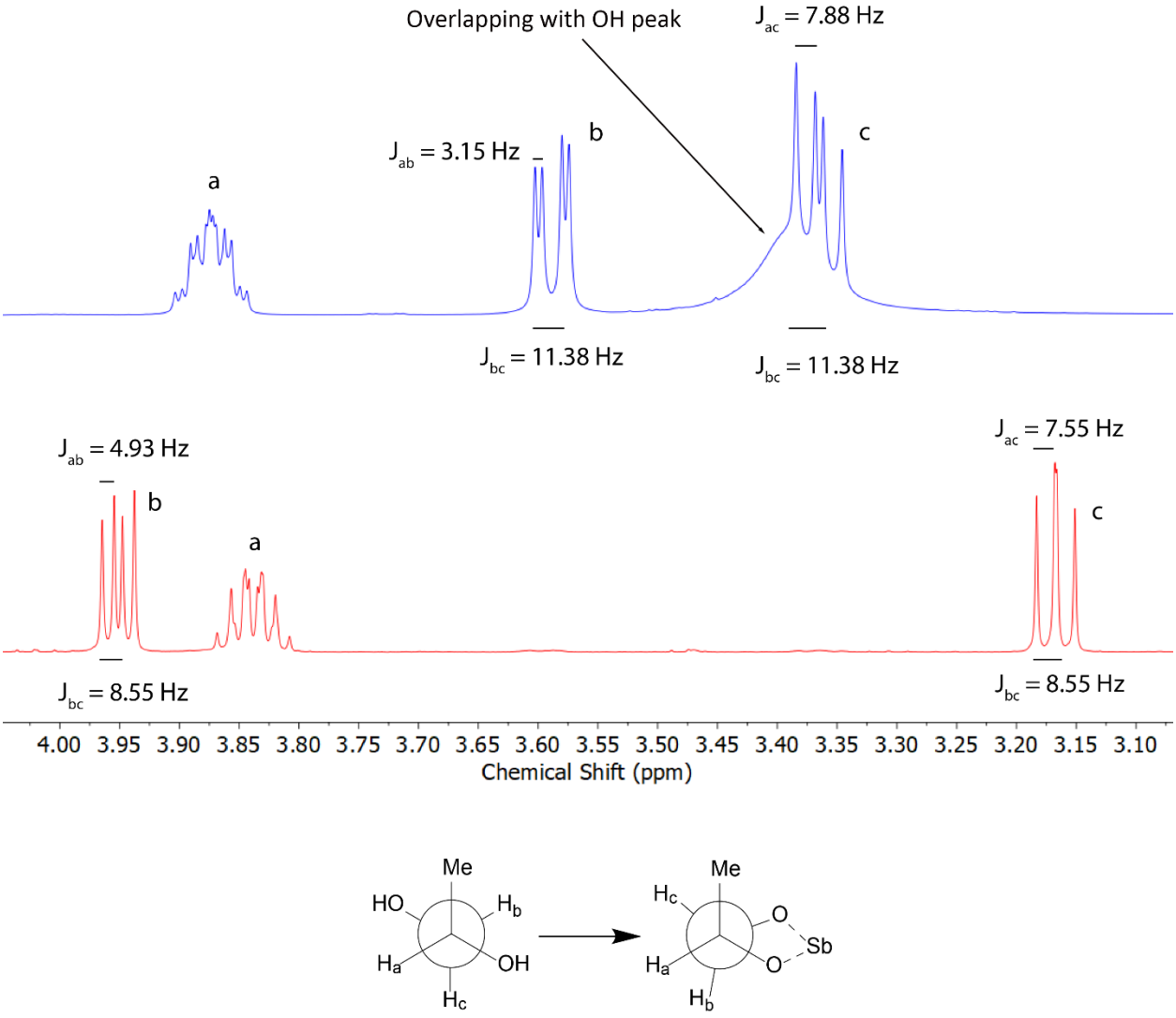


Figure S5. *Top (blue)*: ^{1}H NMR spectrum of free (*S*)-1,2-propanediol. Peaks are arbitrarily labeled based on the labelling scheme used for the Newman projections. *Middle (red)*: ^{1}H NMR spectrum of **6**. *Bottom*: Newman projections displaying conformational change of (*S*)-1,2-propanediol upon binding to Sb.

