

Supporting Information

Synthesis and Antiangiogenic Activity of N-Alkylated Levamisole Derivatives

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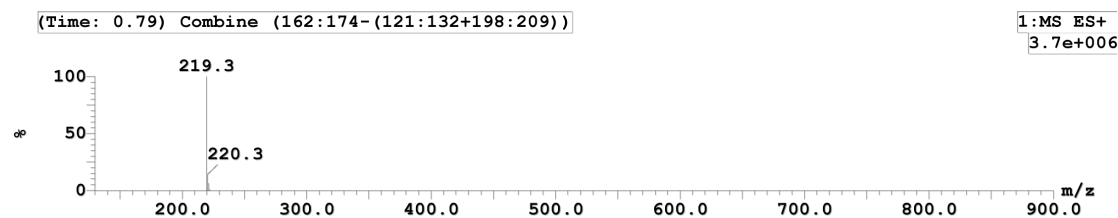
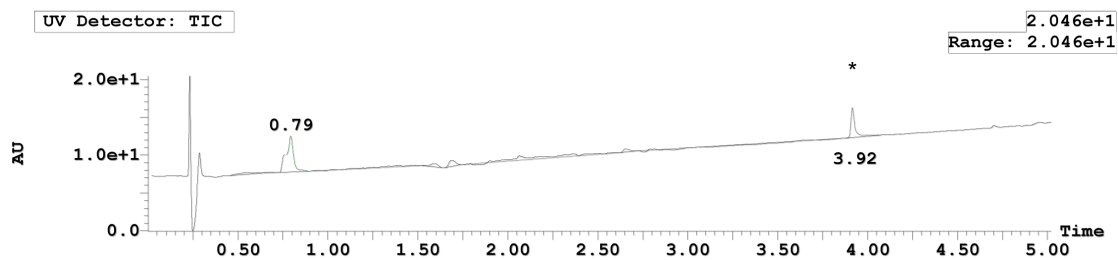
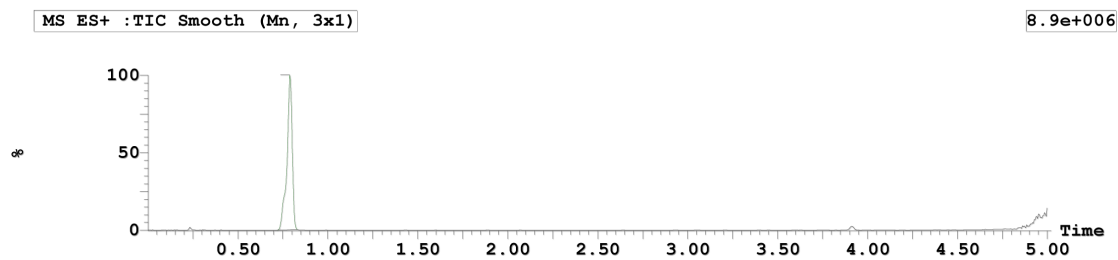
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Compound 7a

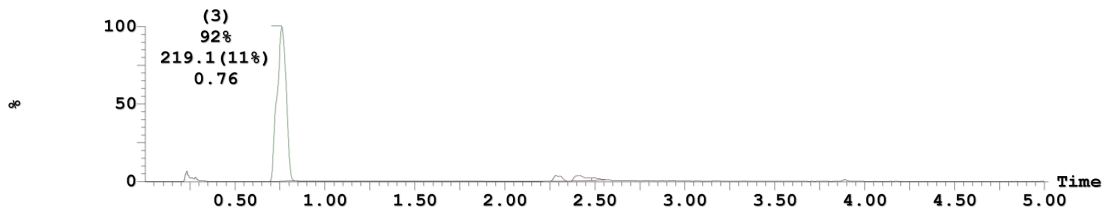


*Ghost peak from the UPLC-MS system.

Compound 7b

MS ES+ :TIC Smooth (Mn, 3x1)

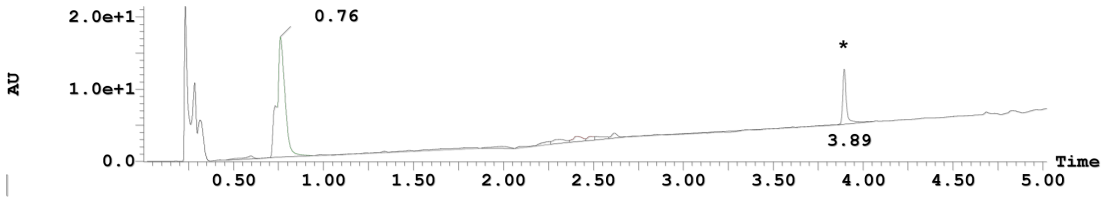
4.1e+007



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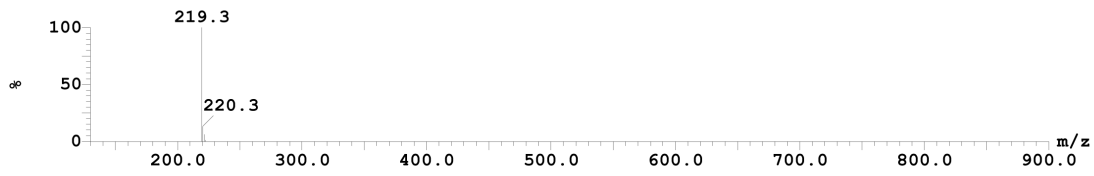
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Range: 2.144e+1



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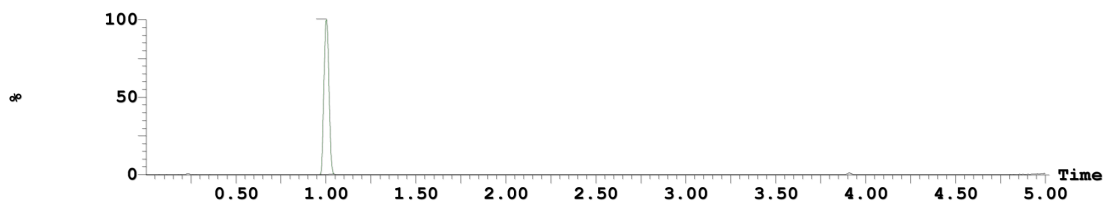
1:MS ES+
2.7e+007



Compound 8a

MS ES+ :TIC Smooth (Mn, 3x1)

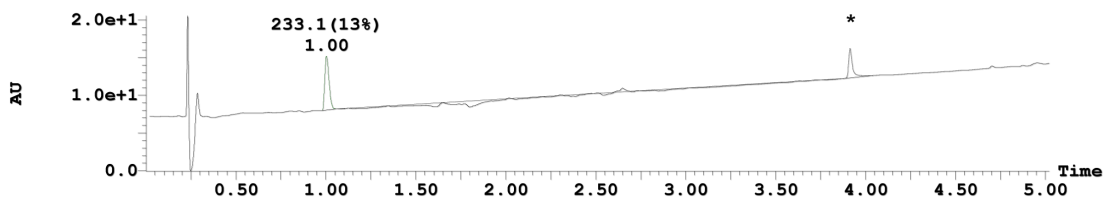
2.7e+007



UV Detector: TIC

2.053e+1

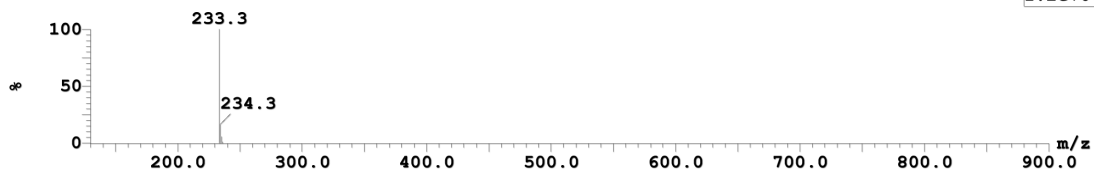
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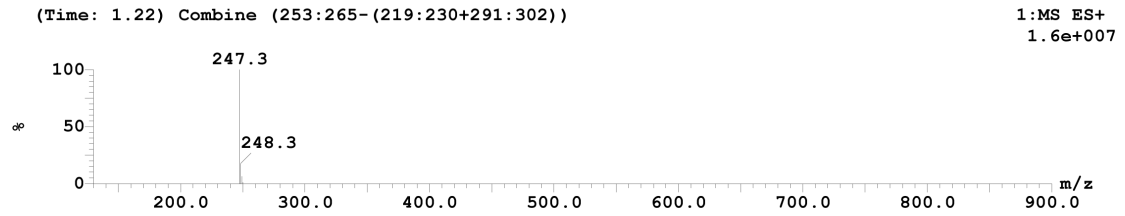
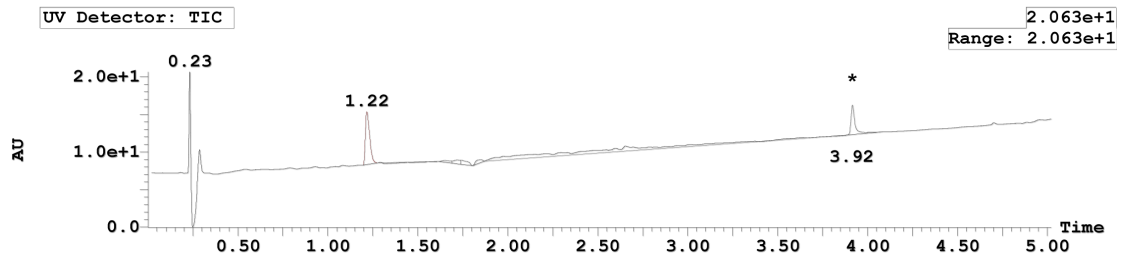
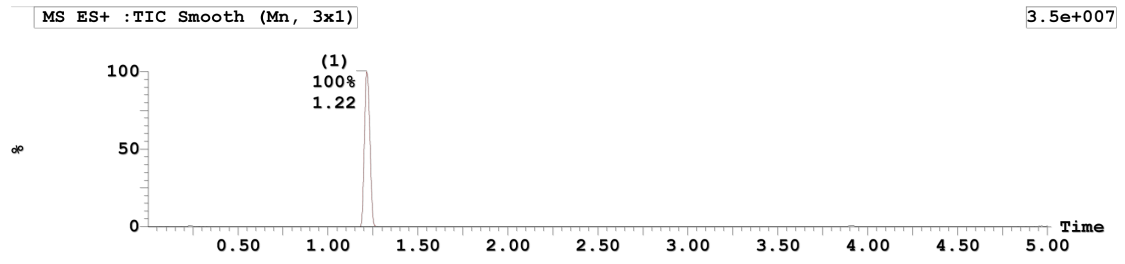
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1:MS ES+

1.2e+007



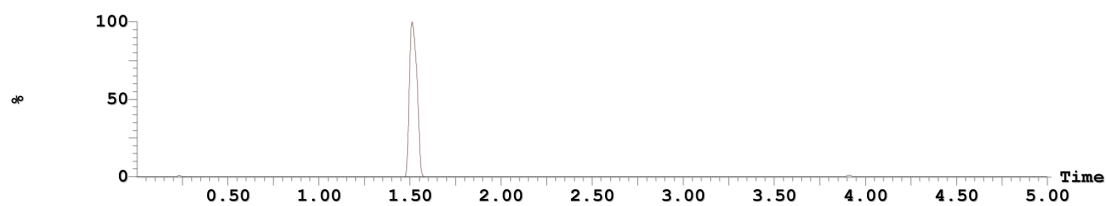
Compound 9



Compound 10

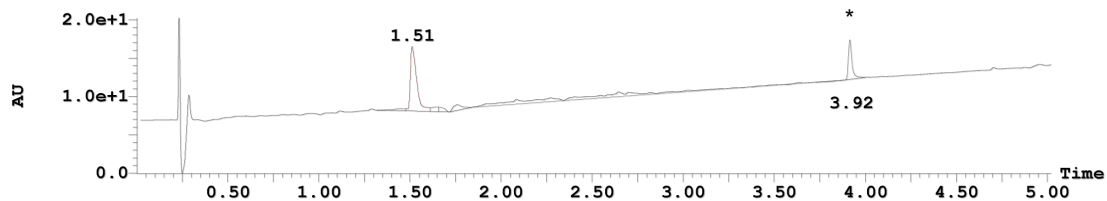
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4.2e+007



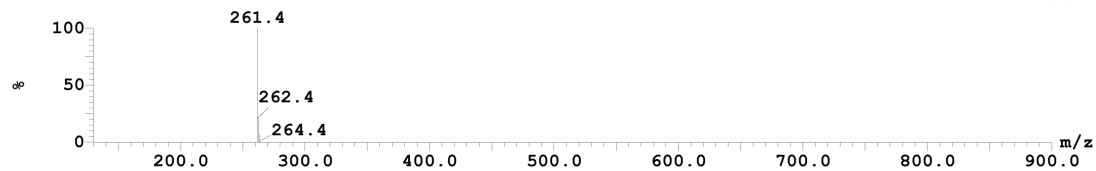
UV Detector: TIC

2.02e+1
Range: 2.019e+1



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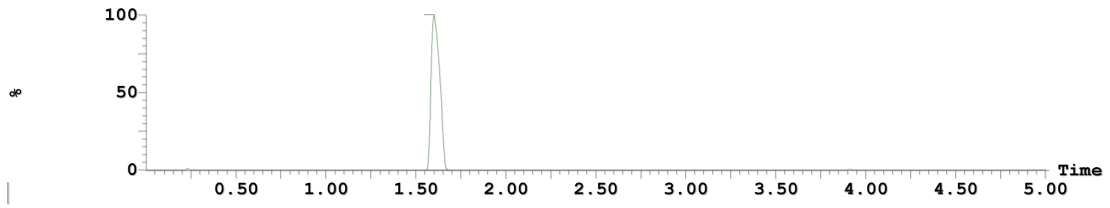
1:MS ES+
2.3e+007



Compound 11a

MS ES+ :TIC Smooth (Mn, 3x1)

