Supplementary Material

Combination of $NH_2OH \cdot HCl$ and $NaIO_4$: a new and mild reagent for the synthesis of vicinal diiodo carbonyl compounds

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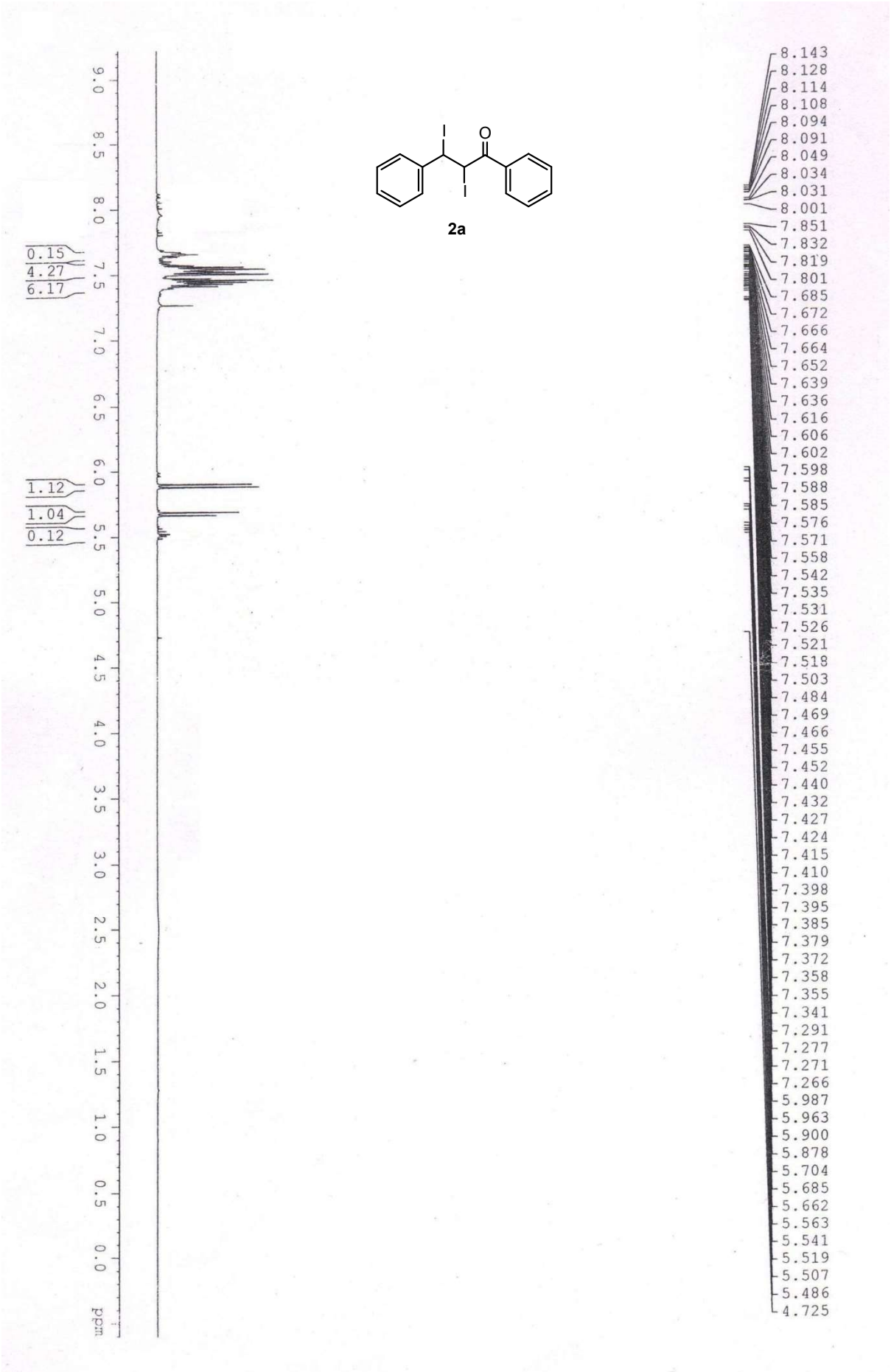

