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for

Phenylnannolones A–C: New Secondary Metabolites and their Biosynthesis from the Myxobacterium *Nannocystis exedens*

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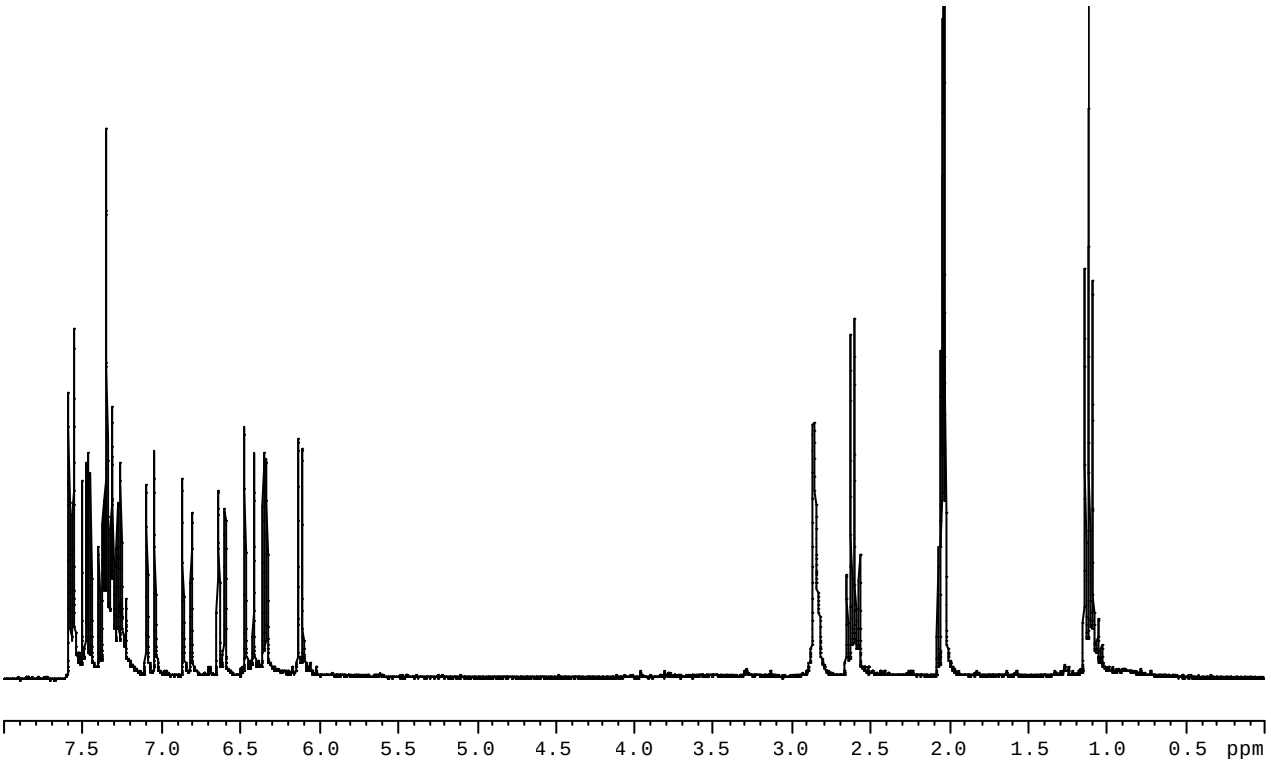
Contents

S1. NMR Spectroscopic Data (300MHz, $(CD_3)_2CO$) for phenylnannolone A (**1**)