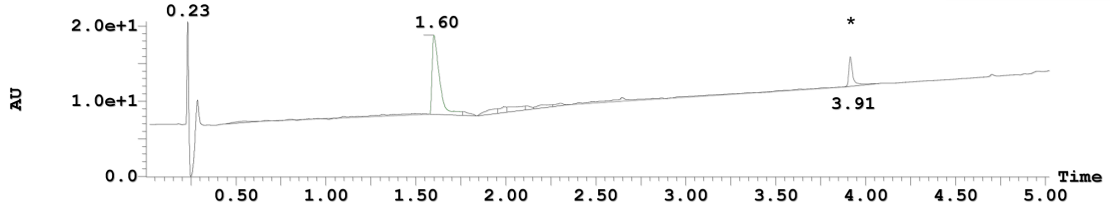
5.6e+007



UV Detector: TIC

2.058e+1

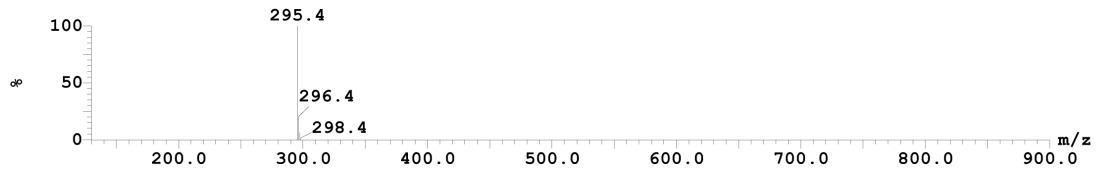
Range: 2.057e+1



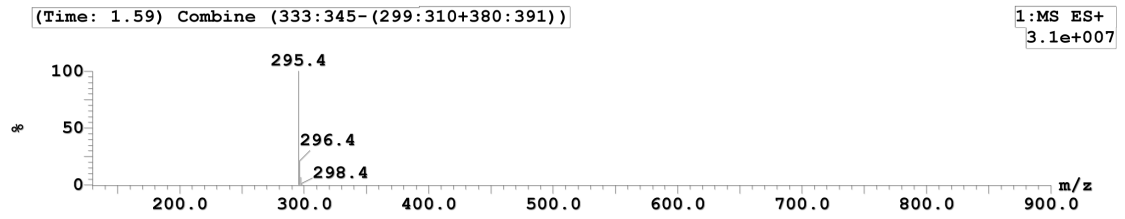
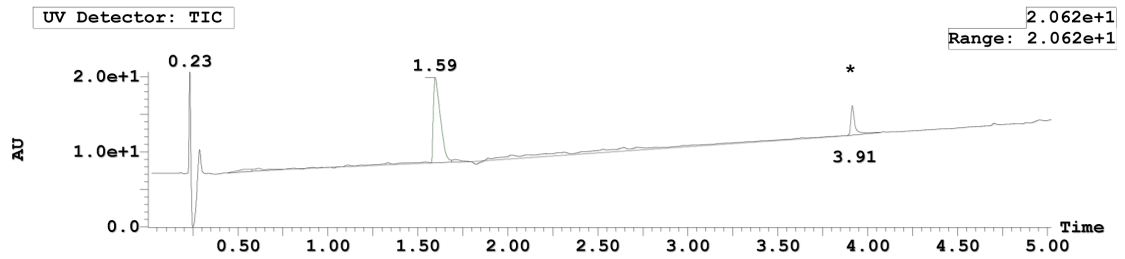
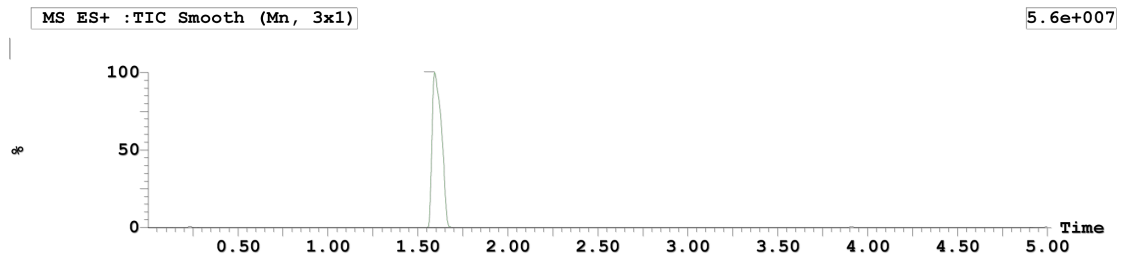
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1:MS ES+

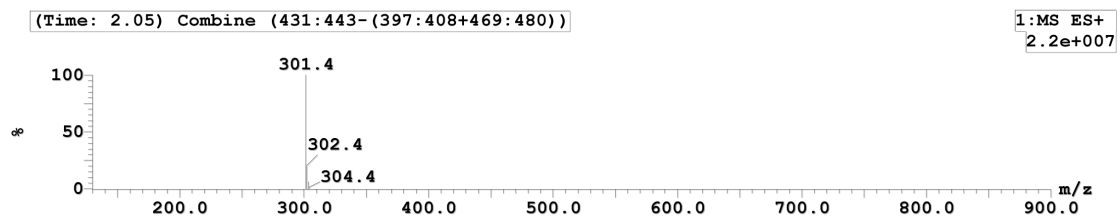
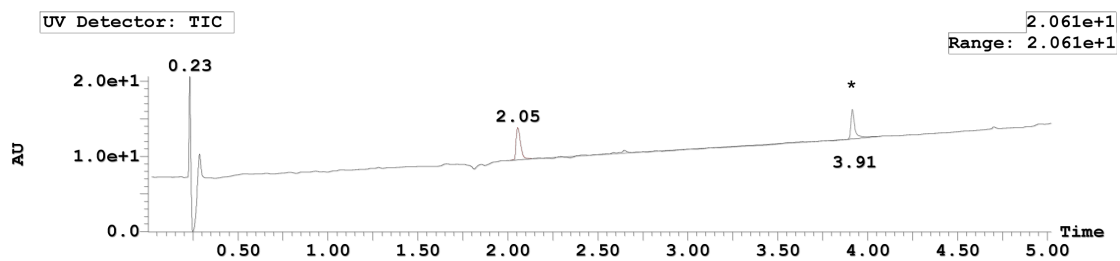
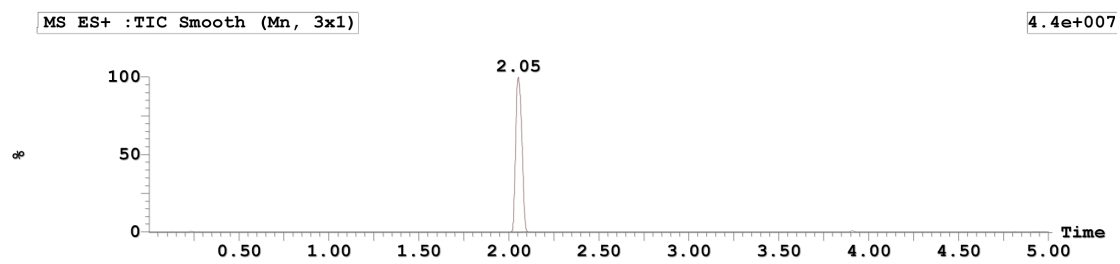
3.3e+007



