

An Efficient Approach to Phosphorylated Isoindoline Fused with Triazoles *via* Zn-Catalyzed Cascade Cyclization of 2-Propynol Benzyl Azides and Diarylphosphine Oxides

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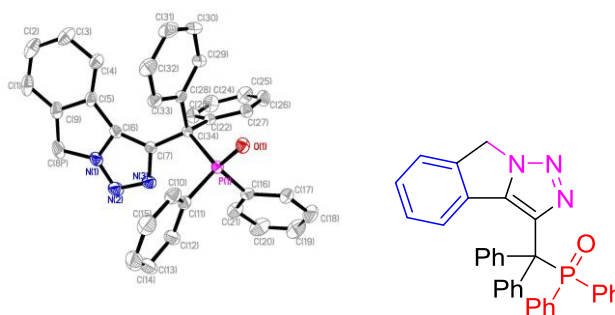
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Table of Contents

1	Crystal preparation and X-ray diffraction analysis of compound 3a	S3
2	^1H NMR and ^{13}C NMR spectra for compounds 3a-3t	S4-S54

Crystal preparation and X-ray diffraction analysis of compound 3a



Datablock: 1

Bond precision: C-C = 0.0047 Å Wavelength=0.71073

Cell: a=10.3355(13) b=15.828(2) c=19.435(2)
 alpha=90.738(2) beta=101.662(2) gamma=107.843(2)

Temperature: 296 K

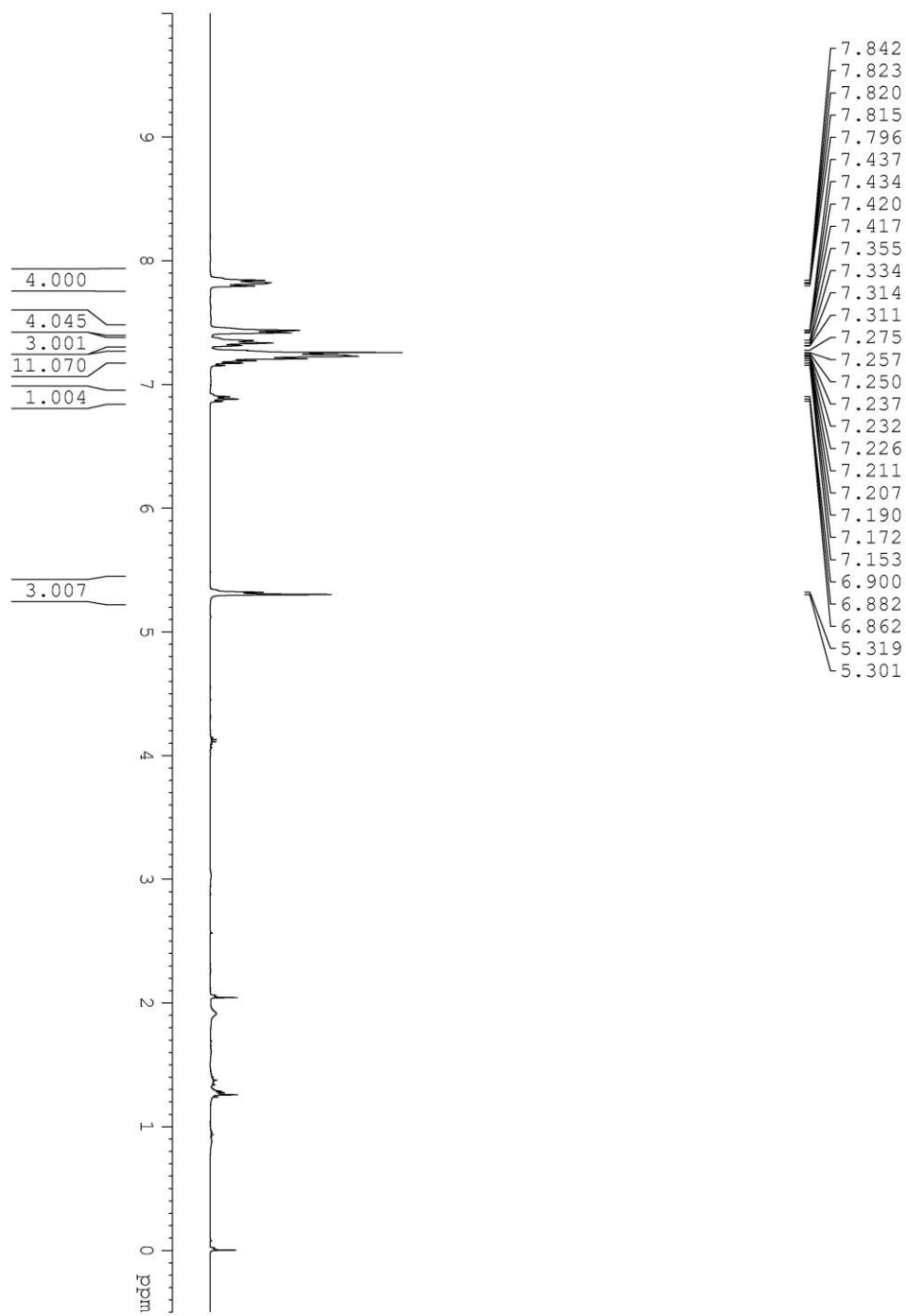
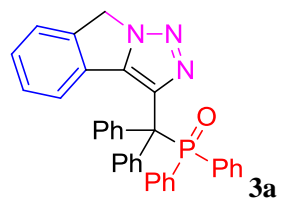
	Calculated	Reported
Volume	2954.4(6)	2954.3(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C ₃₄ H ₂₆ N ₃ O P), C ₄ H ₈ O ₂	?
Sum formula	C ₇₂ H ₆₀ N ₆ O ₄ P ₂	C ₇₂ H ₆₀ N ₆ O ₄ P ₂
Mr	1135.20	1135.20
Dx, g cm ⁻³	1.276	1.276
Z	2	2
Mu (mm ⁻¹)	0.131	0.131
F ₀₀₀	1192.0	1192.0
F ₀₀₀ '	1192.85	
h,k,lmax	12,19,23	12,19,23
Nref	11618	11539
Tmin,Tmax	0.961,0.965	
Tmin'	0.961	

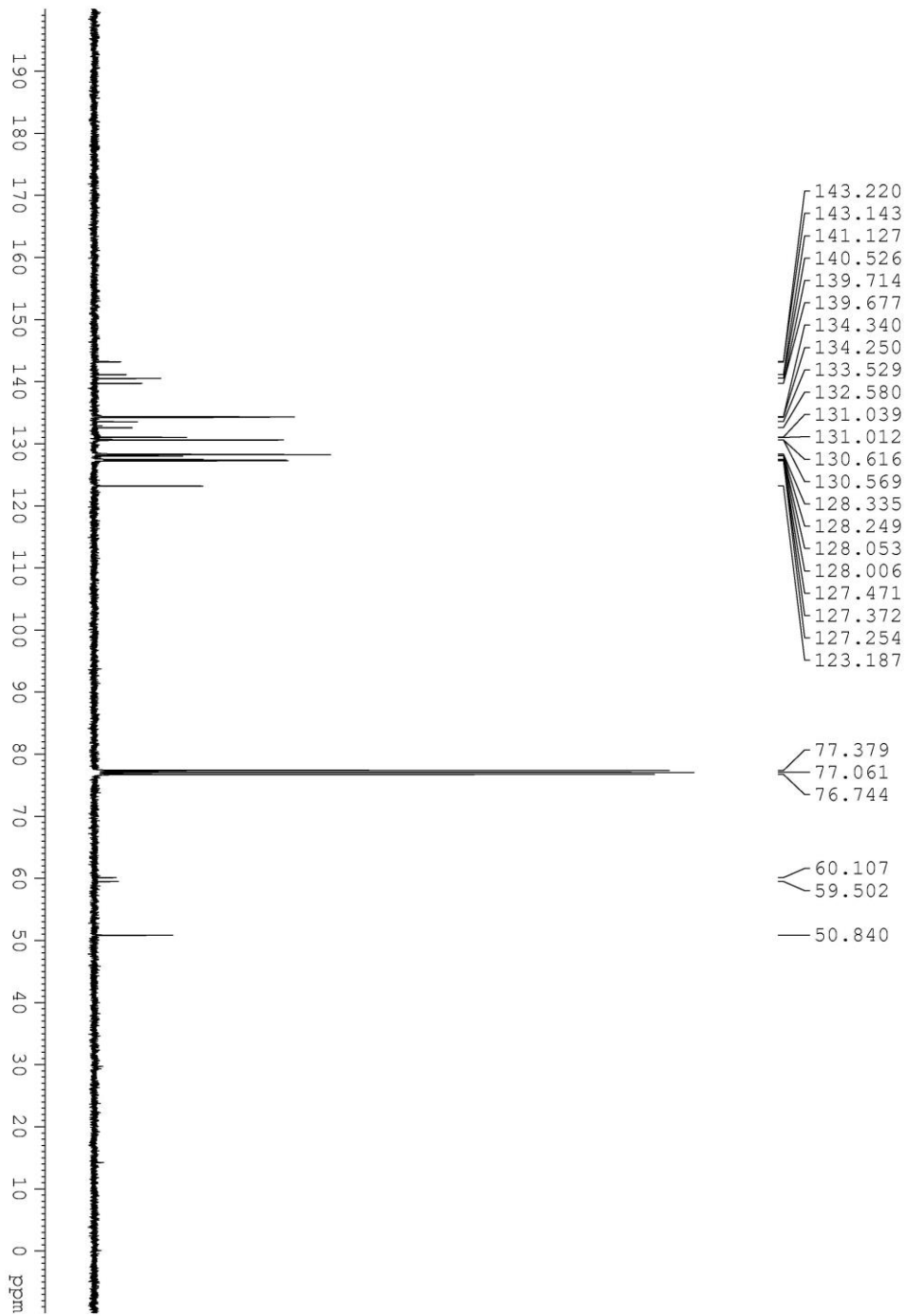
Correction method= Not given

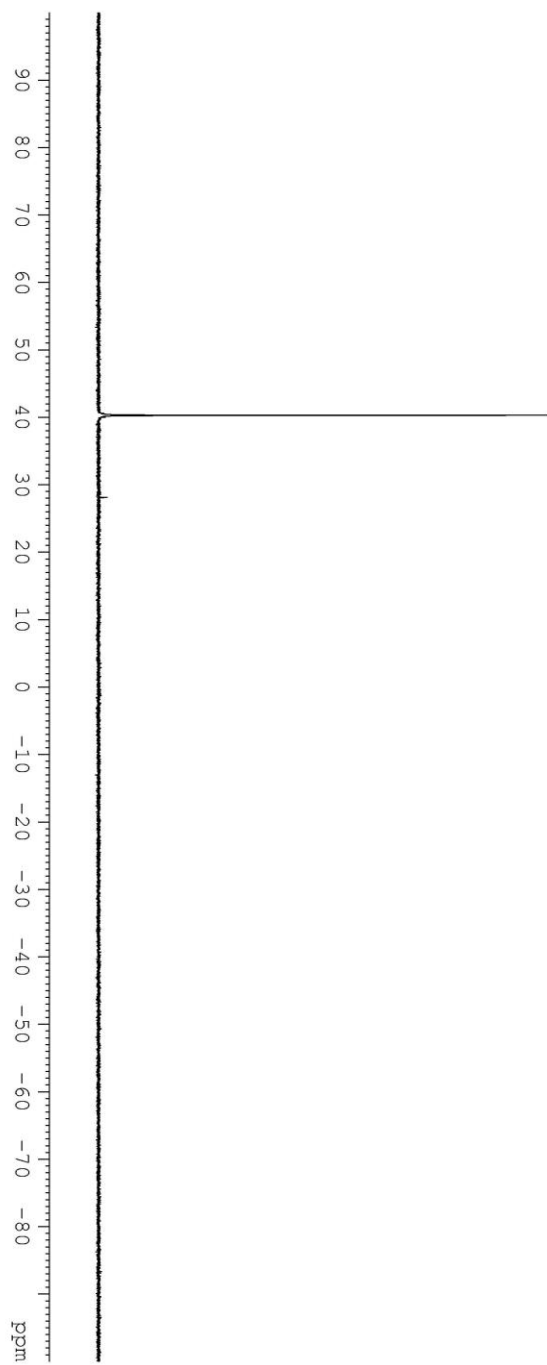
Data completeness= 0.993 Theta(max)= 25.999

R(reflections)= 0.0563(7635) wR2(reflections)= 0.1784(11539)

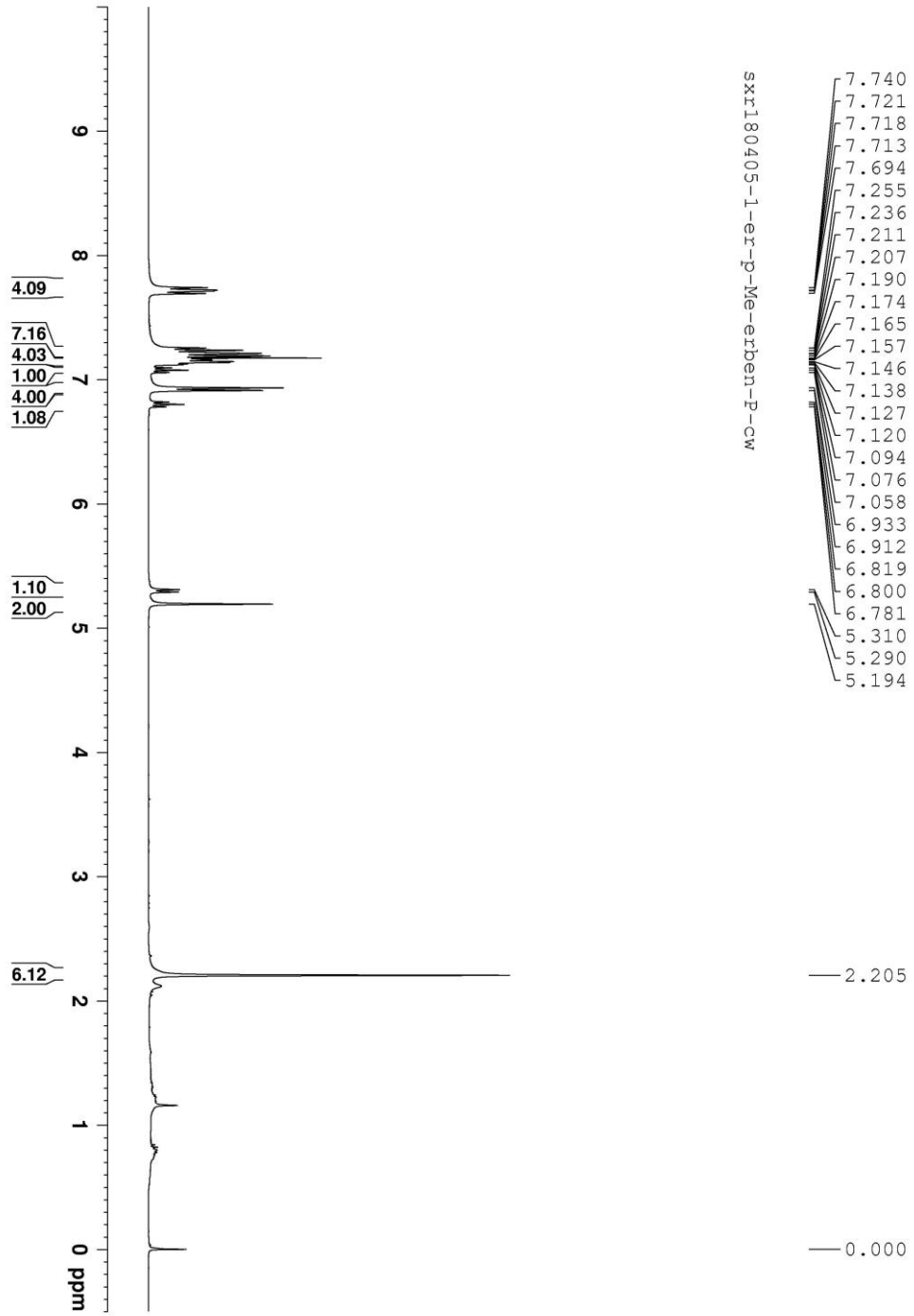
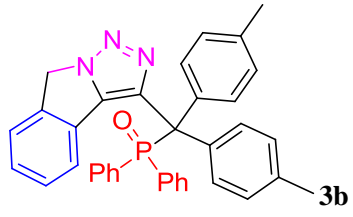
S = 1.007 Npar= 757

