

Supporting Information

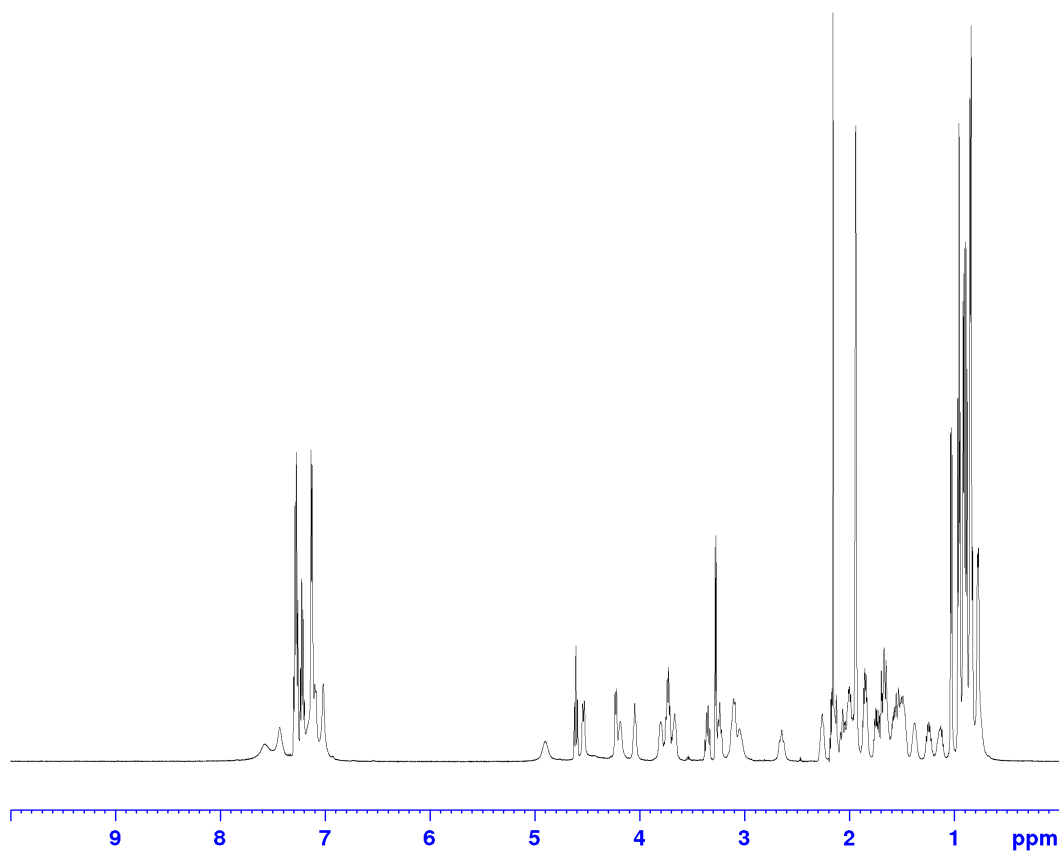


Figure 1: ^1H NMR spectrum of LOB3 dissolved in acetonitrile and collected at 298 K.