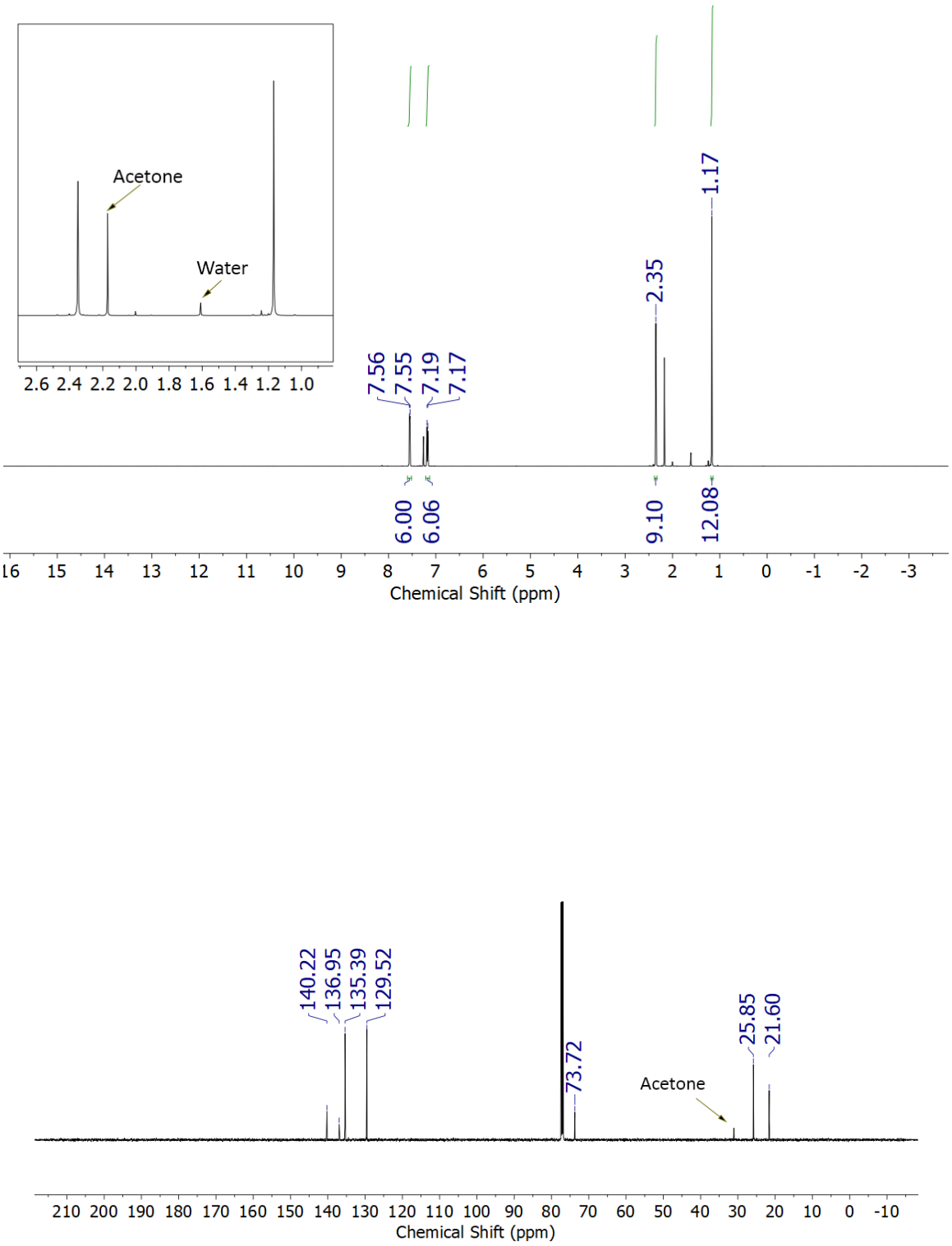


Figure S6. *Top*: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **1**. *Bottom*: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **1**.