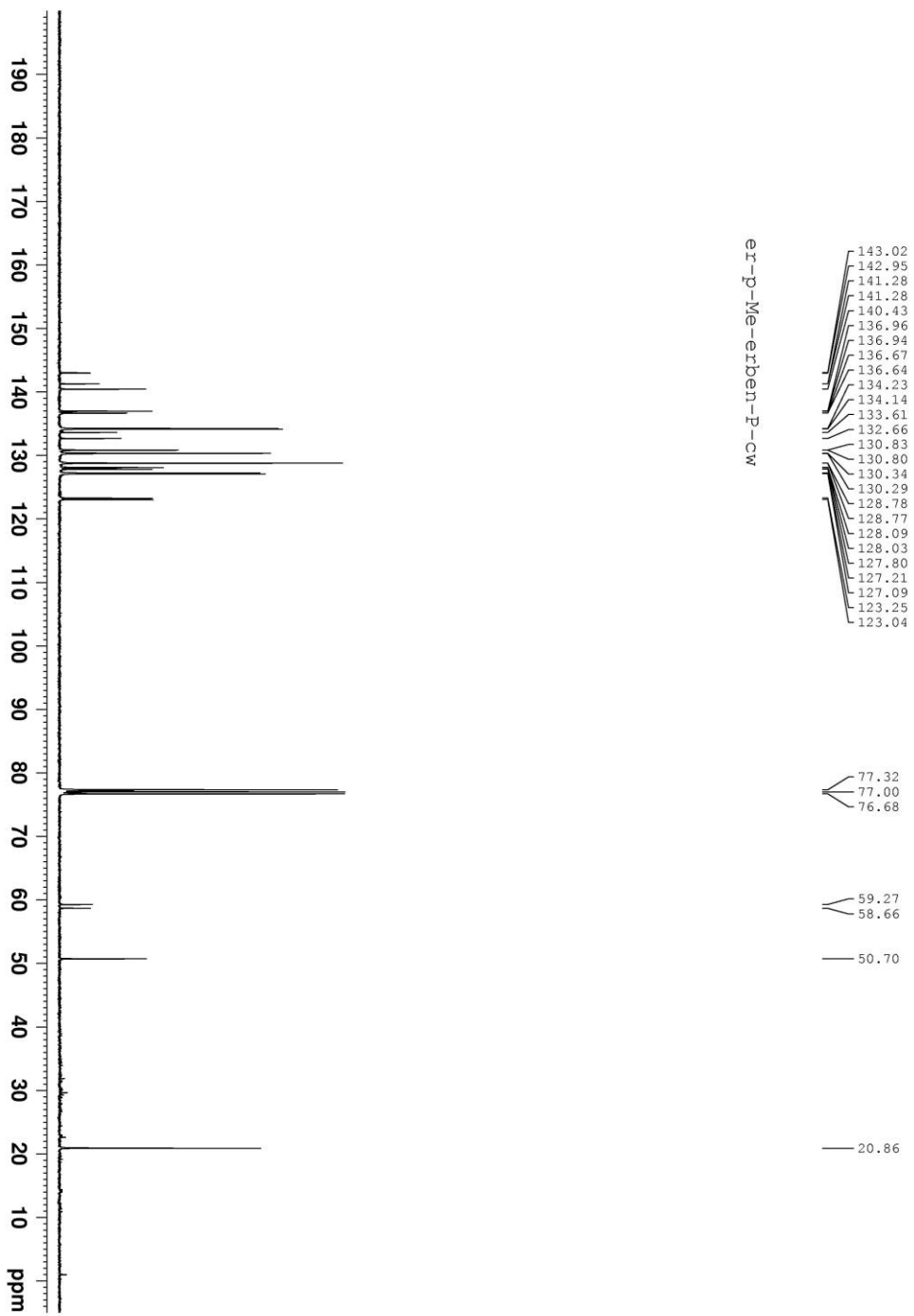


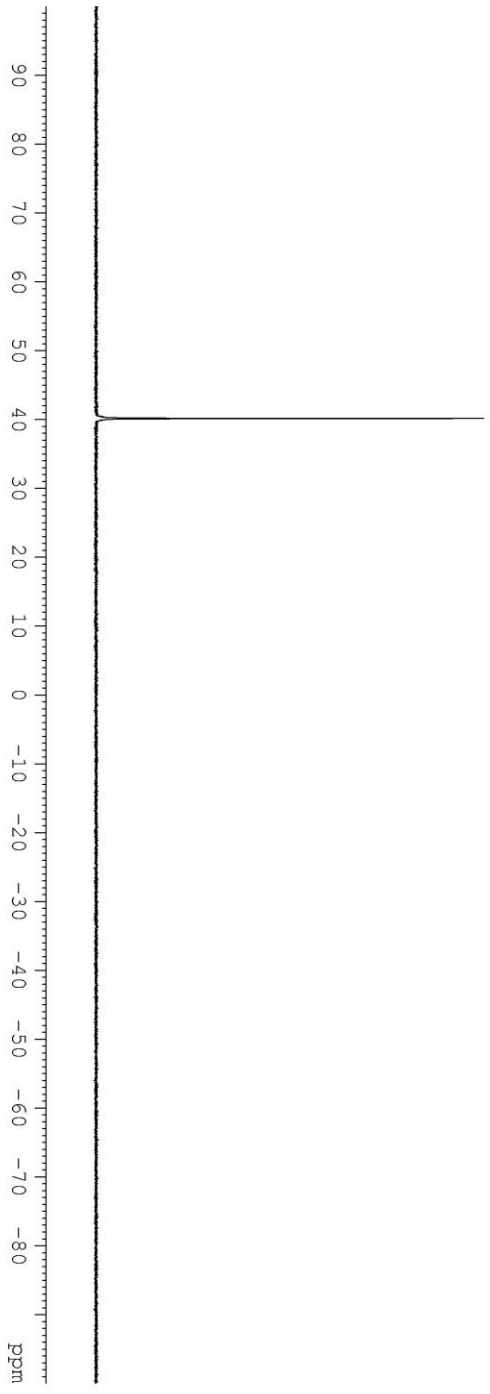




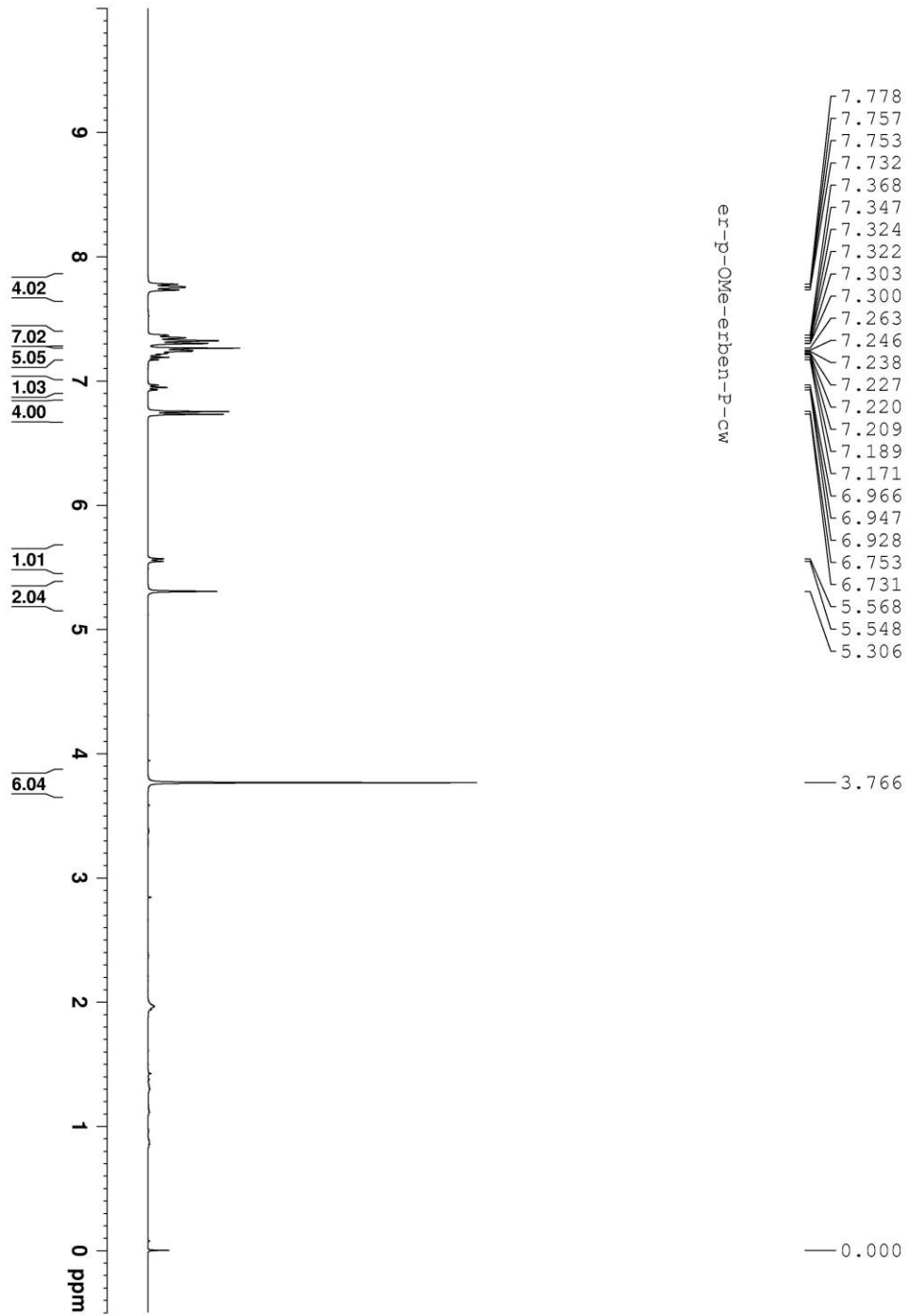
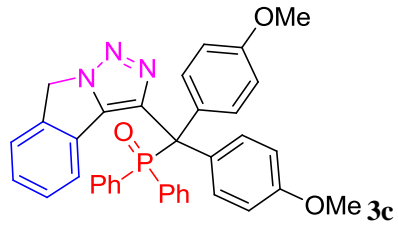
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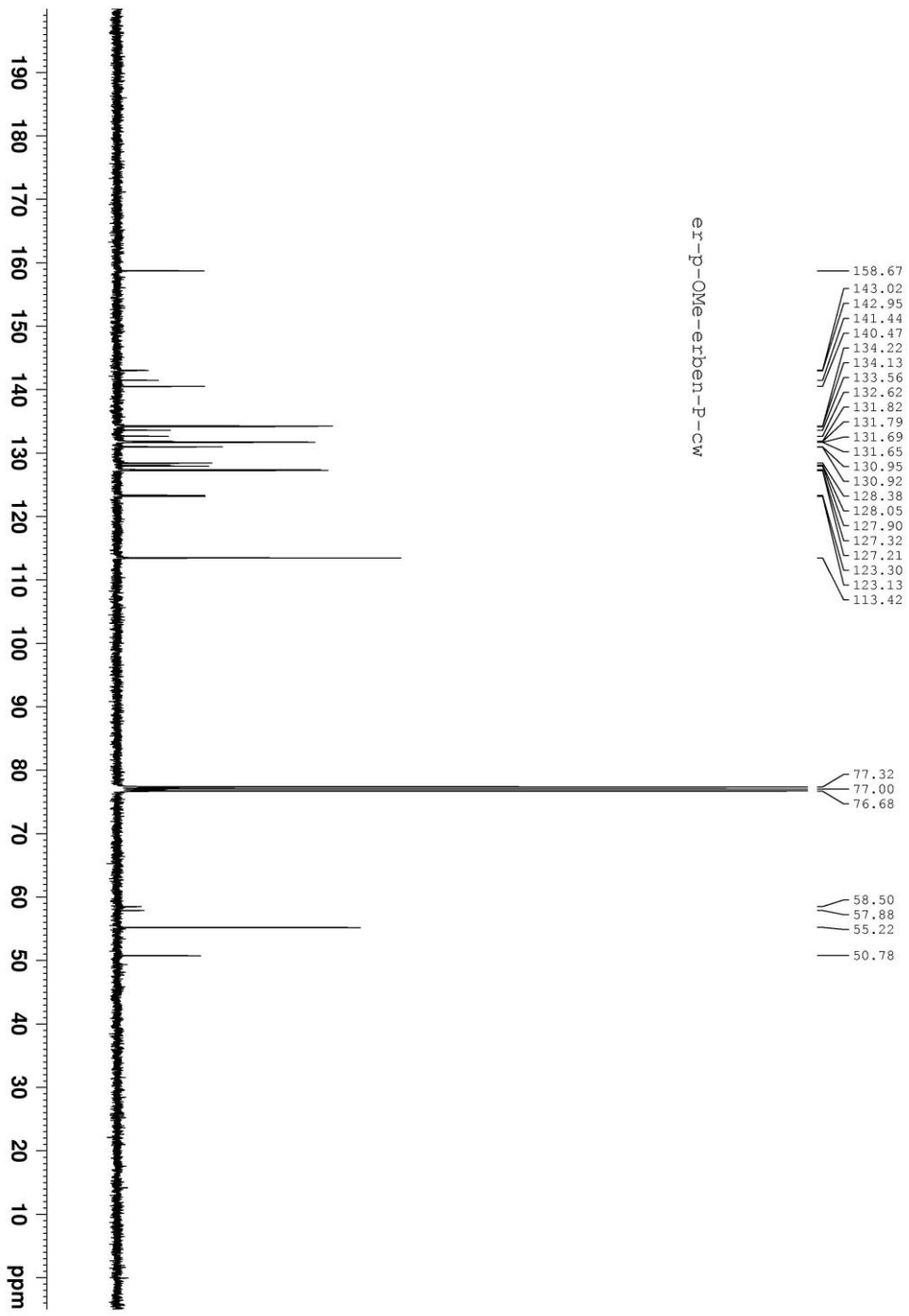


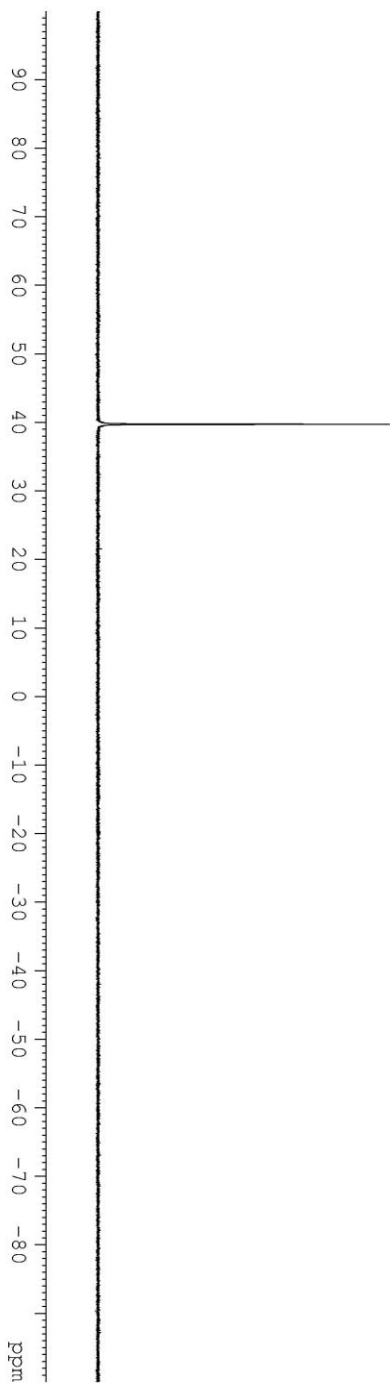




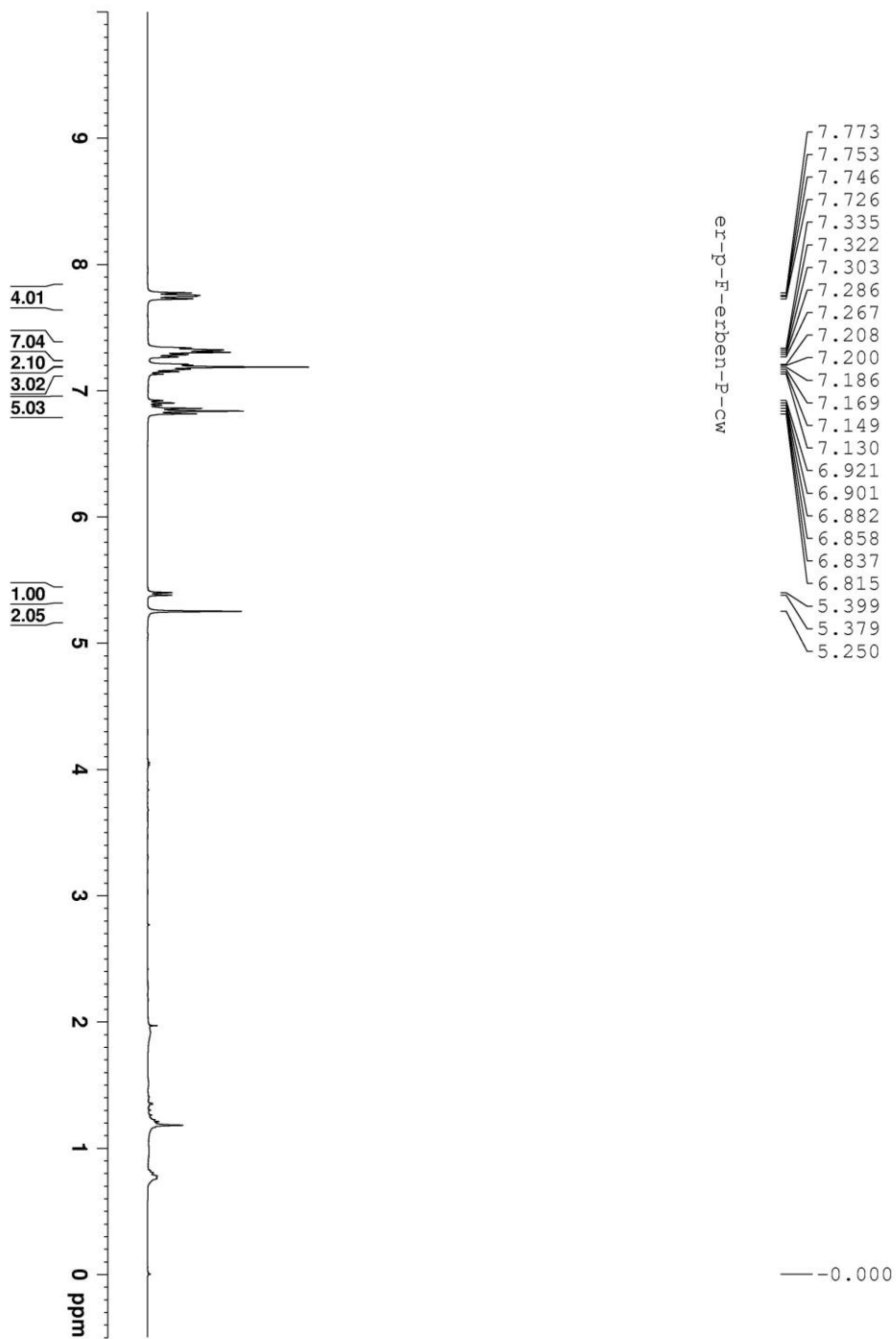
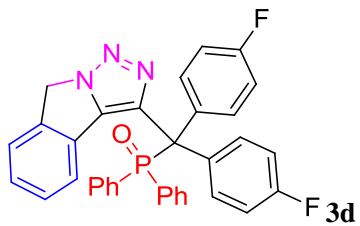
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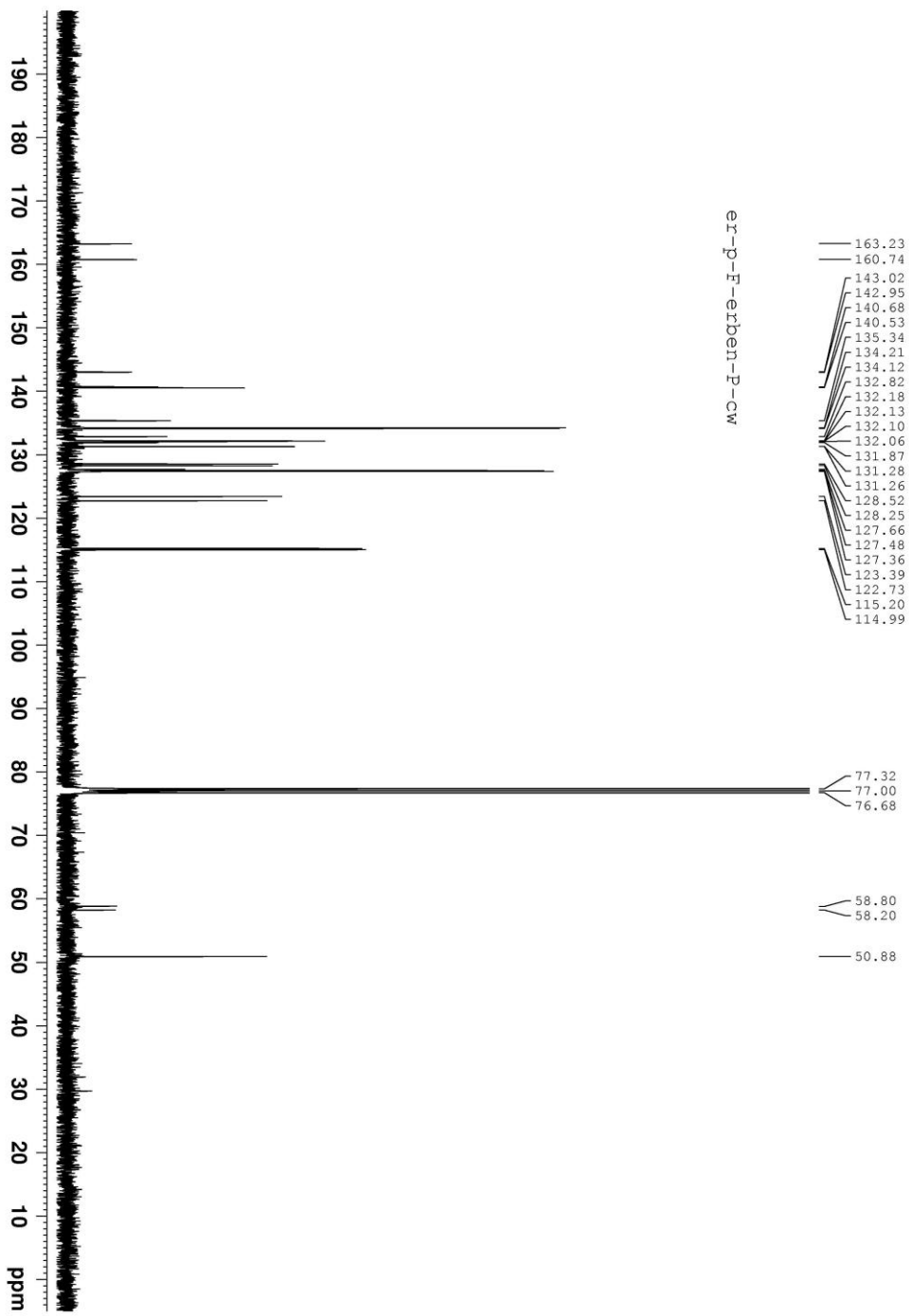