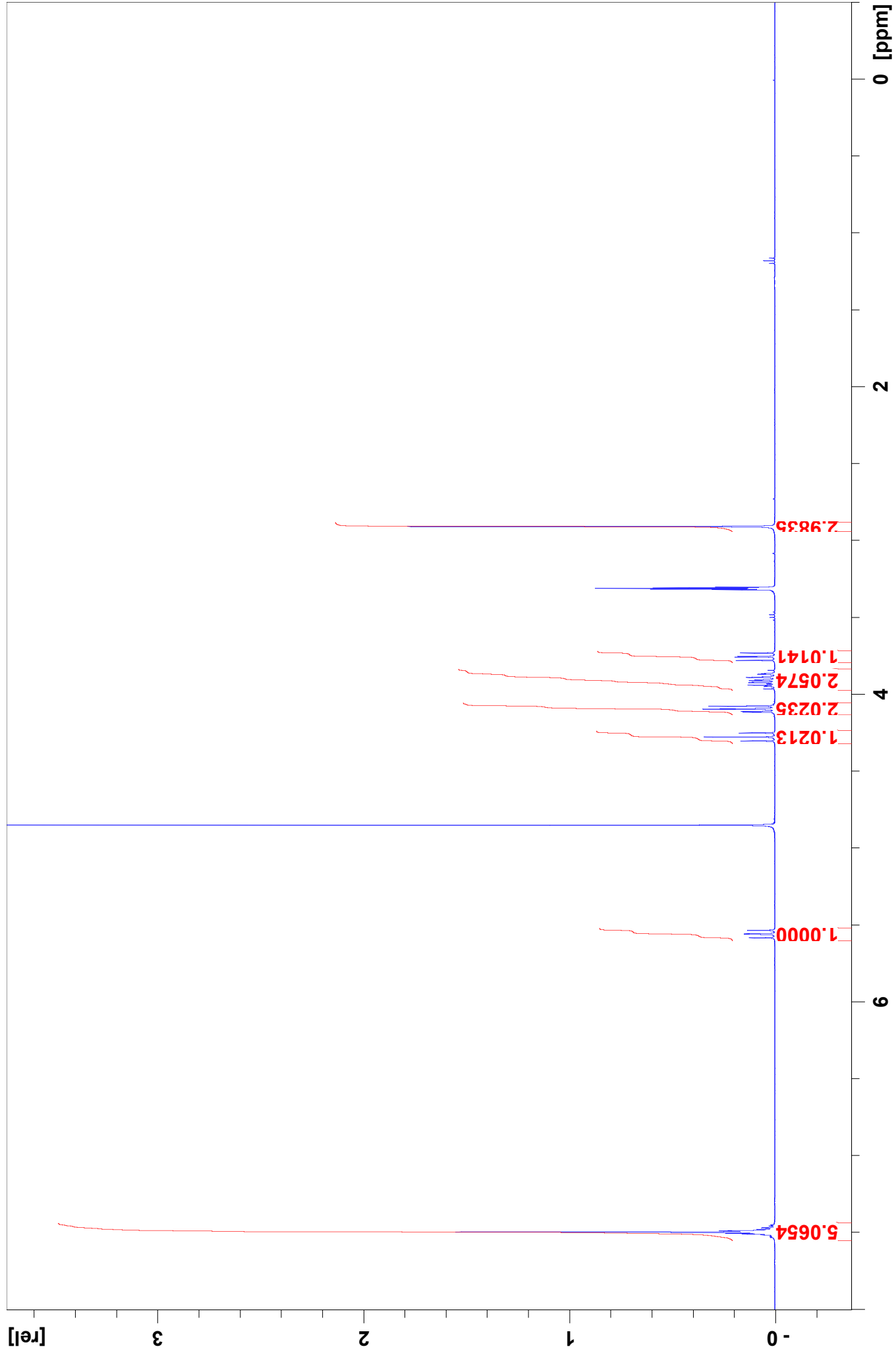
Compound 11b



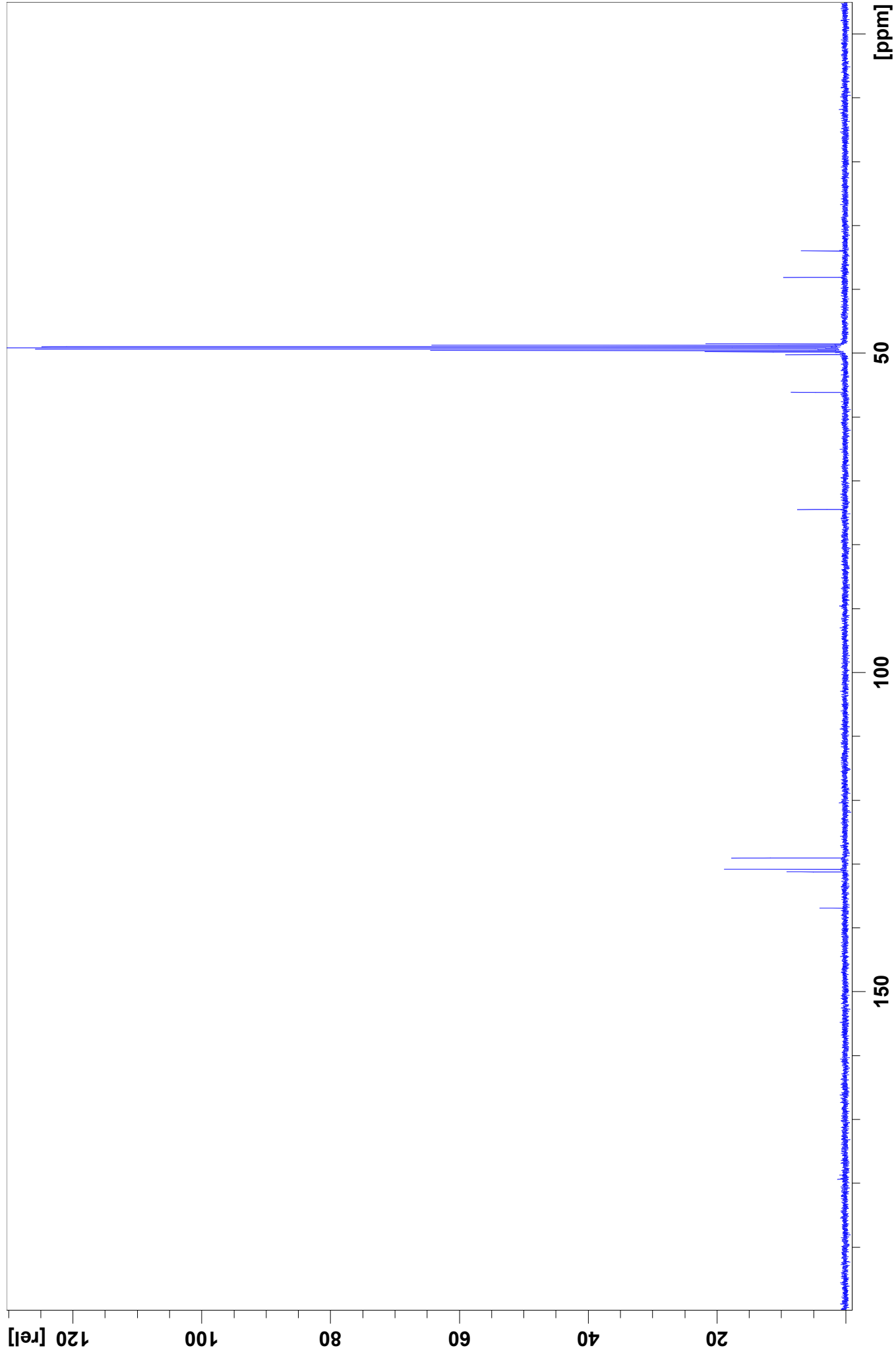
Compound 12



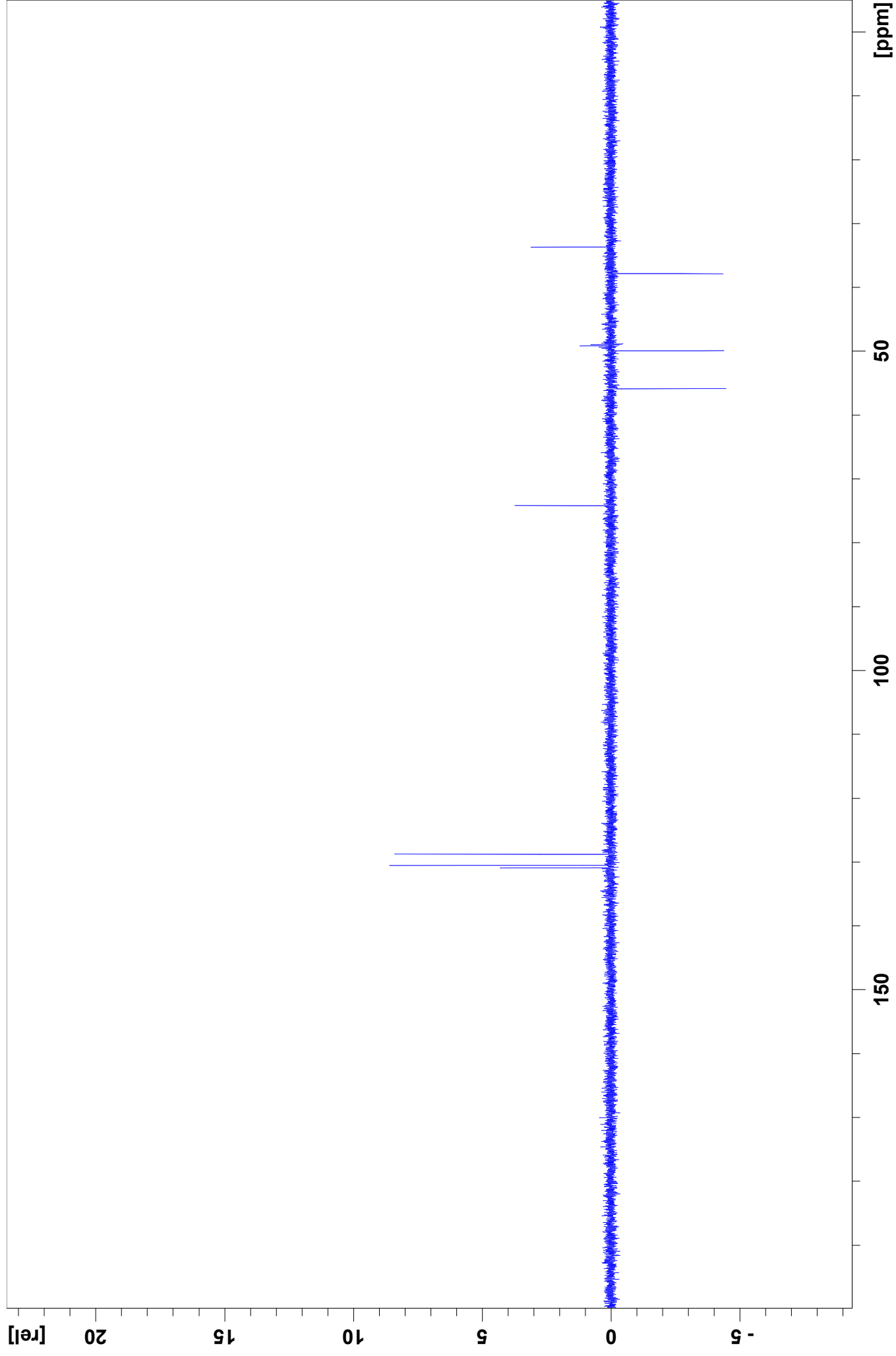
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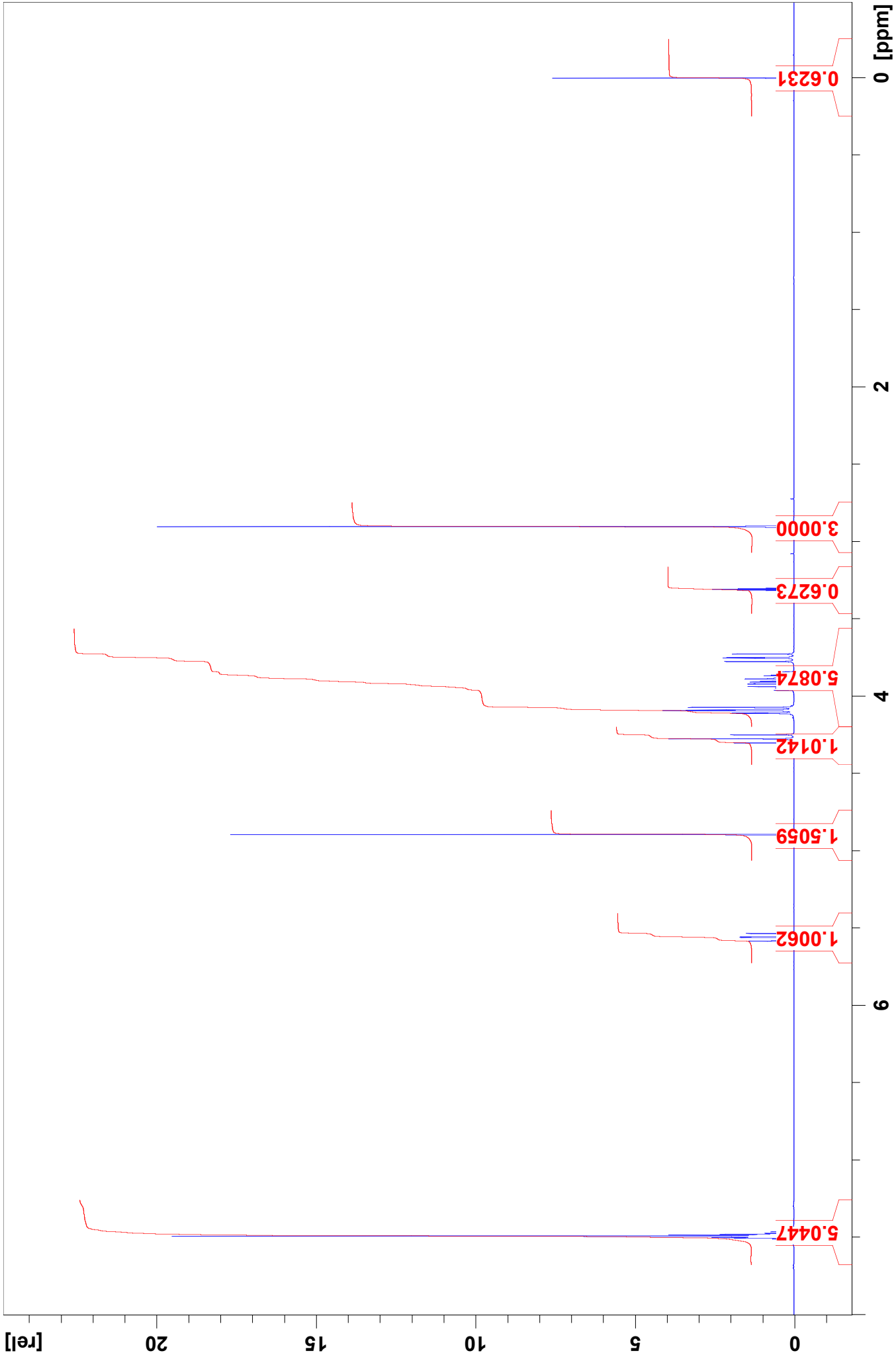
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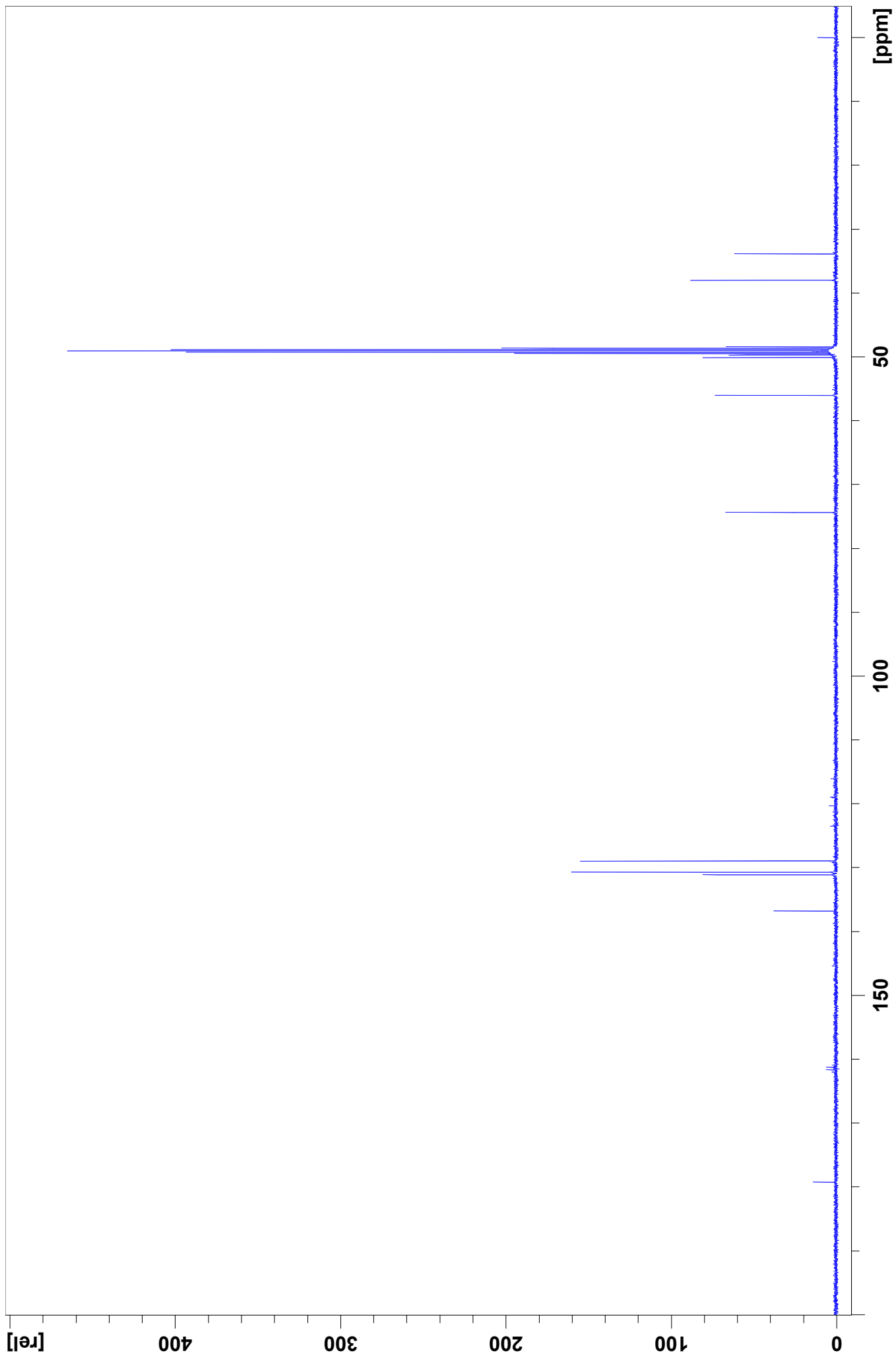
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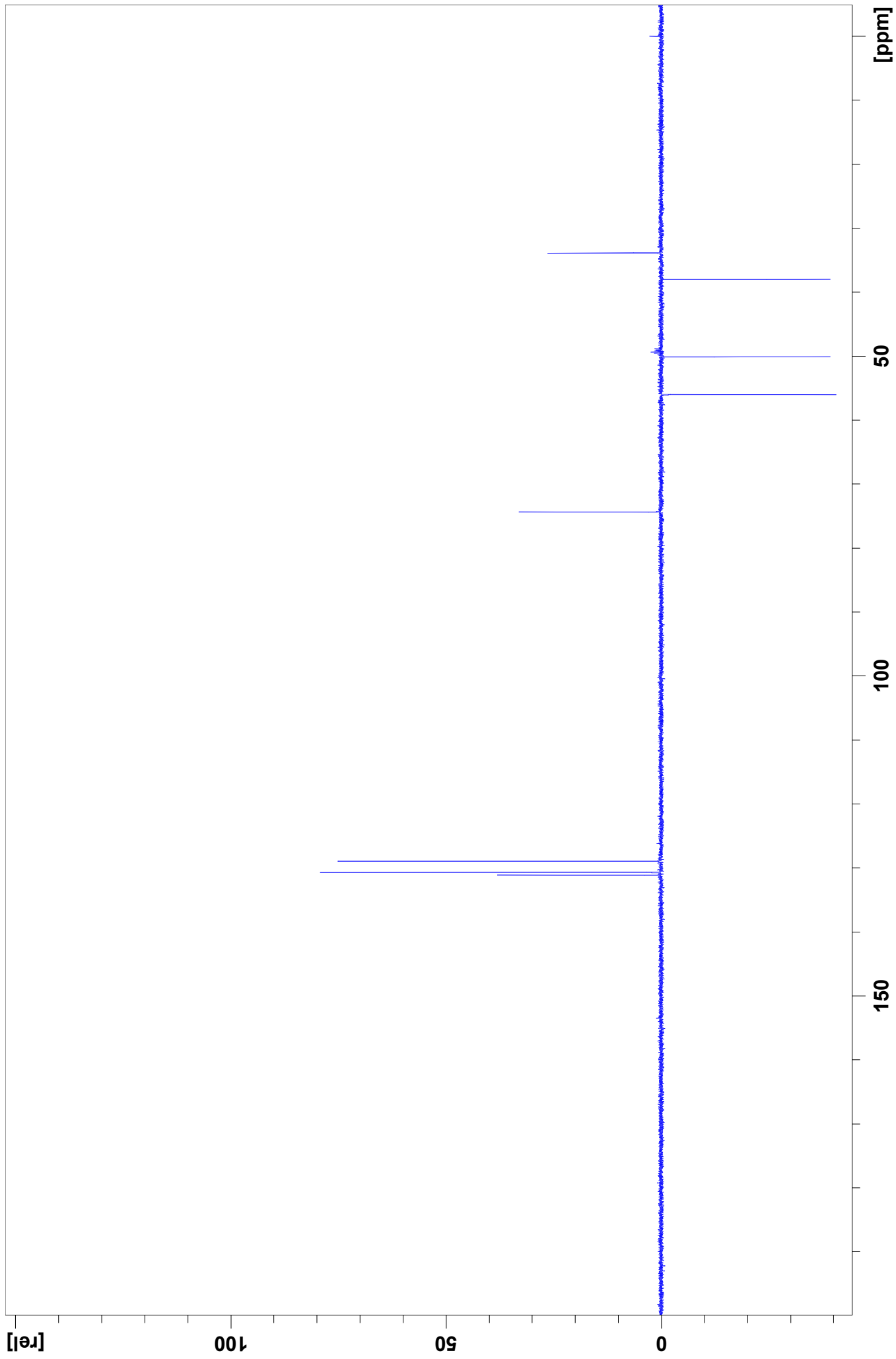
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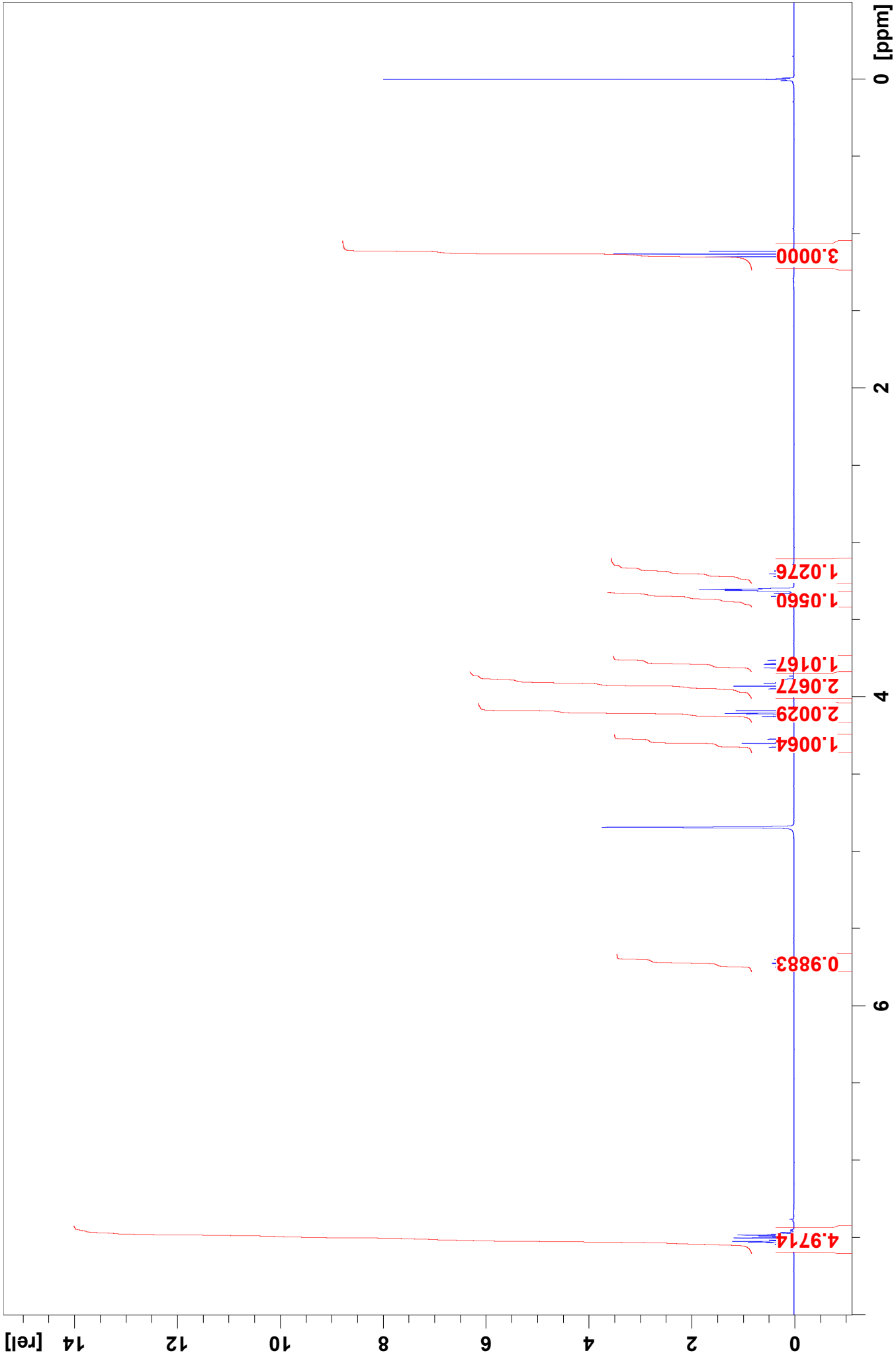
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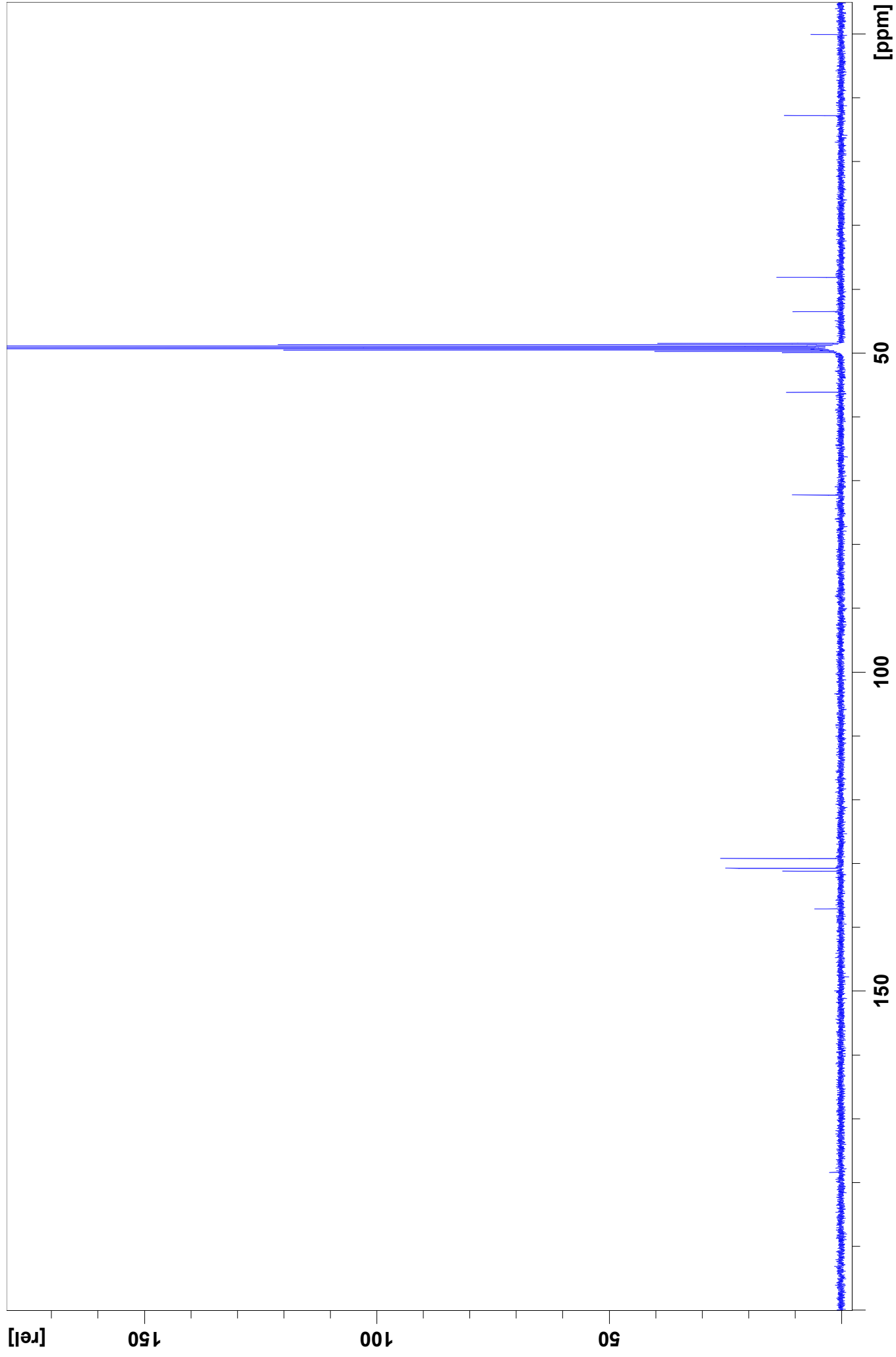