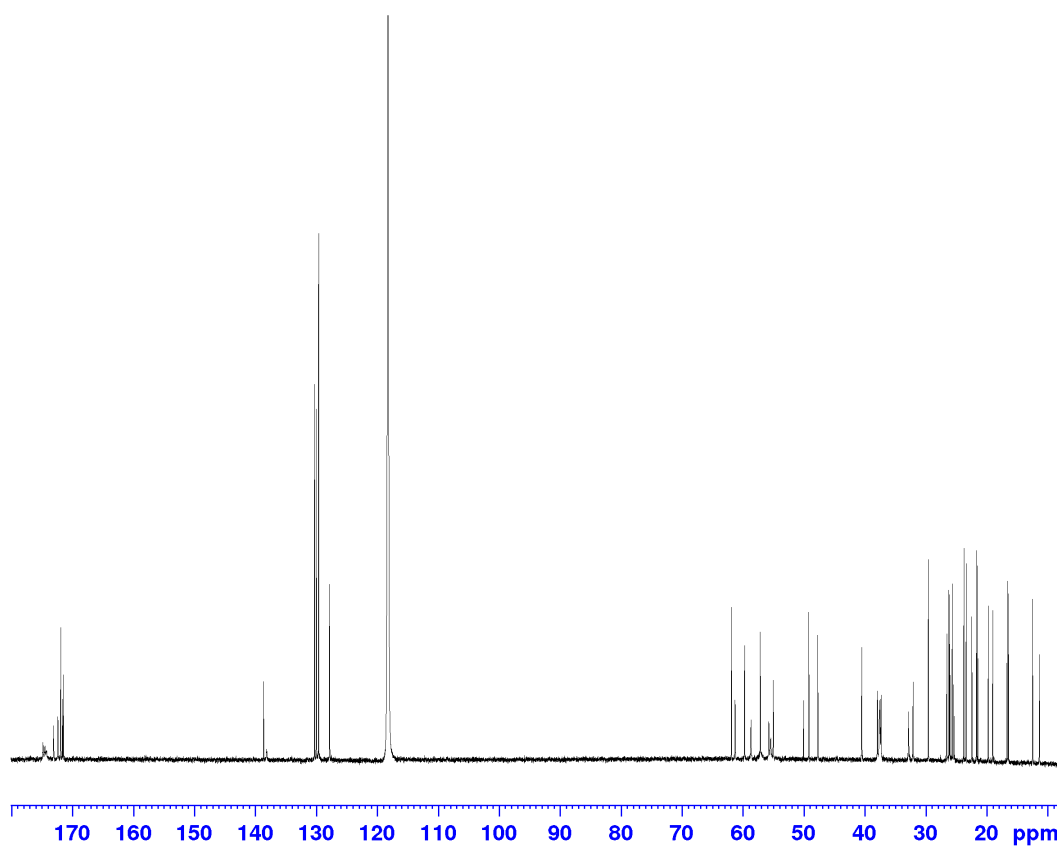


Figure 2: ^{13}C NMR spectrum of LOB3 dissolved in acetonitrile and collected at 298 K.