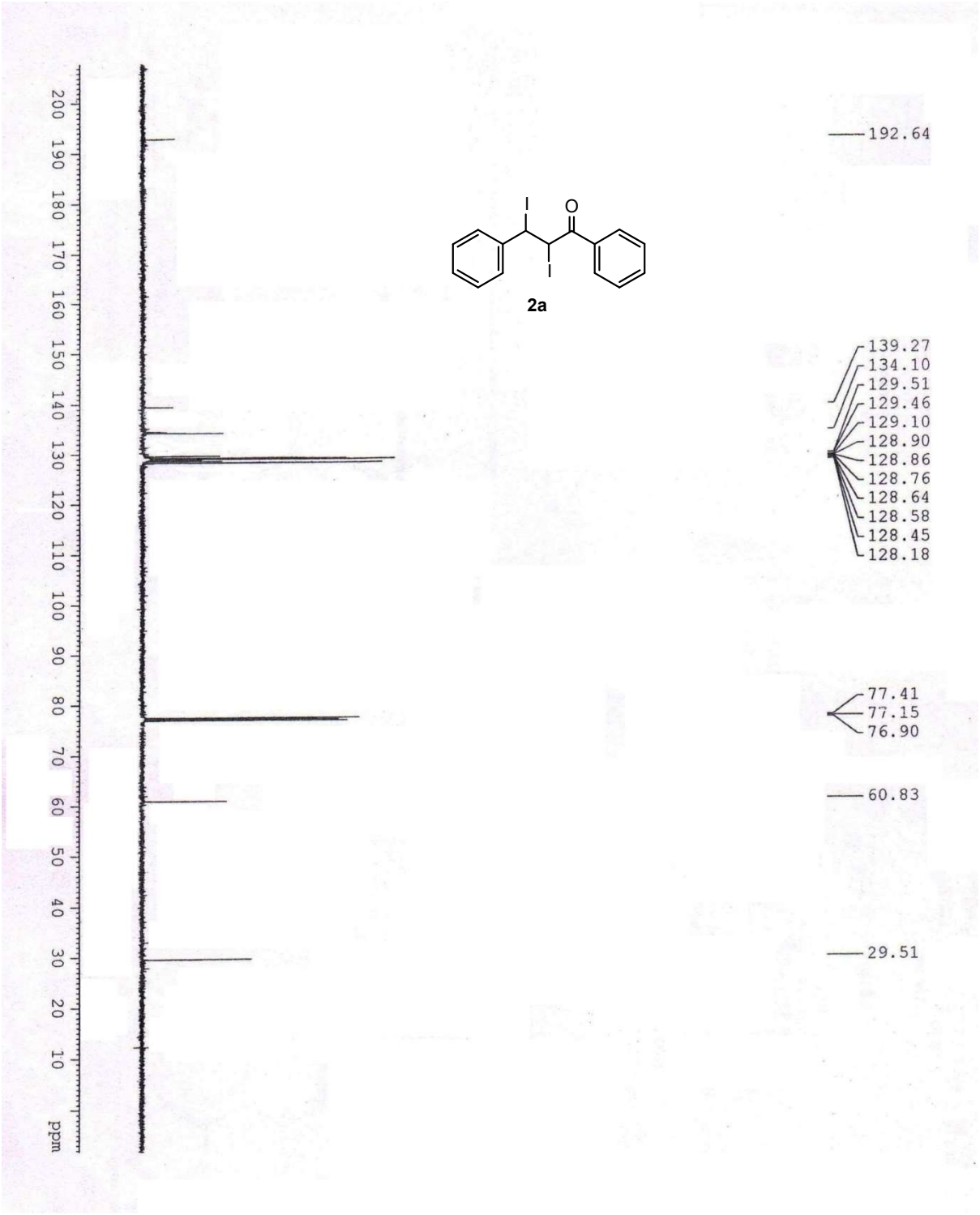

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