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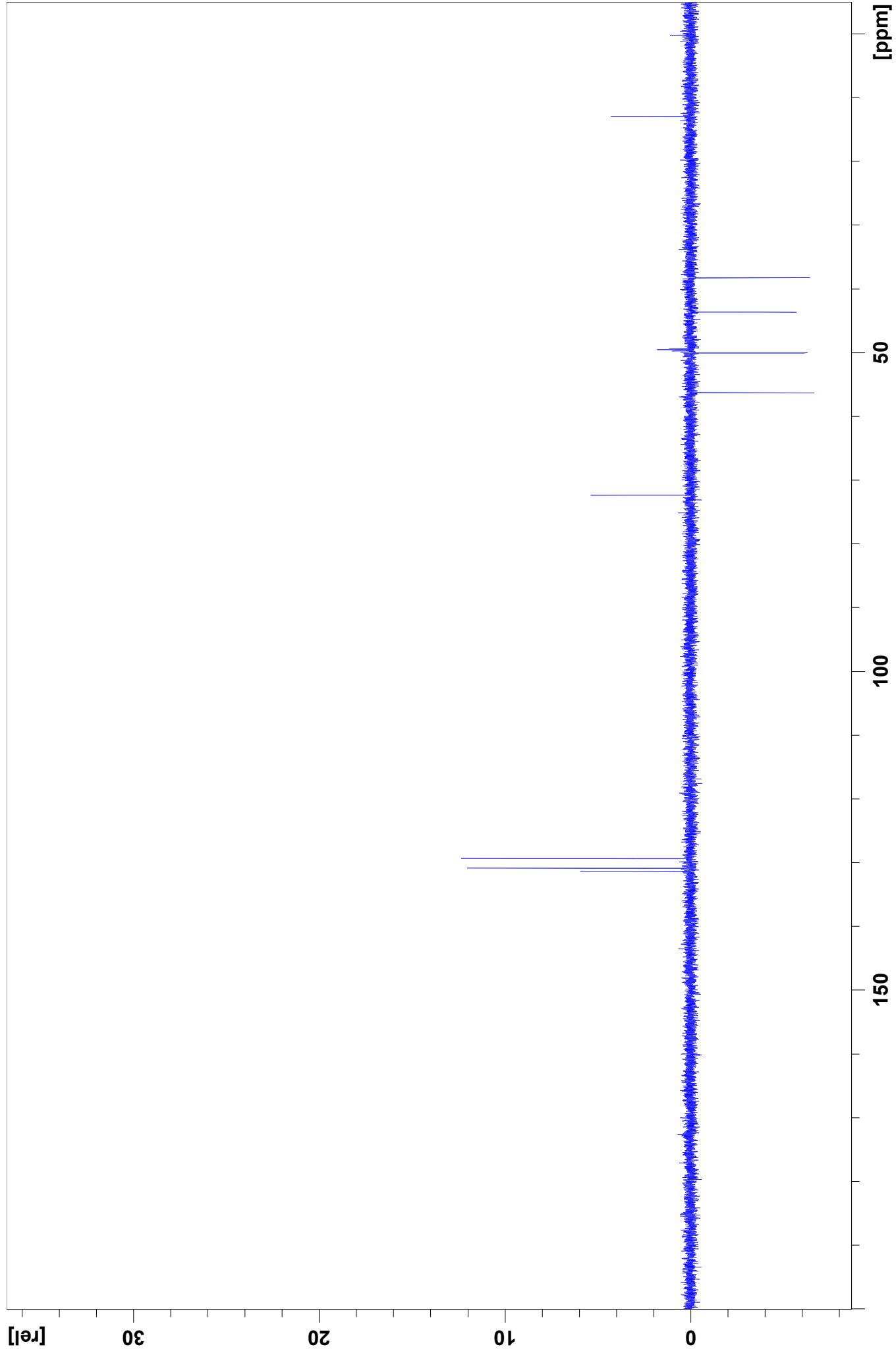
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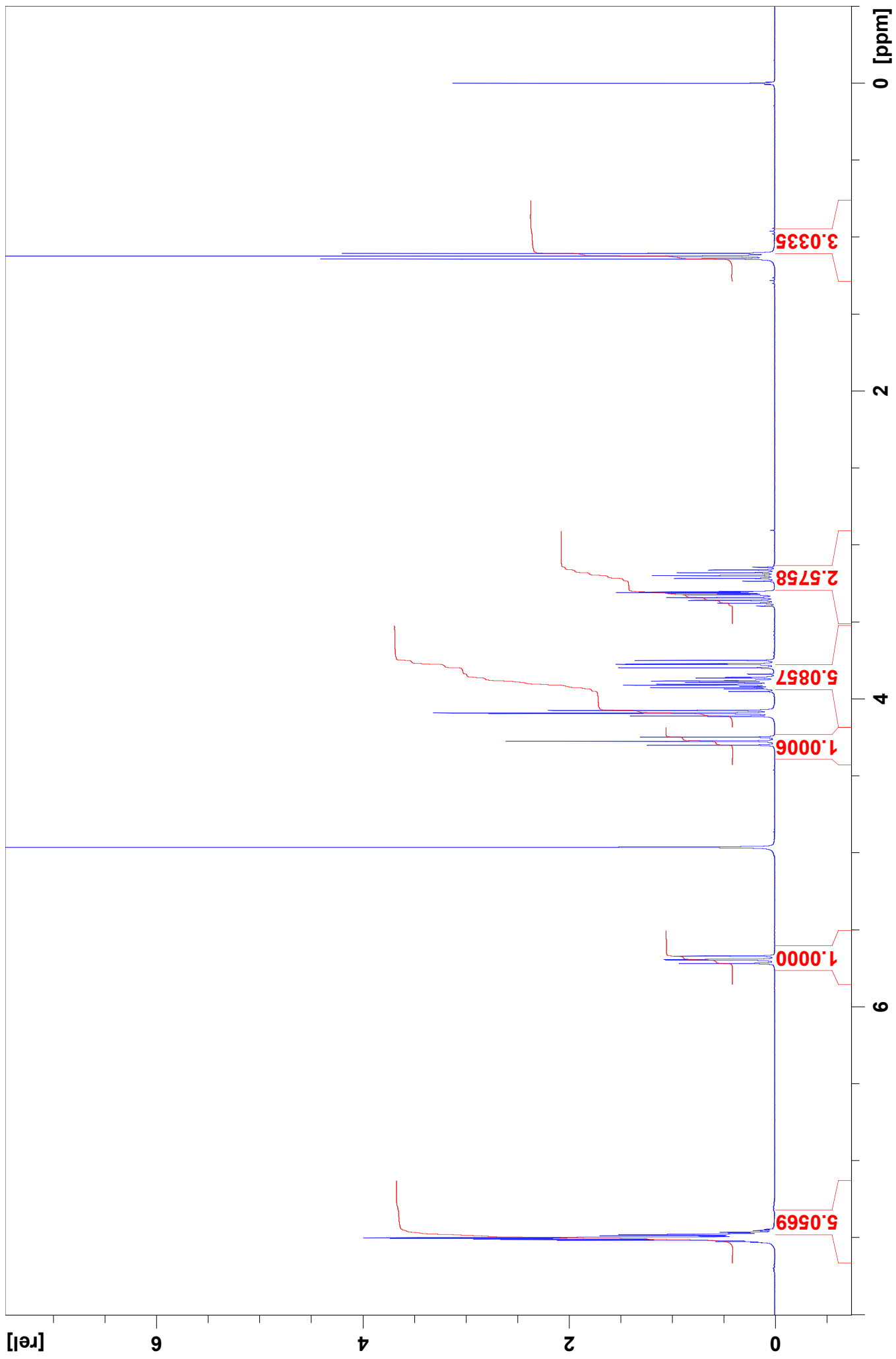
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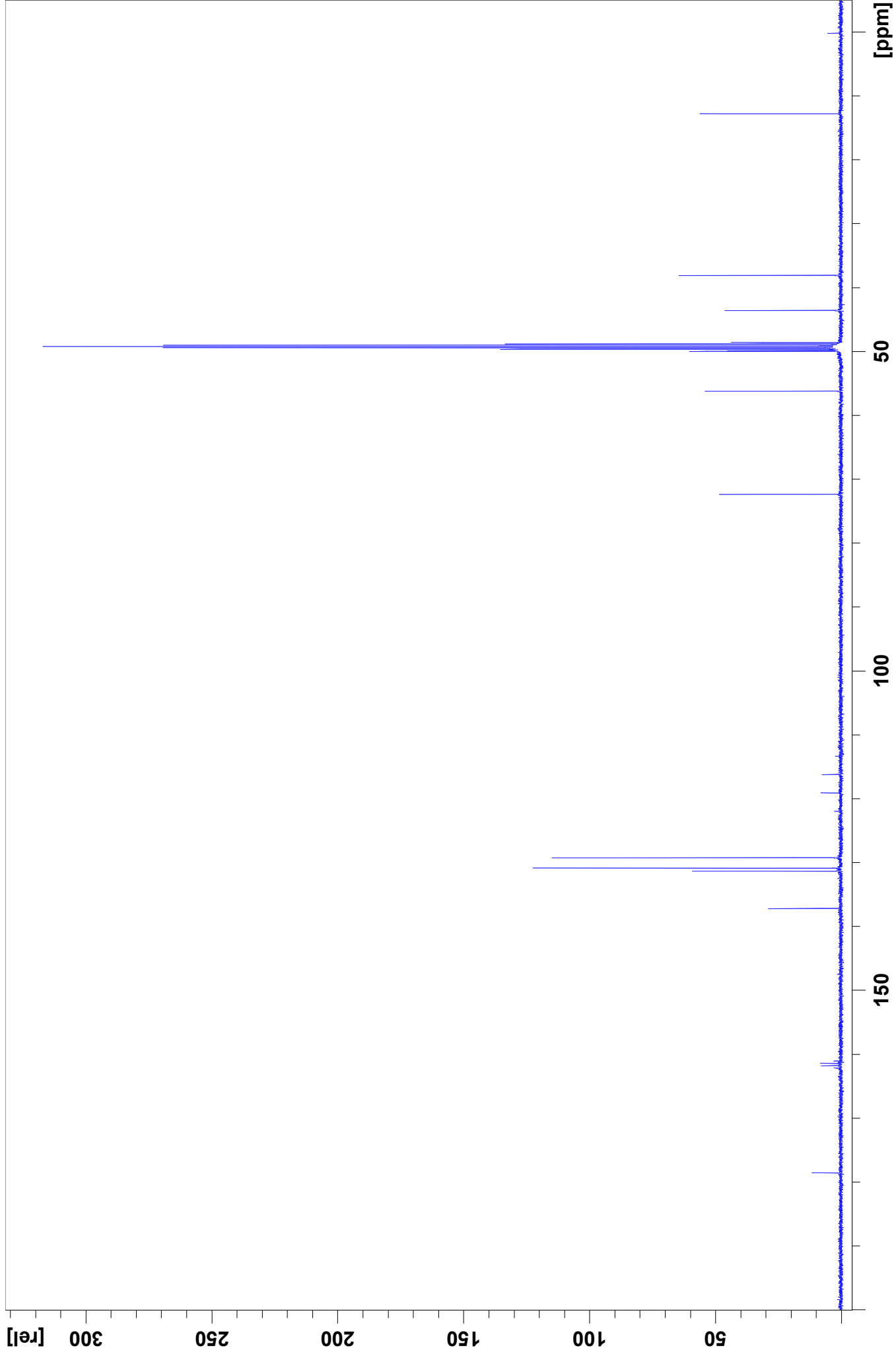
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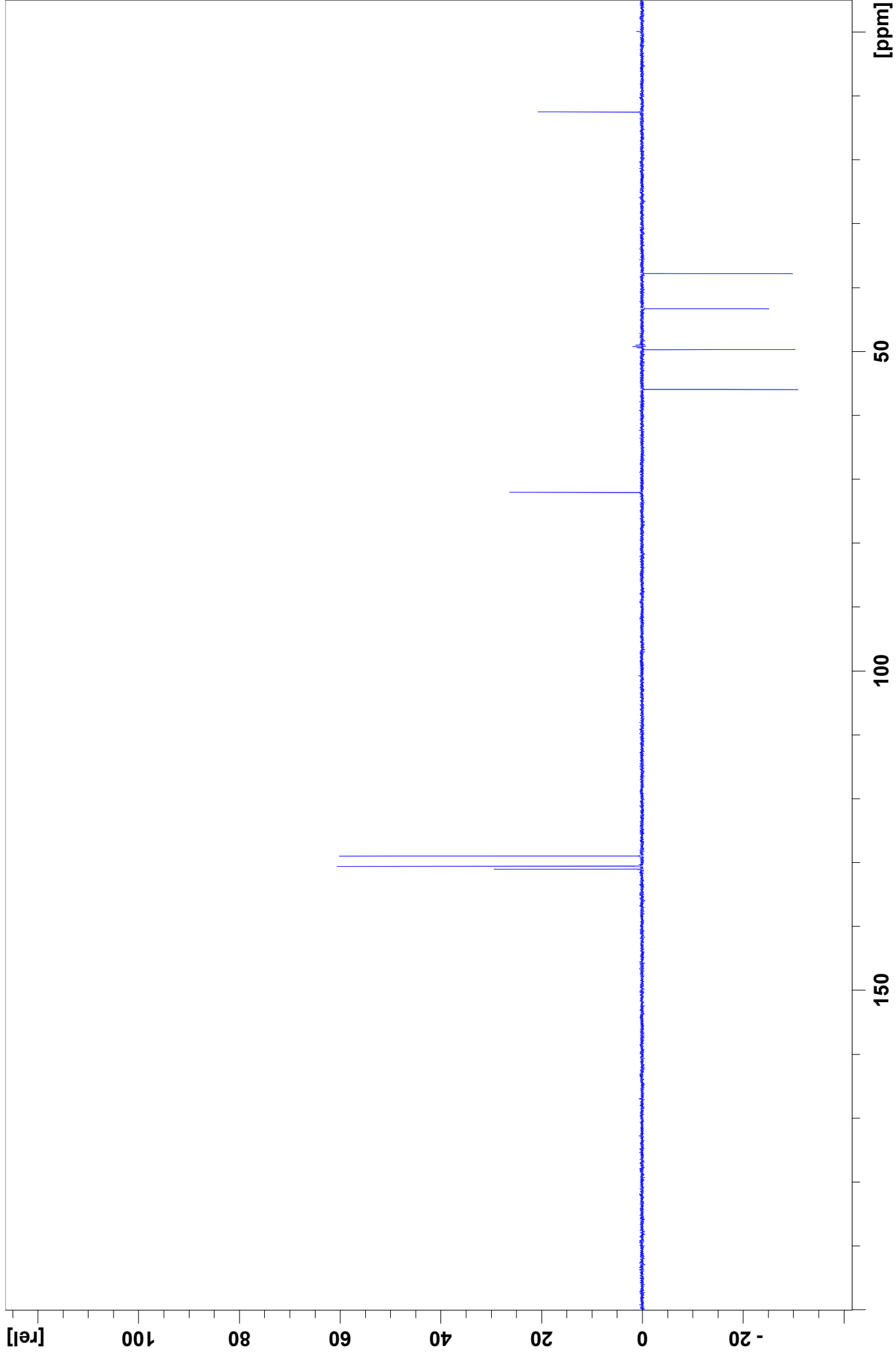
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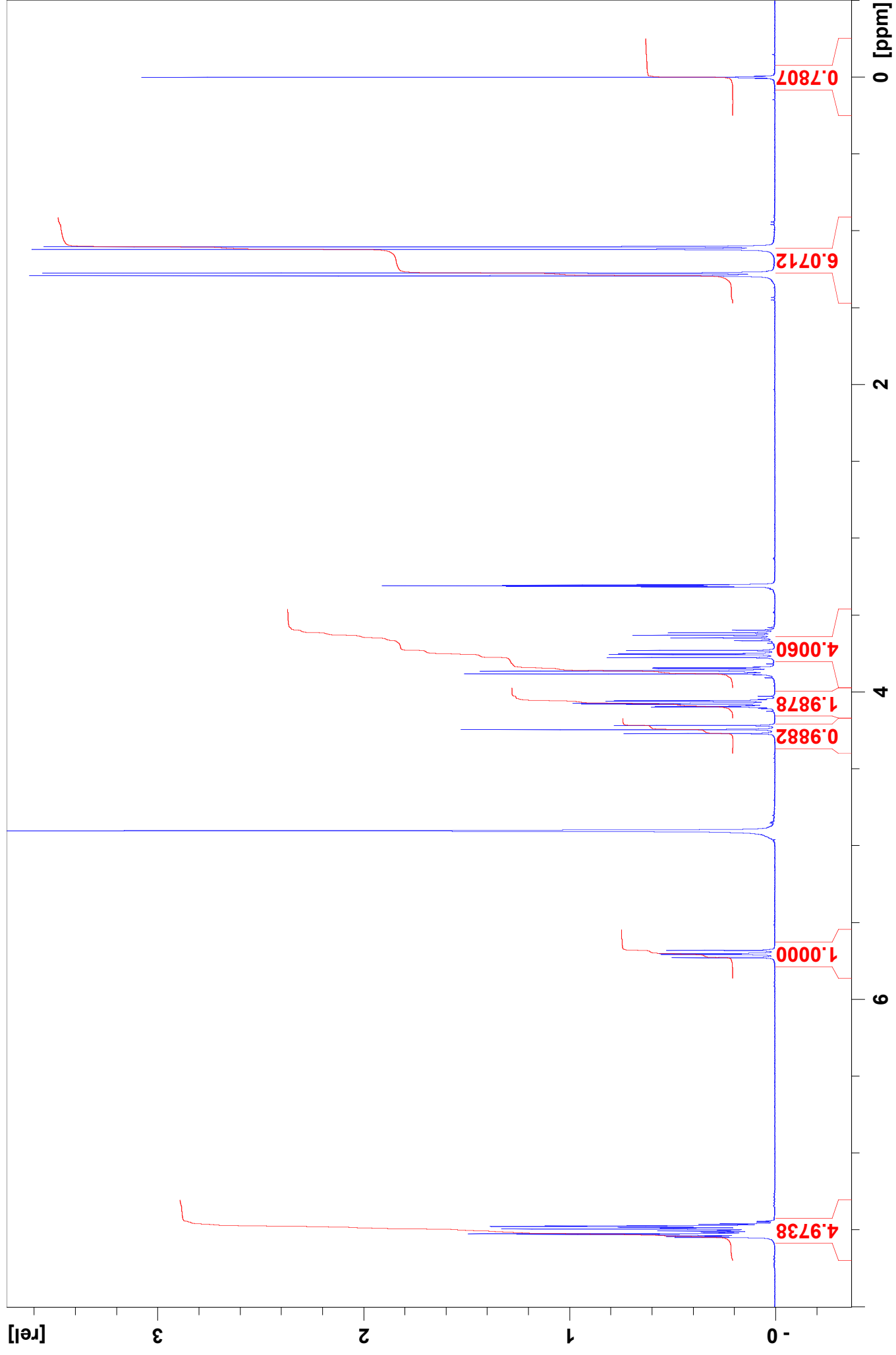
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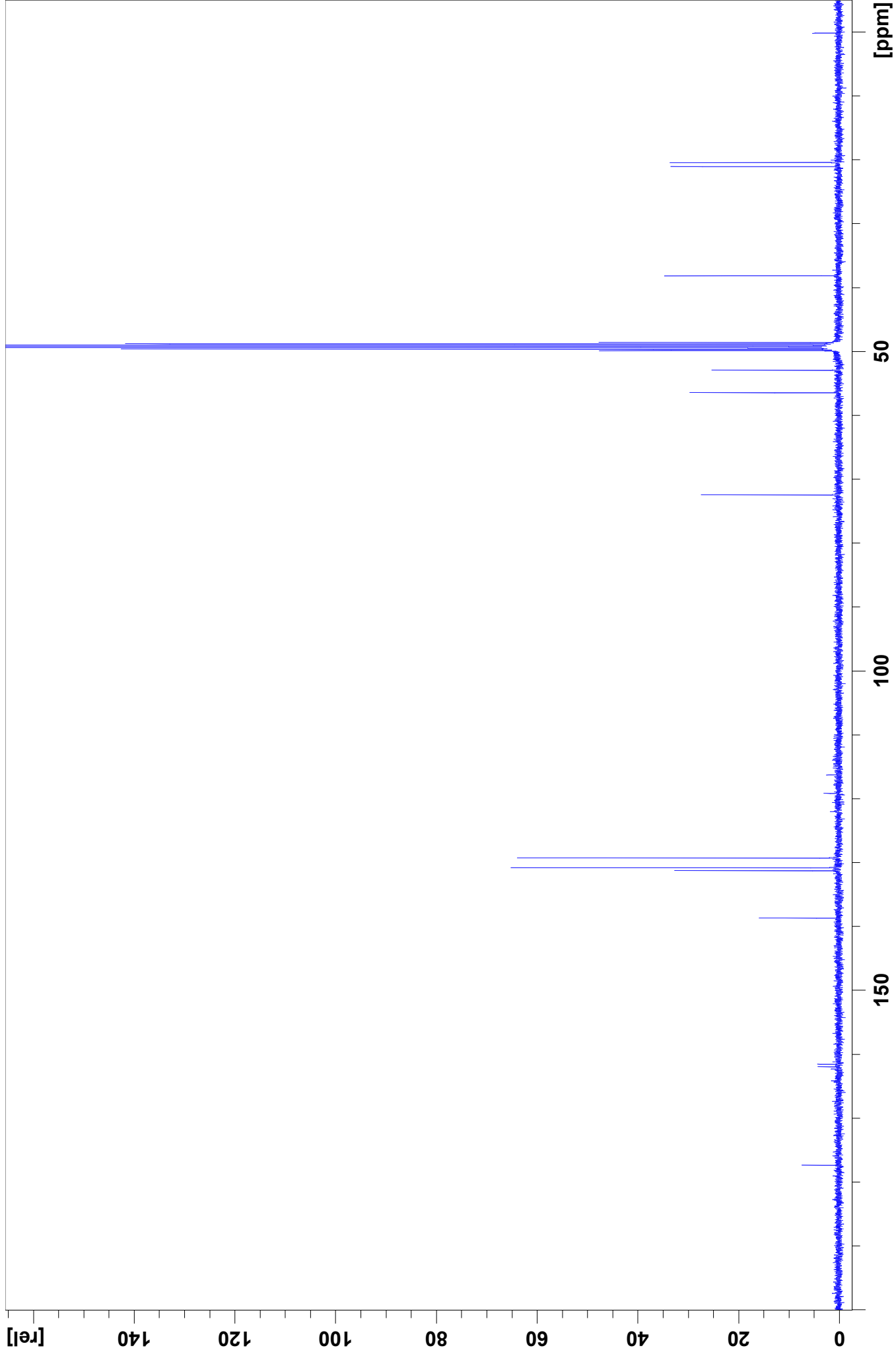