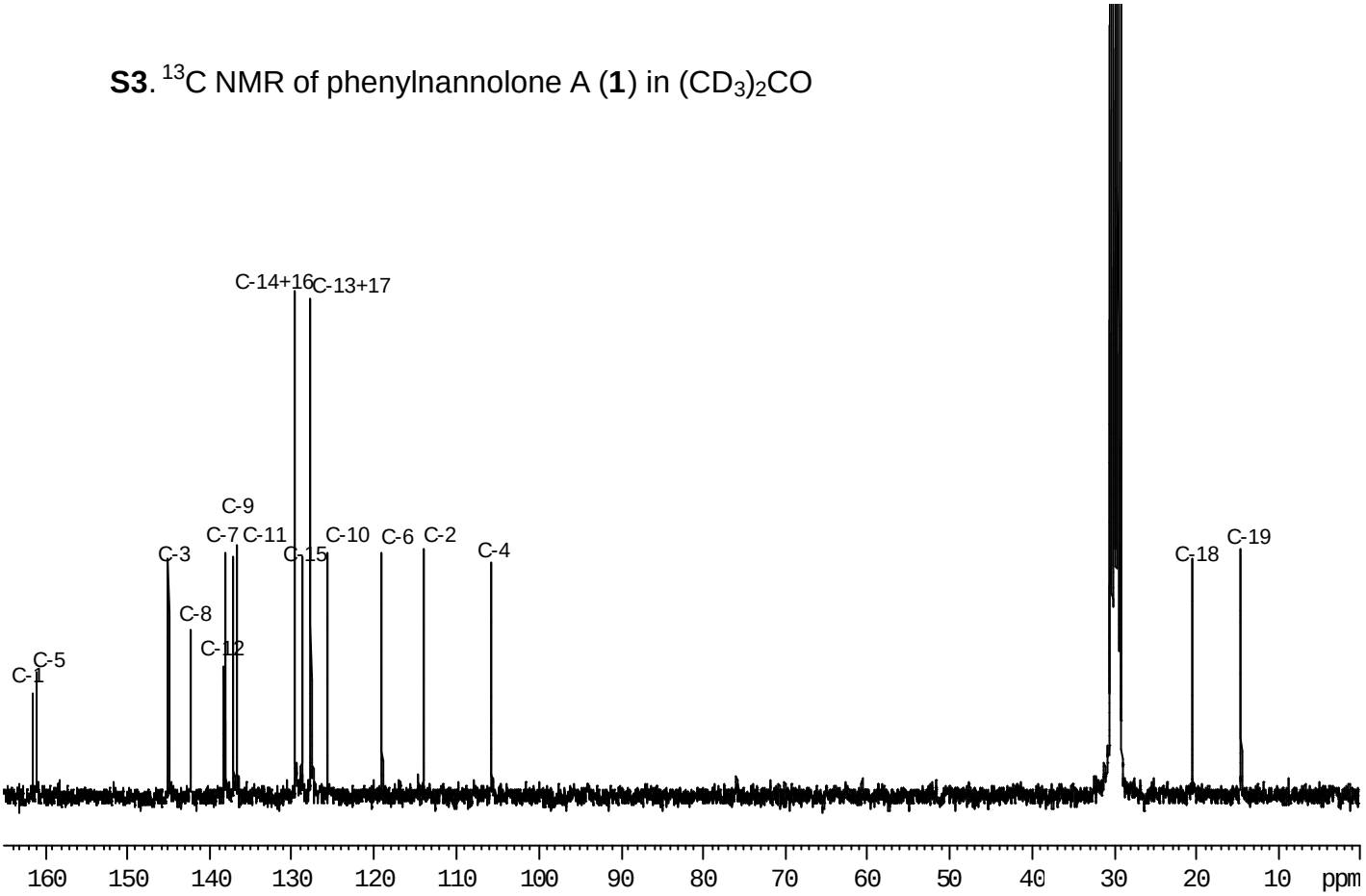
phenylnannolone A (**1**)					
position	$?_C$, mult.	$?_H$ (*J* in Hz)[a]	HMBC	COSY	NOE
1	161.5, qC				
2	114.1, CH	6.12, d (9.2)	1, 4	3, 4	3
3	144.9, CH	7.48, dd (6.6, 9.2)	1, 4, 6	2, 4	2, 4
4	105.7, CH	6.35, d (6.6)	2, 3, 5, 6, 7	3	3, 6, 7
5	161.0, qC				
6	119.0, CH	6.44, d (16.1)	4, 5, 7, 8	7	4, 18, 19
7	138.1, CH	7.07, d (16.1)	4, 5, 6, 8, 9	6	4, 9, 19
8	142.3, qC				
9	137.1, CH	6.62, d (11.7)	7, 8, 10, 11	10, 11	7, 11, 19
10	125.7, CH	7.34, dd (11.7, 15.4)	8, 11, 13/17		
11	136.7, CH	6.84, d (15.4)	8, 9, 10, 13/17	9, 10	9, 13/17, 19
12	138.3, qC				
13/17	127.7, CH	7.57, d (7.7)	11, 15, 14/16	14/16	10, 11, 15
14/16	129.5, CH	7.35, t (7.7)	12, 13/17	15, 13/17	
15	128.9, CH	7.25, t (7.7)	13/17	14/16	14/16
18	20.4, CH_2	2.61, q (7.7)	7, 8, 9, 19	19	6, 10, 19
19	14.6, CH_3	1.12, t (7.7)	8, 18	18	6, 7, 9, 10, 18

[a] assignment was based on extensive 1D and 2D NMR measurements (^1H-^1H COSY, HSQC, ^1H-^{13}C HMBC)