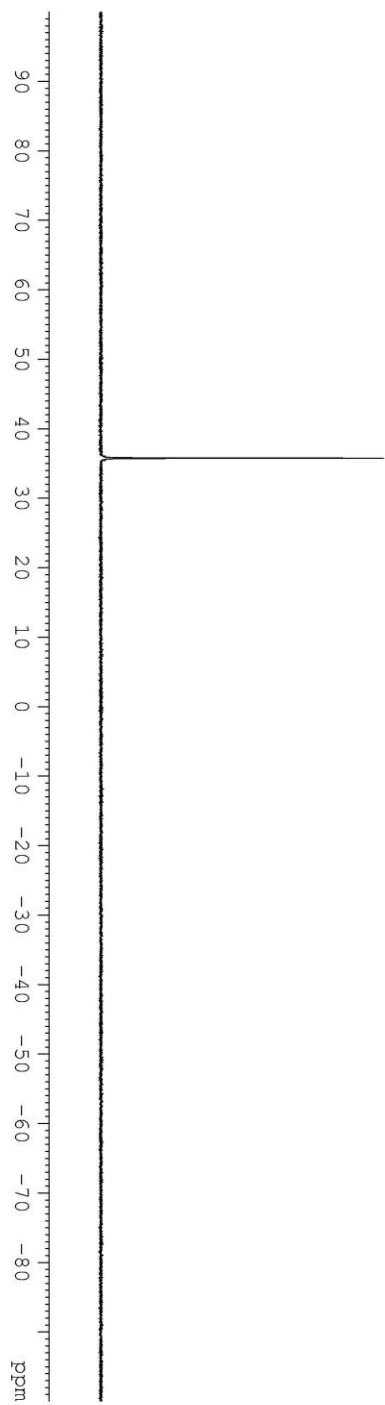




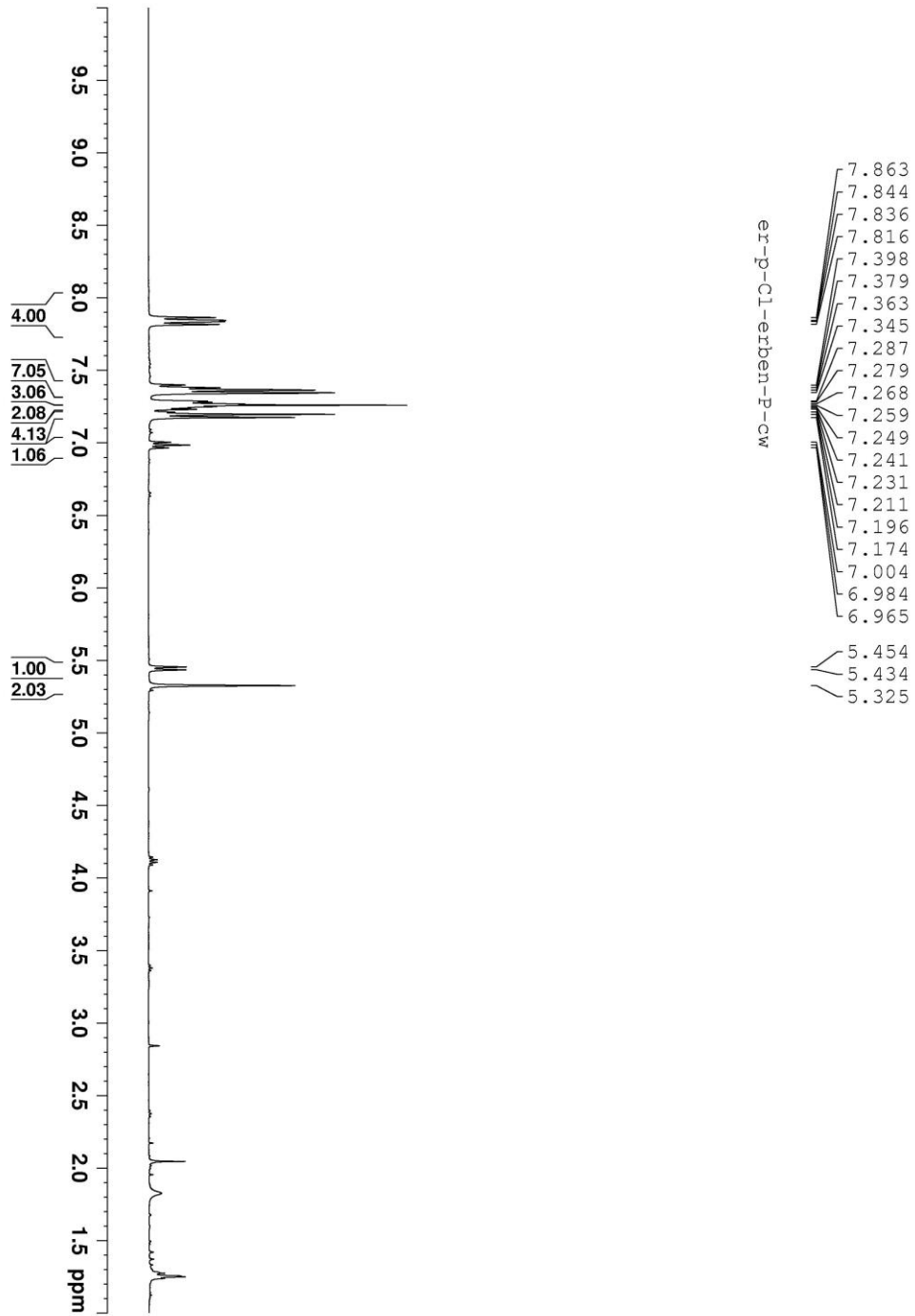
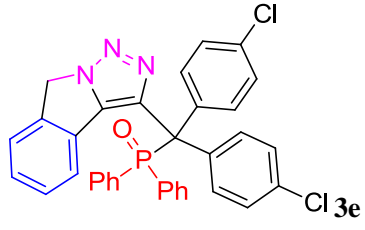
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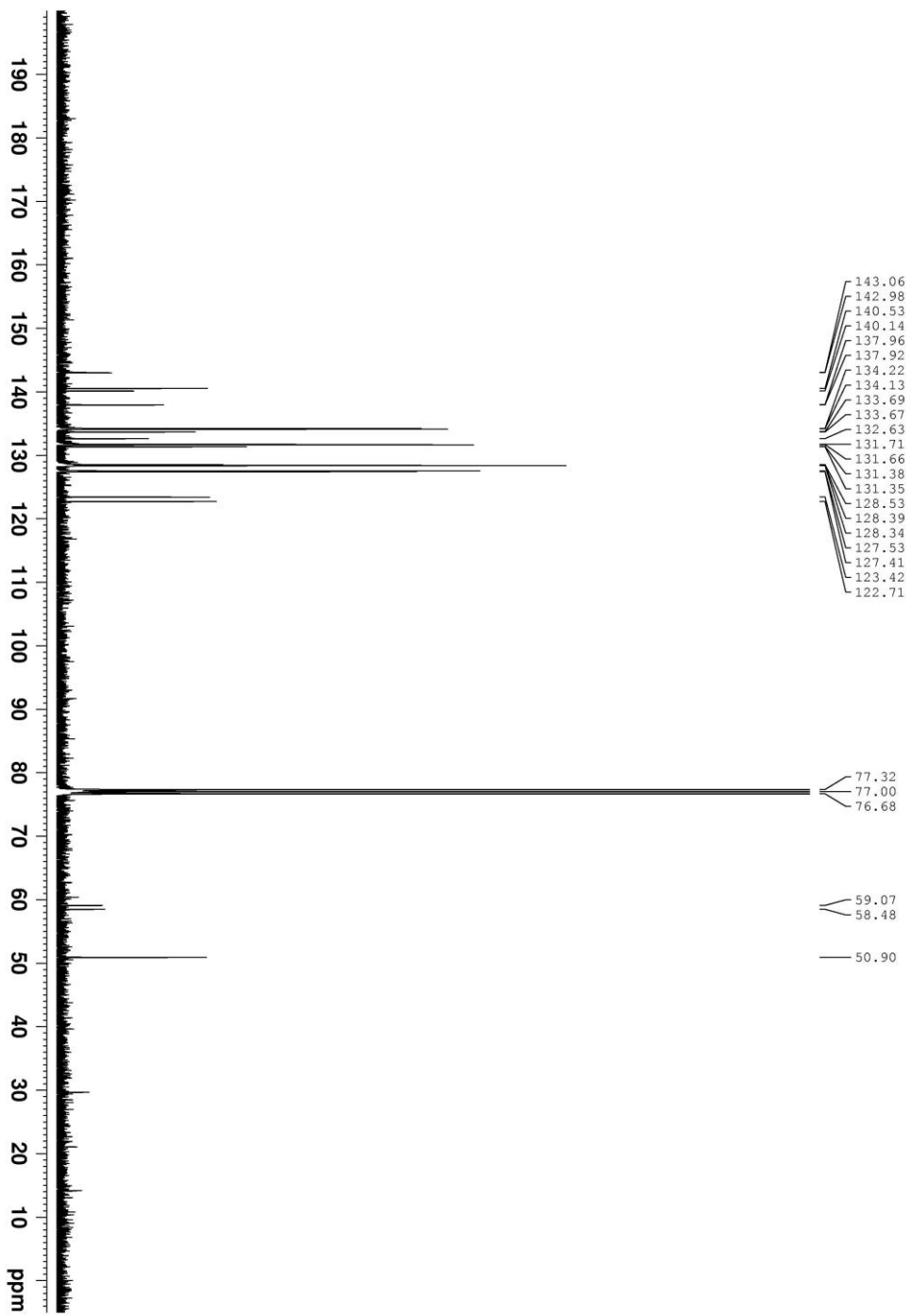


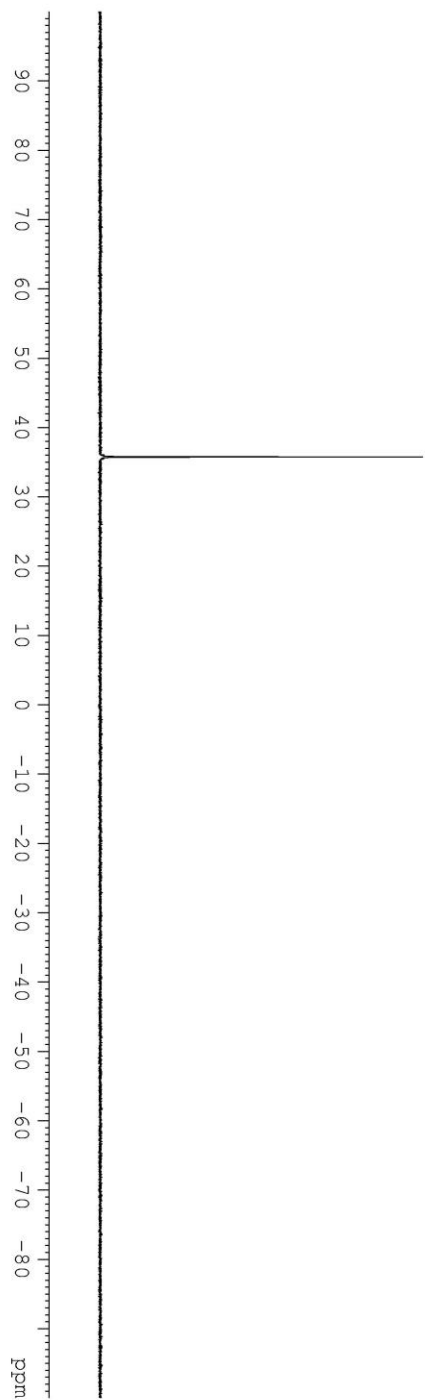




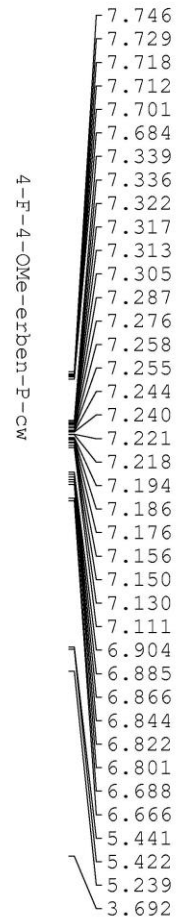
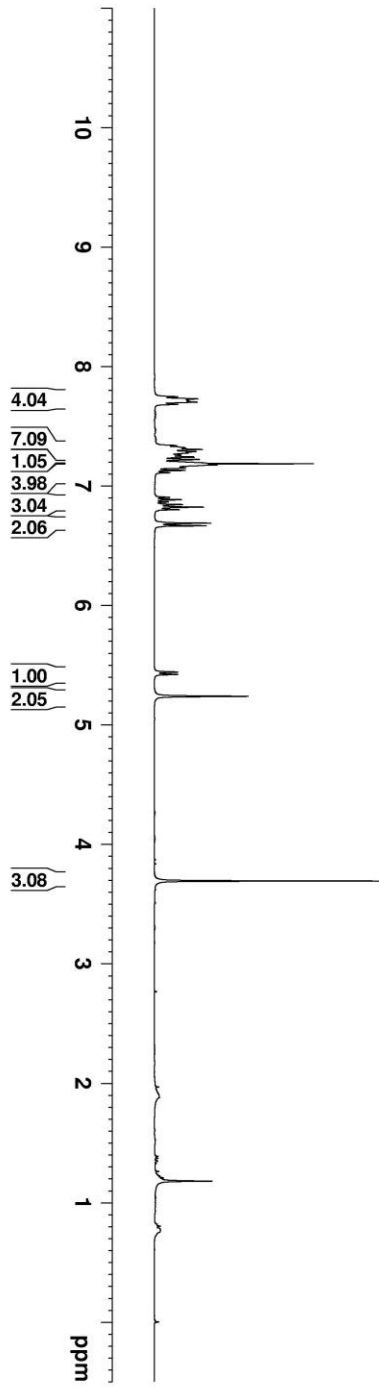
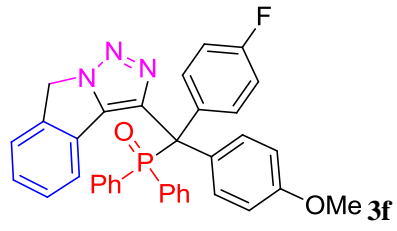
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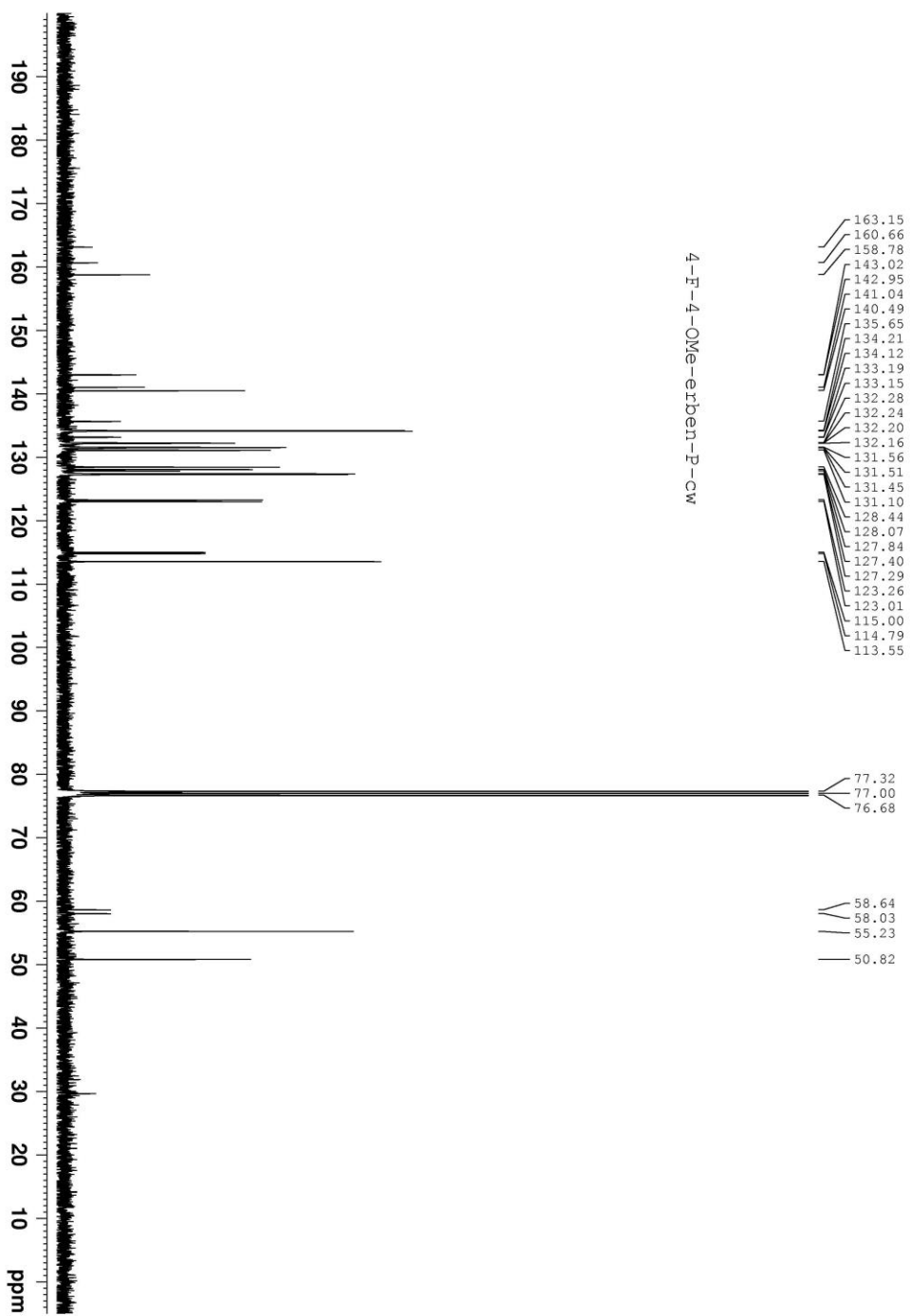


