Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

^{1}H chemical shift differences of Prelog-Djerassi lactone derivatives: A DFT and NMR conformational studies.

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SUPORTING INFORMATION

17 Oct 2014

Acquisition Time (sec)	3.9999	***Comment***	Dimas "DL 2.80 - 17 a 23" CDCl3/Tri-Res dez16djpH1			***Date***	Dec 16 2009
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Number of Transients	16	***Original Points Count***	31999	***Points Count***	32768	***Pulse Sequence***	s2pul
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	8000.00	***Temperature (degree C)***	25.000

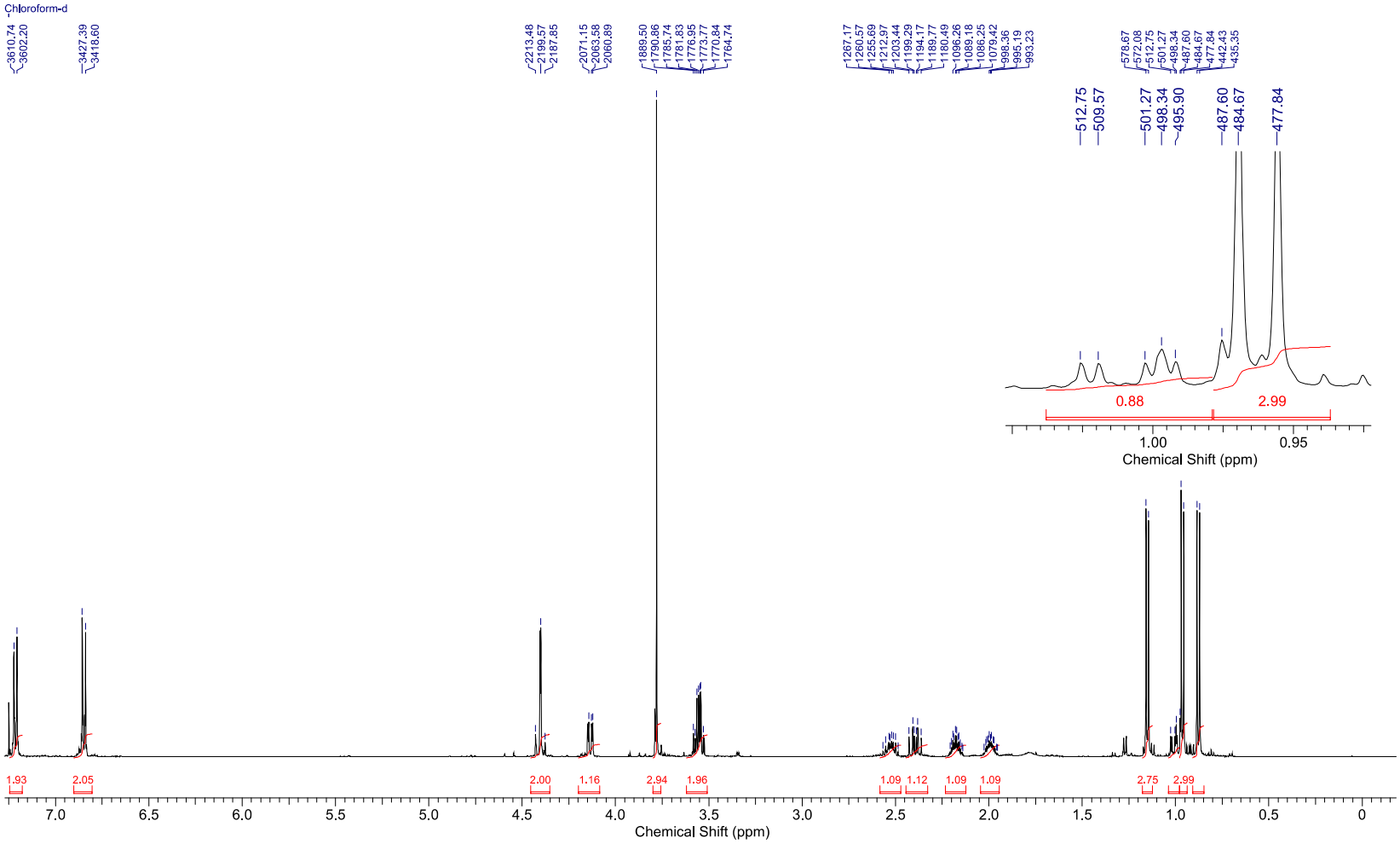
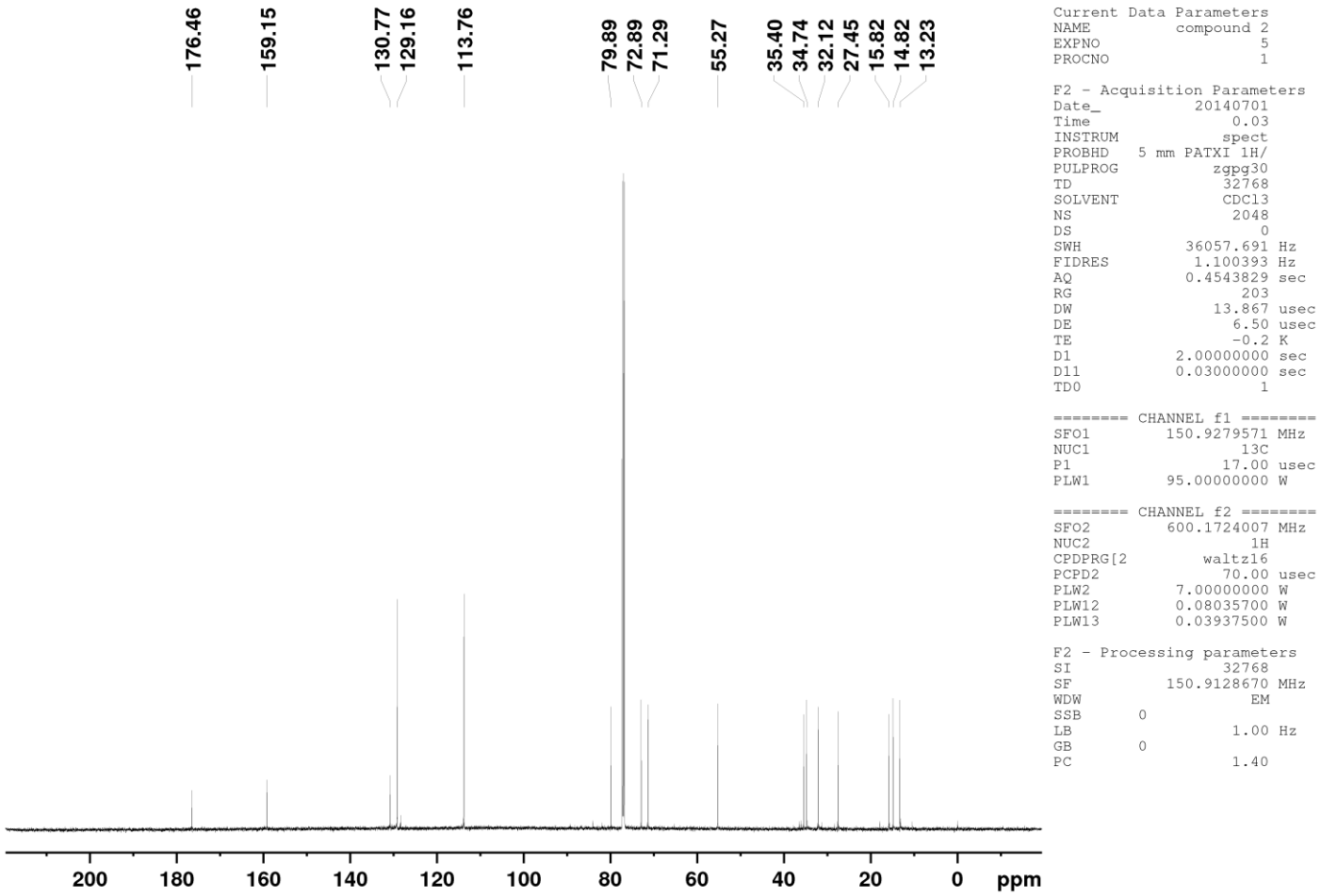


Figure S1. 500 MHz ^{1}H NMR spectrum for compound **2** in CDCl3.