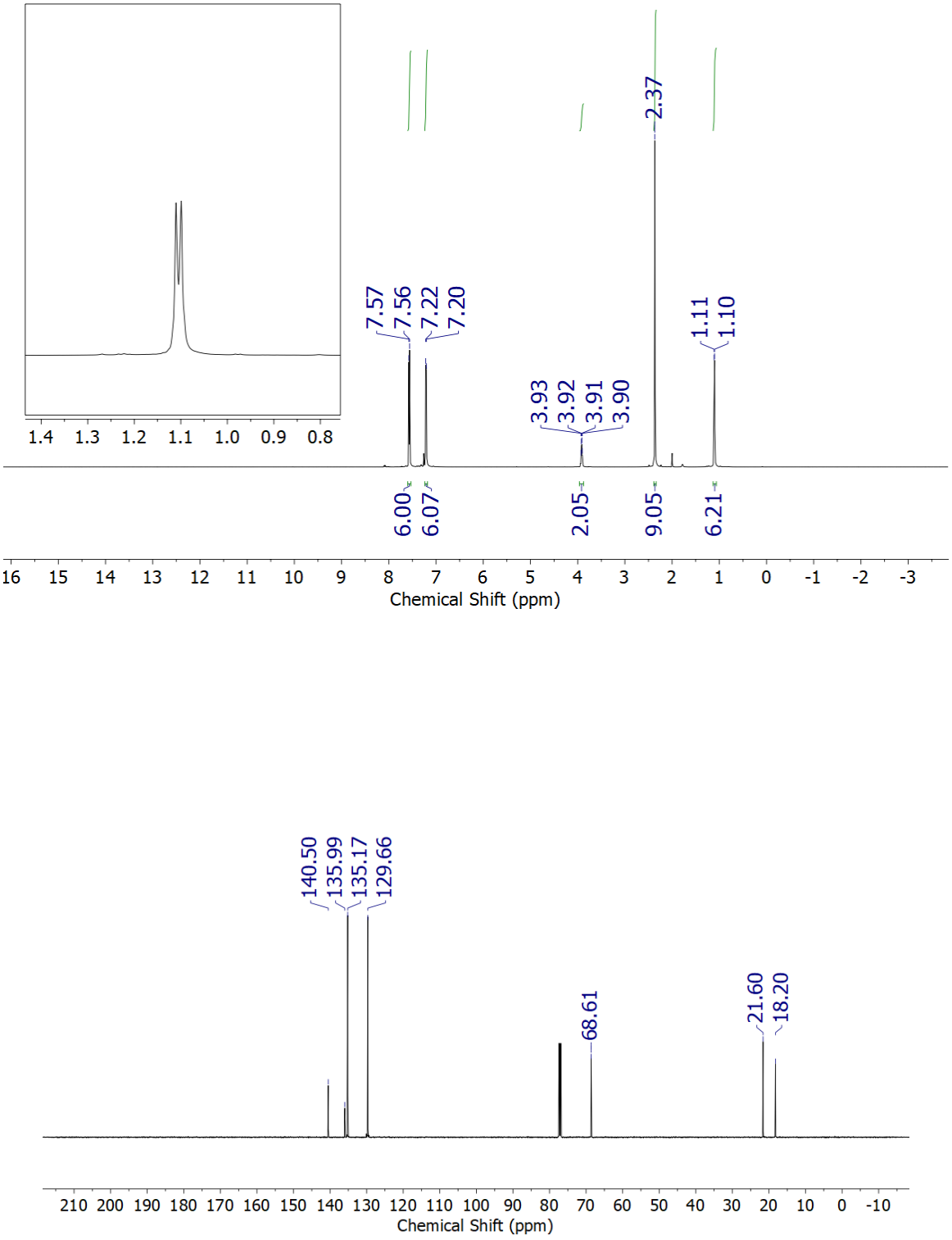


Figure S7. *Top*: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **2**. *Bottom*: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **2**.