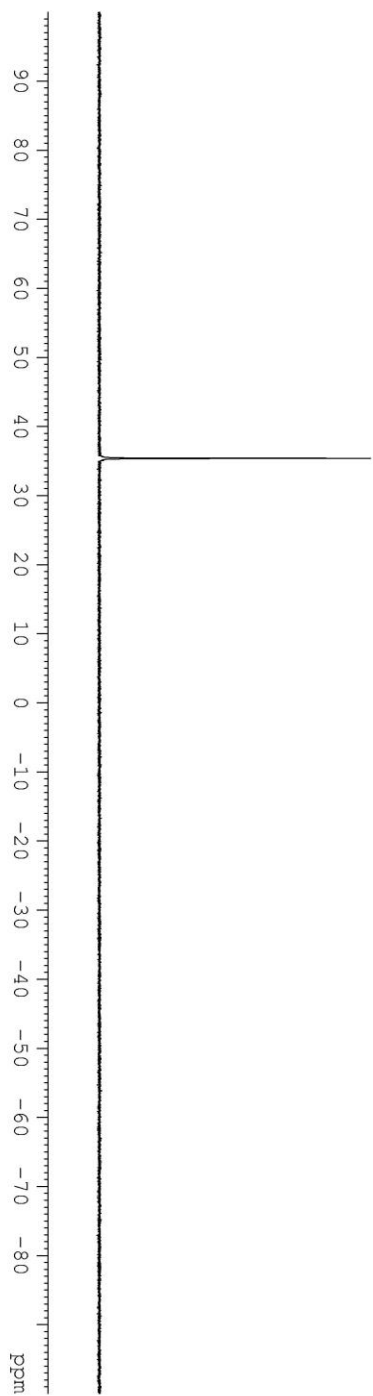




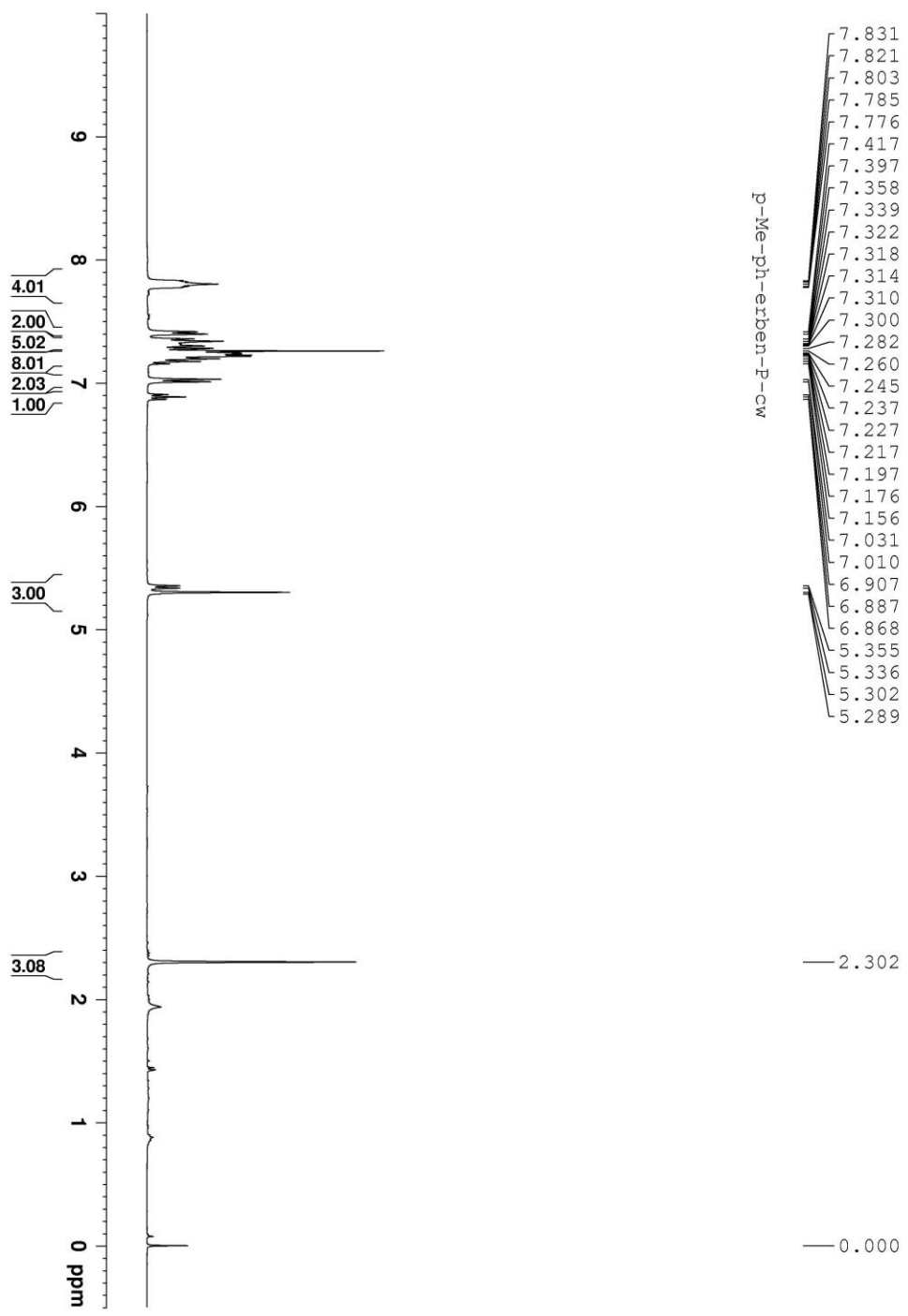
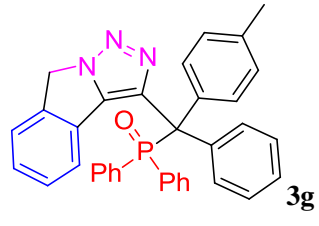
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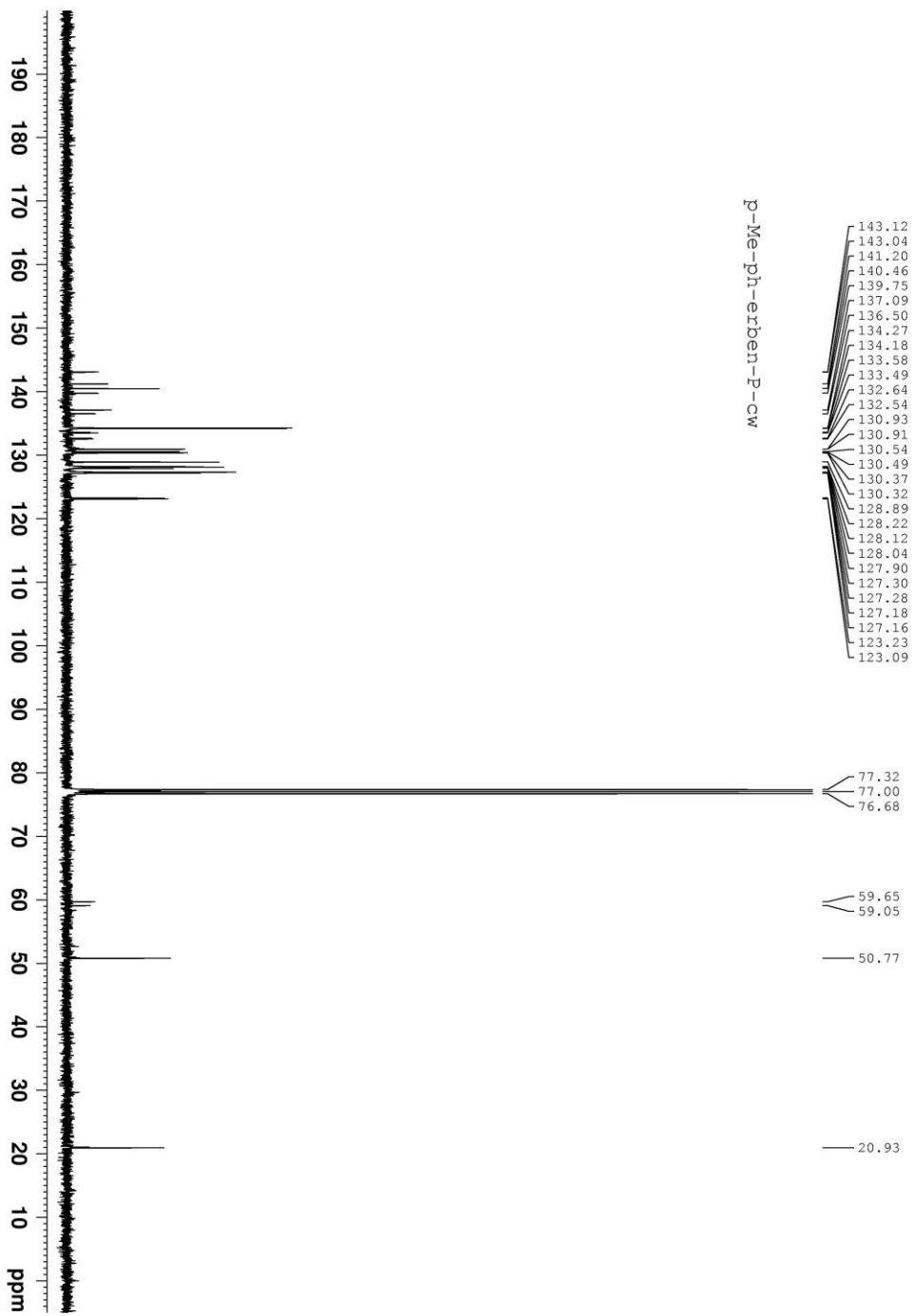


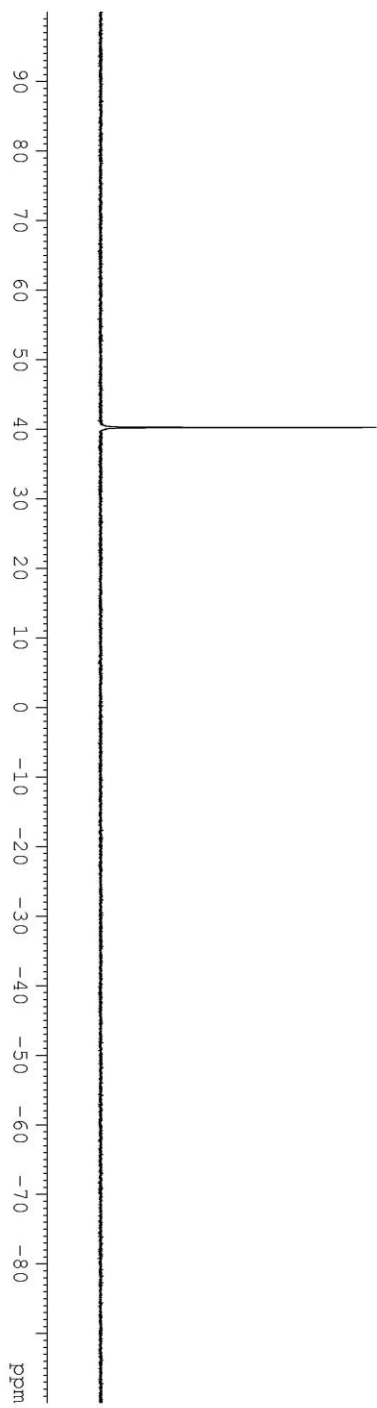




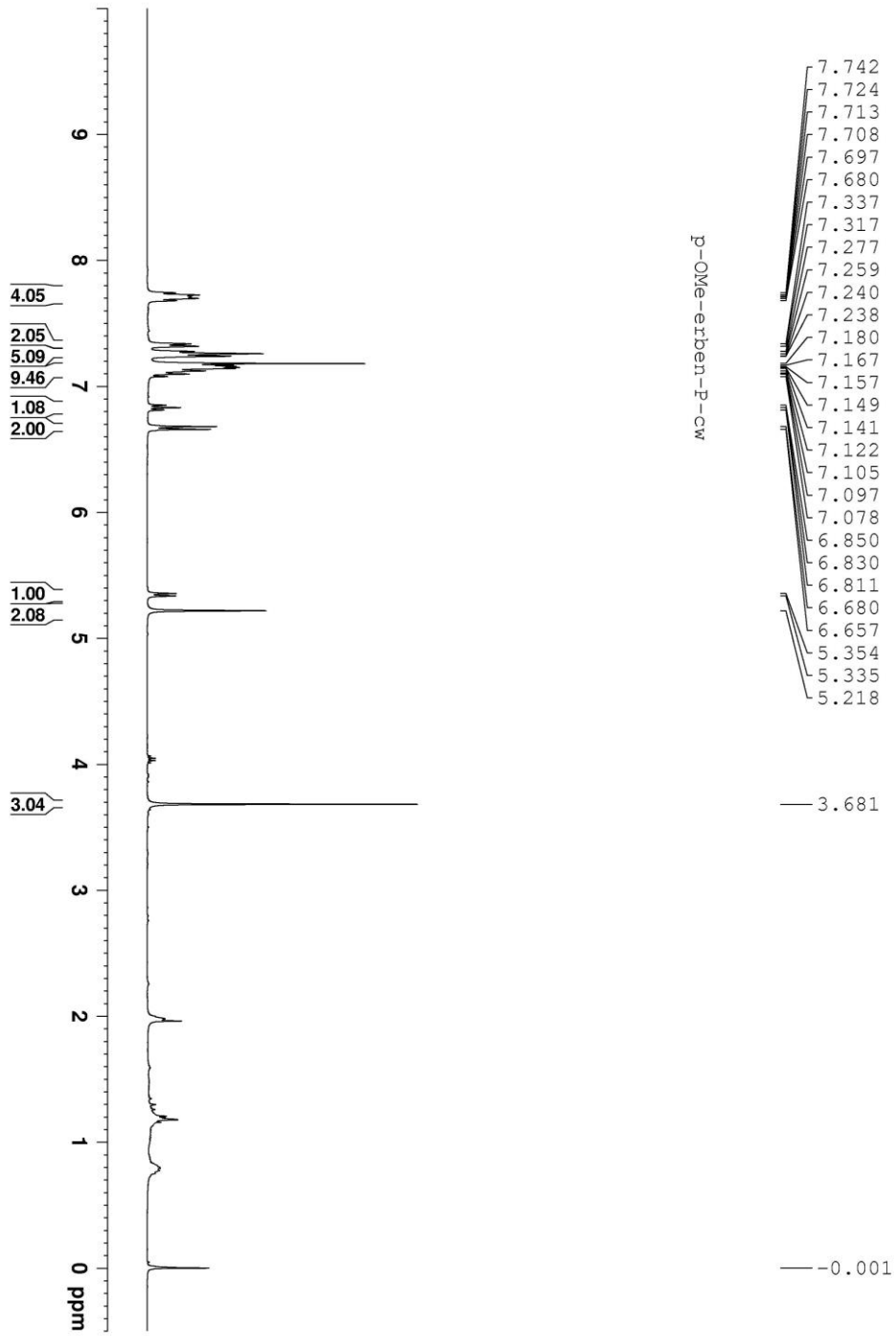
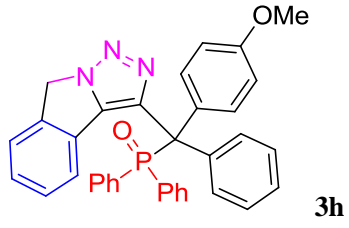
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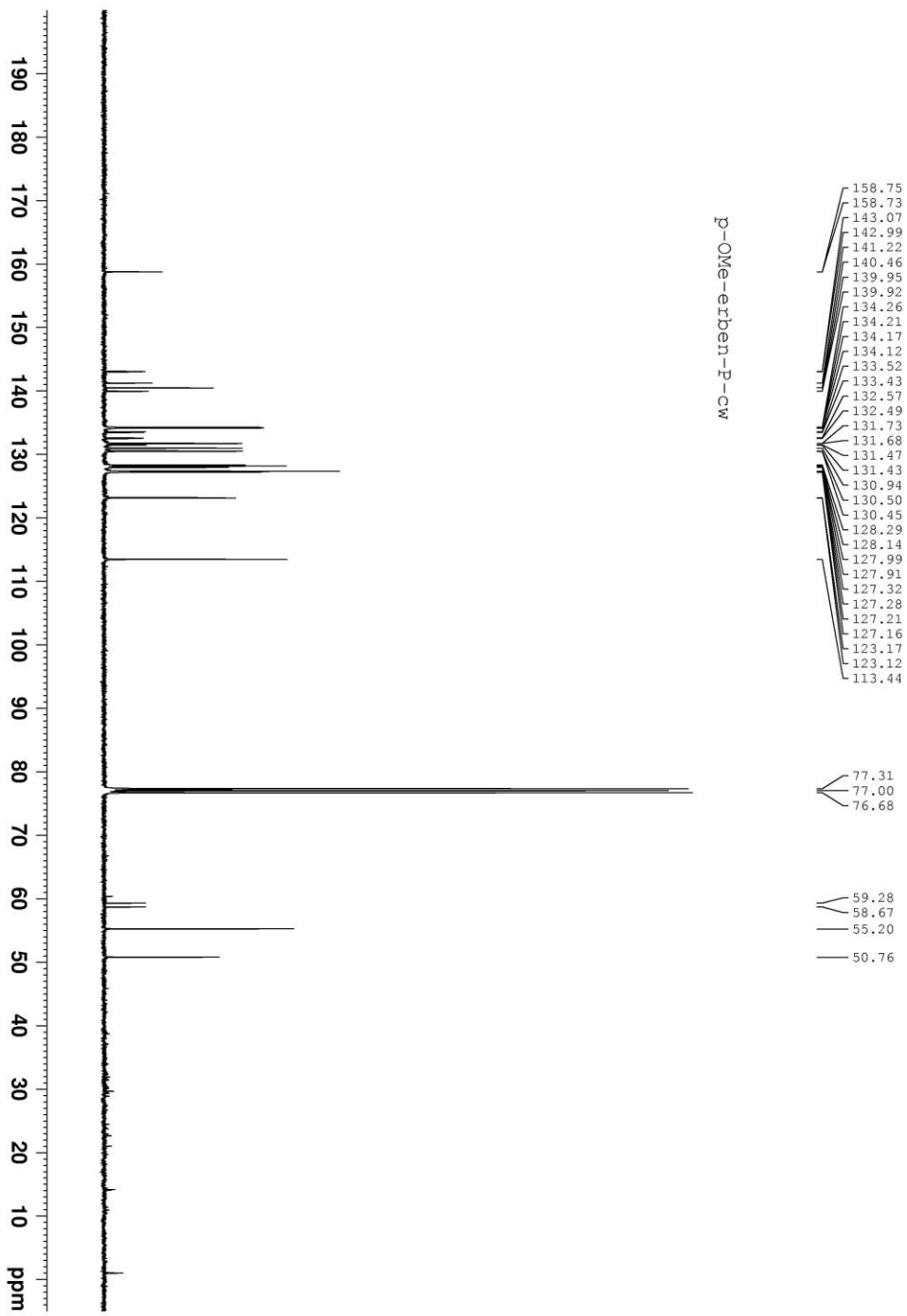