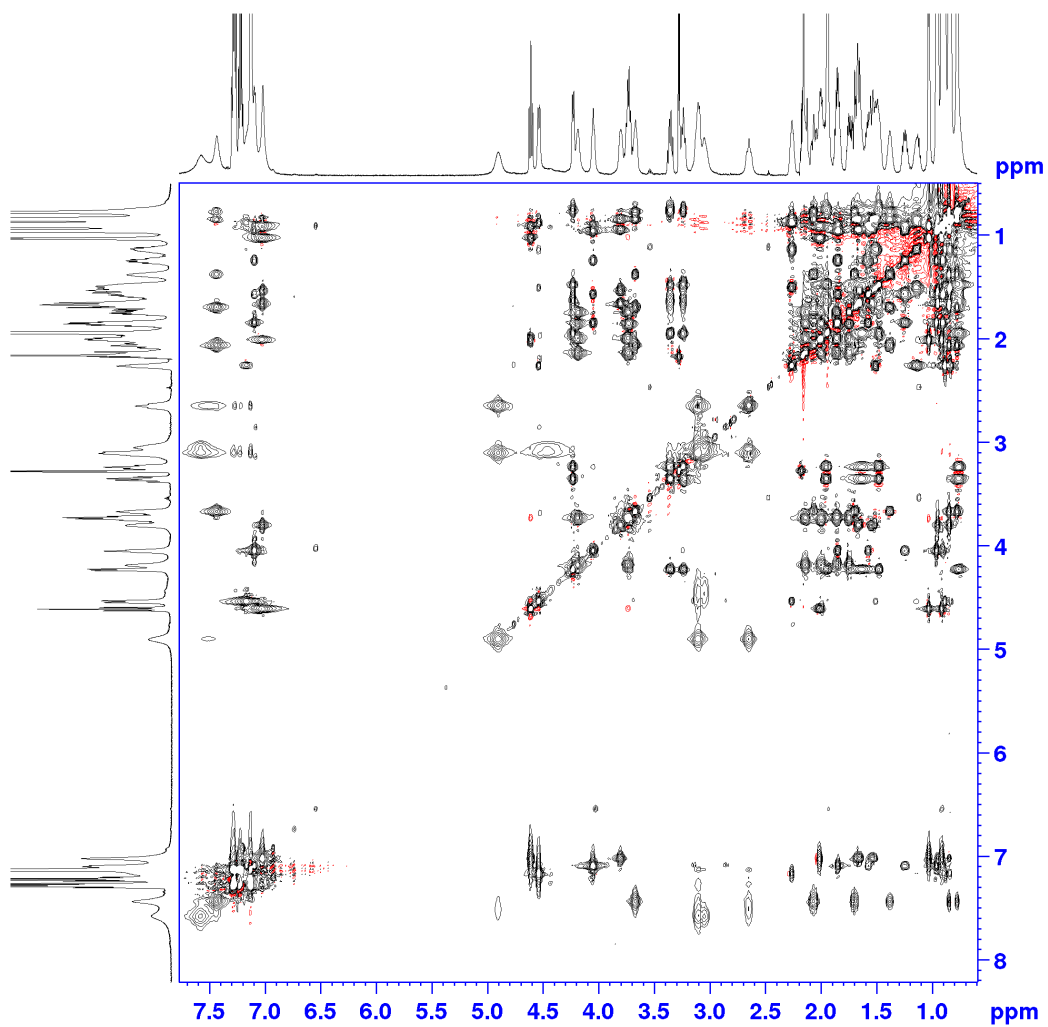


Figure 3: ^1H - ^1H TOCSY spectrum of LOB3 dissolved in acetonitrile and collected at 298 K.