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PROCNO                 1

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FIDRES         1.100393 Hz
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RG                  203
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DE                6.50 usec
TE                -0.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

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P1                17.00 usec
PLW1        95.00000000 W

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NUC2                1H
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PCPD2             70.00 usec
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PLW12         0.08035700 W
PLW13         0.03937500 W

F2 - Processing parameters
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Figure S2. 150 MHZ ^{13}C NMR spectrum for compound in $CDCl_3$.

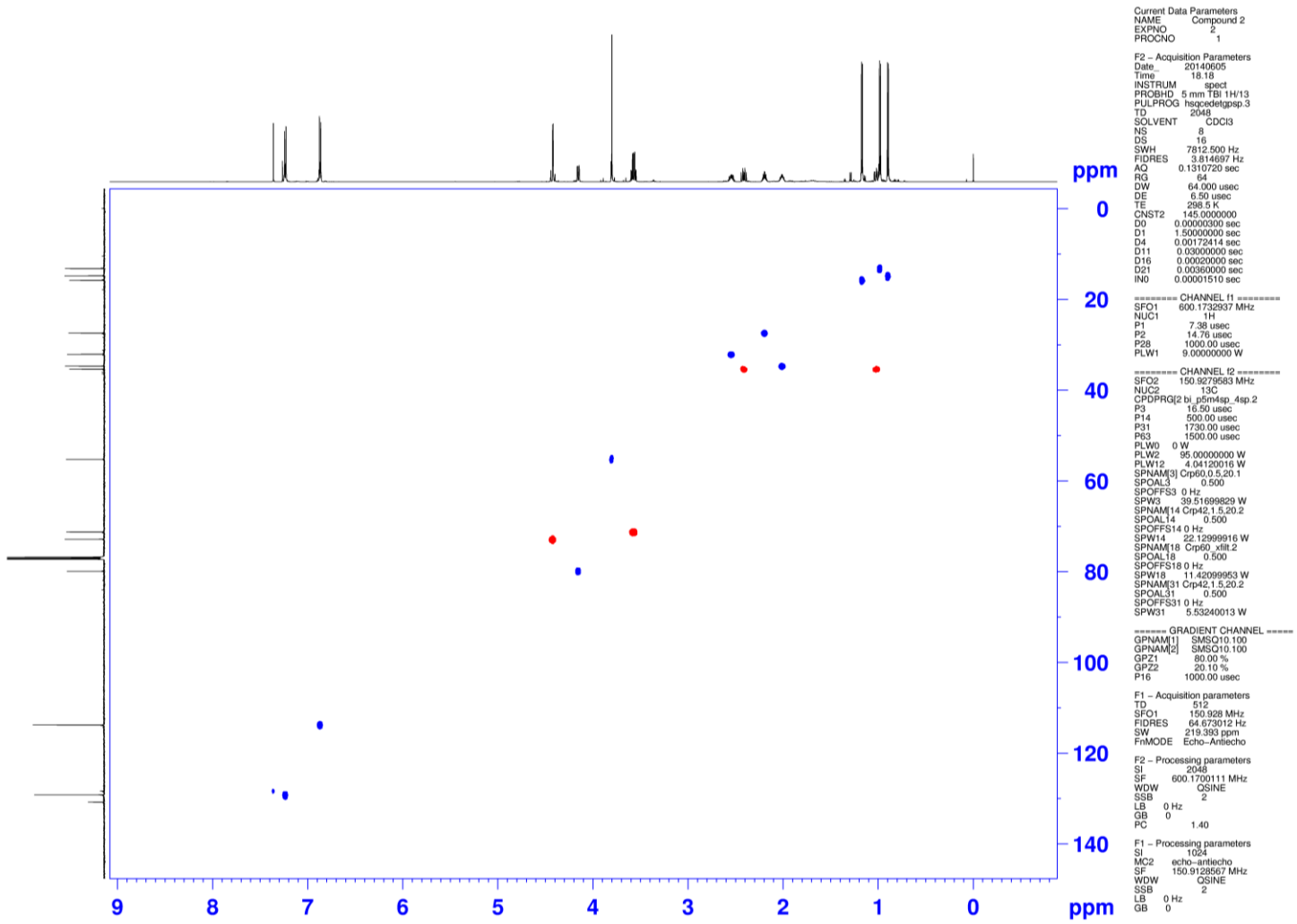

Figure S4. HSQC with multiplicity editing contour plot for compound **2** at 600 MHz in $CDCl_3$