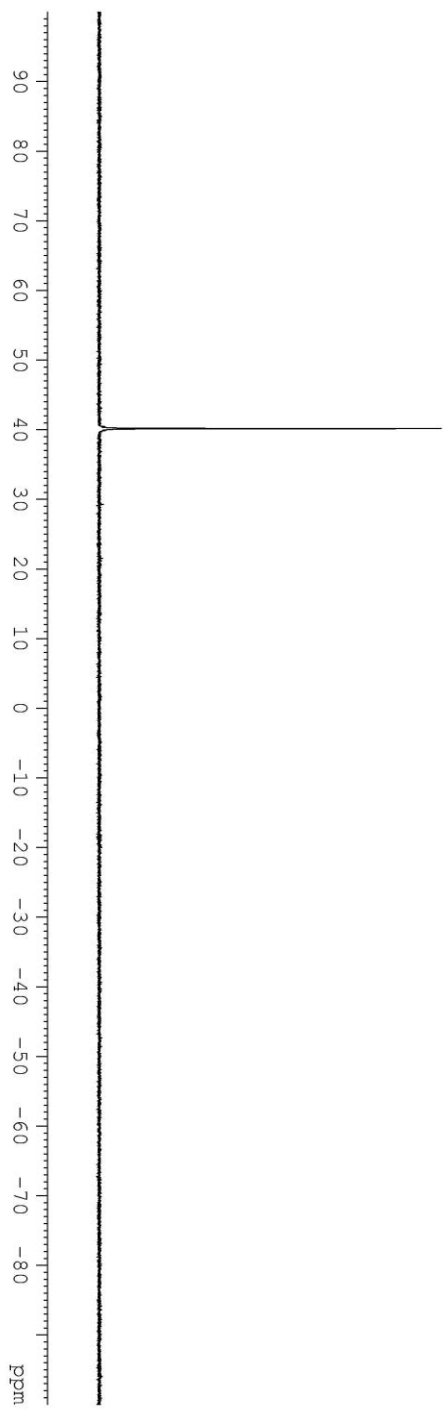




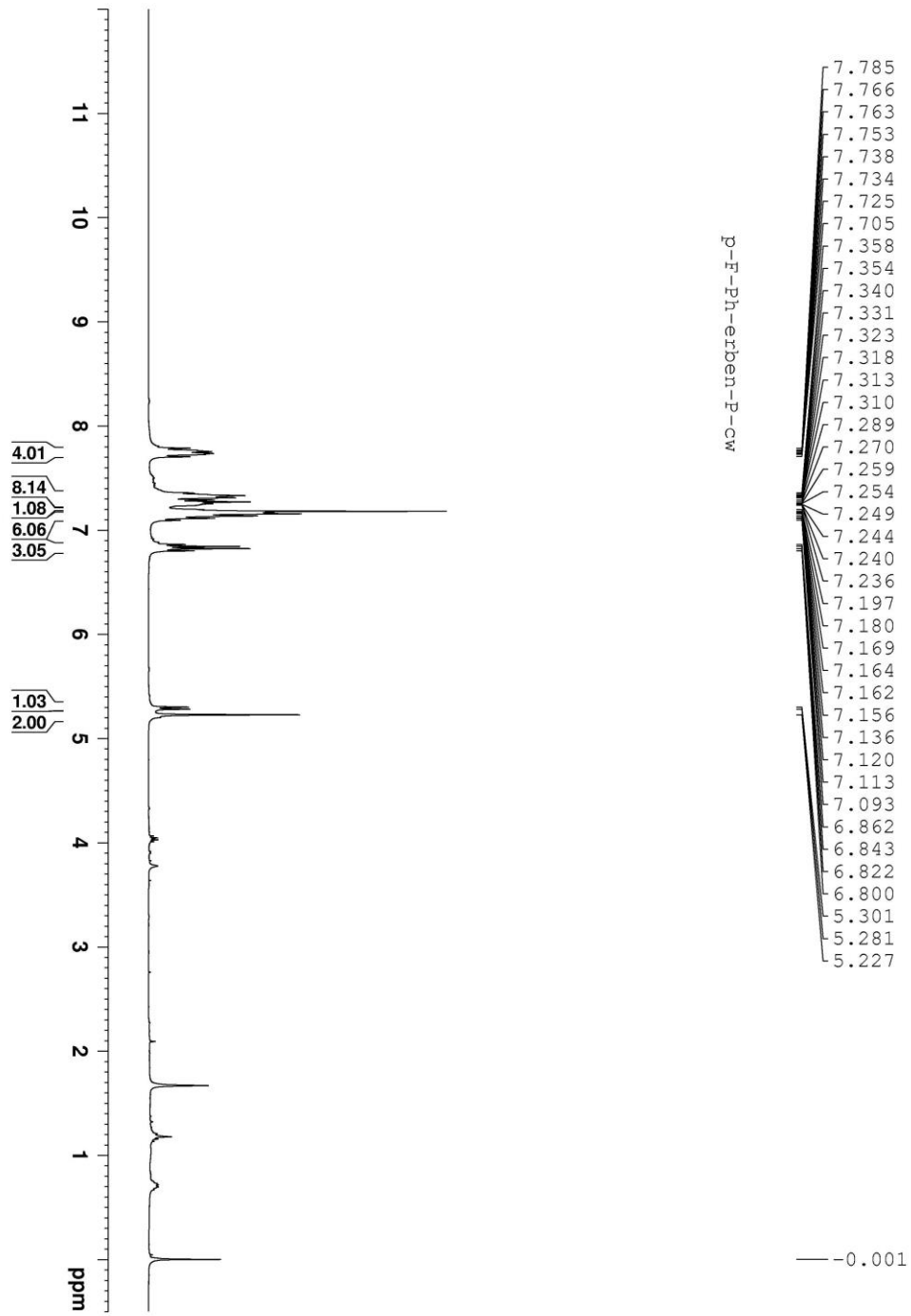
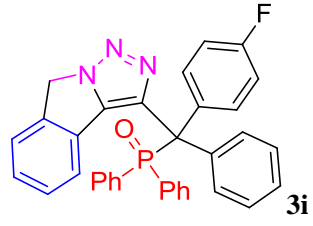
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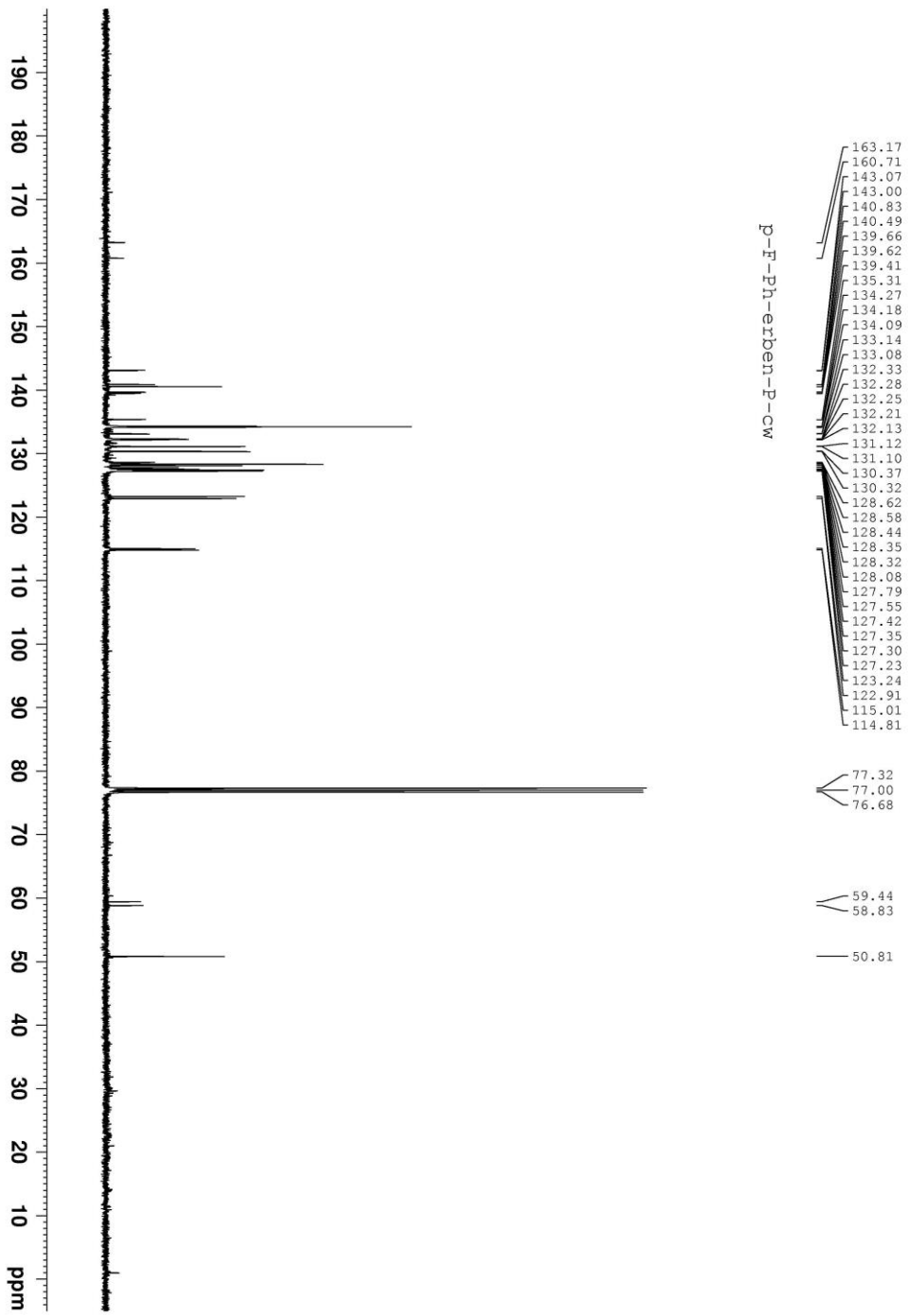


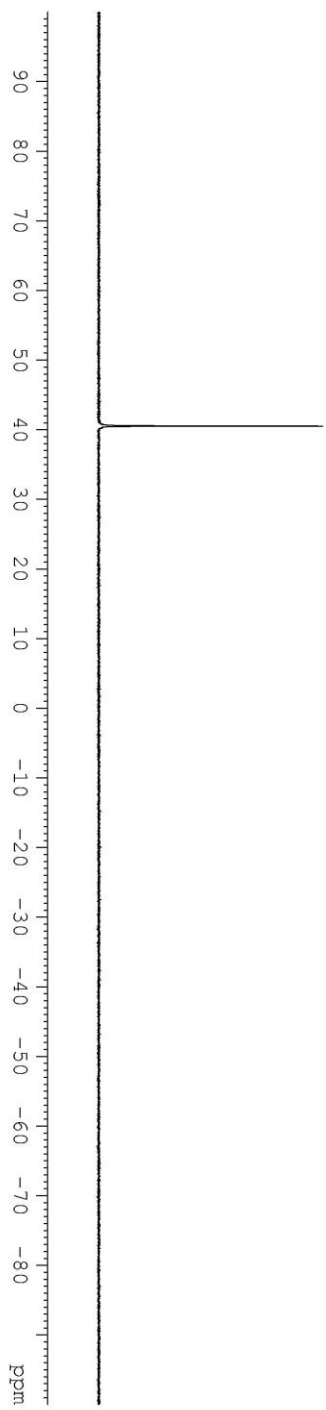




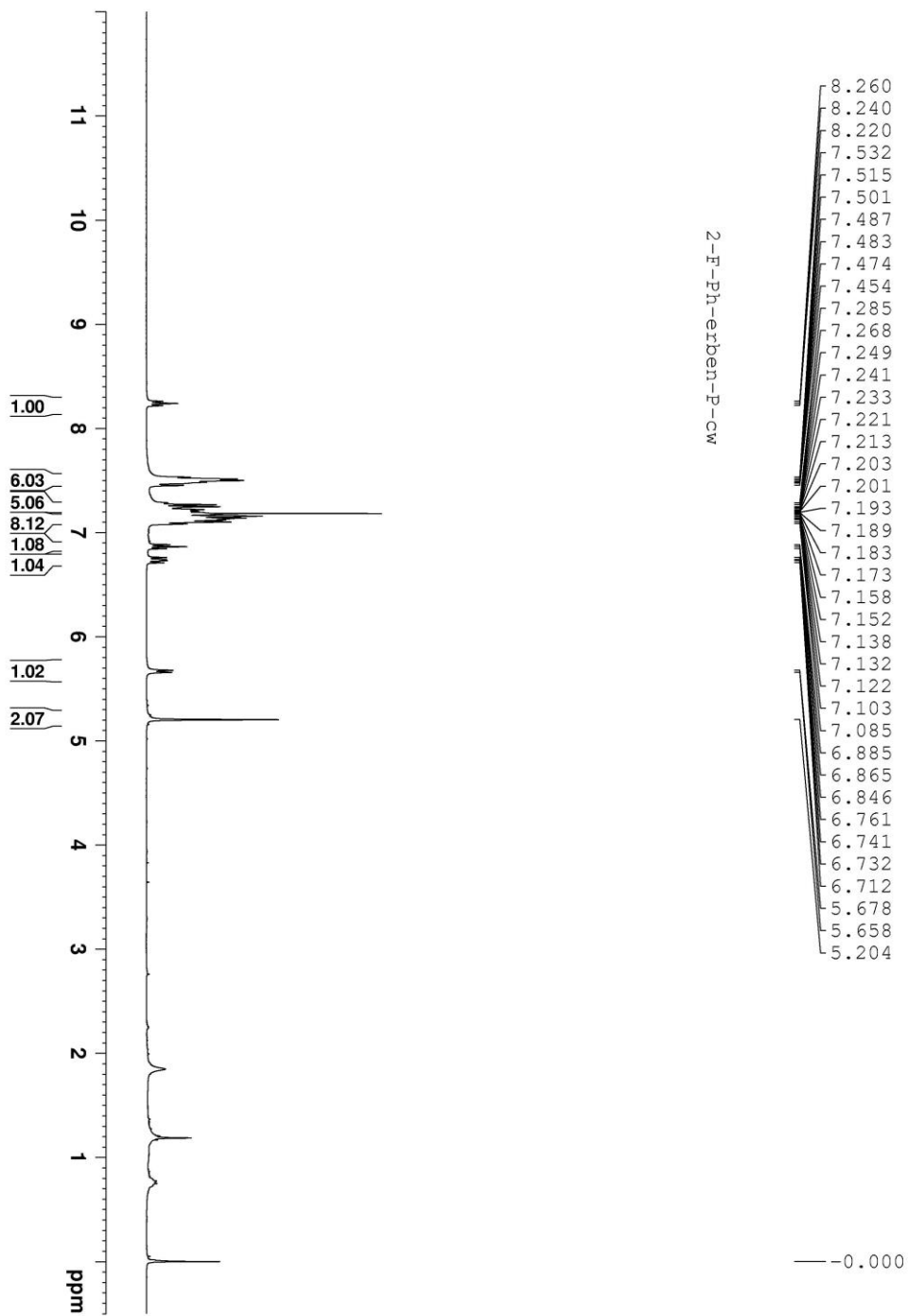
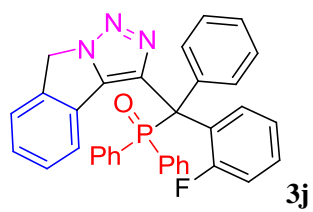
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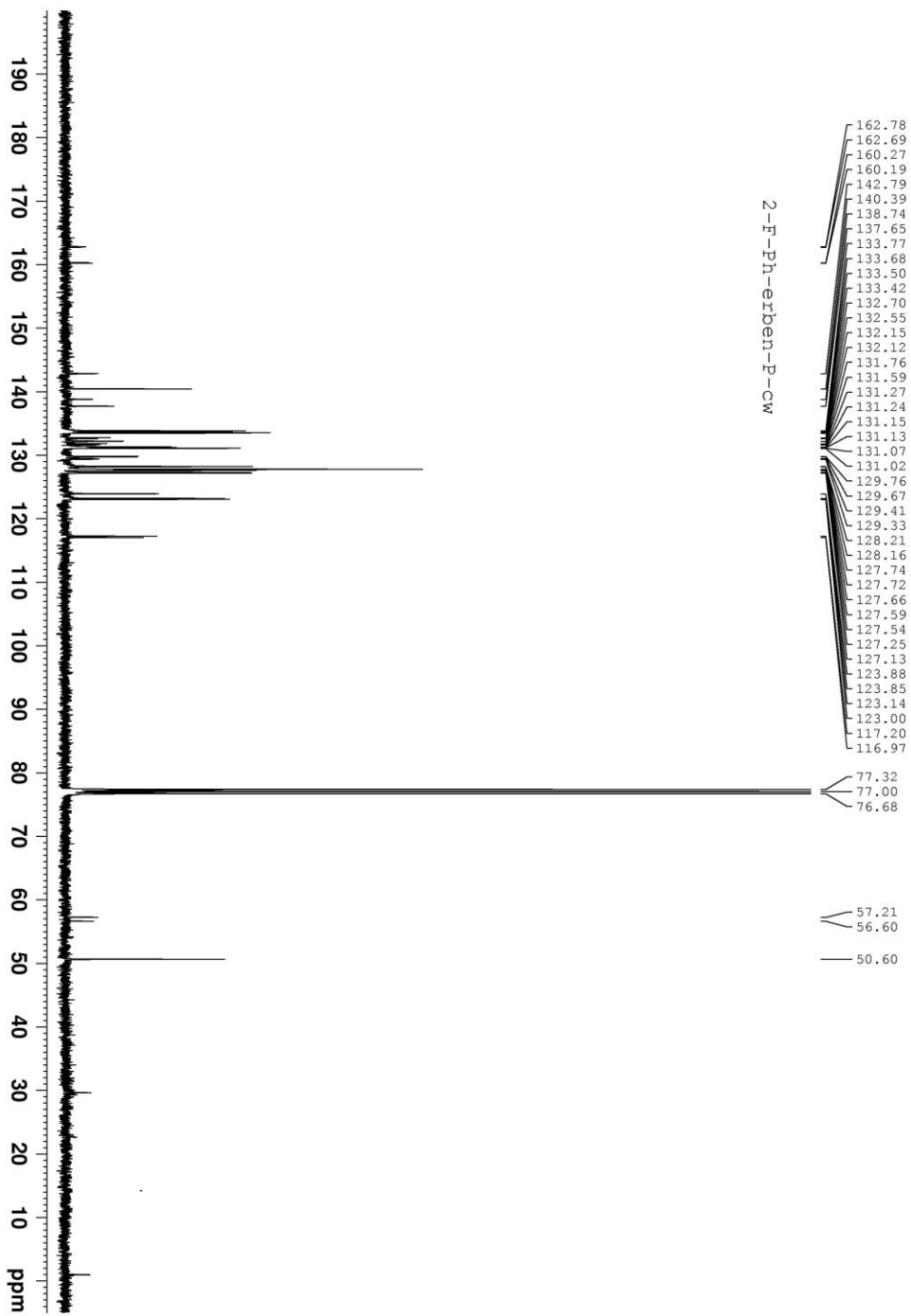






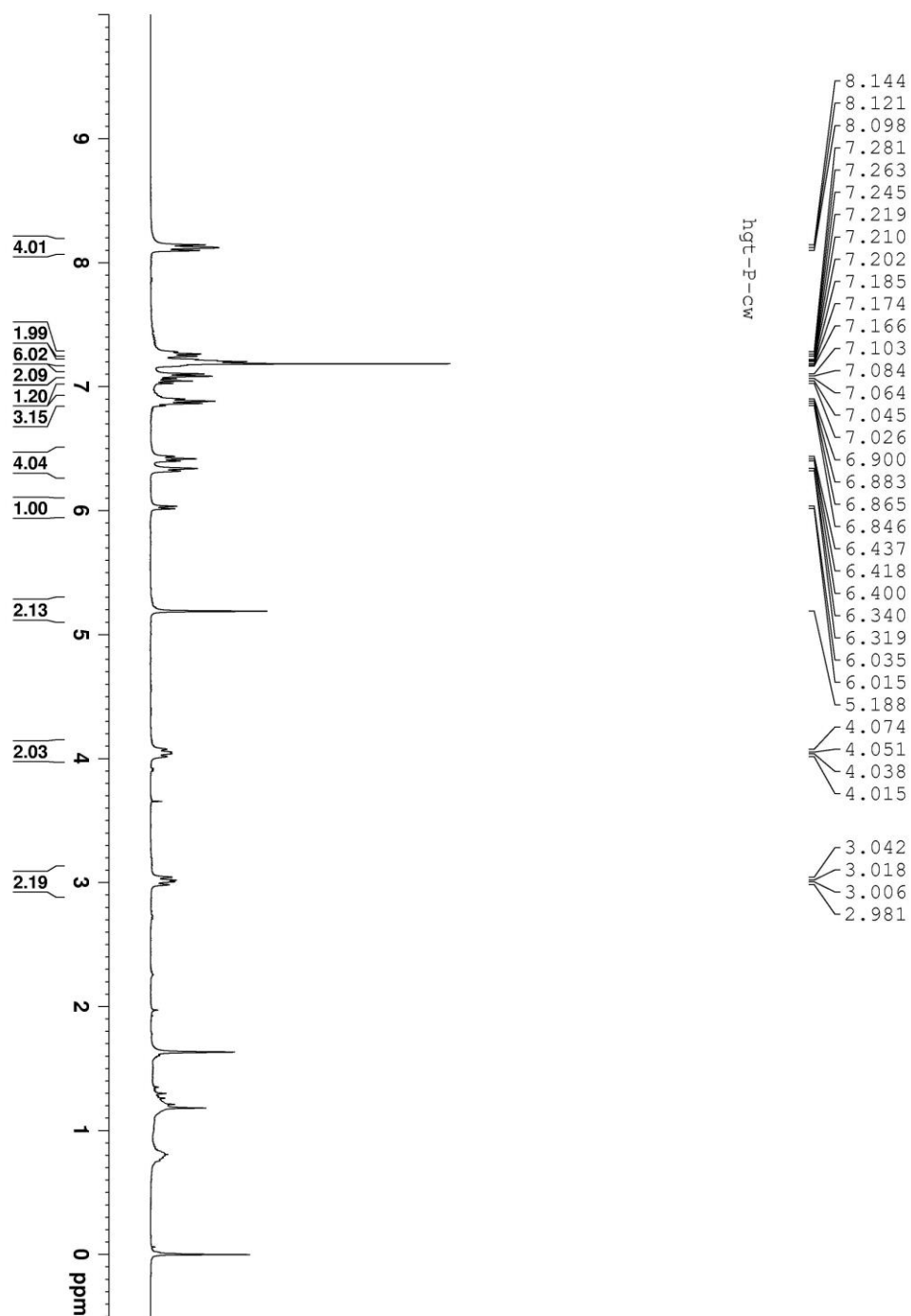
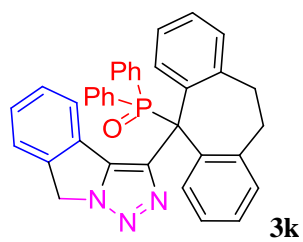
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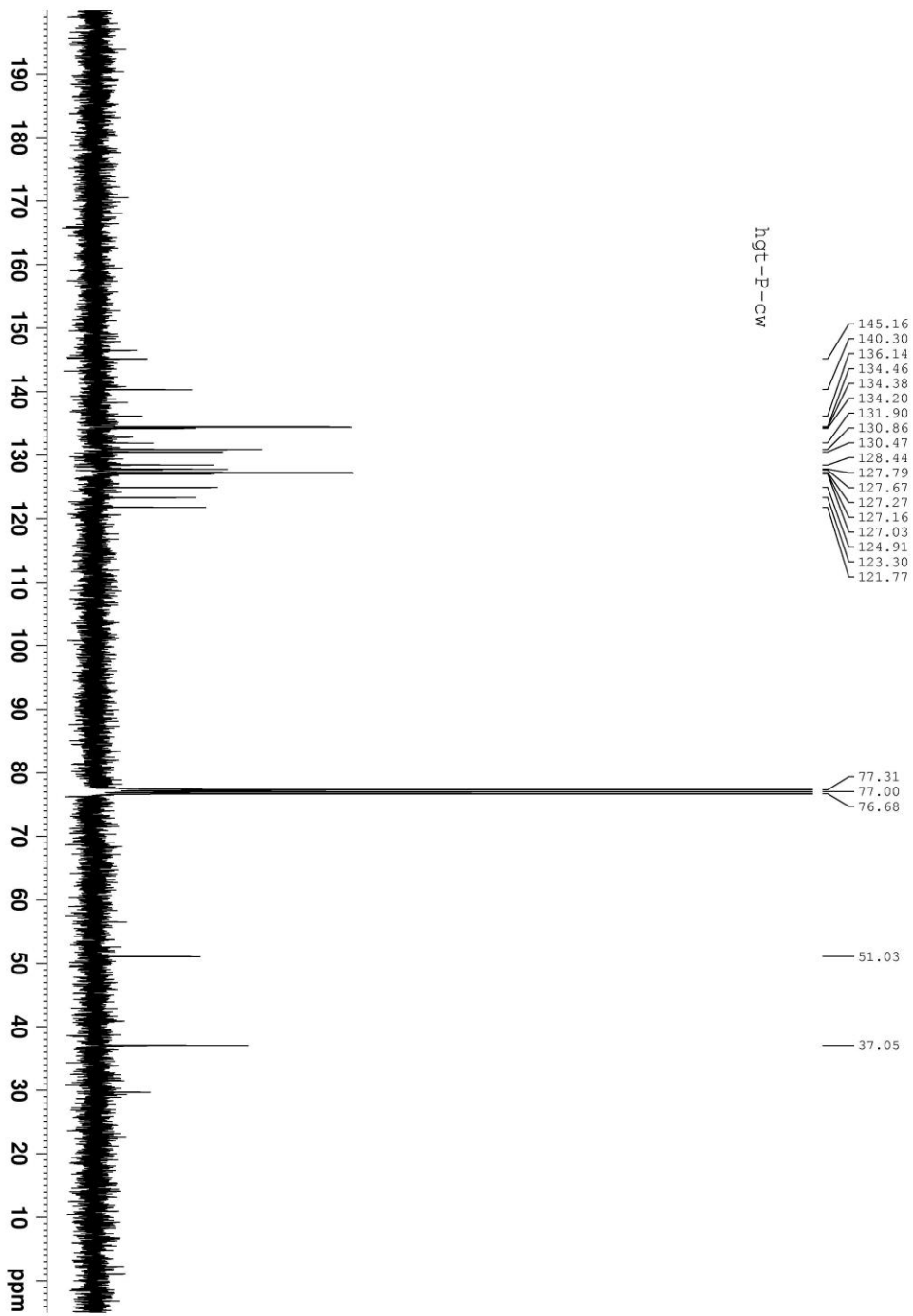