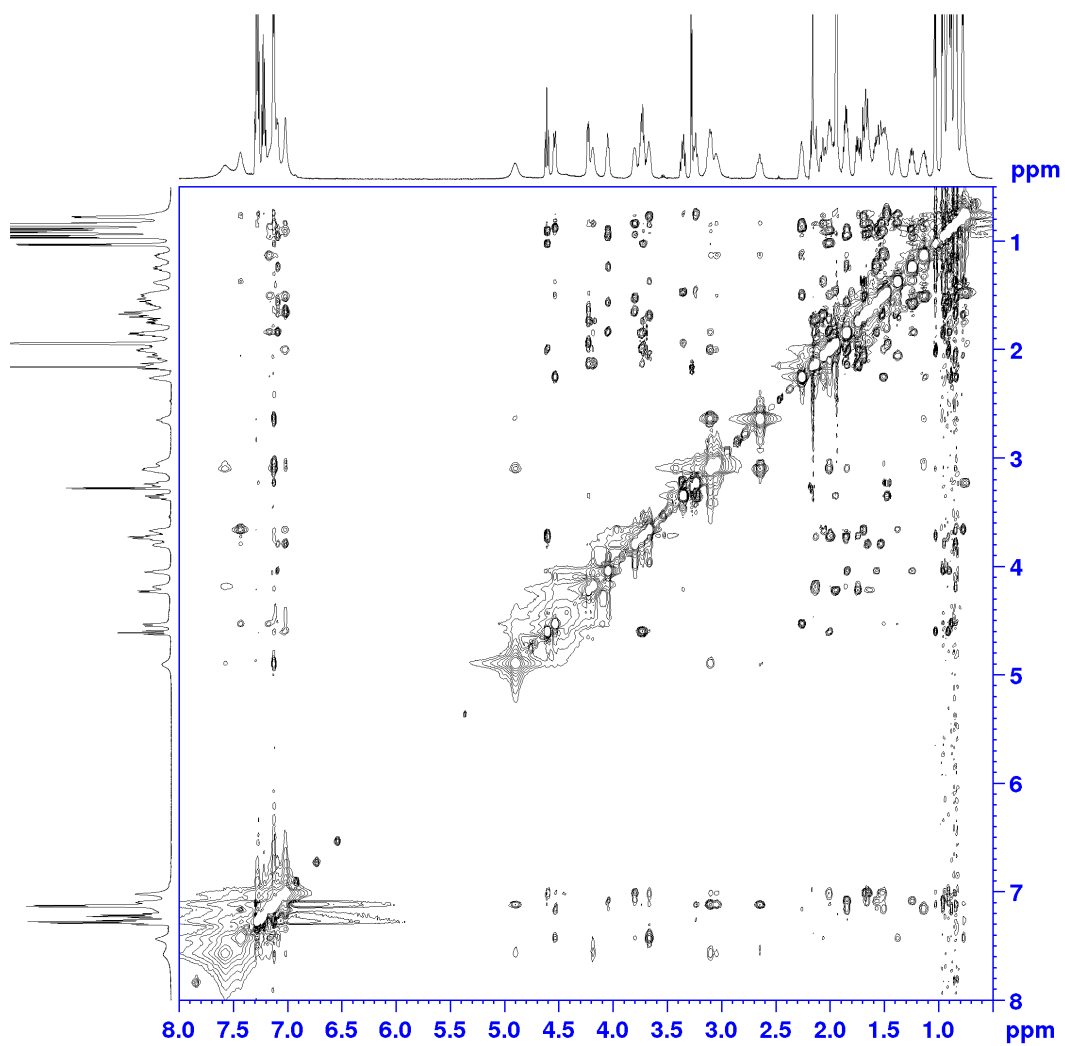


Figure 4: ^1H - ^1H NOESY spectrum of LOB3 dissolved in acetonitrile and collected at 298 K.

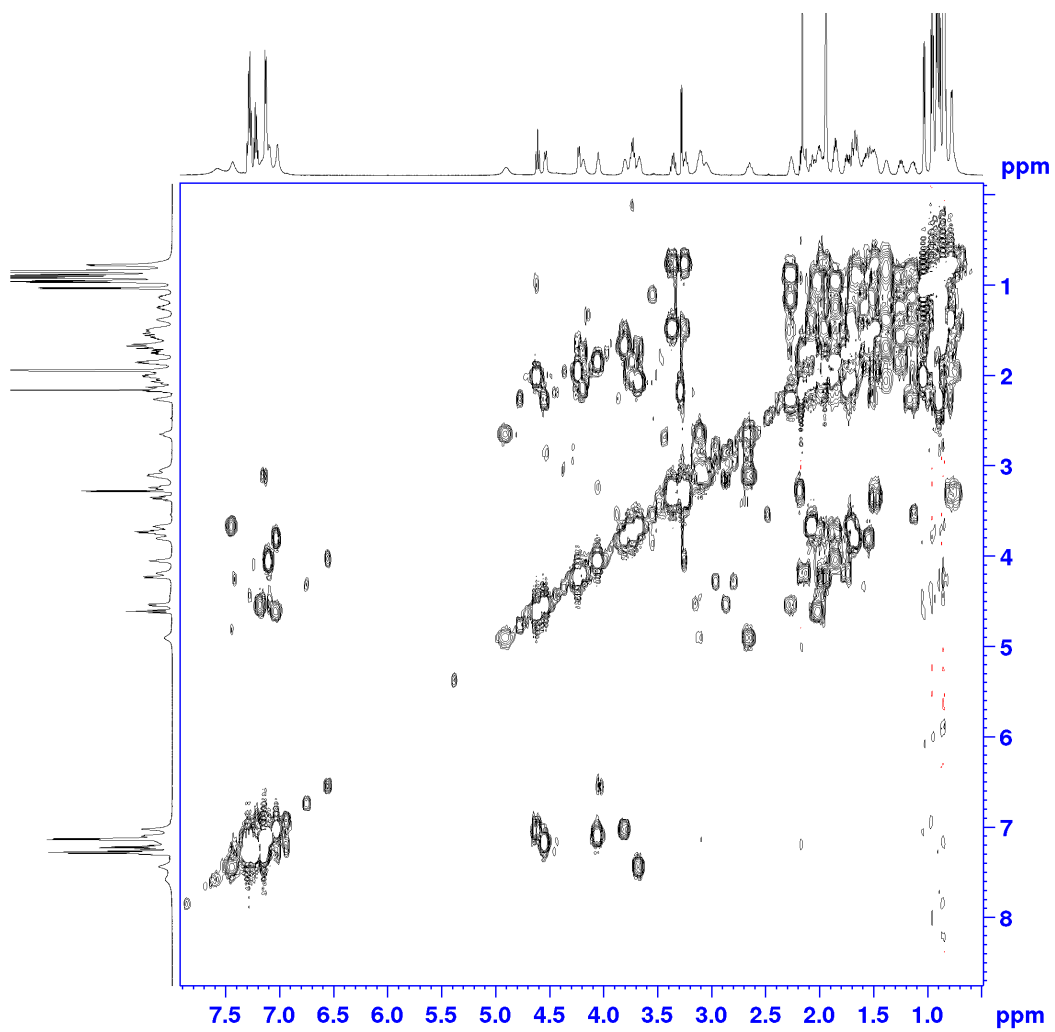


Figure 5: ^1H - ^1H COSY of LOB3.