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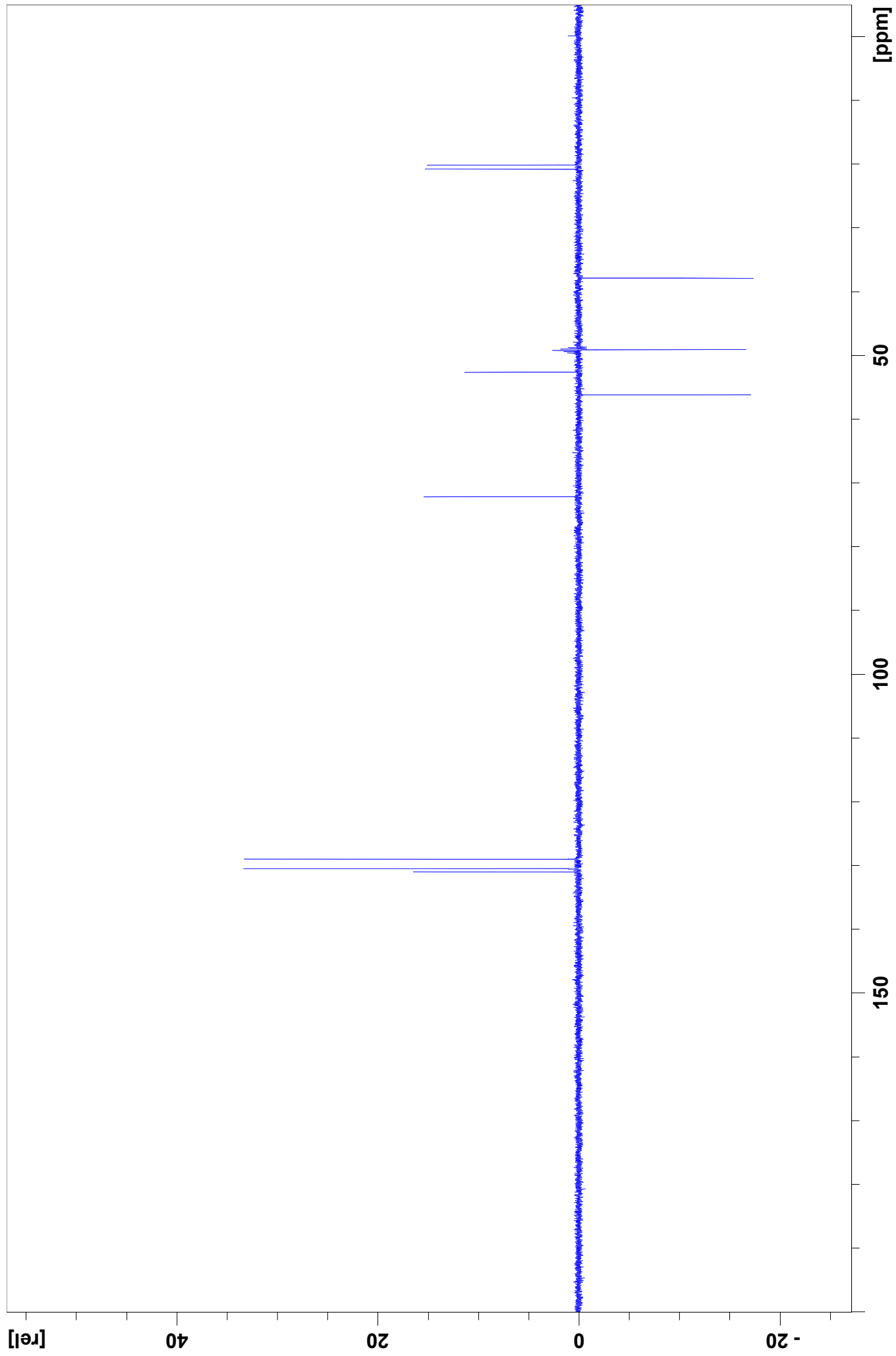
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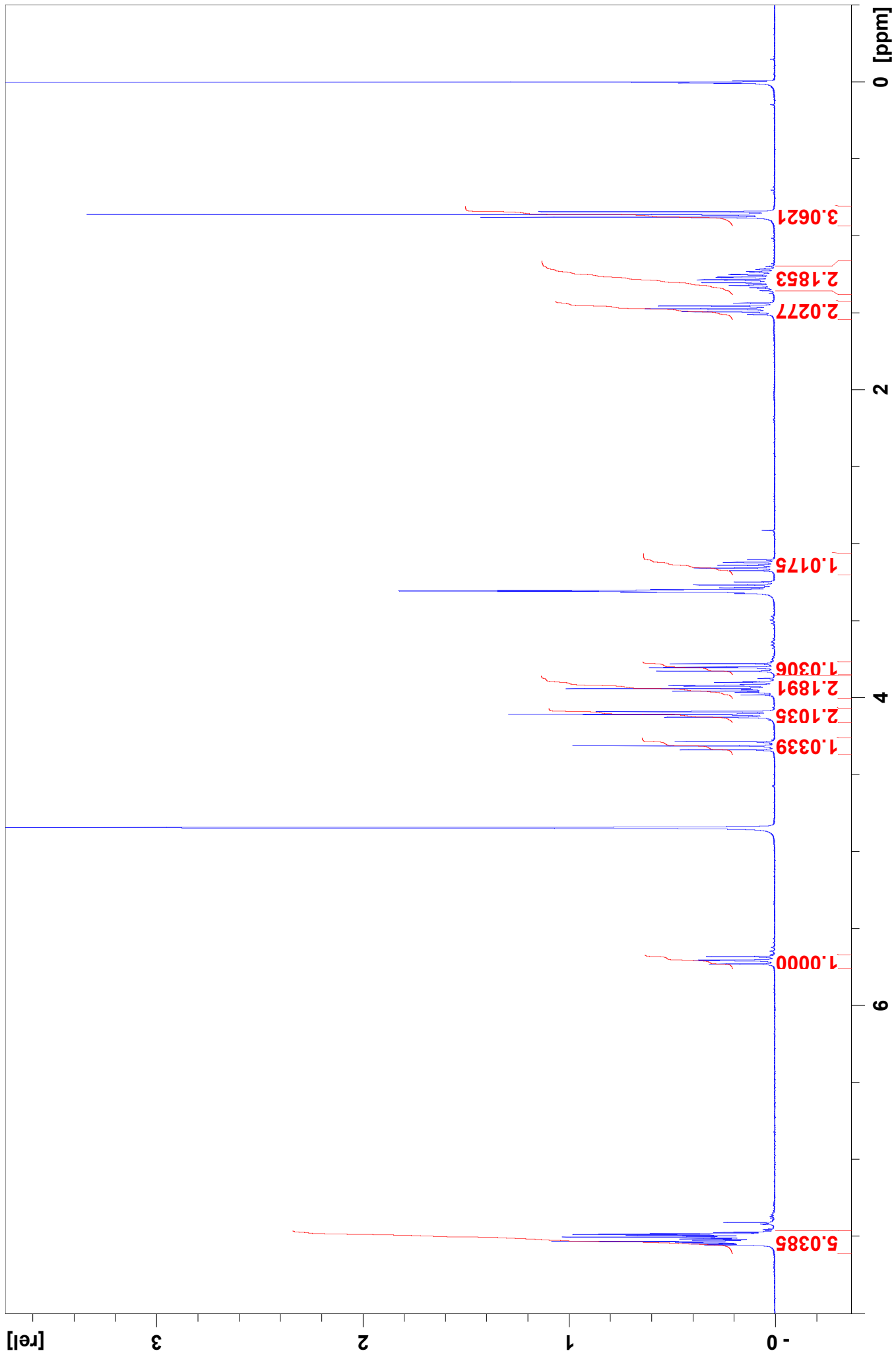
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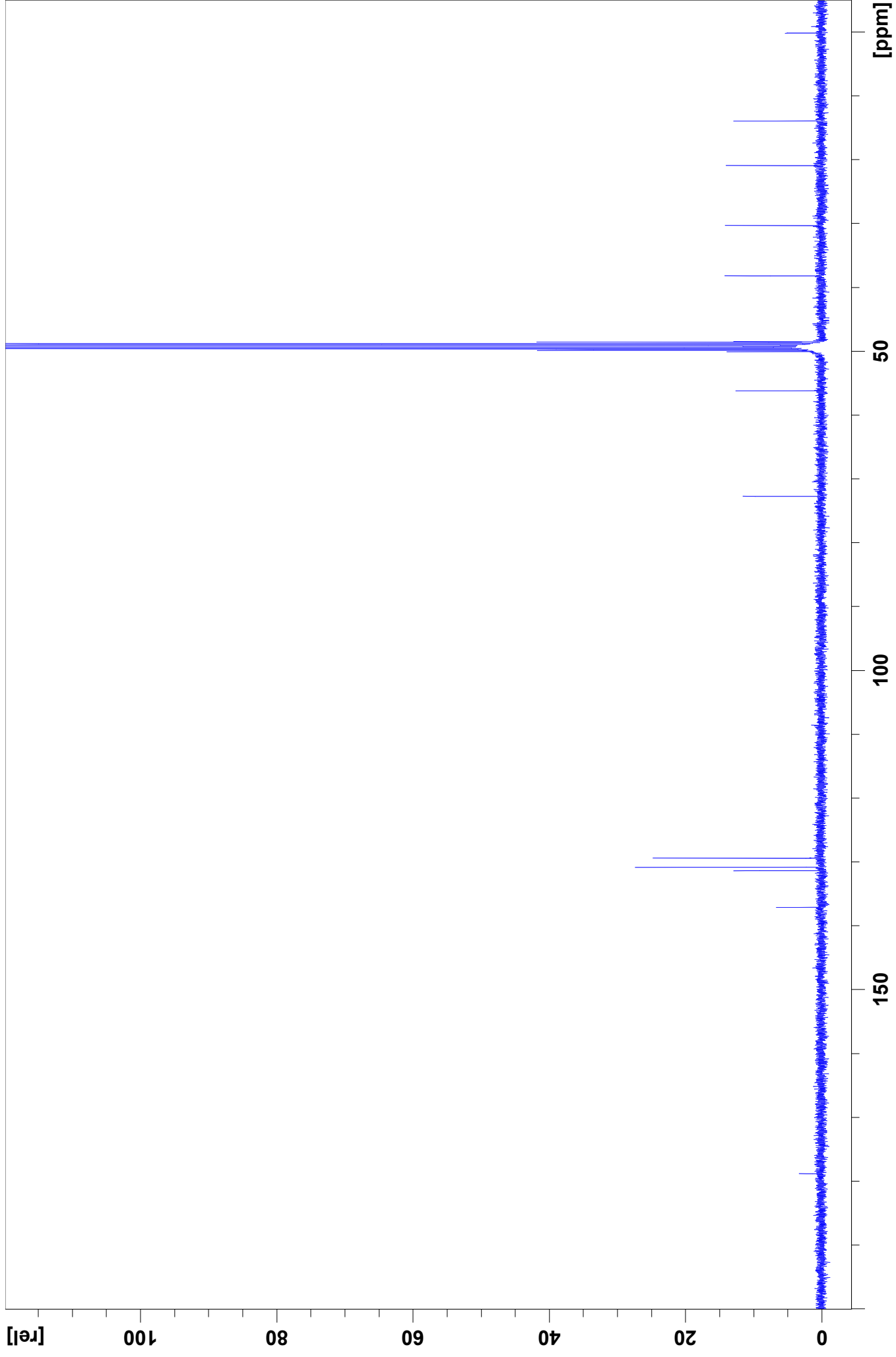
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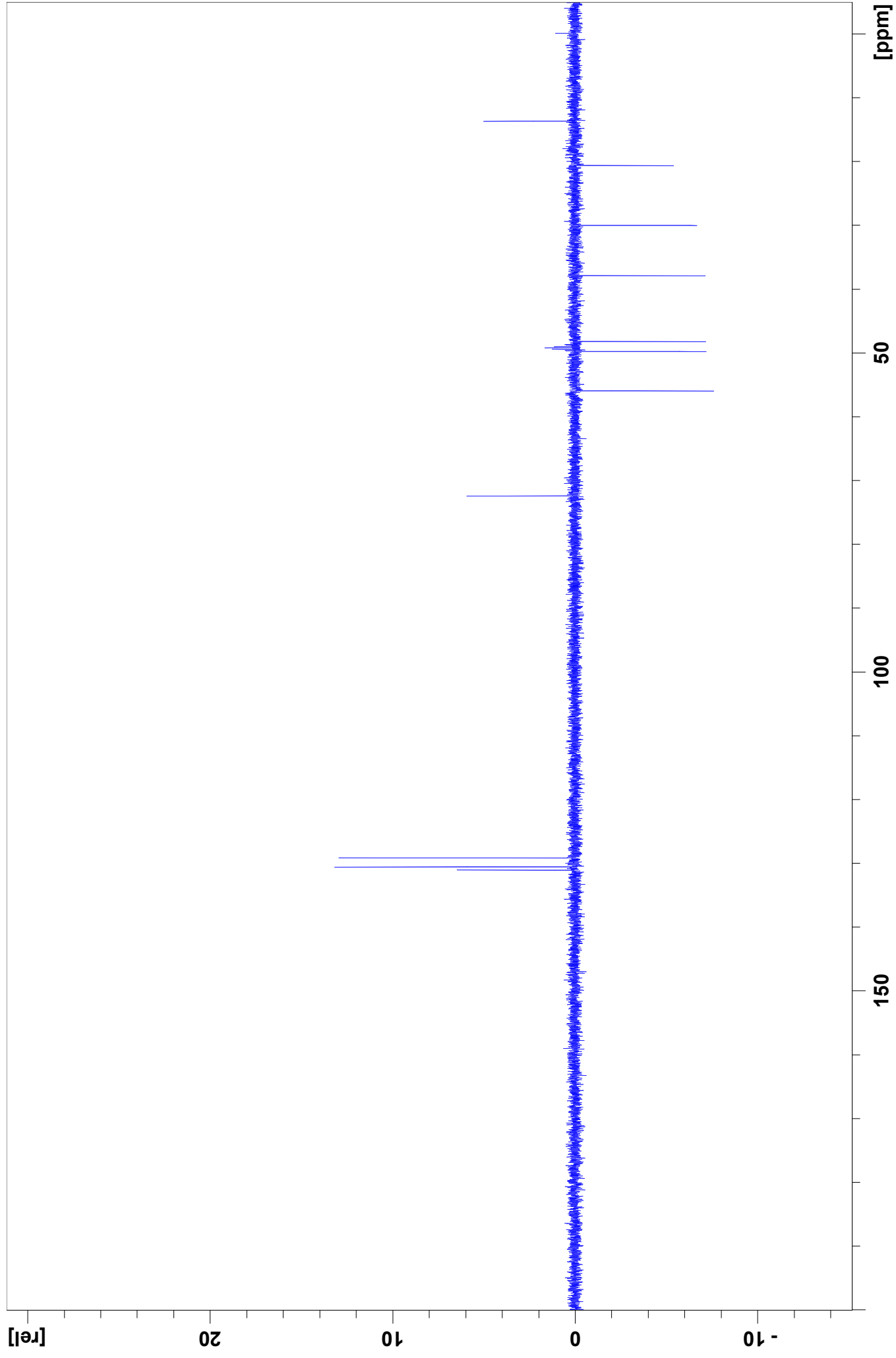
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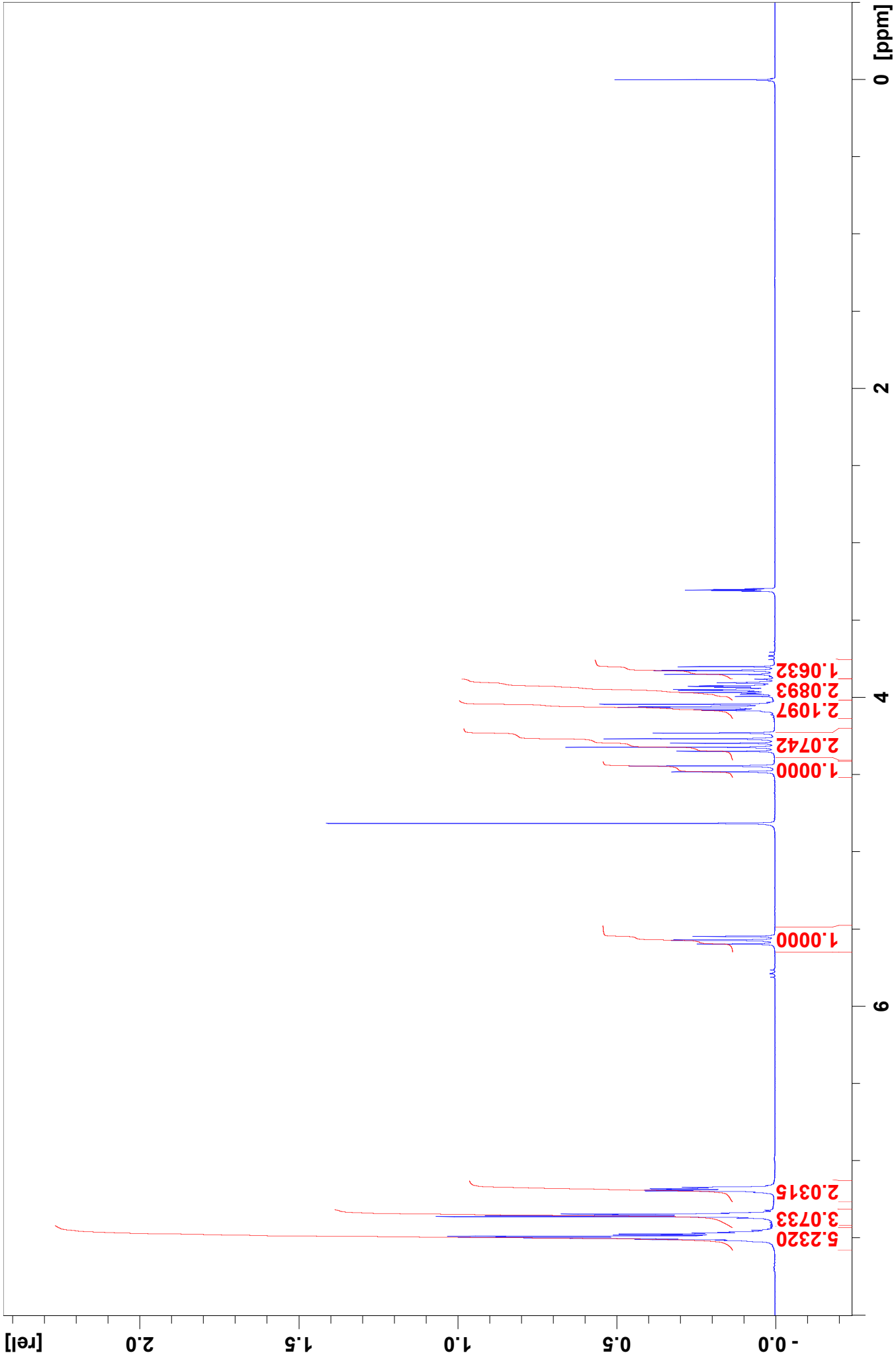
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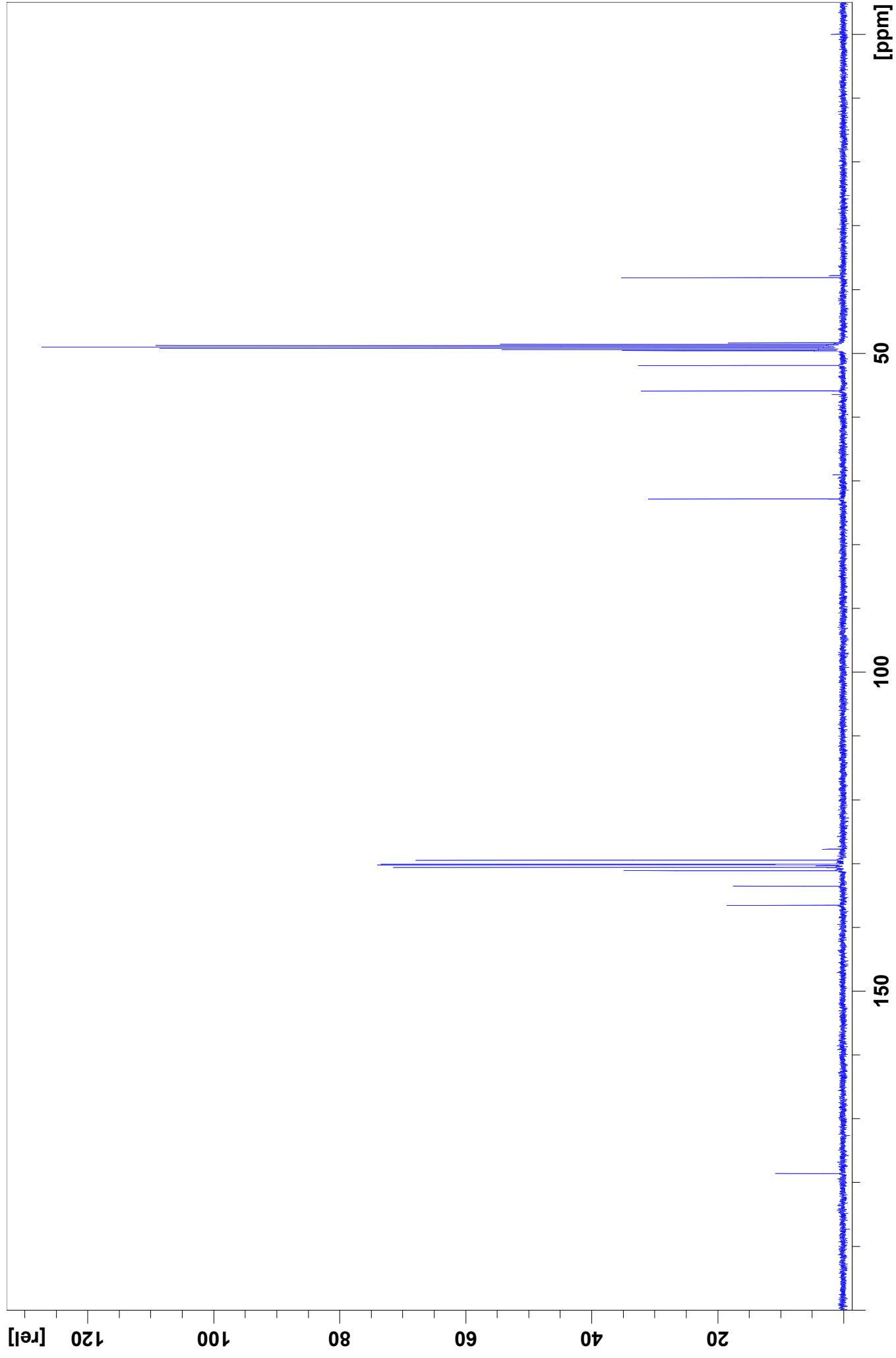