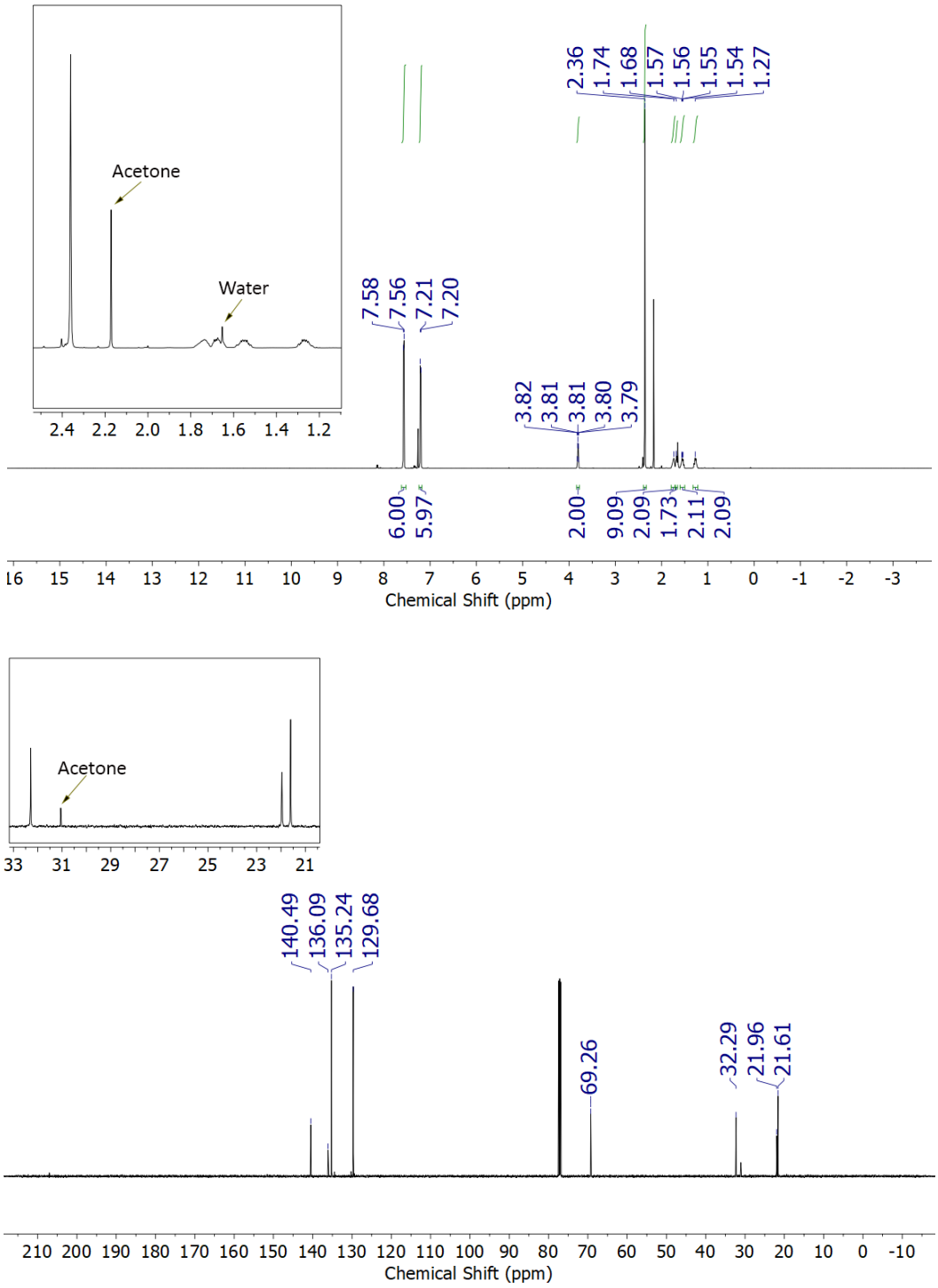
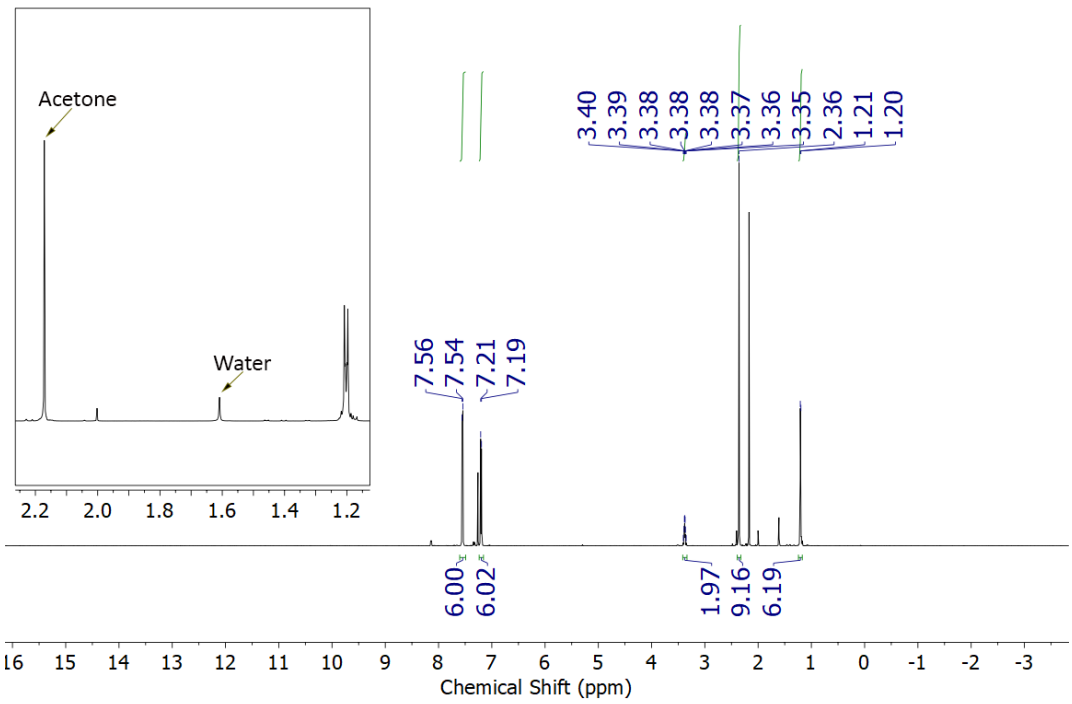