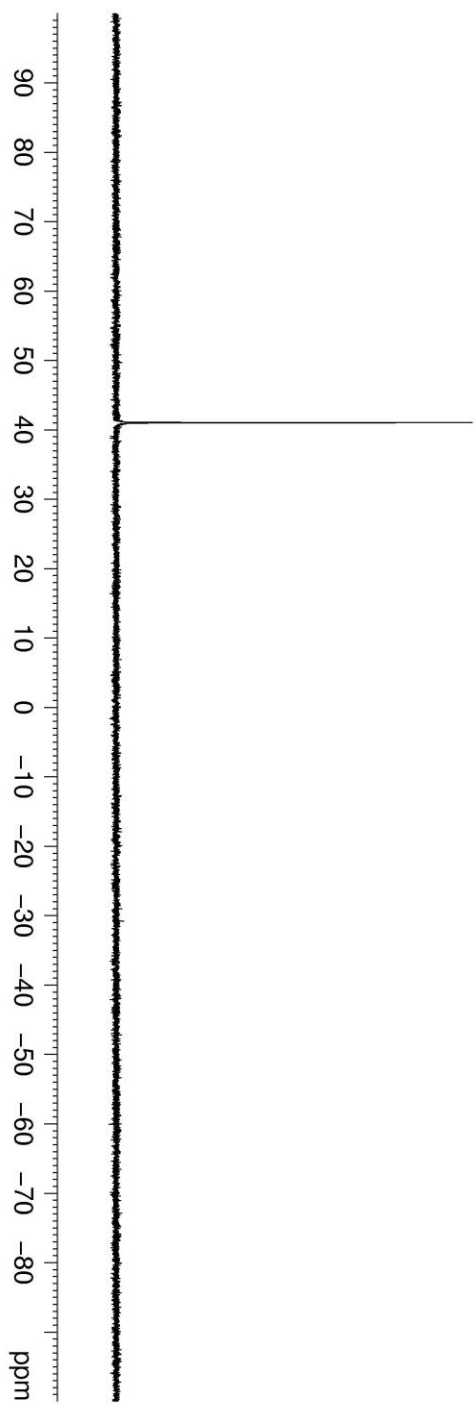




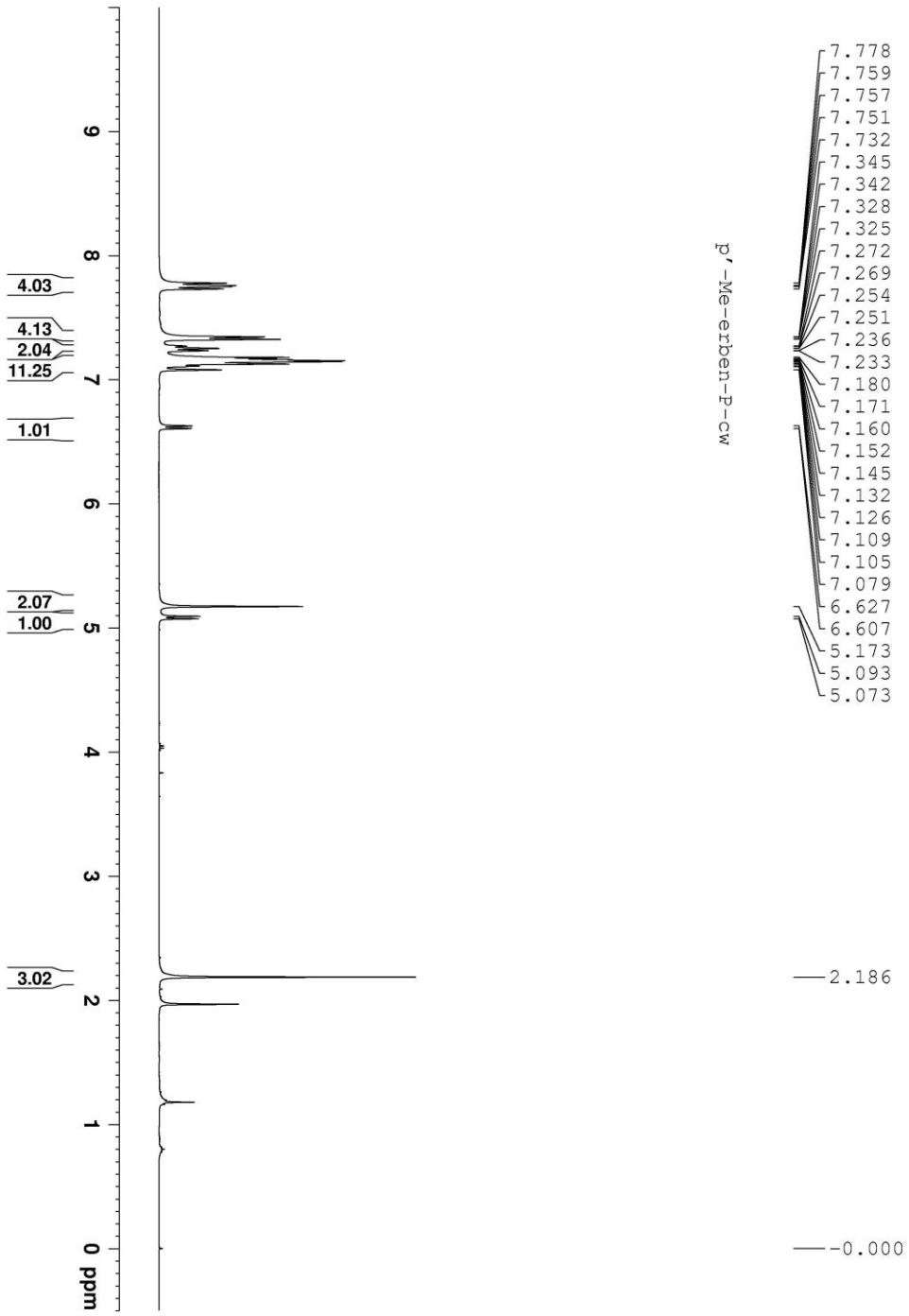
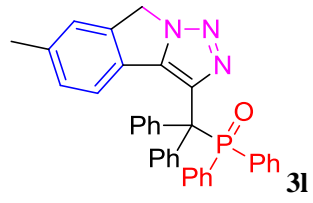
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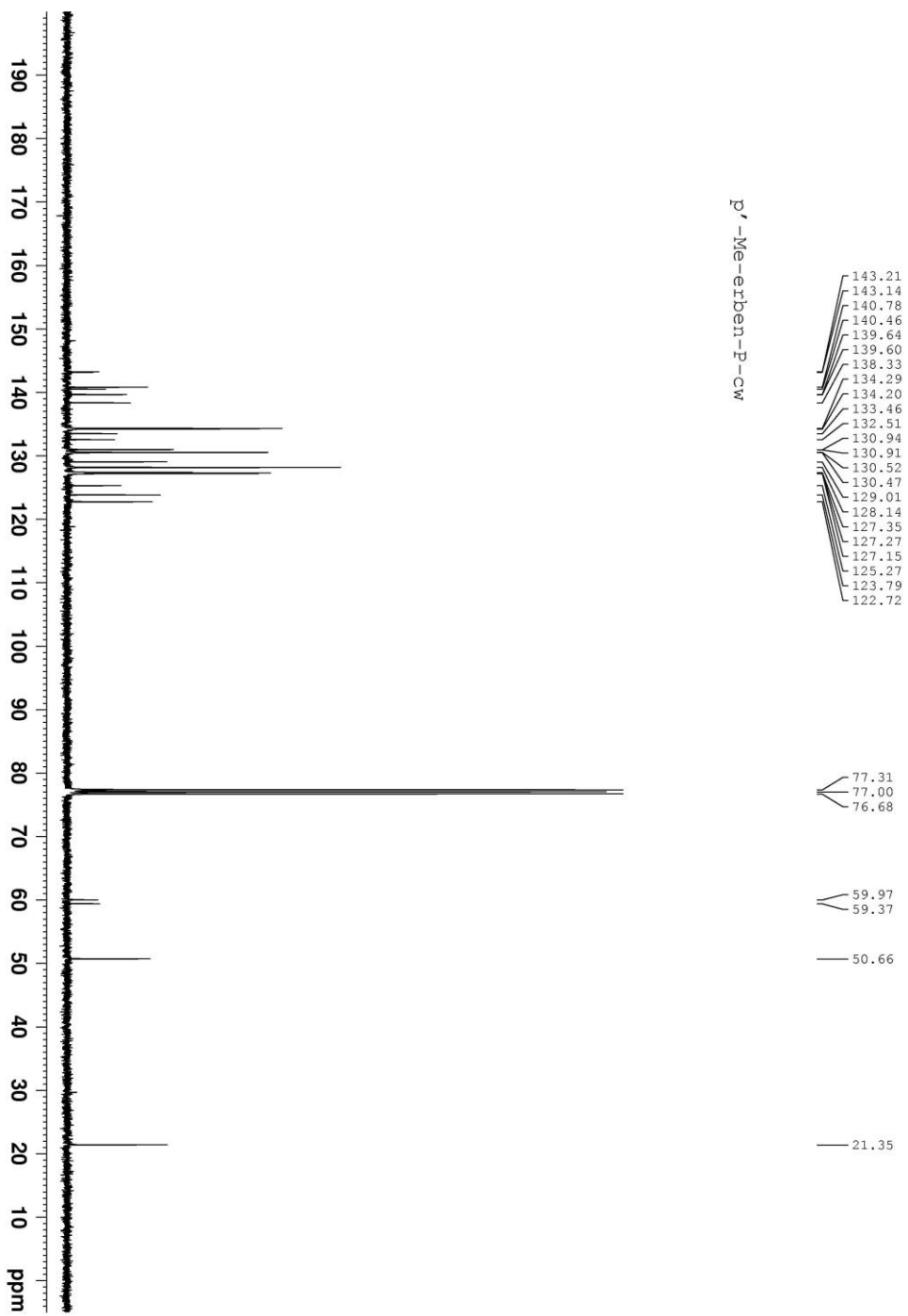


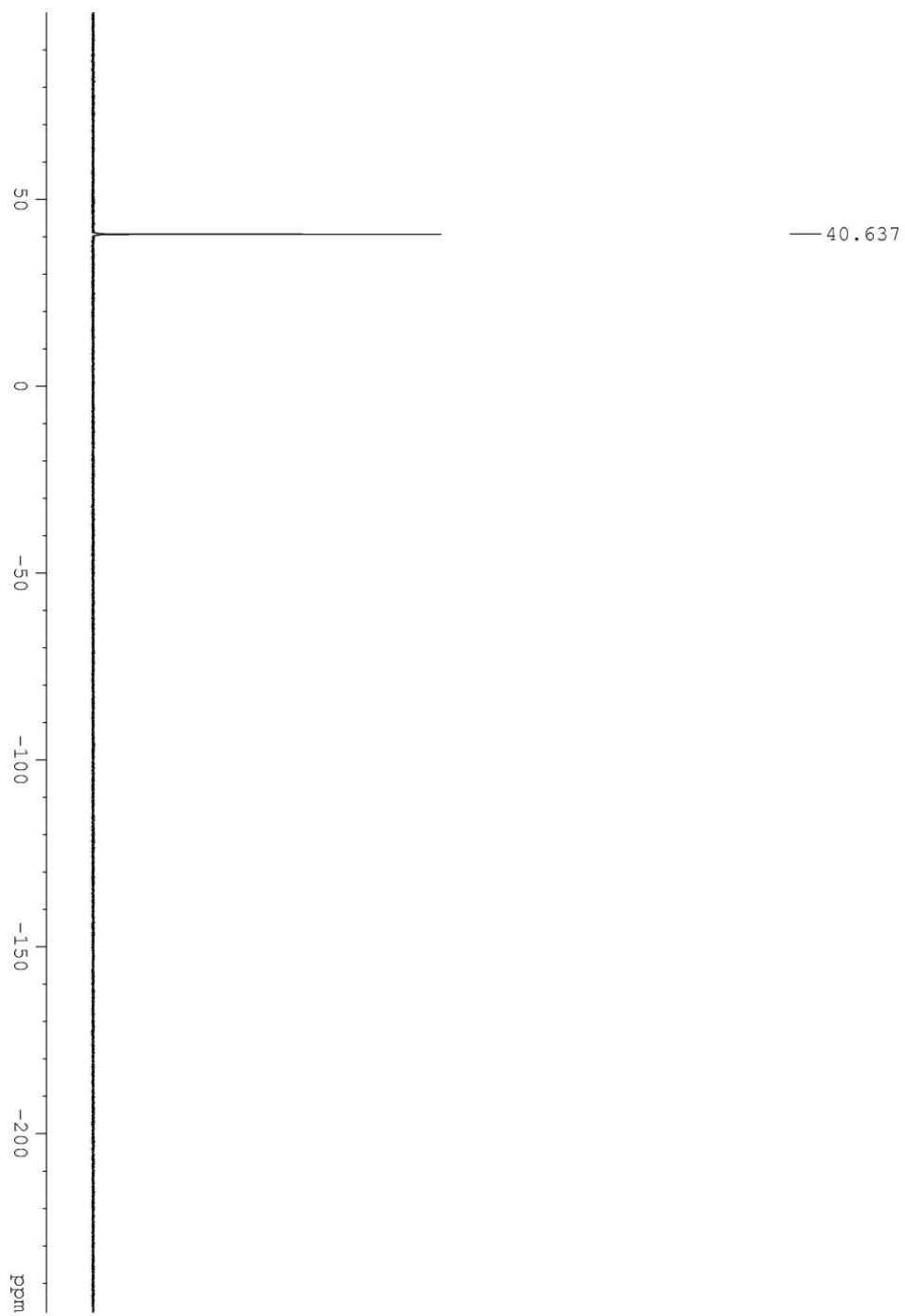


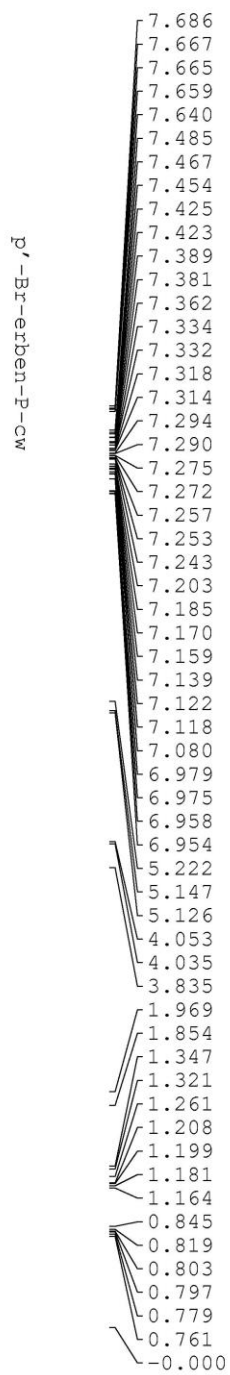
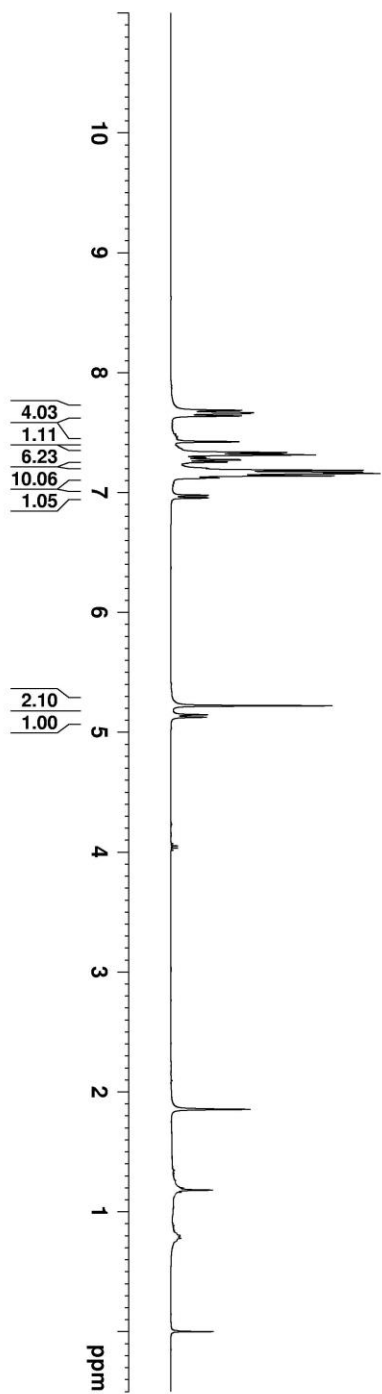
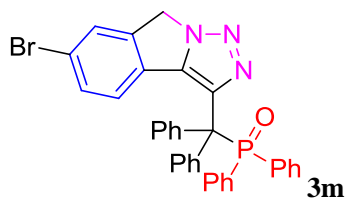


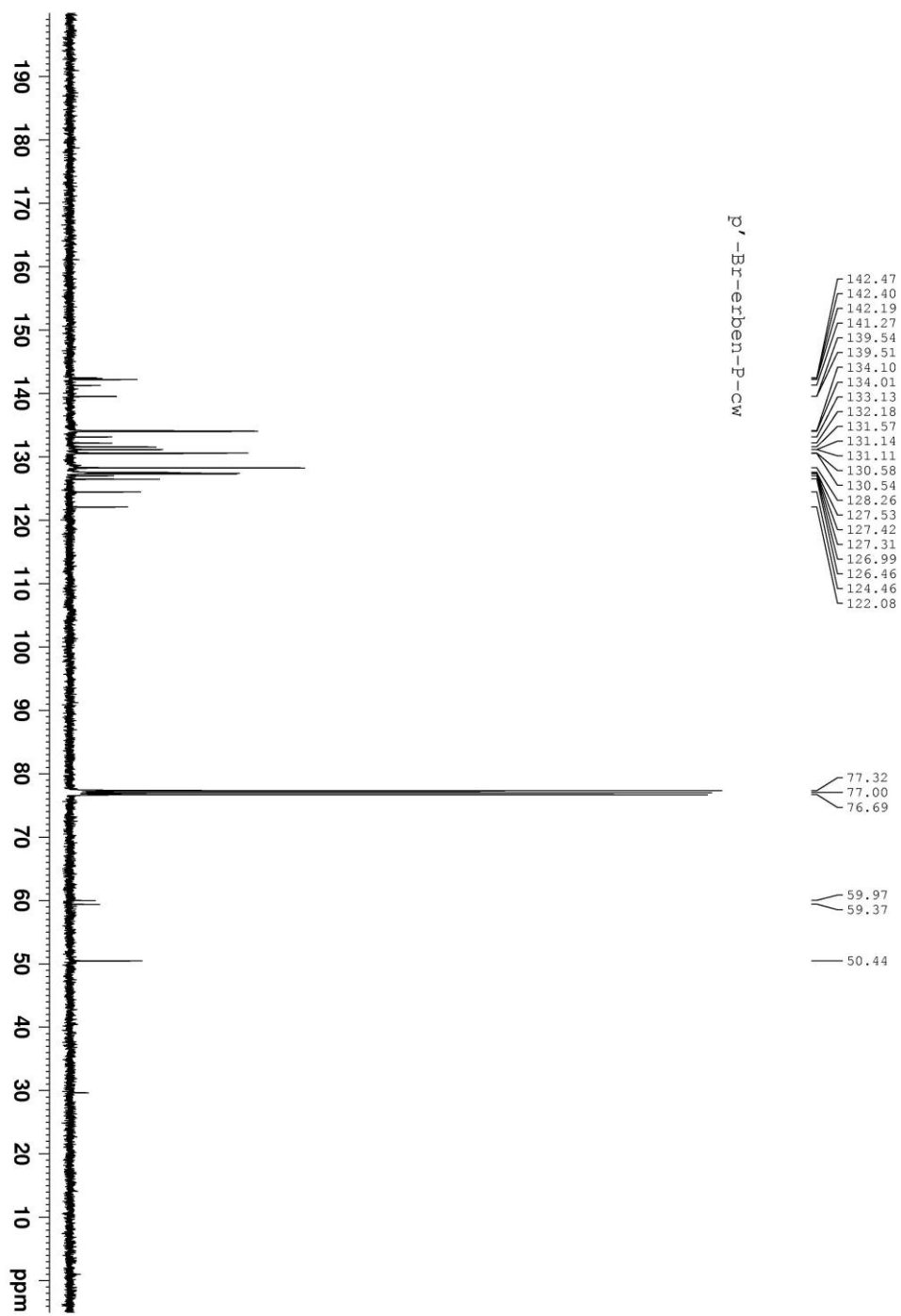
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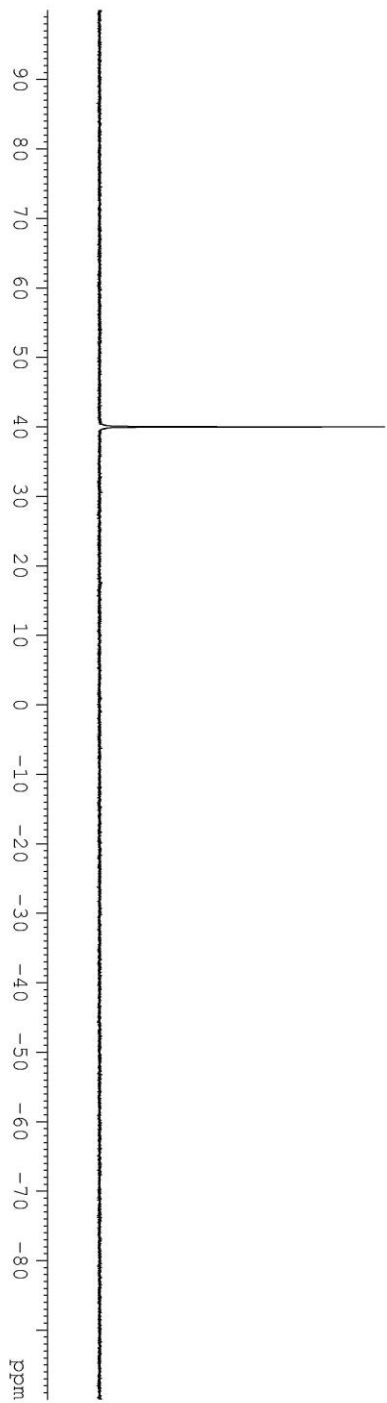