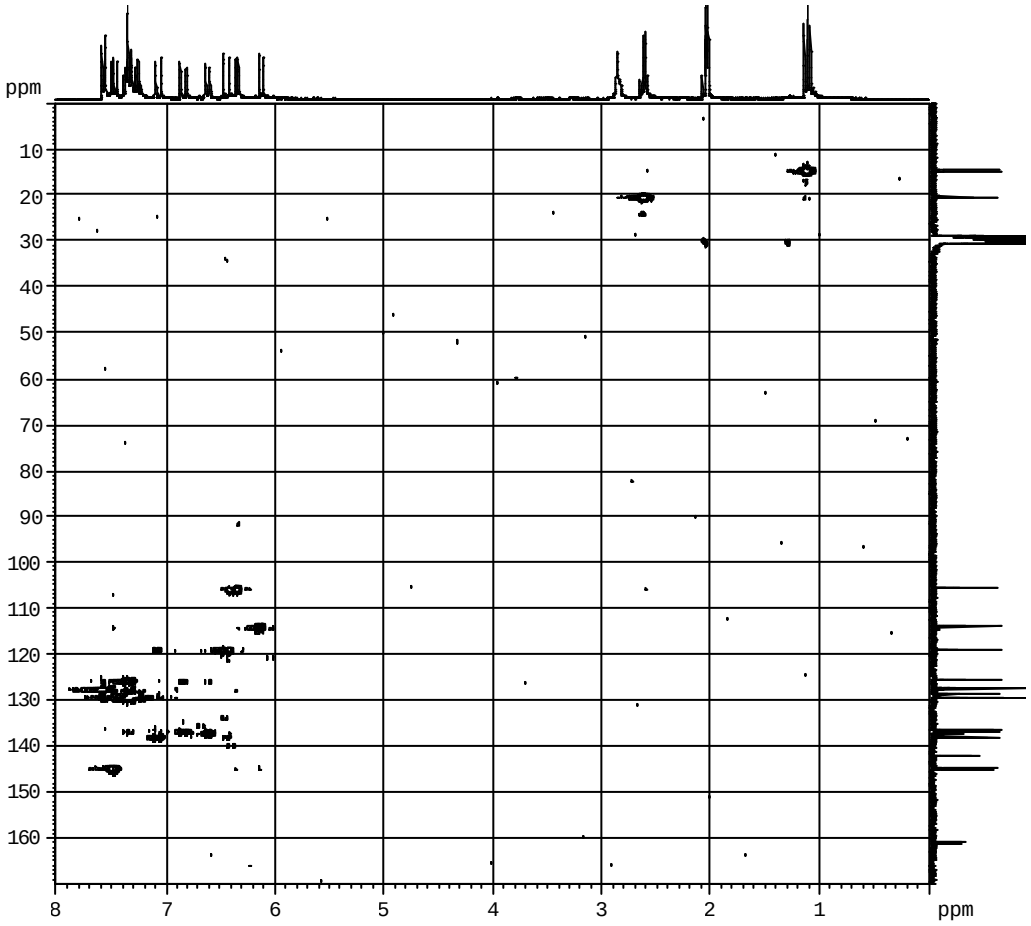
S2. ^1H NMR of phenylnannolone A (**1**) in $(CD_3)_2CO$



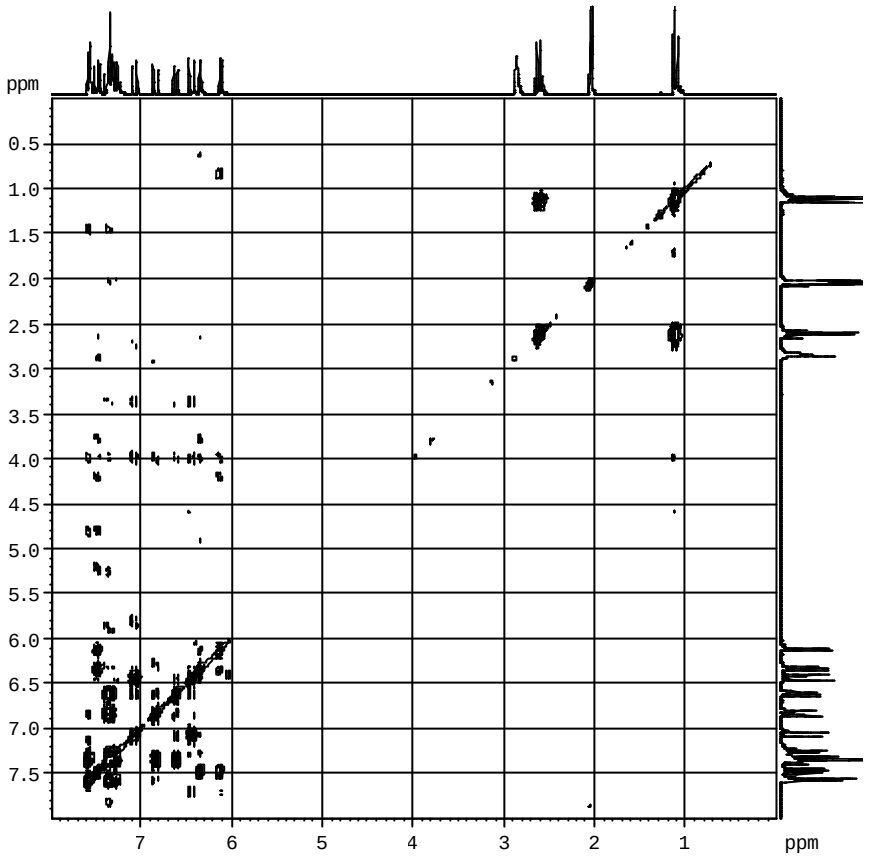
S3. ^{13}C NMR of phenylnannolone A (**1**) in $(CD_3)_2CO$