Figure S8. *Top*: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **3**. *Bottom*: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **3**.



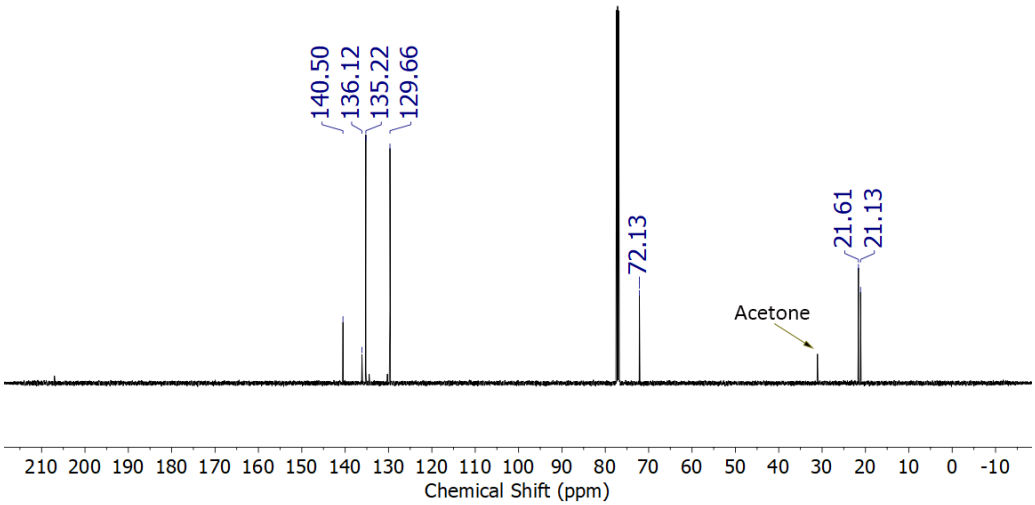


Figure S9. *Top*: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **4**. *Bottom*: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **4**.