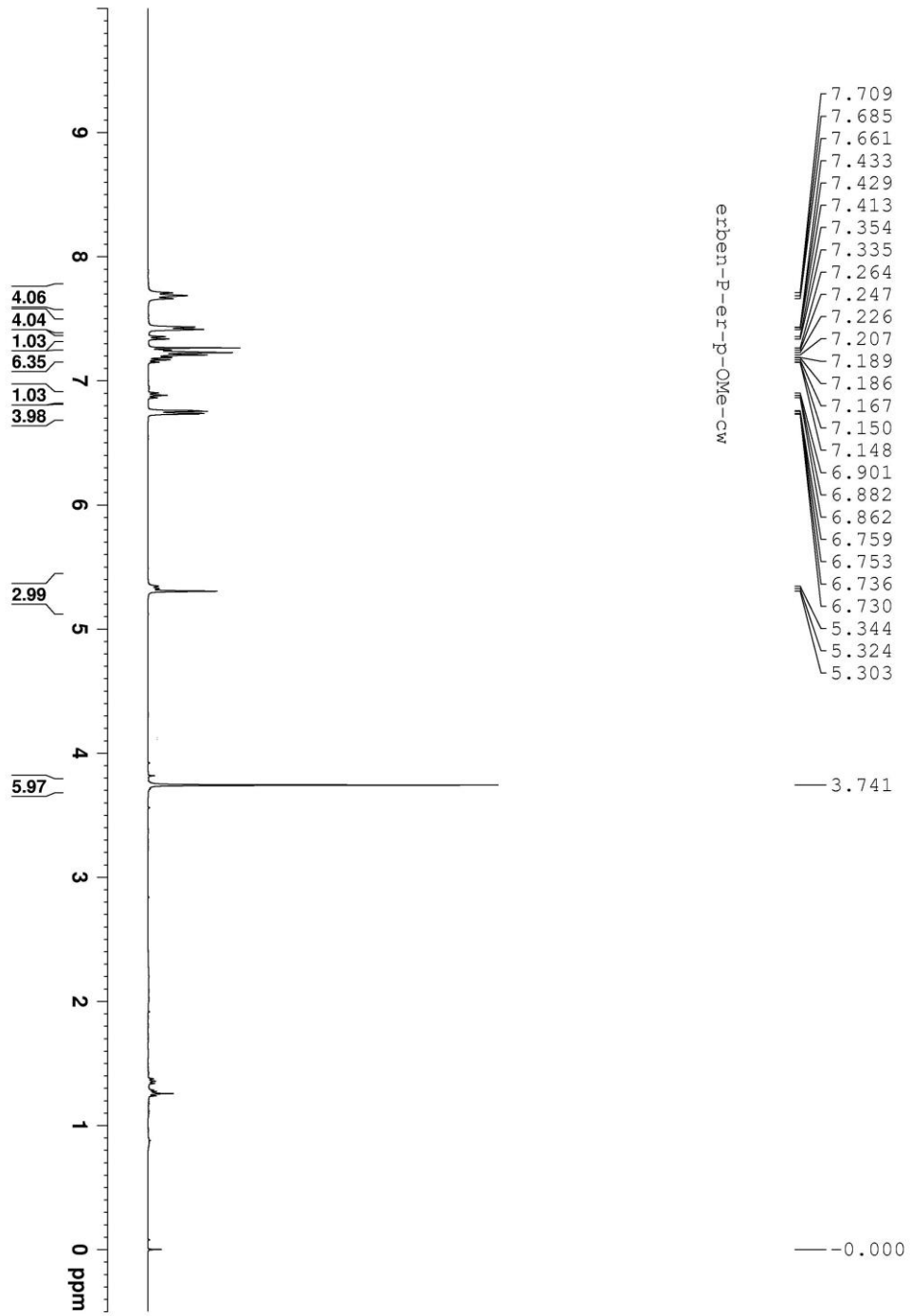
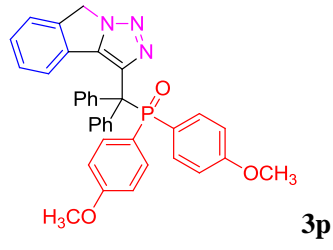


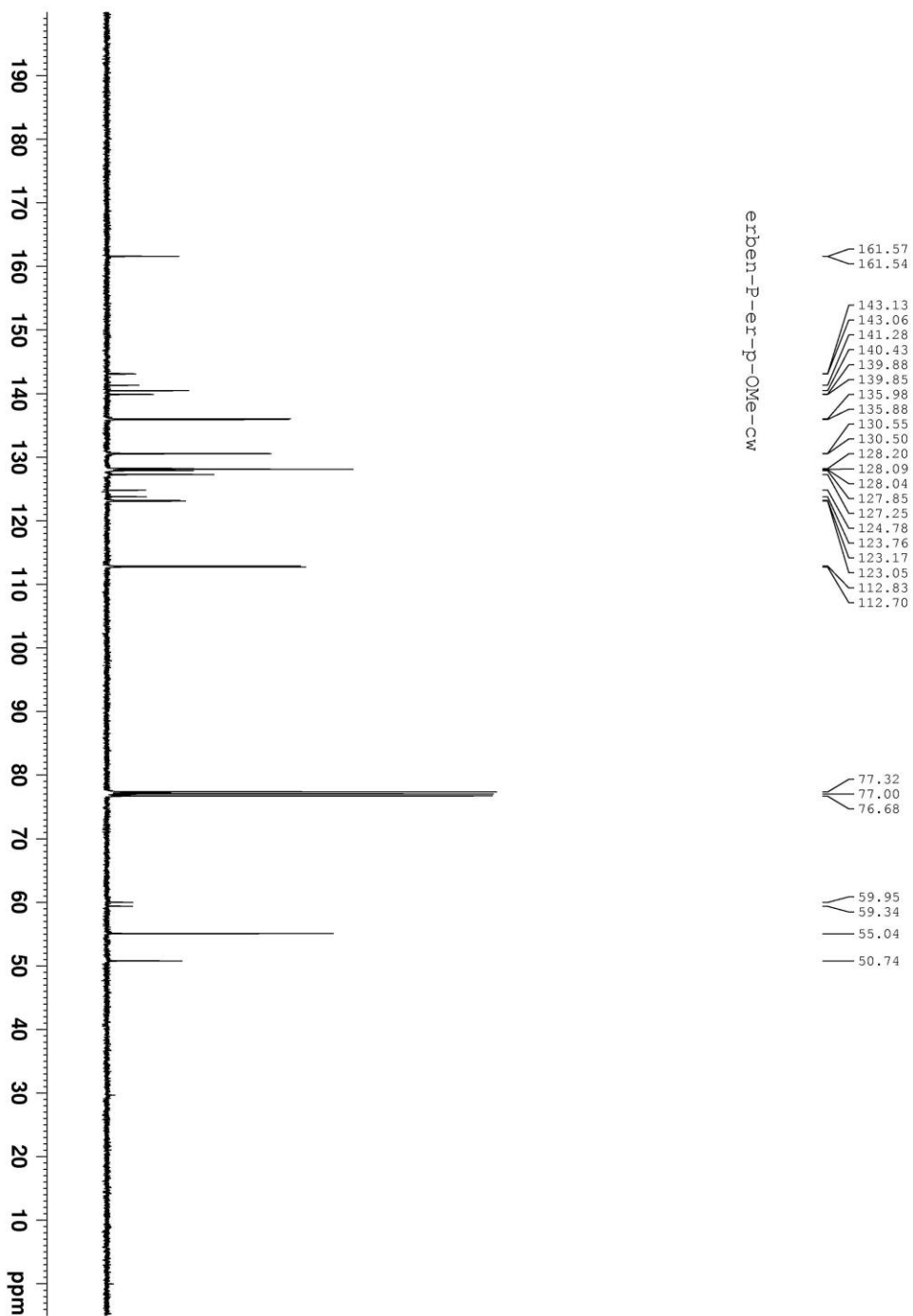


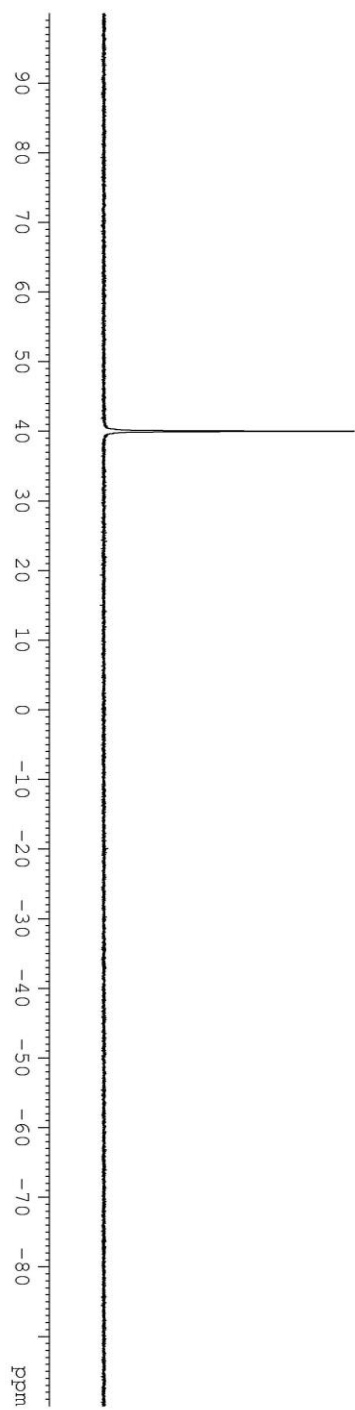




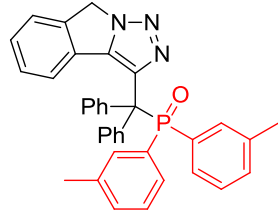
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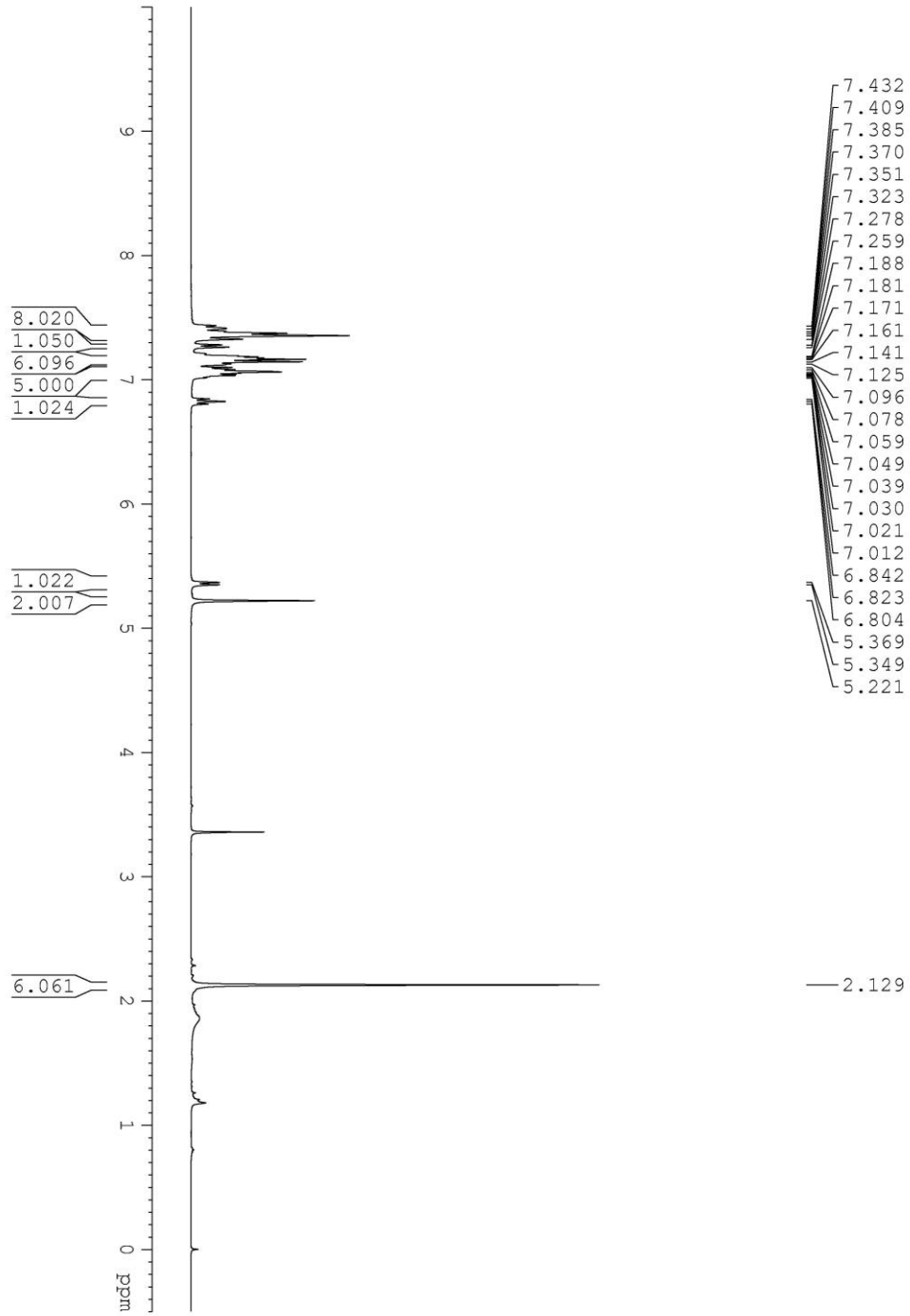