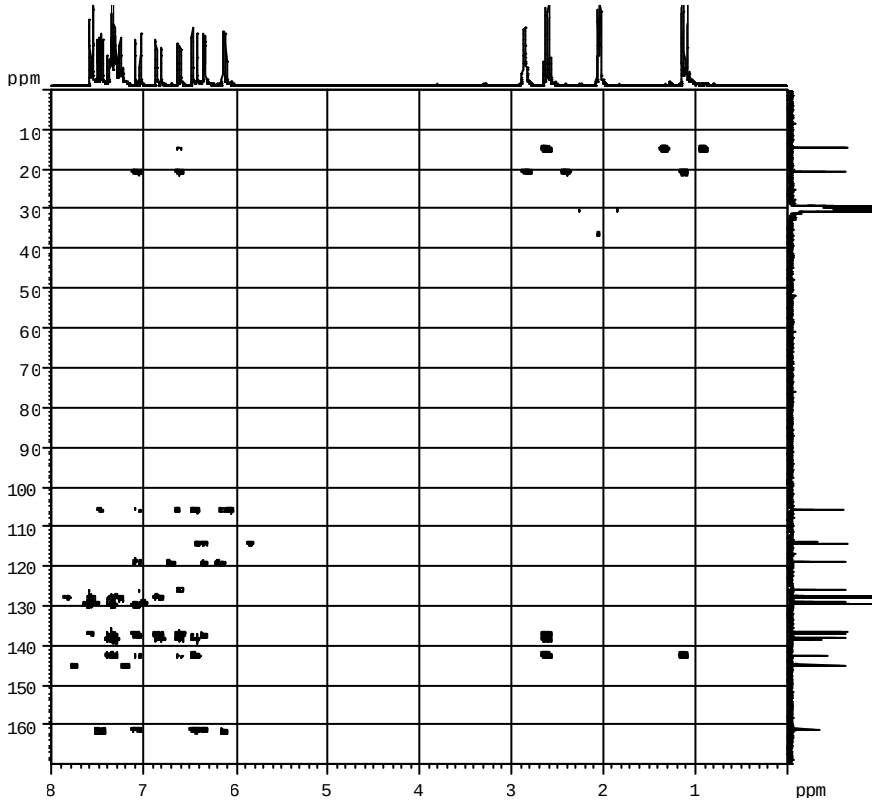
S4. HSQC of phenylnannolone A (**1**) in $(CD_3)_2CO$



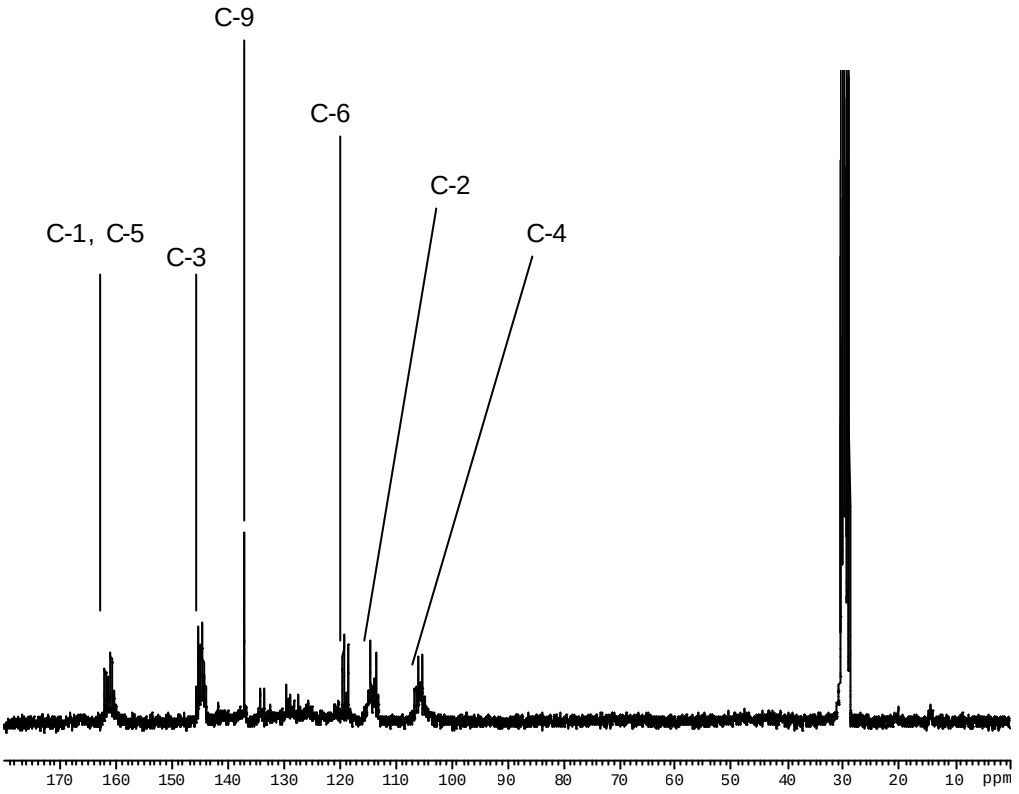
S5. $^{1}H,^{1}H$ COSY of phenylnannolone A (**1**) in $(CD_3)_2CO$