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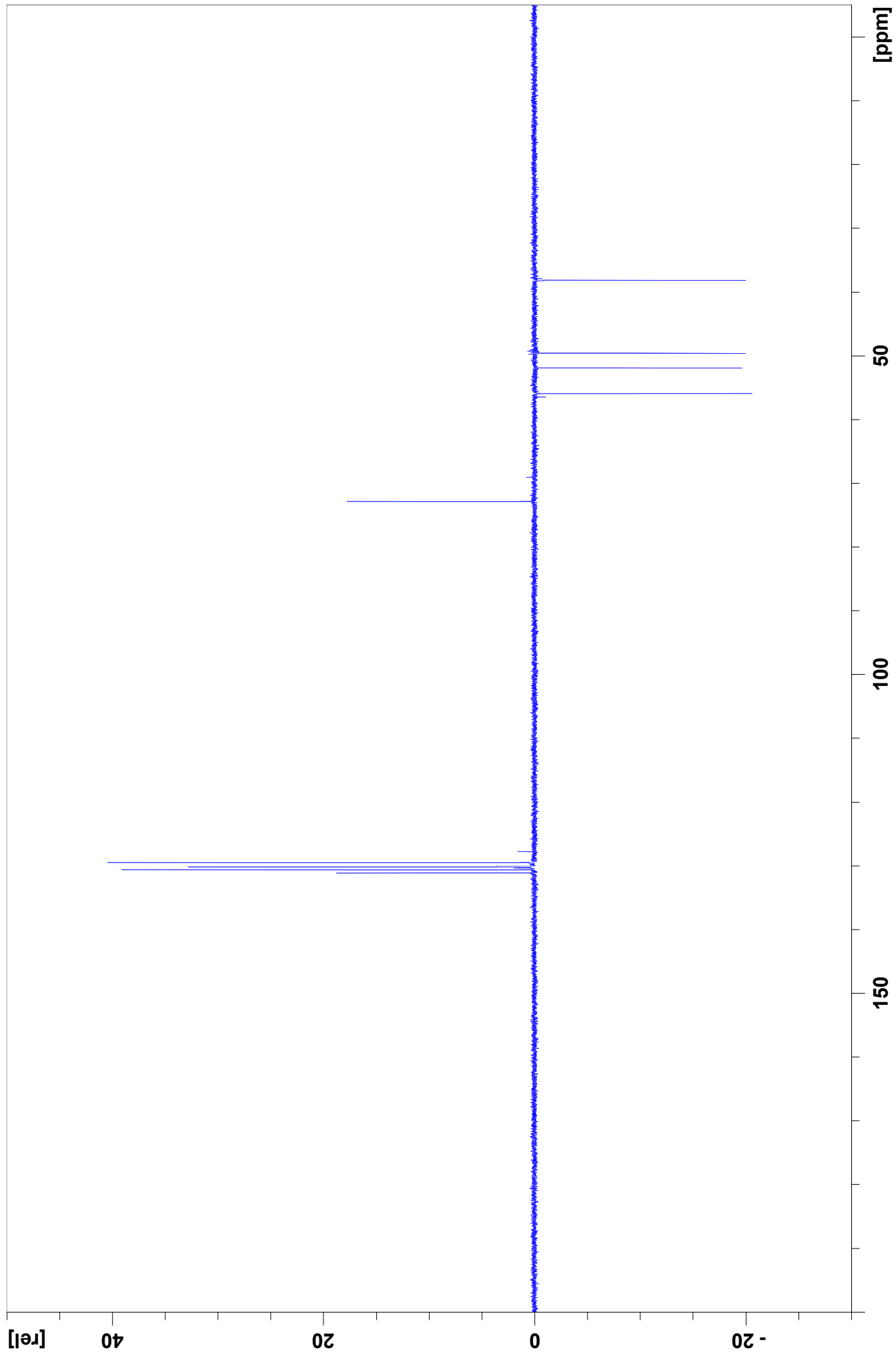
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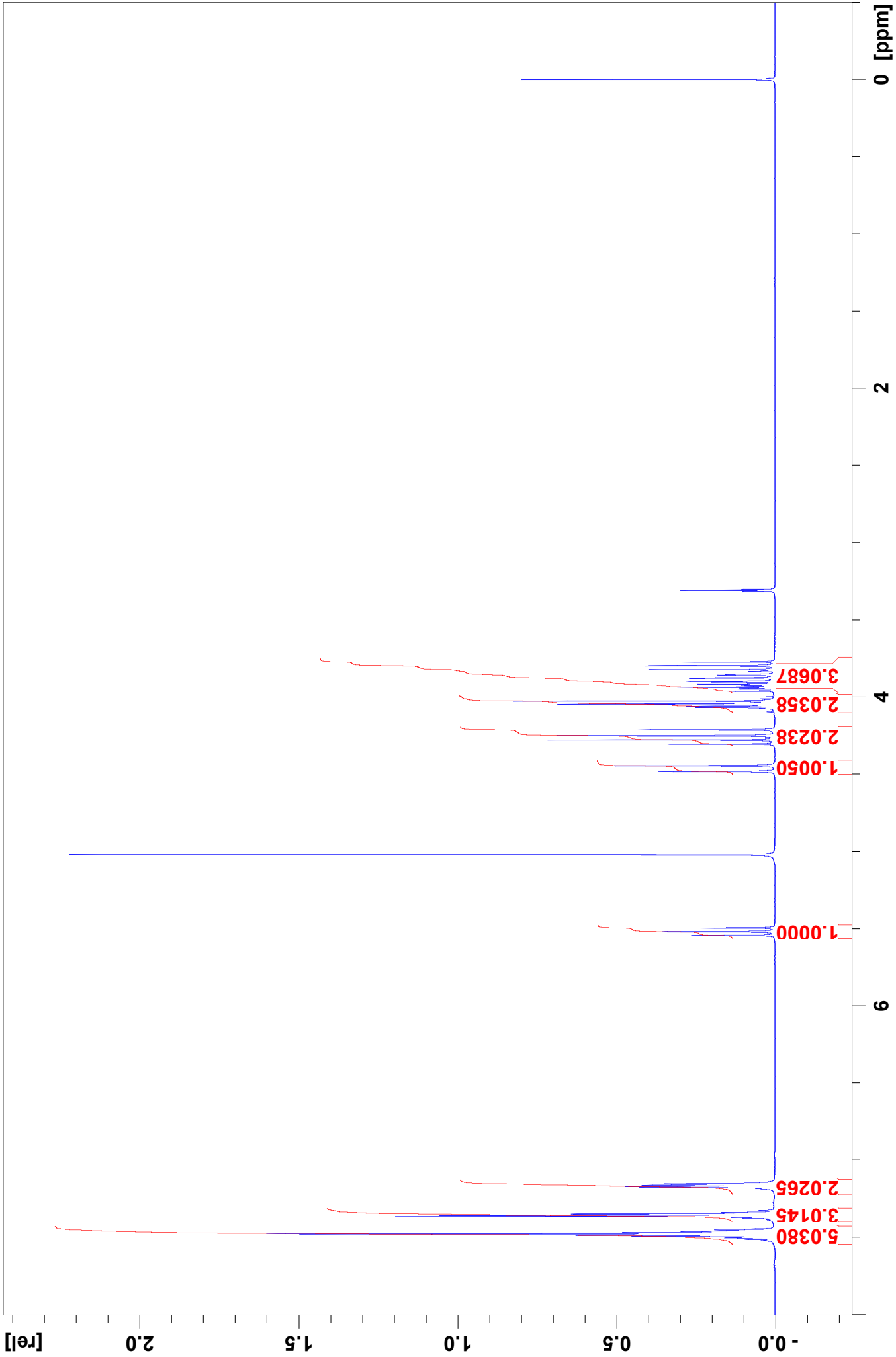
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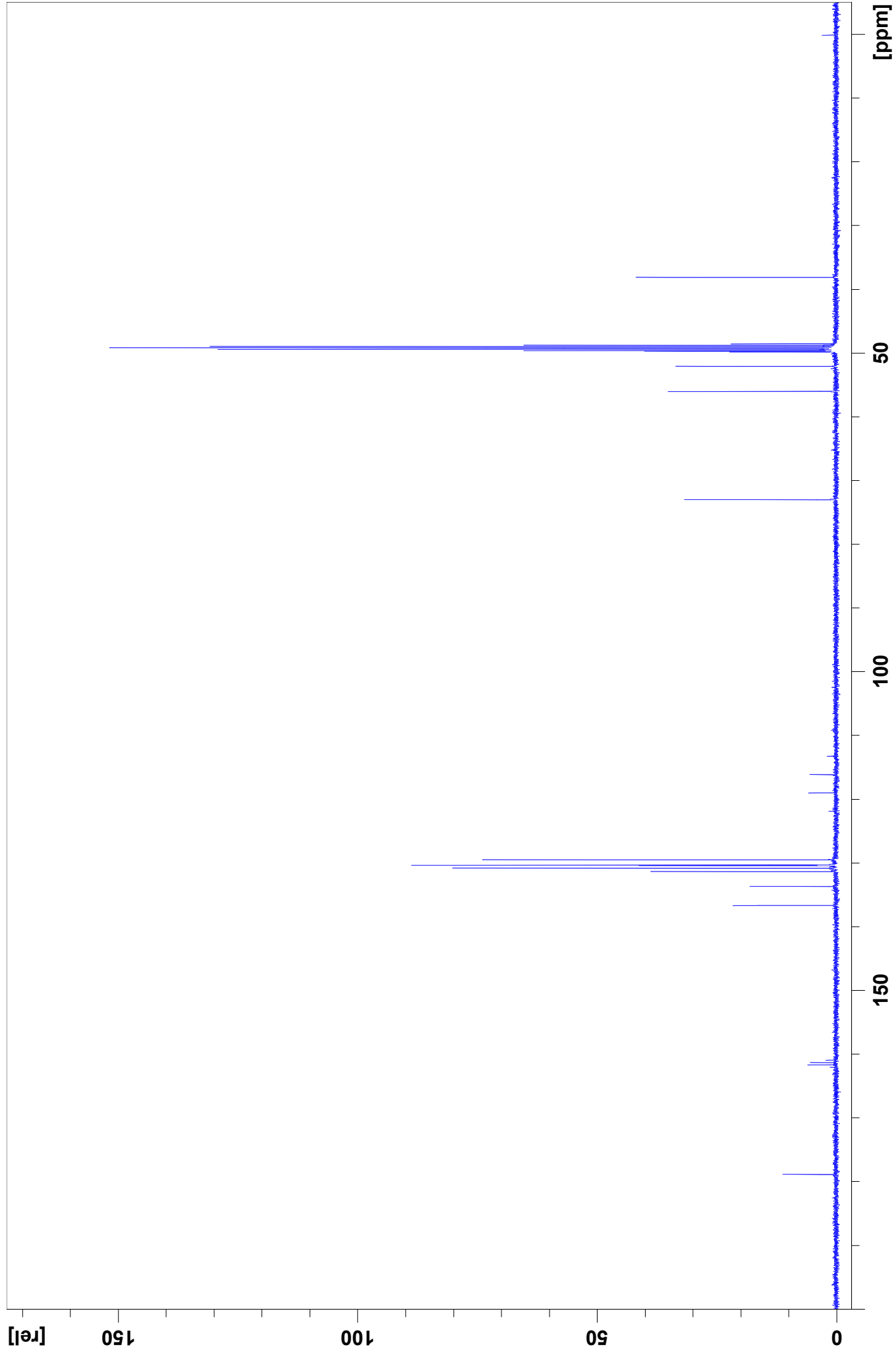
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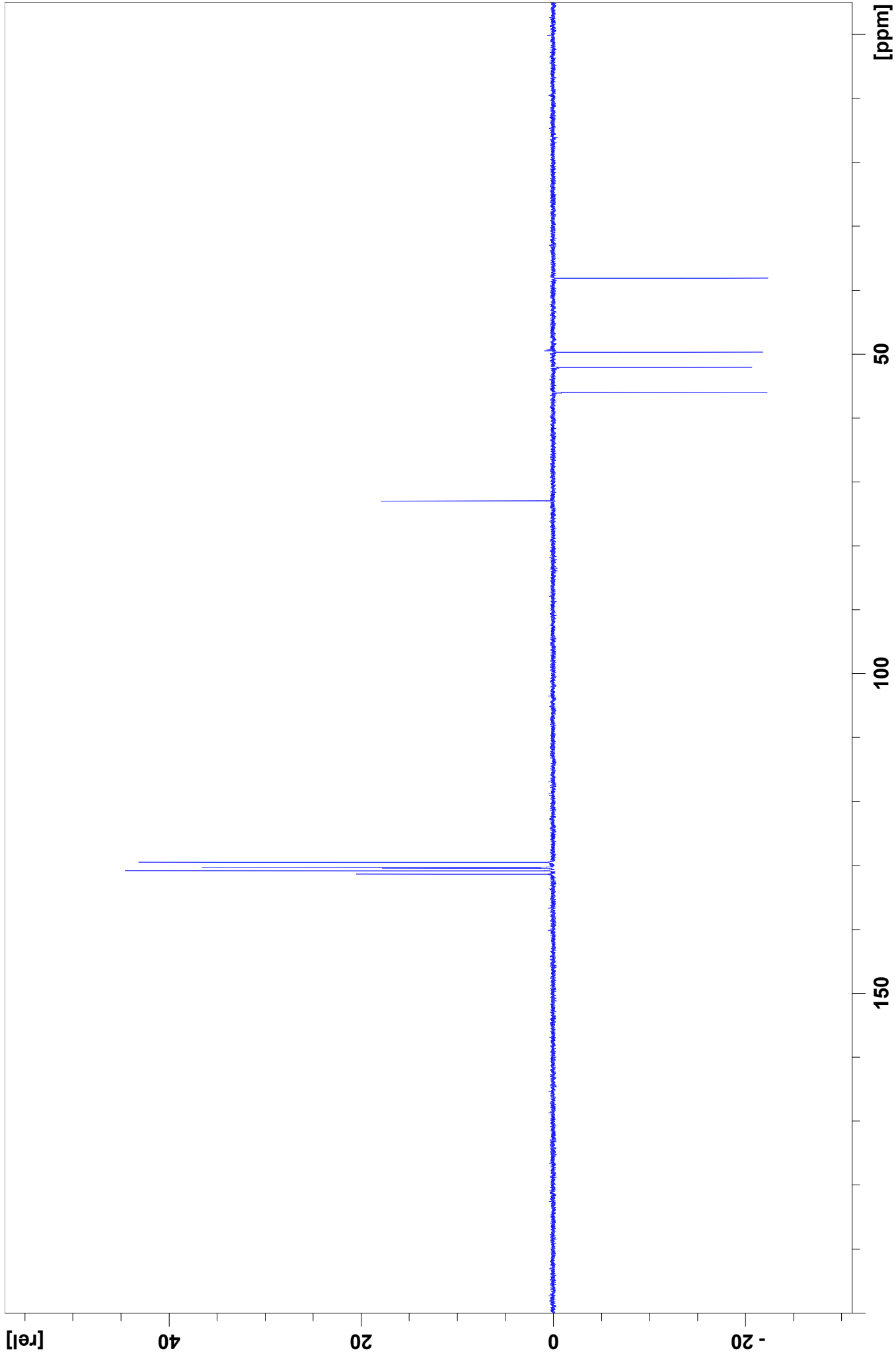
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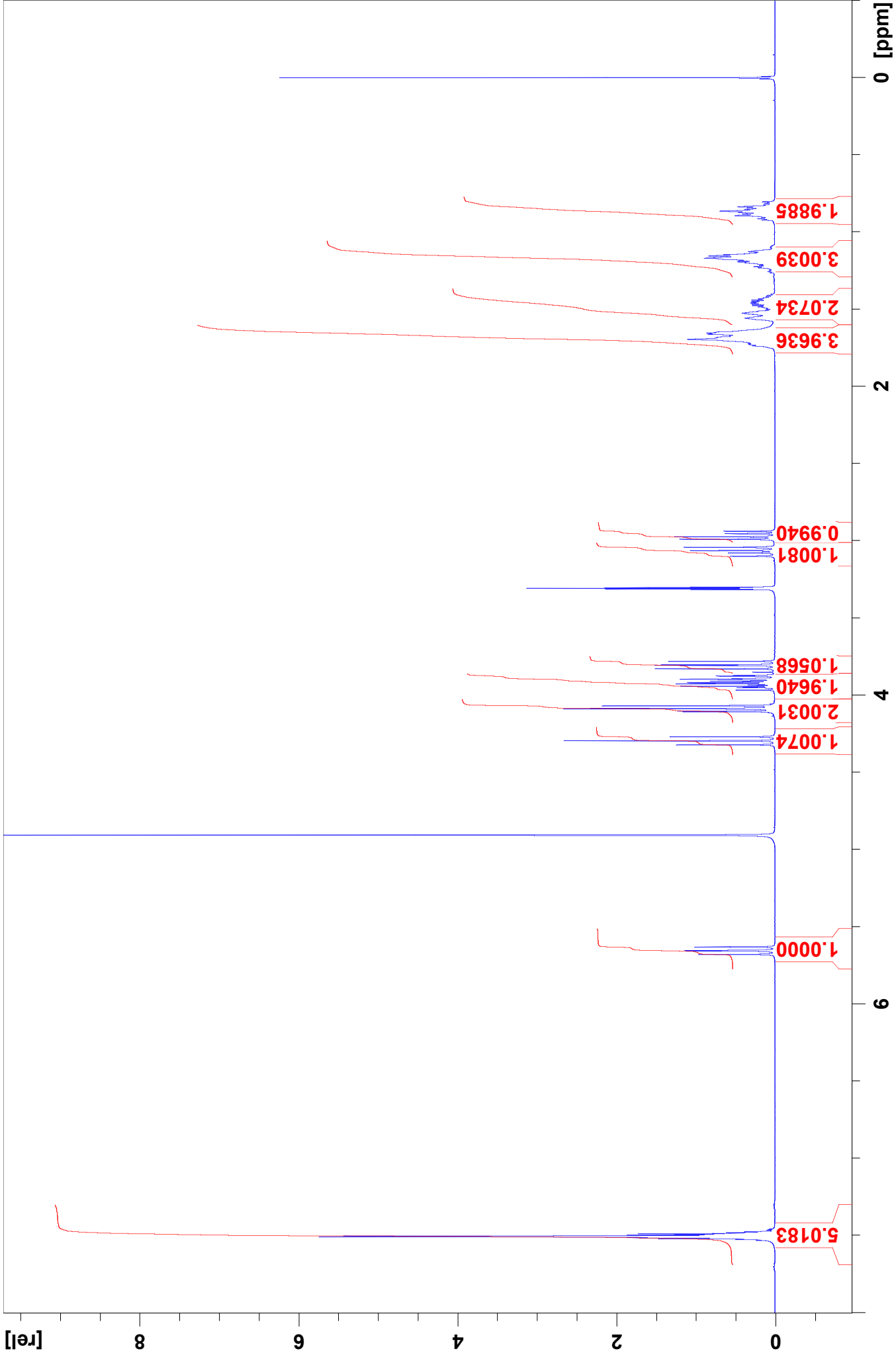
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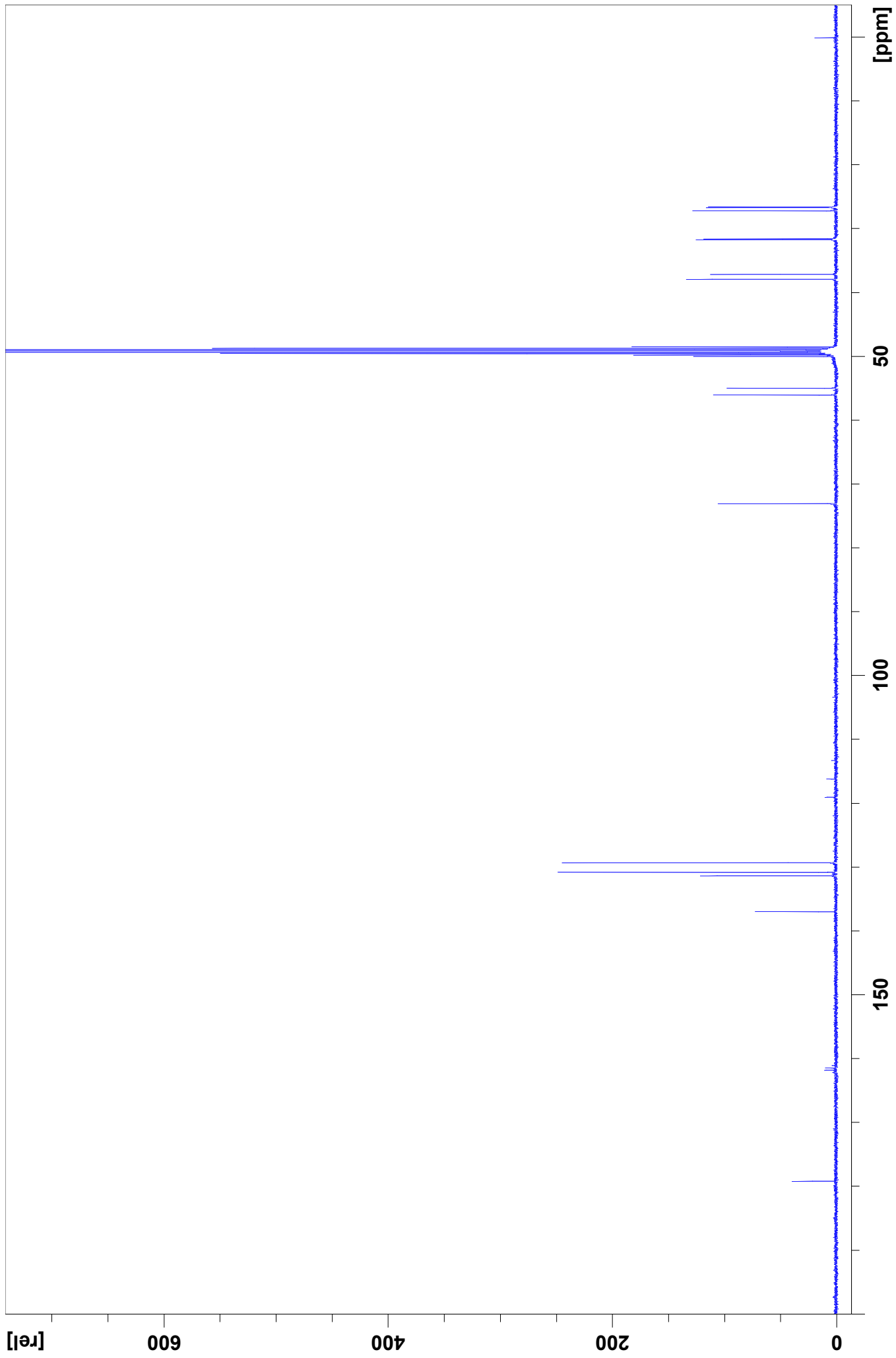
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anh.240107 11 1 d: dan