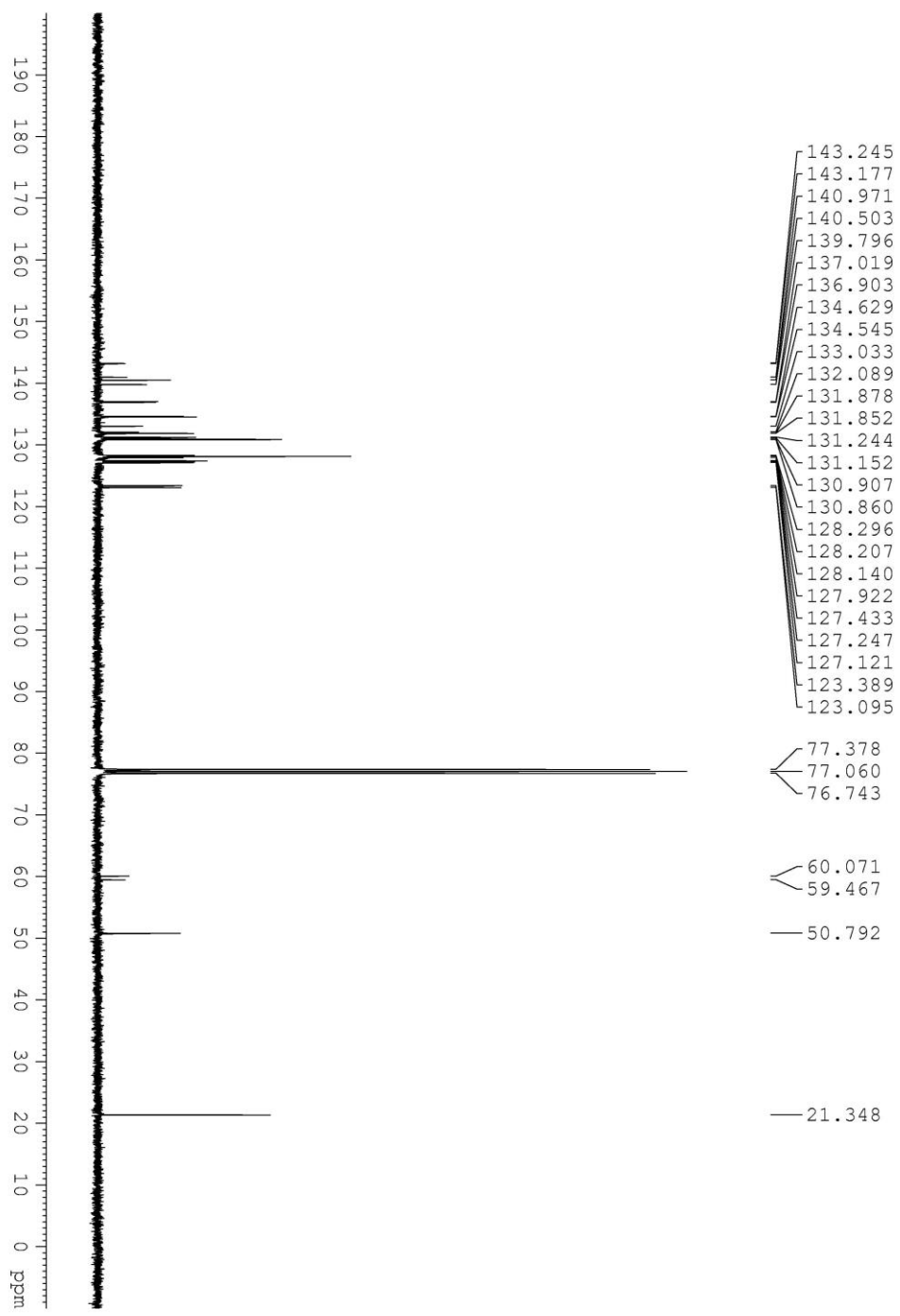


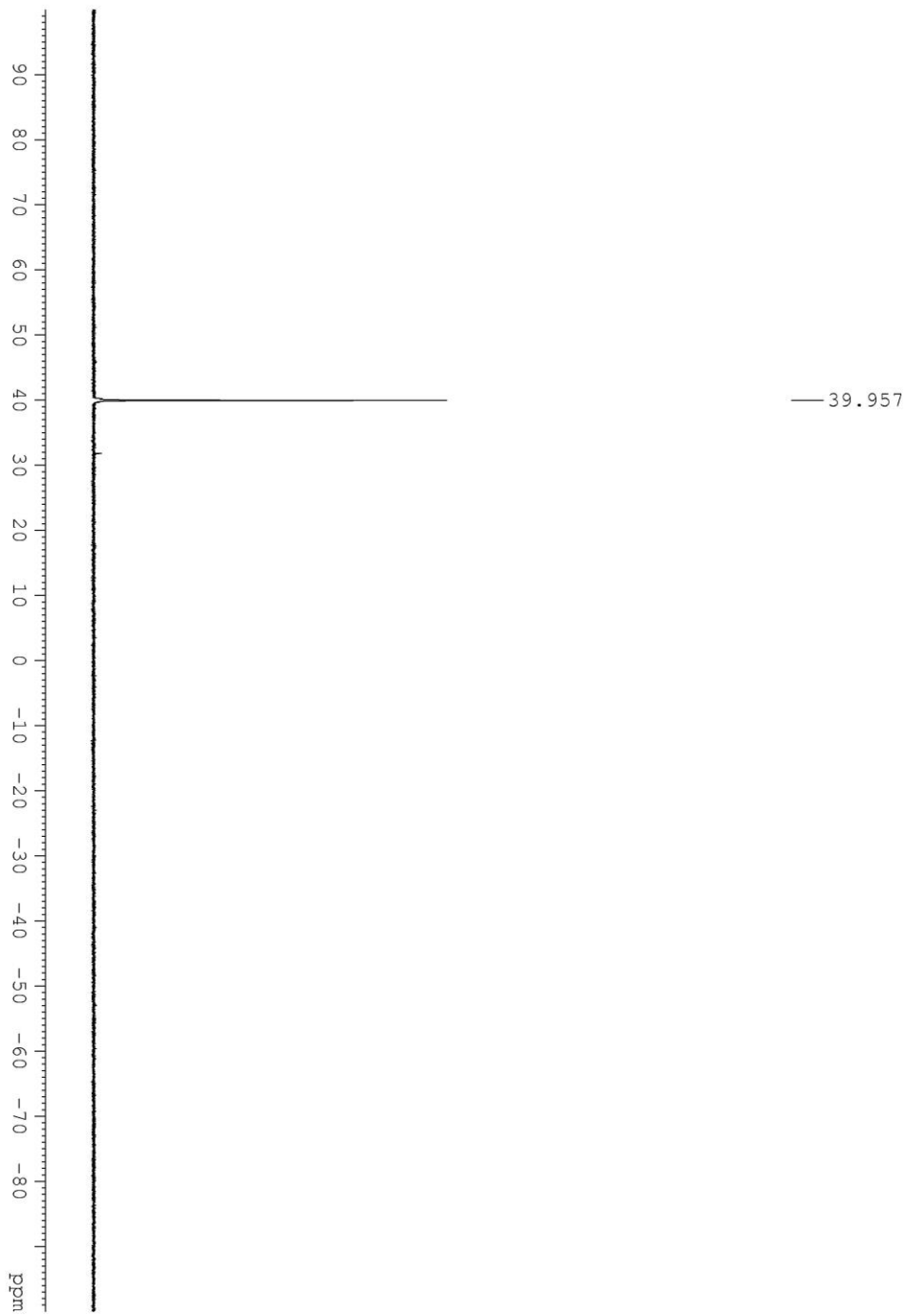
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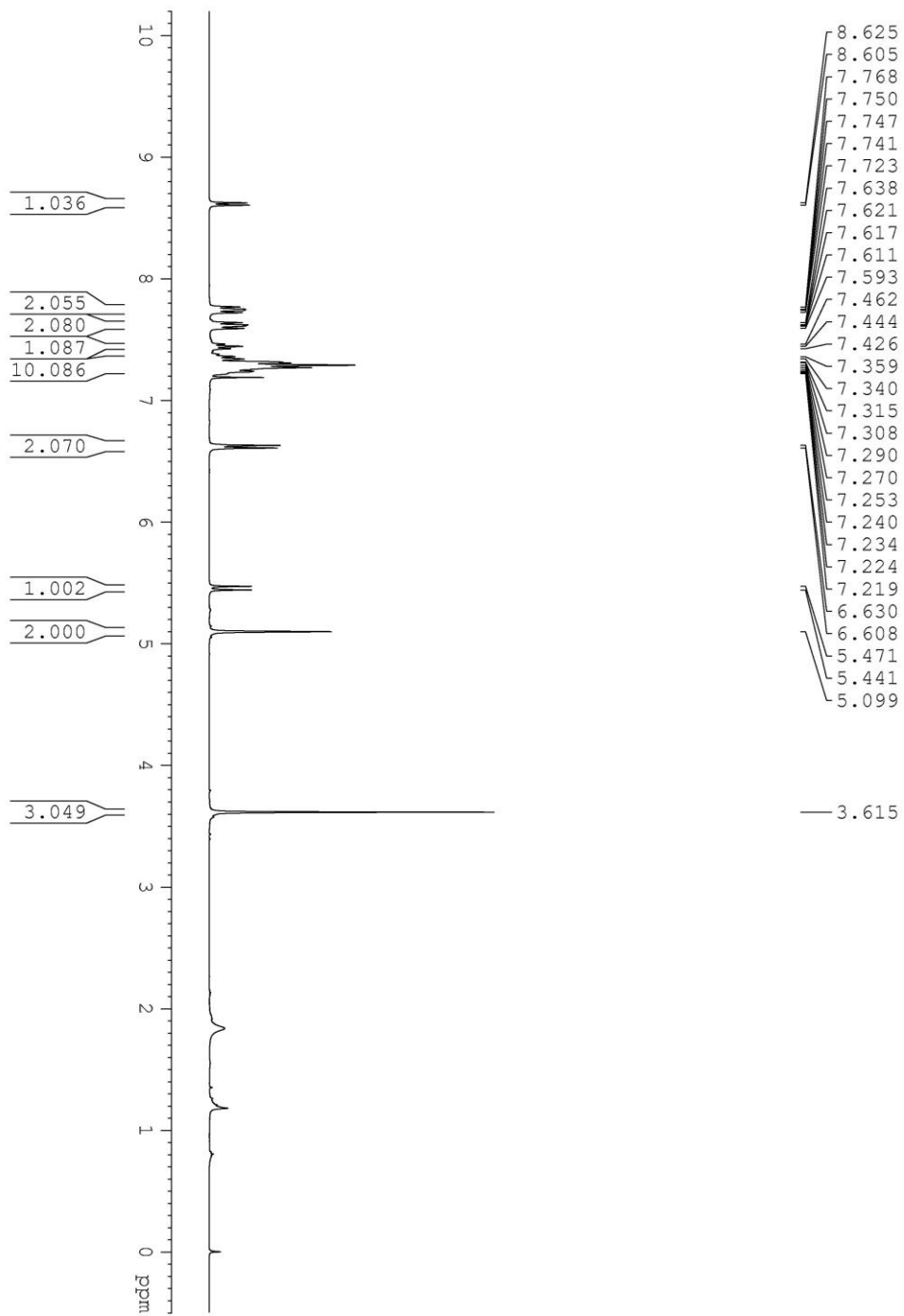
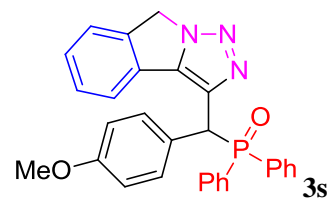


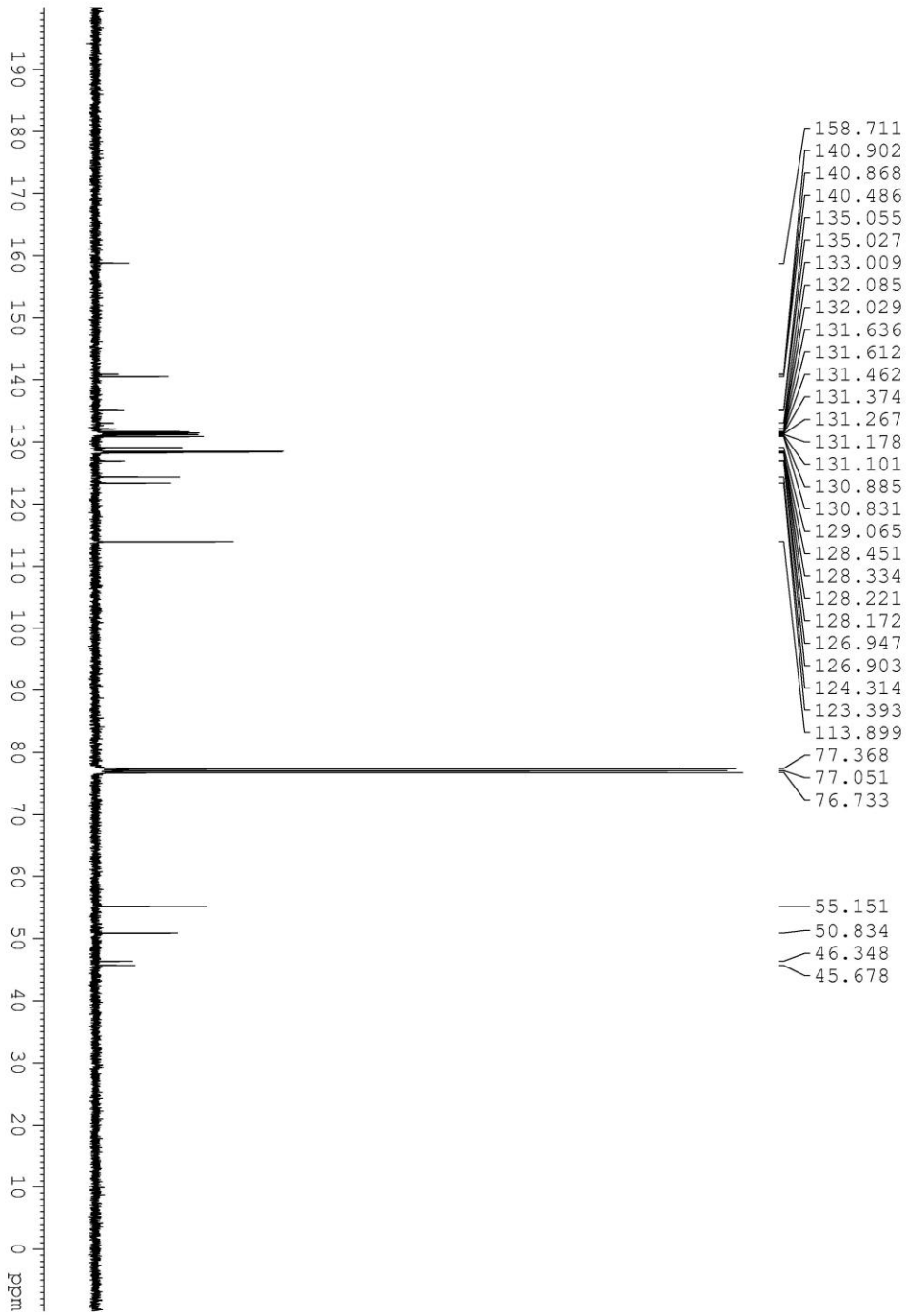
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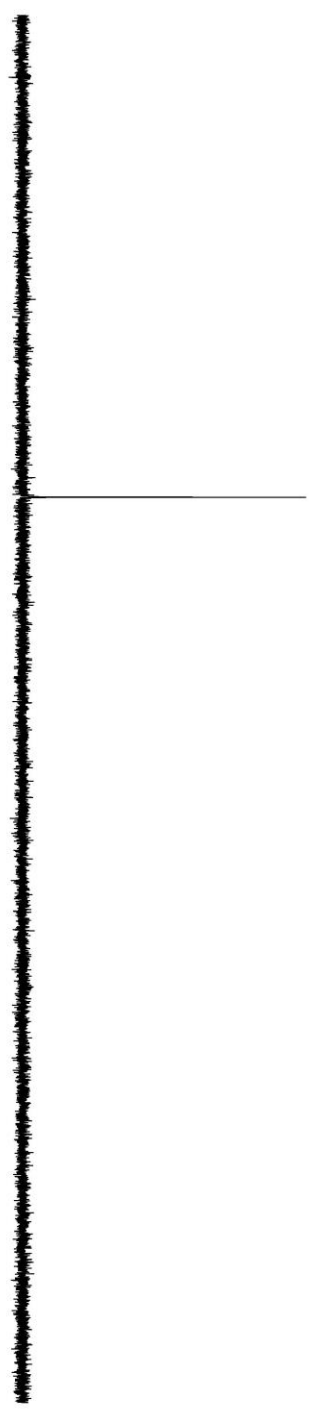




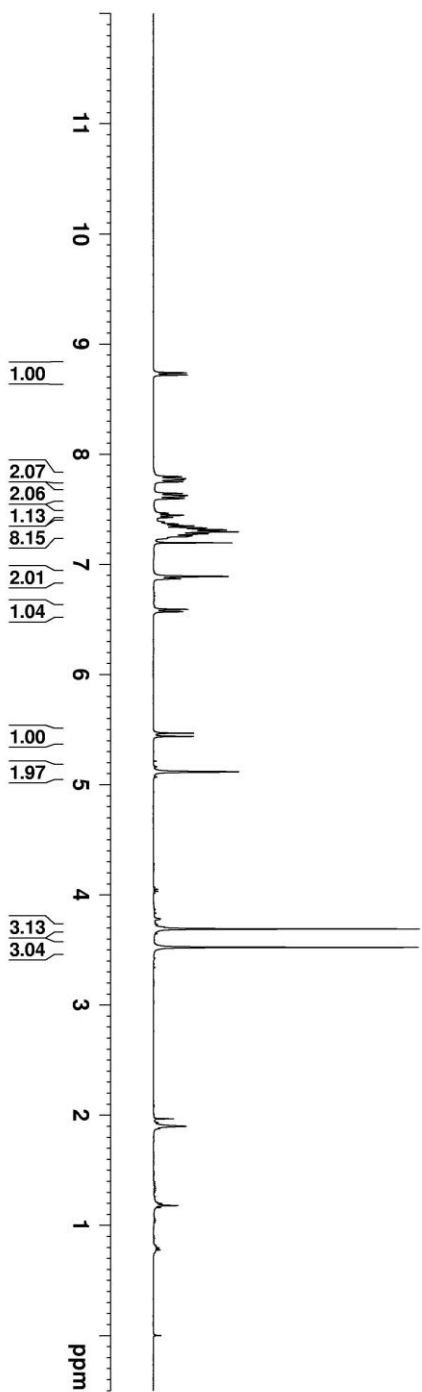
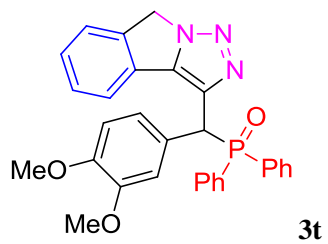




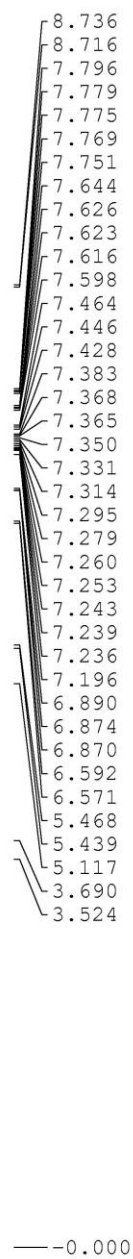
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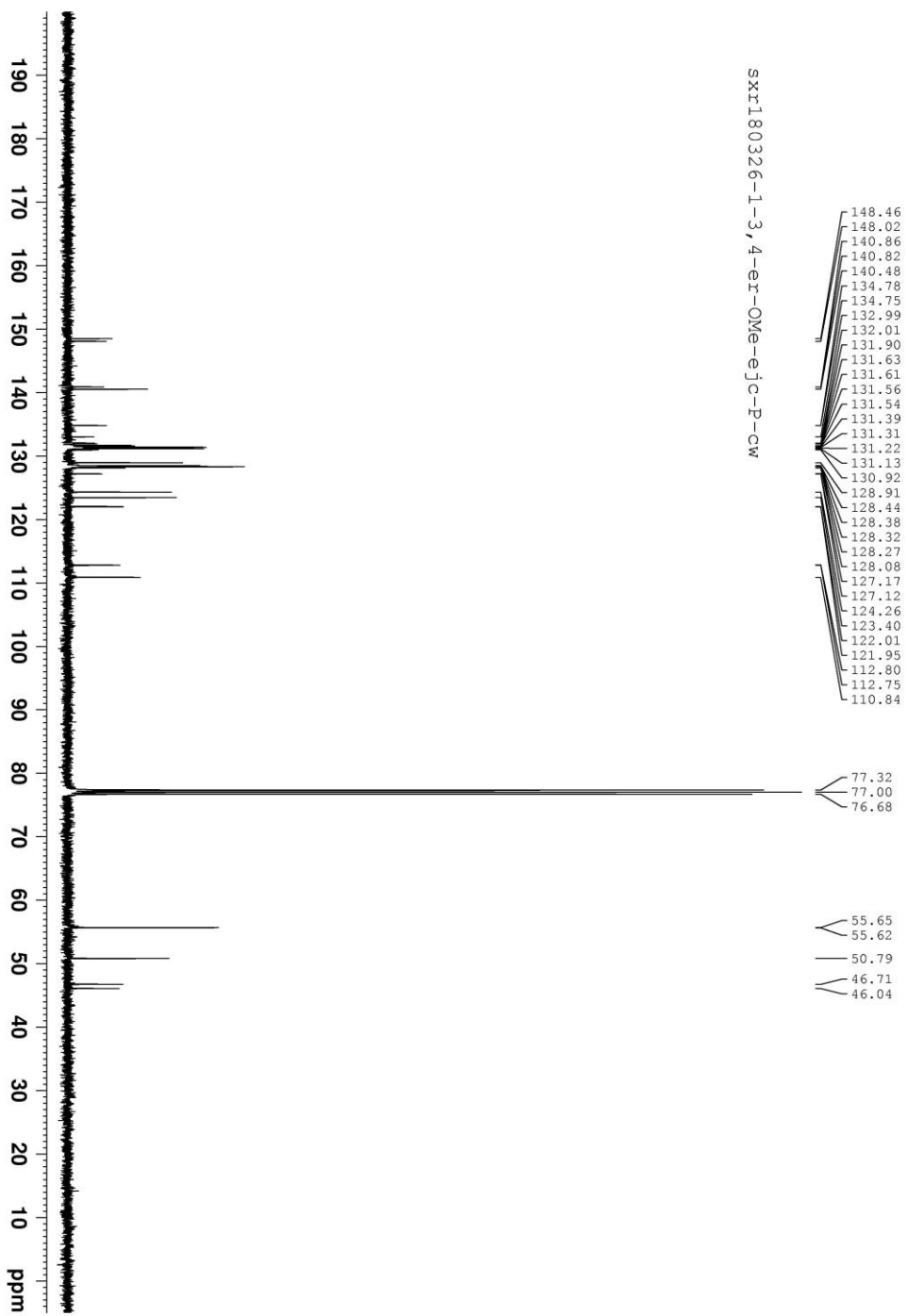


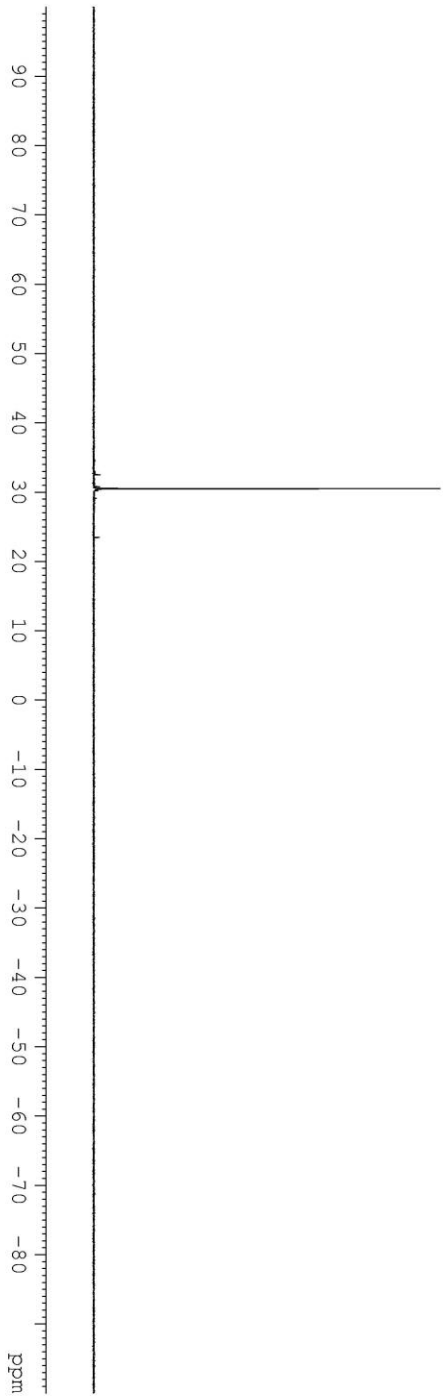
— 30.501



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— 30.506