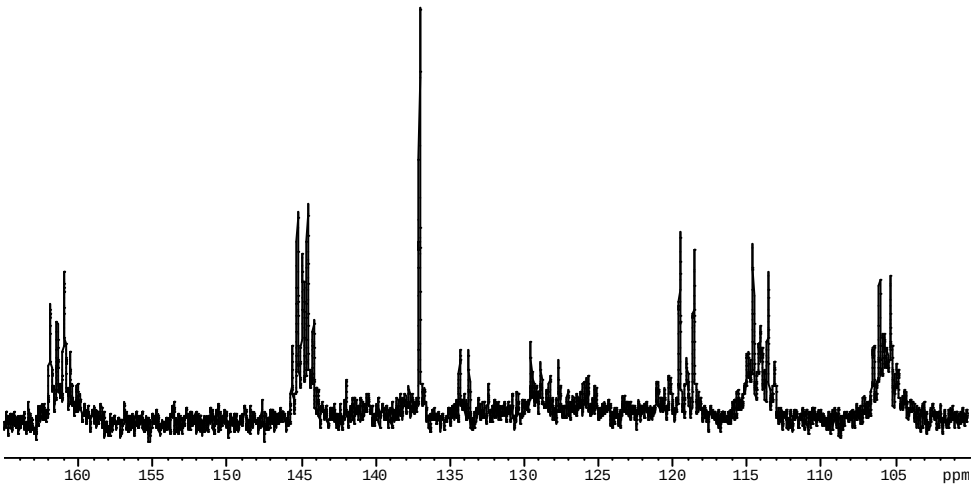
S6. $^{1}H,^{13}C$ HMBC of phenylnannolone A (**1**) in $(CD_3)_2CO$



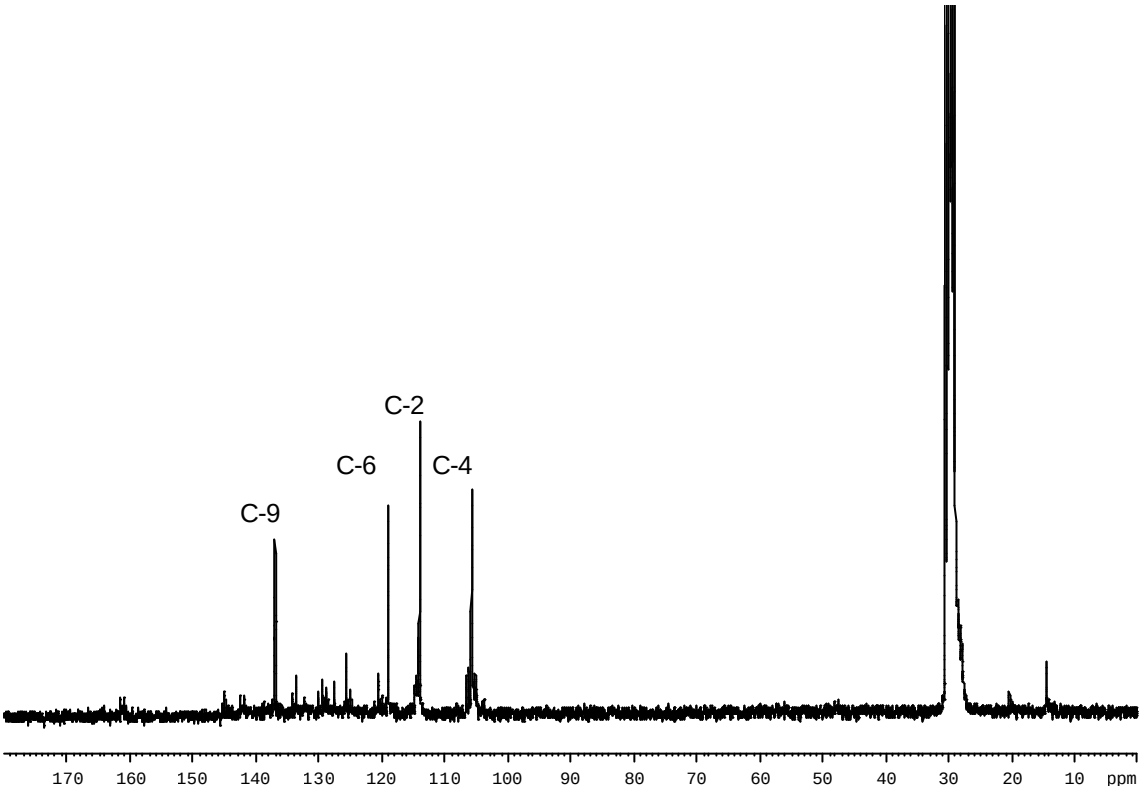
S7. ^{13}C NMR of phenylnannolone A after labeling with 1, 2-$^{13}C_2$-acetate, in $(CD_3)_2CO$



carbons	*J* (in Hz)
C-1, C-2	73.5
C-3, C-4	52.1
C-5, C-6	67.5



S8. ^{13}C NMR of phenylnannolone A after labeling with 2-^{13}C-acetate, in $(CD_3)_2CO$