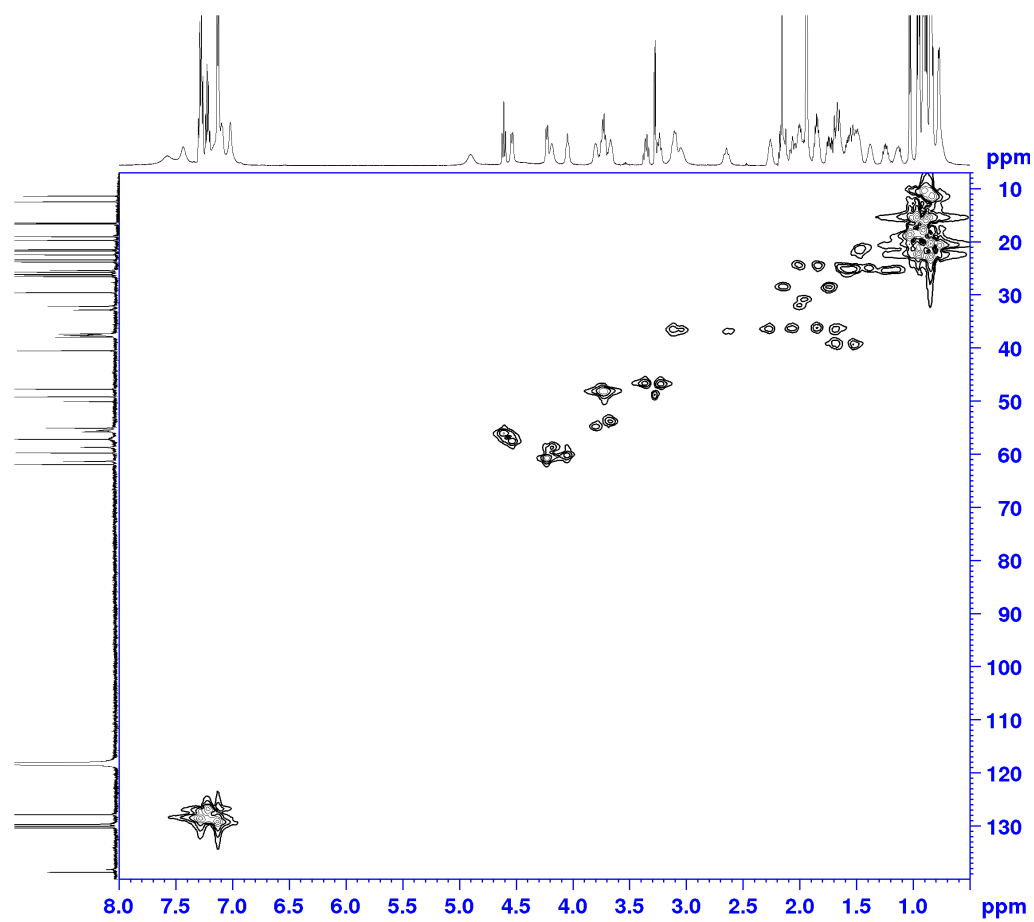


Figure 6: ^1H - ^{13}C HSQC of LOB3.