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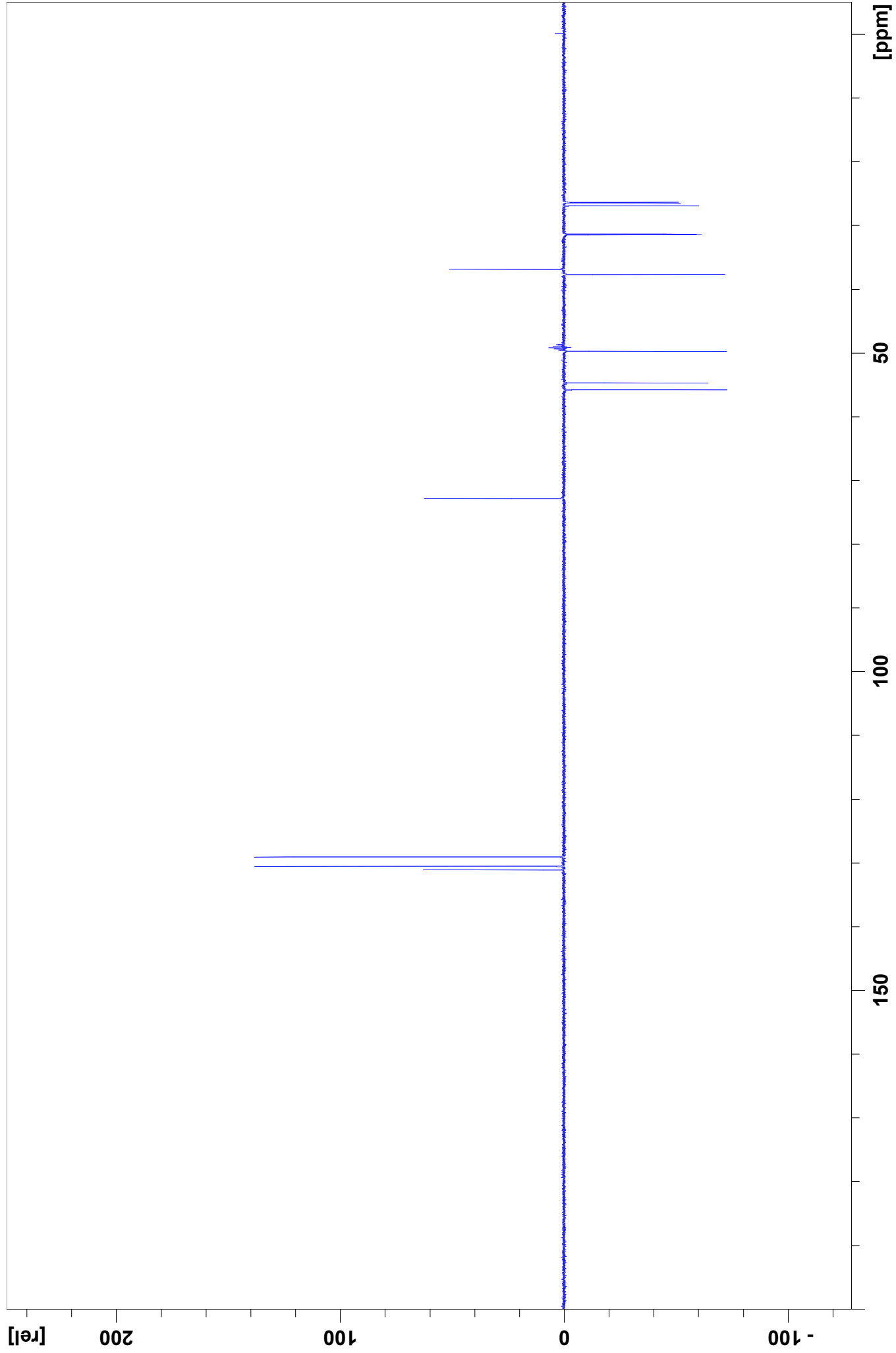
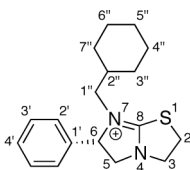