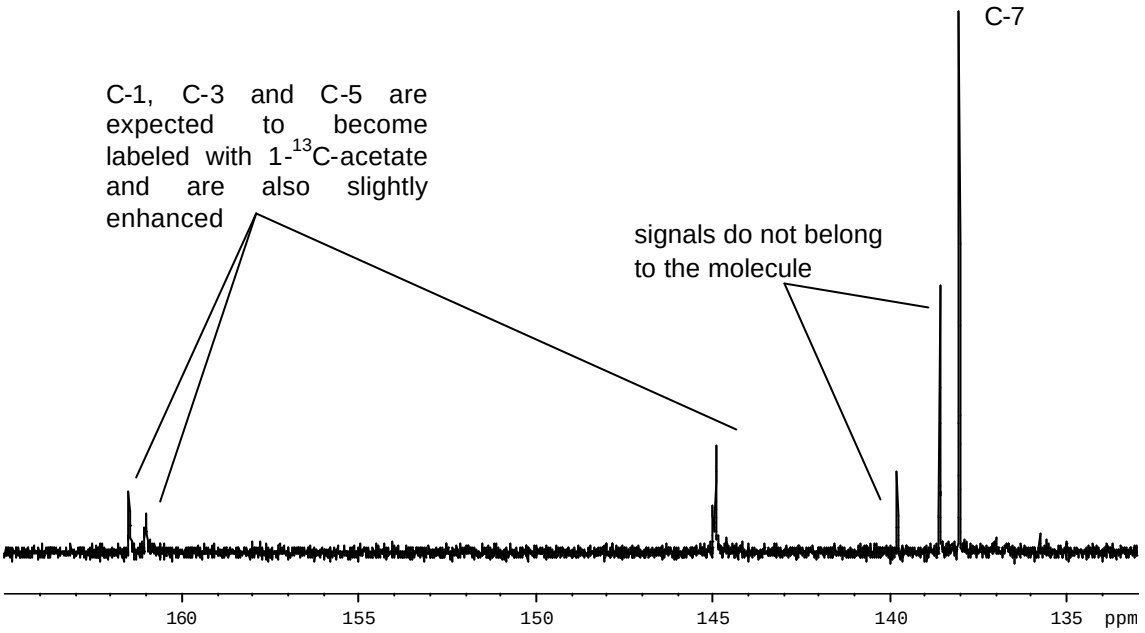


Enrichment = enhancement of the signal x 1.1% - 1.1%

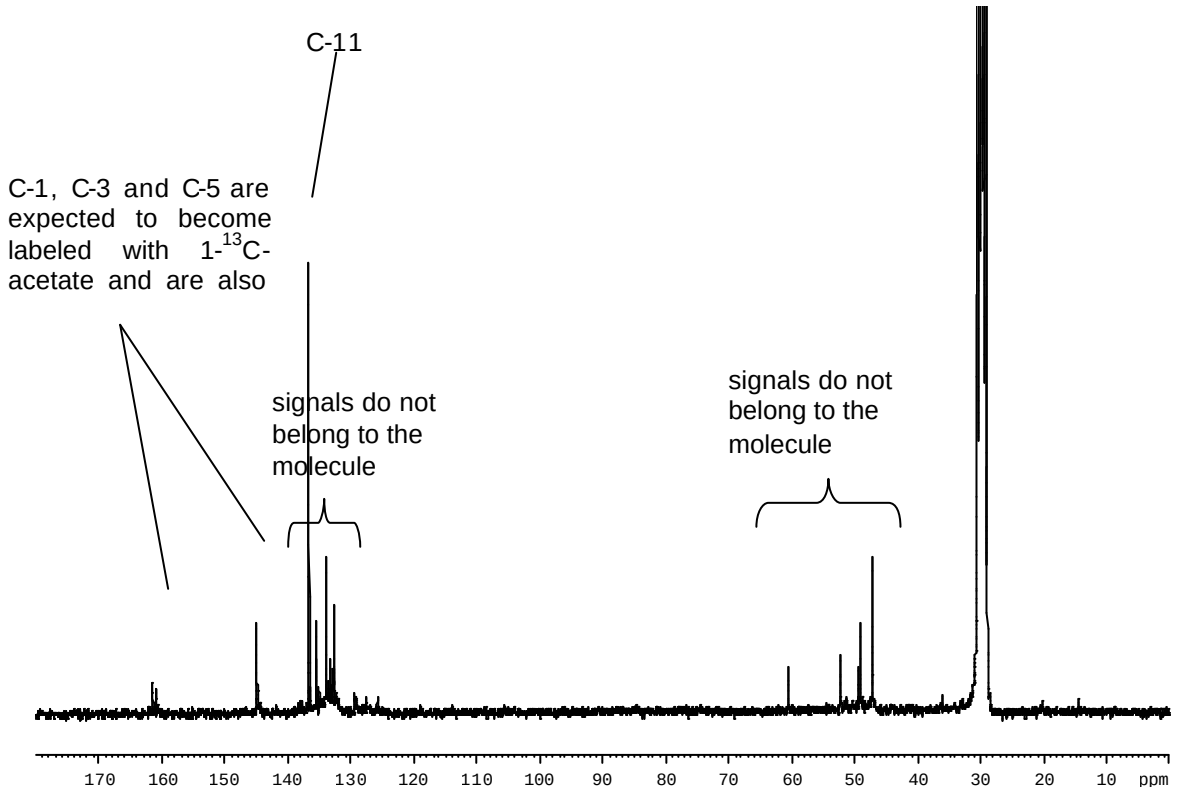
The integral of carbon 19 was set to 1.000 for every spectrum and subsequently the integrals of the other carbons were compared in the spectra of the labeled and the non labeled compound.