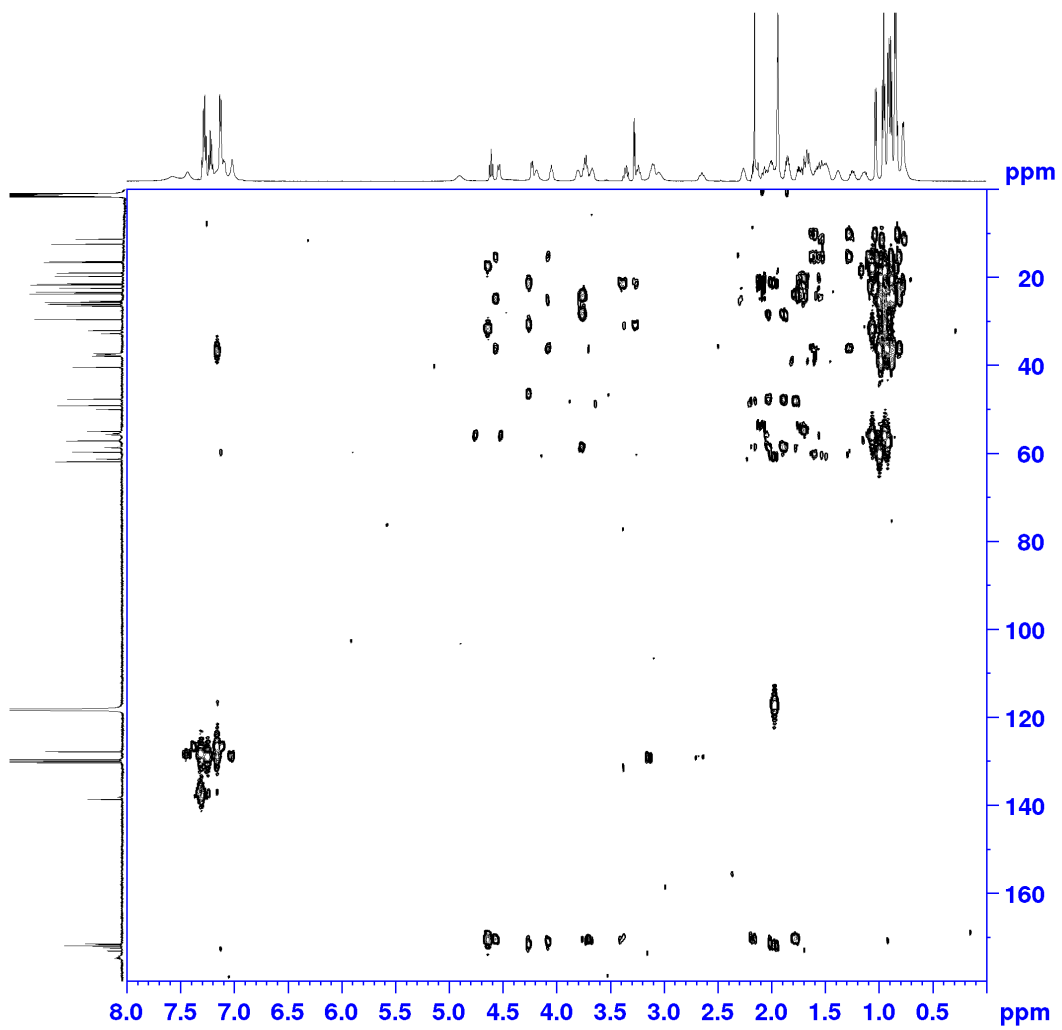


Figure 7: ^1H - ^{13}C HMBC of LOB3.