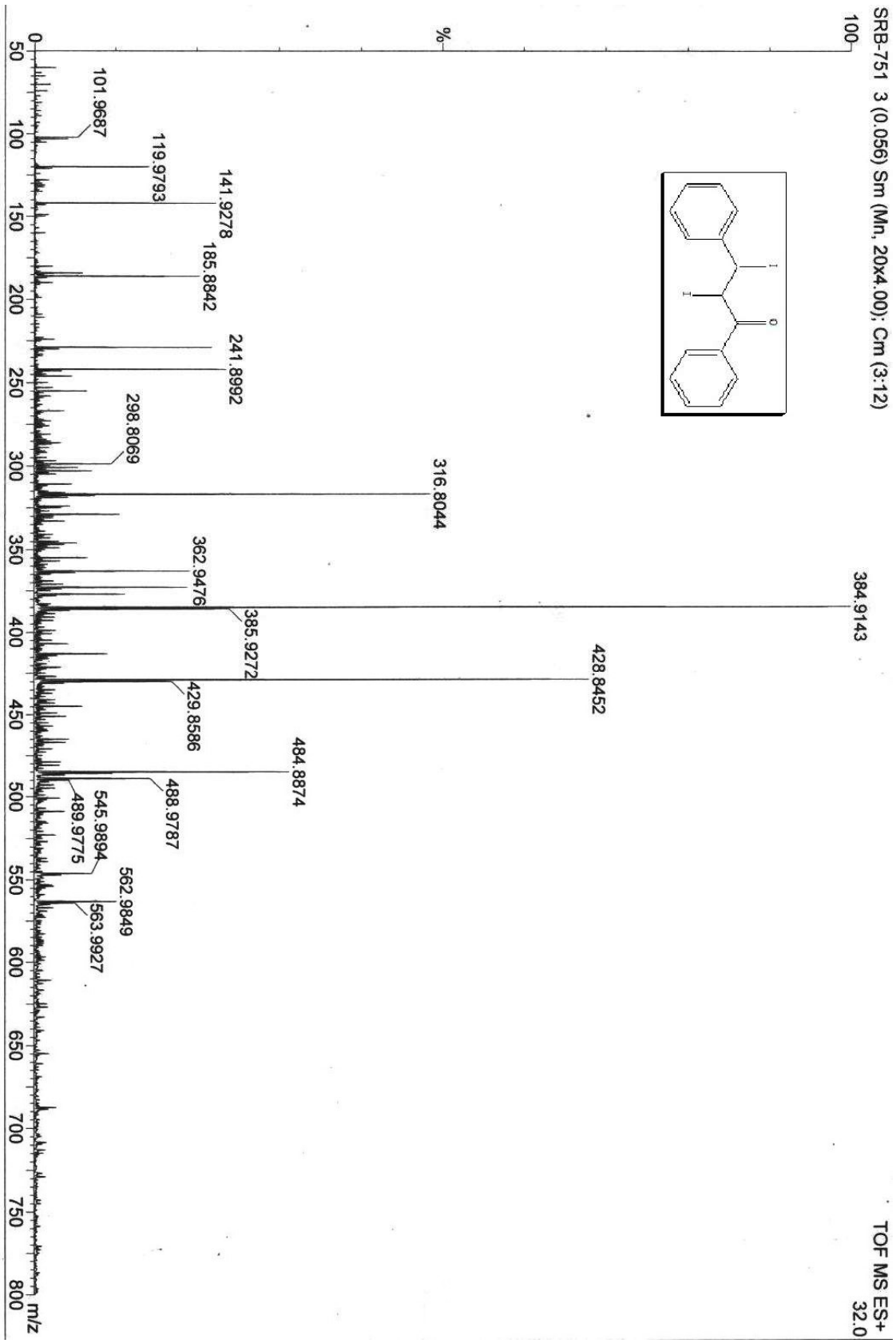