carbon	1. integral (spectrum of the labeled compoud)	2.integral (spectrum of the non-labeled compound)	quotient of the integrals (enriched/ not enriched)	enrrichment (%) (calculation see above)
2	7.60	0.91	8.33	8.1
4	6.30	0.88	7.26	6.9
6	6.37	0.90	7.08	6.7
8	0.37	0.64	0.58	
9	4.20	0.91	4.61	4.0
10	1.05	0.94	1.11	
13+17	0.53	1.85	0.29	
14+16	0.58	2.00	0.29	
19	1.00	1.00	1.00	

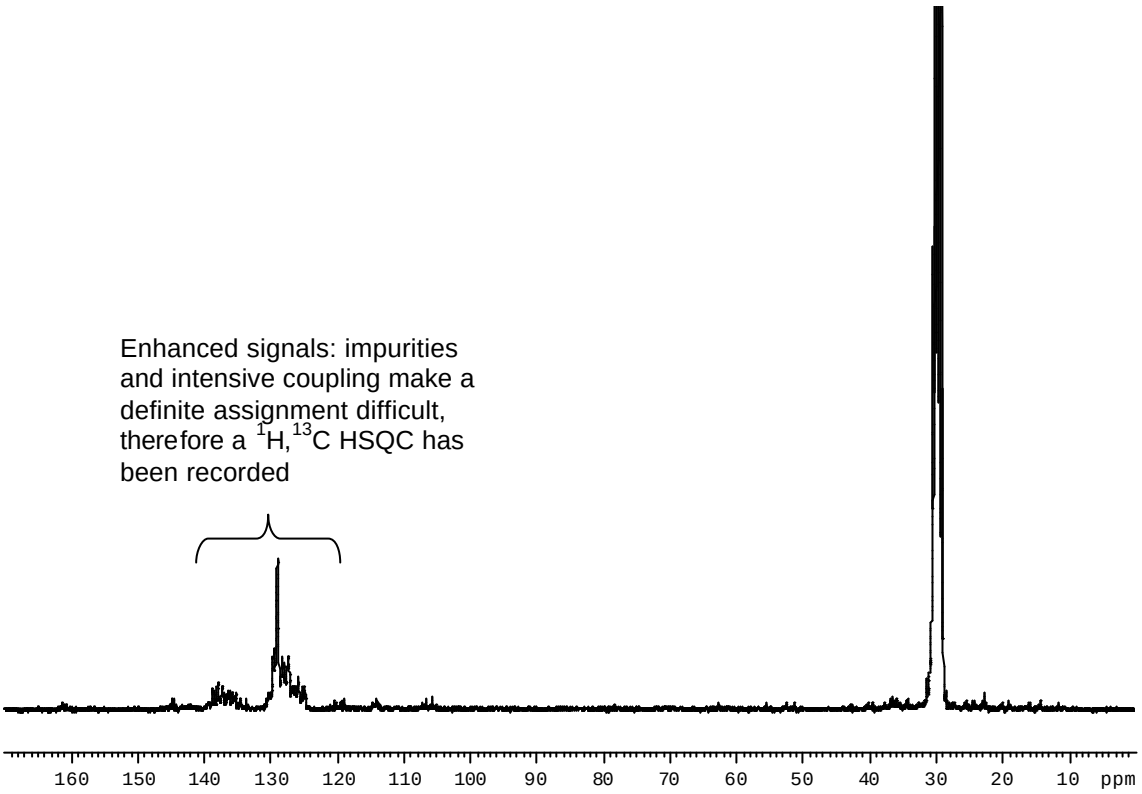
S9. ^{13}C NMR of phenylnannolone A (VLC fraction) after labeling with 1-^{13}C-butyrate