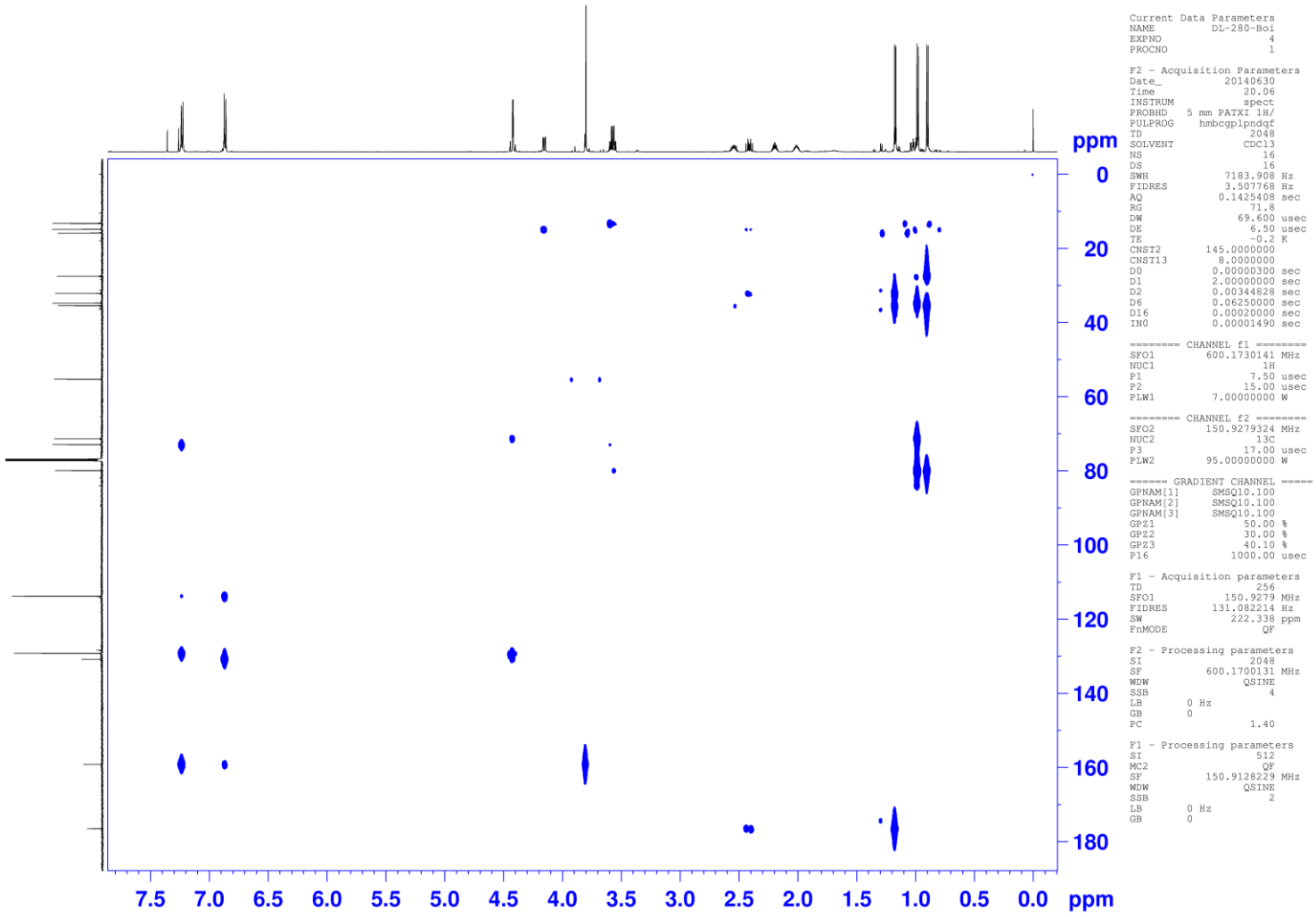

Figure S5. HMBC contour plot for compound **2** at 600 MHz in $CDCl_3$.