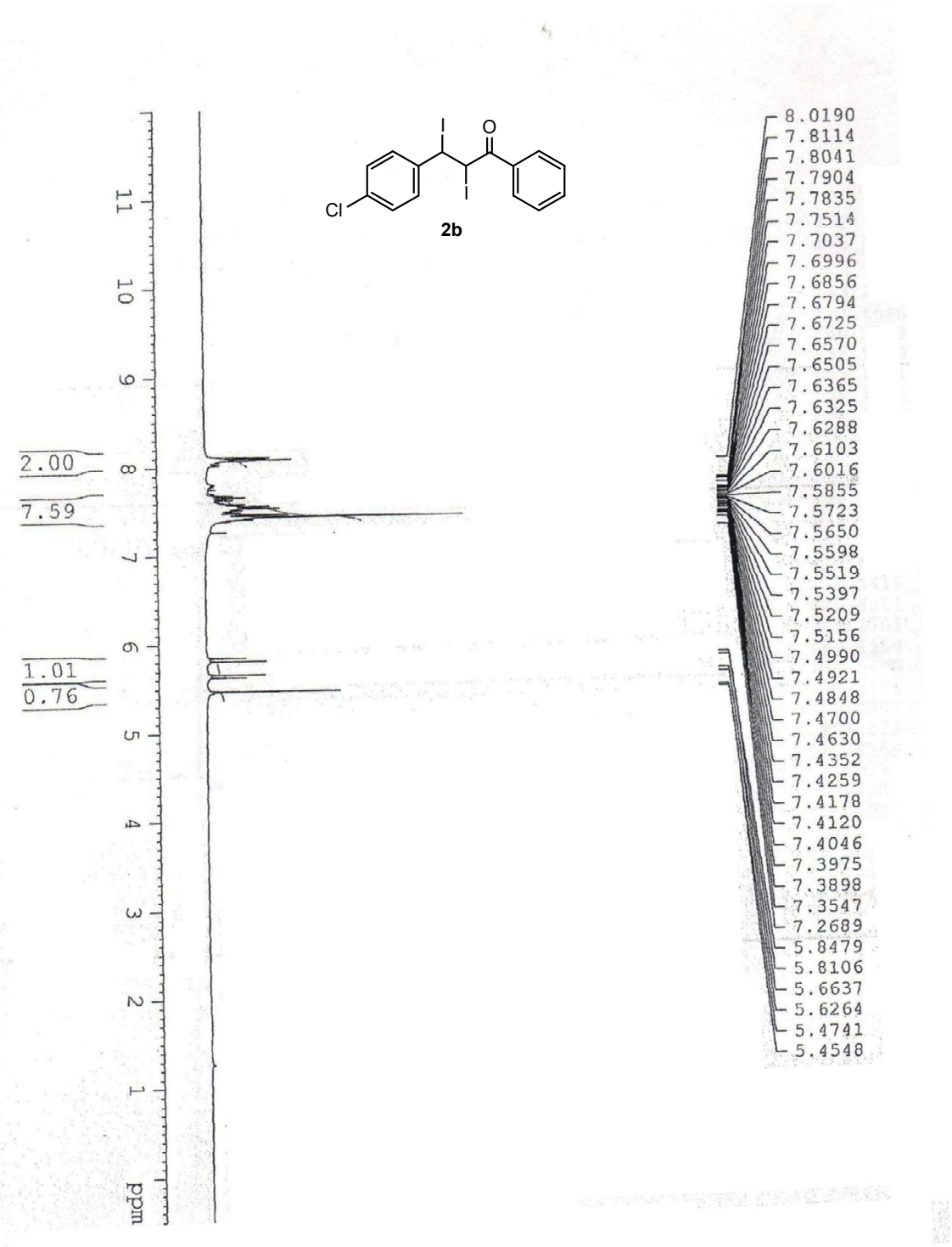

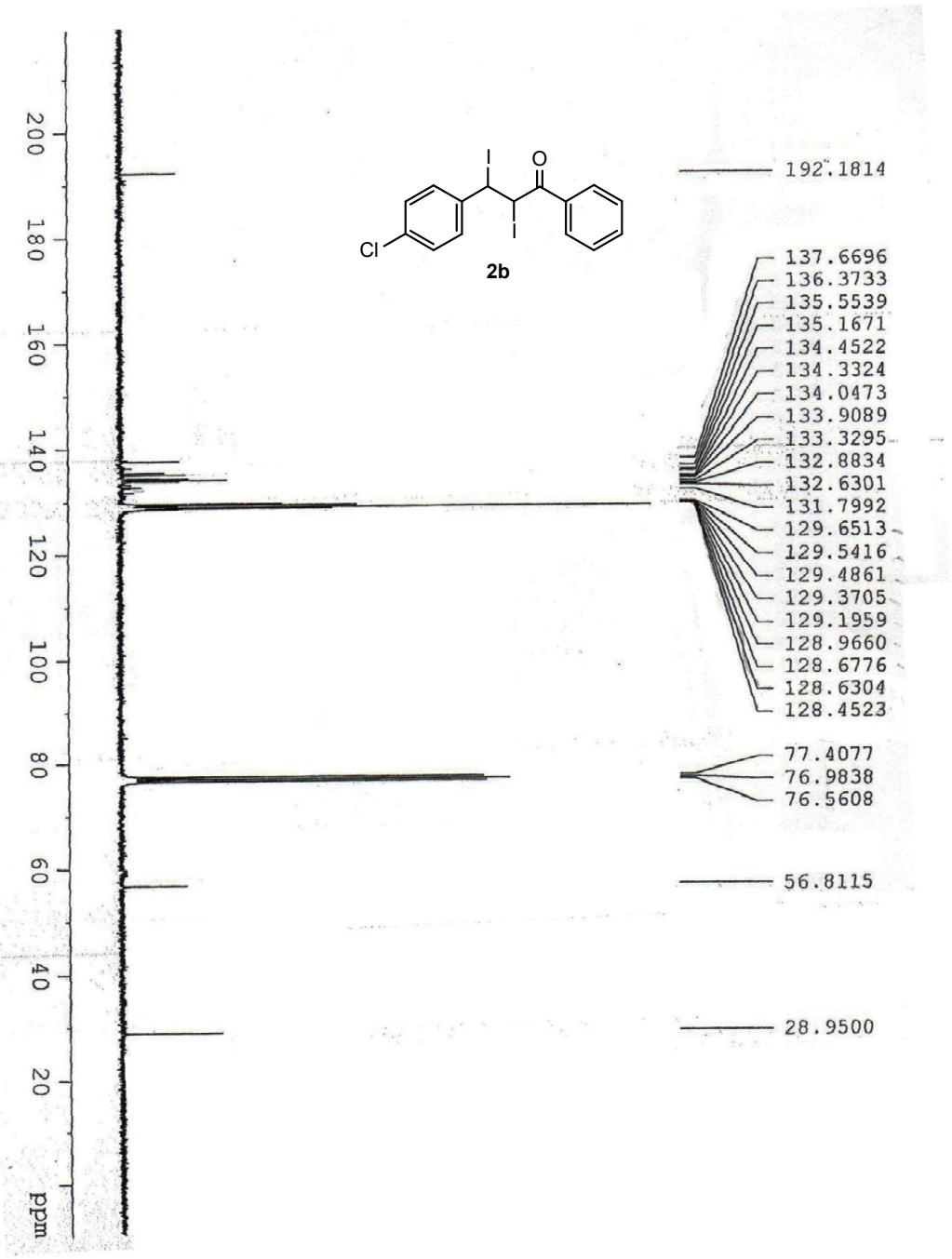