Table S1. Full assignment of the NMR spectral data obtained for compound 12.



Position	¹³ C ^a	¹ H ^{a,b}	COSY ^{a,c}	NOESY ^{a,c,d}	HSQC ^{a,c,e}	HMBC ^{a,c,f}
2	49.9	3.87 (m, A/B part of a larger spin system)	H-3A, H-3B	H-3A, H-3B	C-2	C-3, C-8
		3.93 (m, A/B part of a larger spin system)				
3	37.8	4.08 (m, A/B part of a larger spin system)	H-2	H-2	C-3	C-2, C-8
		4.10 (m, A/B part of a larger spin system)	H-2	H-2	C-3	
5	55.9	α: 3.80 (dd, $J_{5\alpha, 5\beta} = 10.4$, $J_{5\alpha, 6} = 8.8$)	H-5β, H-6	H-5β, H-2'	C-5	C-6, C-8, C-1'
		β: 4.29 (t, $J_{5\beta, 5\alpha} = 10.4$, $J_{5\beta, 6} = 10.4$)	H-5α, H-6	H-5α	C-5	C-6, C-8, C-1'
6	73.0	5.66 (dd, $J_{6, 5\beta} = 10.4$, $J_{6, 5\alpha} = 8.8$)	H-5α, H-5β, H-2', H-6'	H-2', H-5α, H-5β	C-6	C-5, C-2', C-6', C-1''
8	179.1					
1'	136.9					
2'	129.2	7.51 (m)	H-6	H-6, H-5α	C-2'	C-6
3'	130.7	7.49 (m)			C-3'	
4'	131.3	7.48 (m)			C-4'	
1''	54.9	α: 2.96 (dd, $J_{1''\alpha, 1''\beta} = 14.4$, $J_{1''\alpha, 2''} = 6.29$)	H-2'', H-1''β	1''β	C-1''	C-6, C-8, C-2'', C-7''
		β: 3.07 (dd, $J_{1''\beta, 1''\alpha} = 14.4$, $J_{1''\beta, 2''} = 8.44$)	H-2'', H-1''α	1''α	C-1''	
2''	37.0	1.46 (m)	H-1''α, H-1''β		C-2''	C-1''
3''	26.6	A: 1.55 (m)			C-3''	
		B: 1.15 (m)			C-3''	
4''	27.1	1.16 (m)	H-5''		C-4''	
5''	31.6	0.86 (m)	H-4''		C-5''	
6''	26.5	1.69 (m)			C-6''	
7''	31.5	A: 1.54 (m)			C-7''	C-1''
		B: 1.67 (m)			C-7''	

^a ¹H (400 MHz) and ¹³C (100 MHz) NMR spectral data obtained in CD₃OD. ^b Signal multiplicity and coupling constants in Hz are given in parentheses. ^c Signals correlate with ¹H resonance. ^d Mixing time 500 milliseconds. ^e Optimized for $^1J_{C,H} = 145$ Hz. ^f Optimized for $^nJ_{C,H} = 7.7$ Hz.