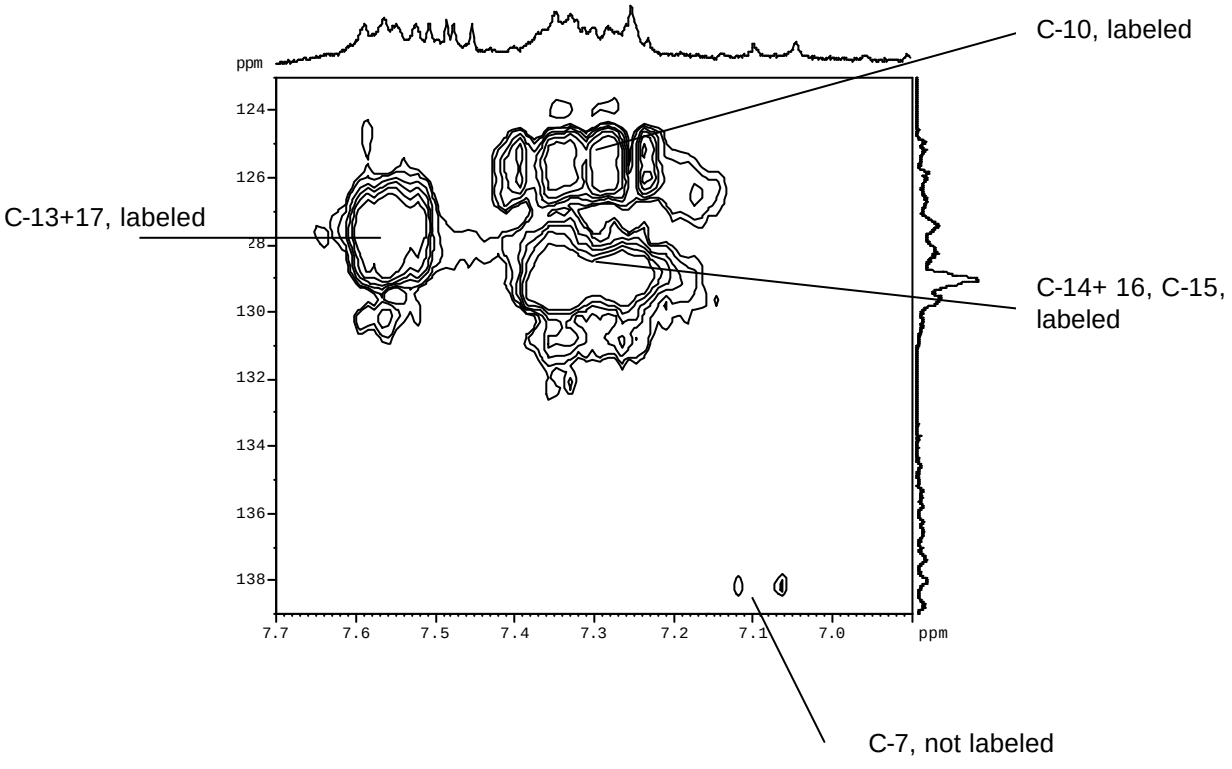
S10. ^{13}C NMR of phenylnannolone A (VLC fraction) after labeling with 3-^{13}C-L-phenylalanine



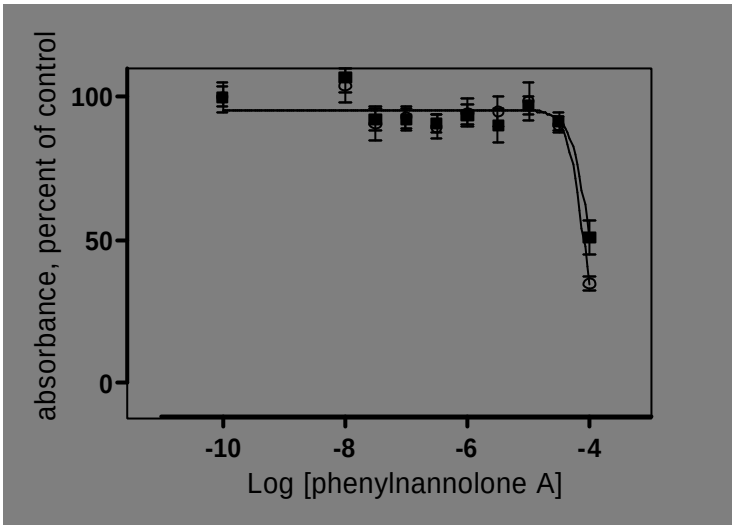
S11. ^{13}C NMR of phenylnannolone A (VLC fraction) after labeling with U-$^{13}C_9$-^{15}N-L-phenylalanine



S12. $^{1}H,^{13}C$ HSQC of phenylnannolone A (VLC fraction) after labeling with U-$^{13}C_9$-^{15}N-L-phenylalanine



S13. Concentration effect curve of phenylnannolone A



Concentration effect curve of phenylnannolone A in the resistant A2780 ADR (squares) and the sensitive A2780 WT (circles) cell line. Presented data are averages ± SD of three independent experiments.