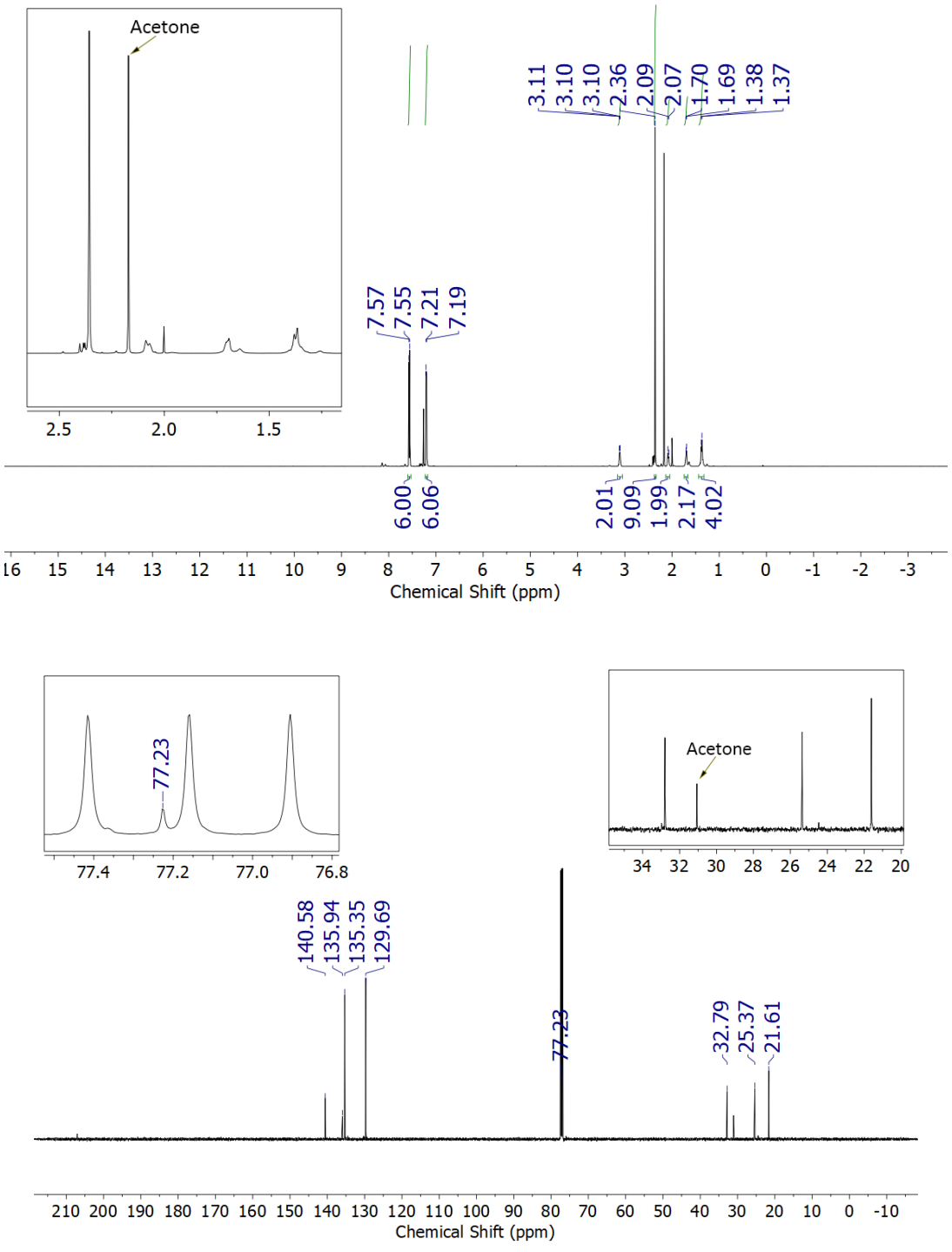
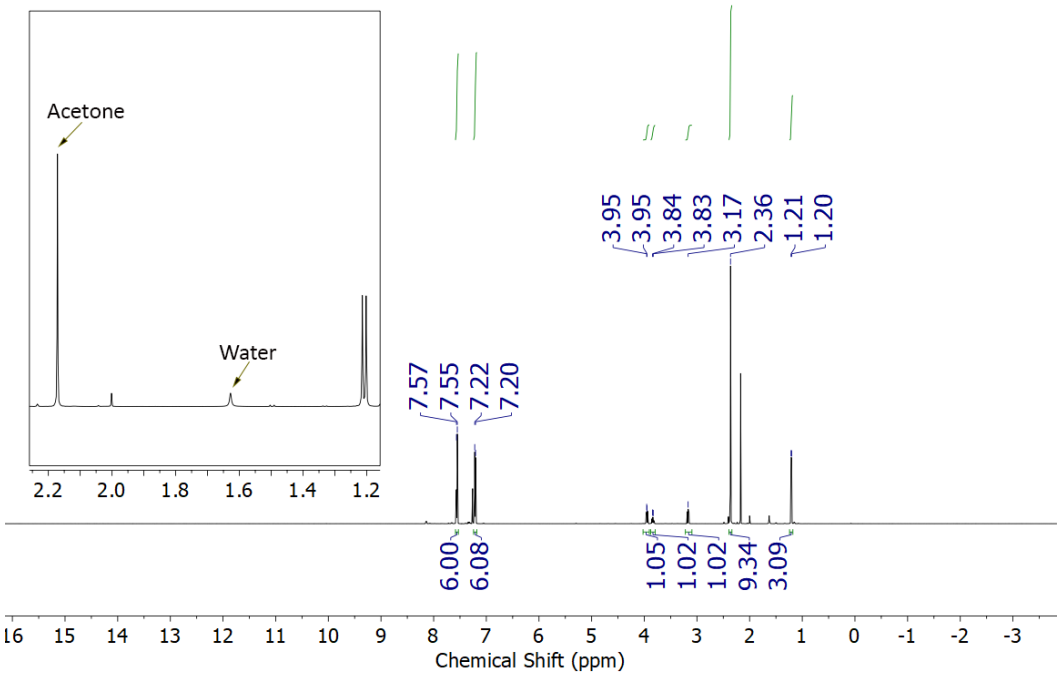