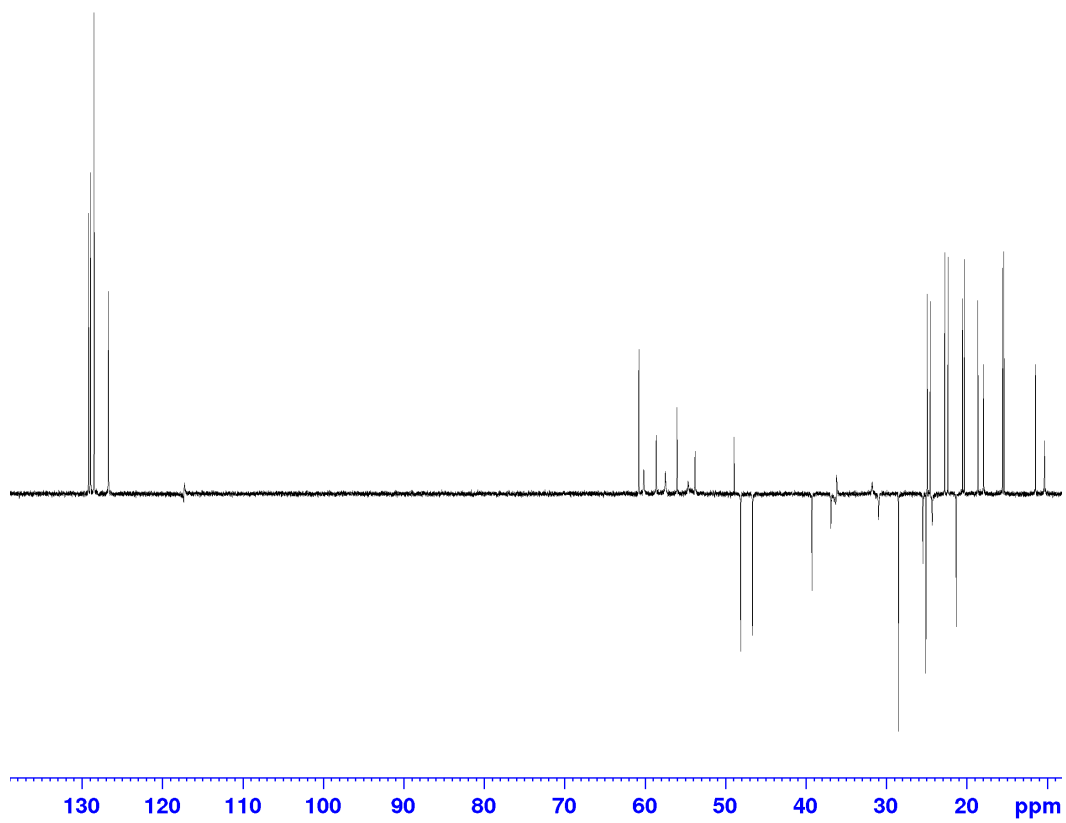


Figure 8: ^{13}C -DEPT of LOB3.

Table 1: ^1H and ^{13}C -NMR assignments for LOB3

Assignment	δ_{H}	δ_{C}		δ_{H}	δ_{C}
Ile¹			δ	3.35 (1H, m)	47.70
α	4.53 (1H, m)	58.66		3.23 (1H, m)	
β	2.26 (1H, m)	37.32	C=O		173.11
γ	1.49 (1H, m)	26.18			
	1.13 (1H, m)		Phe⁶		
γ_{Me}	0.89 (3H, d, 6.6)	16.63	α	4.90 (1H, m)	55.43
δ_{Me}	0.82 (3H, d, 6.6)	12.45	β	3.05 (1H, m)	37.91
NH	7.16 (1H, br.s)			2.64 (1H, m)	
C=O		172.41	γ		138.16
			δ	7.12 (2H, m)	130.02
Leu²			ϵ	7.21 (1H, m)	129.62
α	3.66 (1H, m)	55.02	ζ	7.27 (2H, m)	127.81
β	2.06 (1H, m)	37.61	NH	7.43 (1H, br.s)	
	1.69 (1H, m)		C=O		171.93
γ	1.37 (1H, m)	25.65			
δ_{Me}	0.84 (3H, d, 6.6)	23.73	Phe⁷		
	0.77 (3H, d, 6.6)	21.69	α	4.53 (1H, m)	58.66
NH	7.30 (1H, br.s)		β	3.10 (2H, m)	37.61
C=O		171.64	γ		138.67
			δ	7.12 (2H, m)	130.29
Val³			ϵ	7.21 (1H, m)	129.62
α	4.60 (1H, t, 9.6)	57.14	ζ	7.27 (2H, m)	127.84
β	2.00 (1H, m)	32.79	NH	7.58 (1H, br.s)	
δ_{Me}	1.03 (3H, d, 6.6)	19.72	C=O		174.87
δ_{Me}	0.91 (3H, d, 6.6)	18.97			
NH	7.02 (1H, br.s)		Ile⁸		
C=O		172.41	α	3.80 (1H, m)	55.74
			β	1.67 (2H, m)	40.49
Pro⁴			γ	1.54 (1H, m)	26.06
α	4.18 (1H, m)	59.72	δ_{Me}	0.94 (3H, d, 6.6)	23.36
β	2.15 (1H, m)	29.57		0.84 (3H, d, 6.6)	21.46
	1.98 (1H, m)		NH	7.02 (1H, br.s)	
γ	1.85 (1H, m)	25.39	C=O		174.54
	1.74 (1H, m)				
δ	3.73 (2H, m)	49.17	Ile⁹		
C=O		171.49	α	4.04 (1H, m)	61.28
			β	1.84 (1H, m)	37.32
Pro⁵			γ	1.56 (1H, m)	26.51
α	4.23 (1H, m)	61.88		1.24 (1H, m)	
β	1.94 (1H, m)	32.07	γ_{Me}	0.96 (3H, d, 6.6)	16.42
	1.67 (1H, m)		δ_{Me}	0.88 (3H, d, 6.6)	11.34
γ	1.49 (1H, m)	22.41	NH	7.09 (1H, d, 7.2)	
	0.77 (1H, m)		C=O		174.27