Figure S10. *Top*: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **5**. *Bottom*: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **5**.



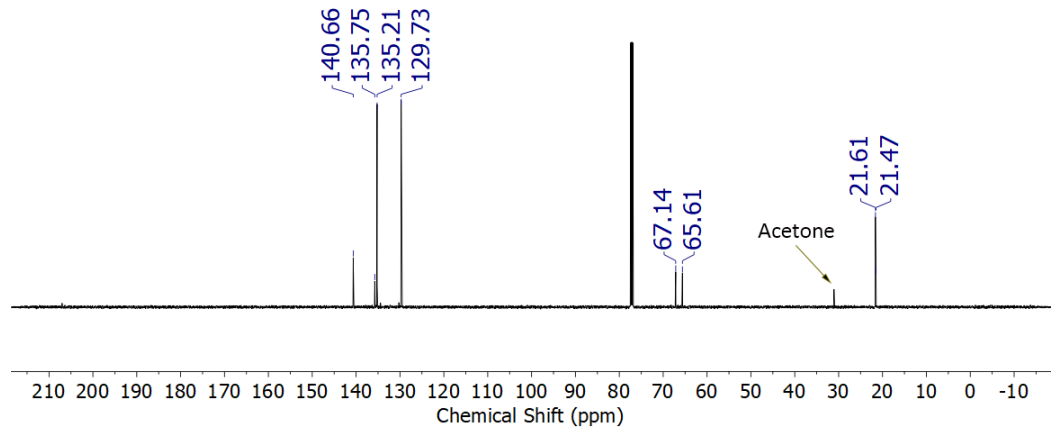


Figure S11. *Top*: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **6**. *Bottom*: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **6**.