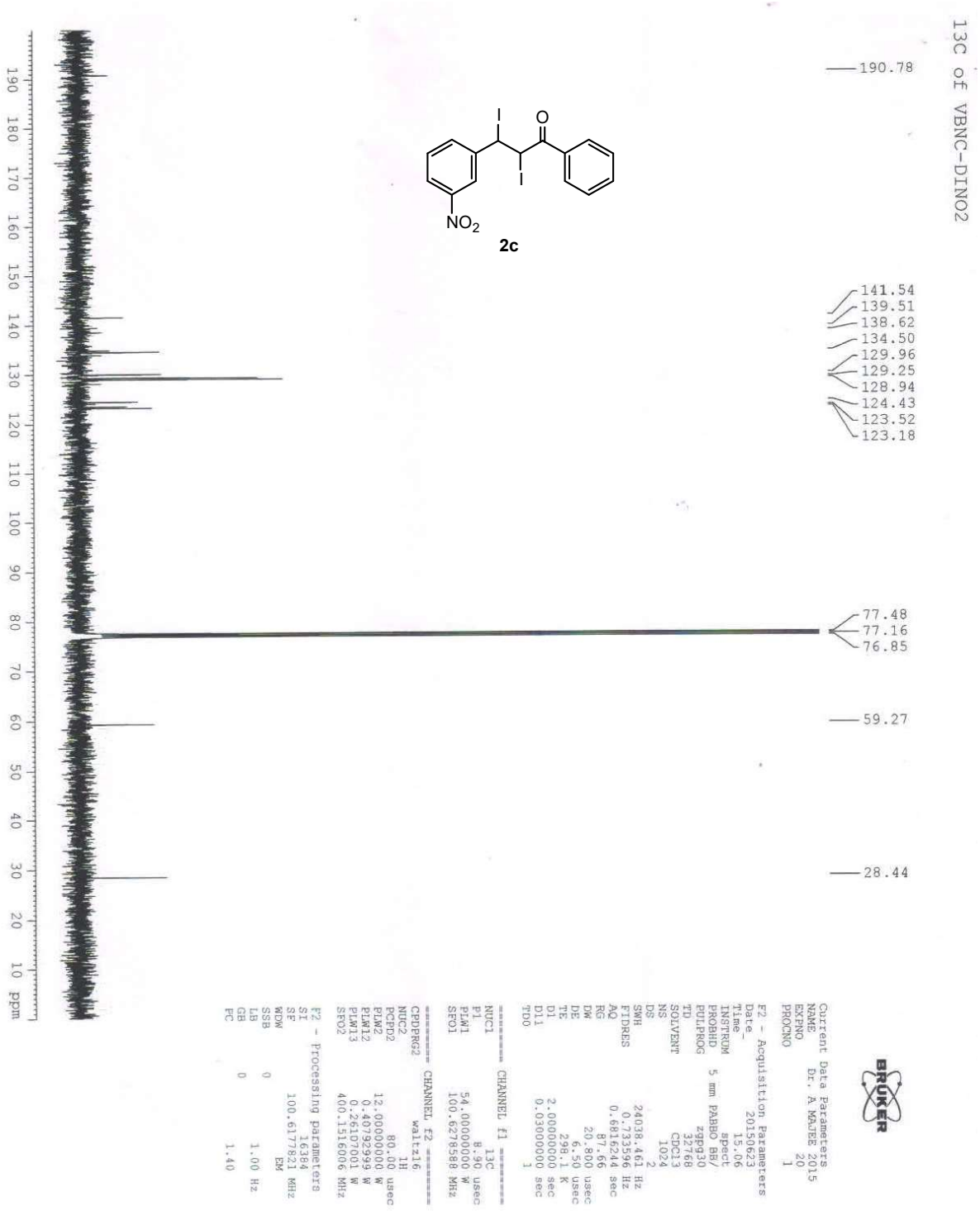

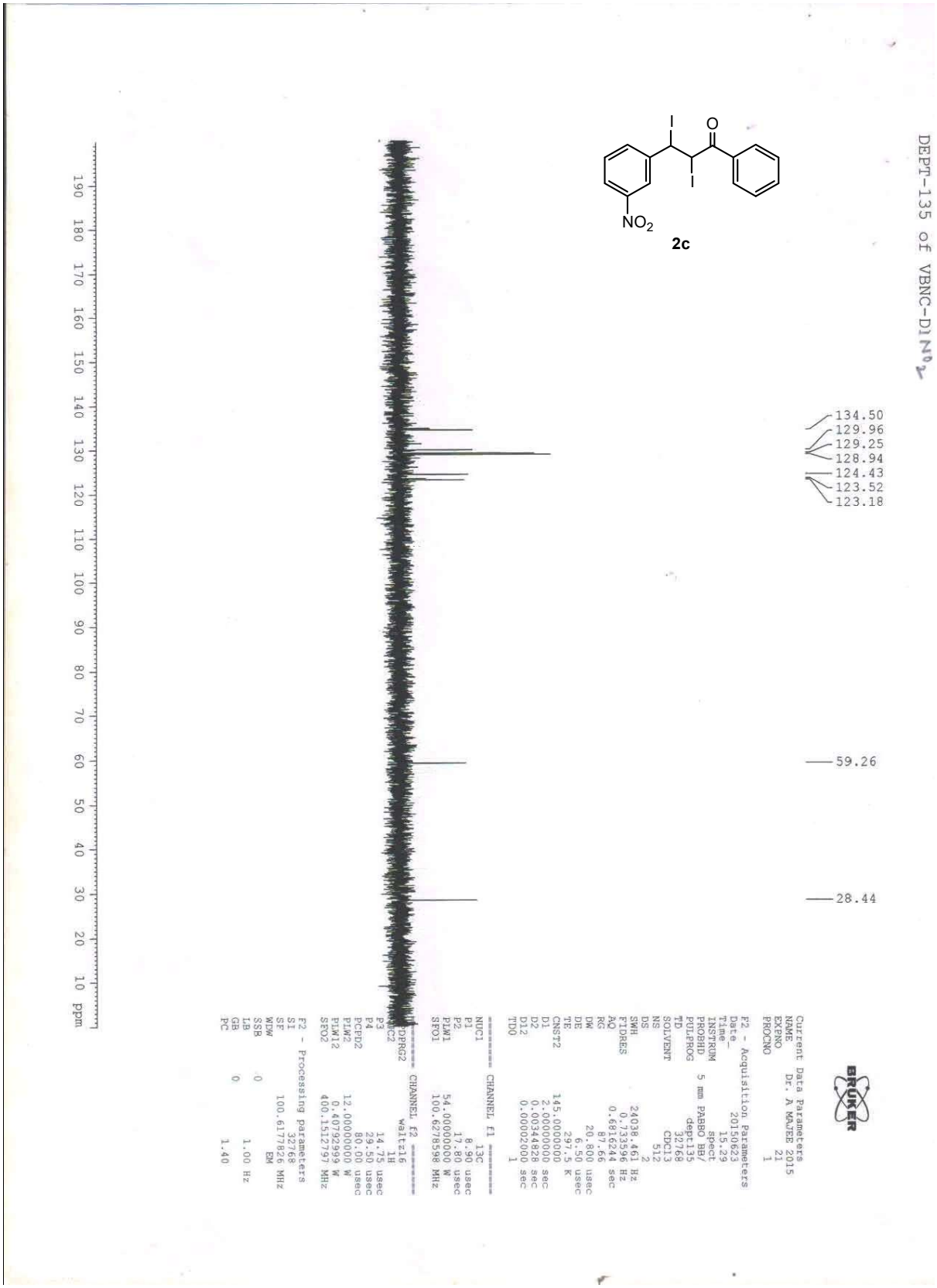

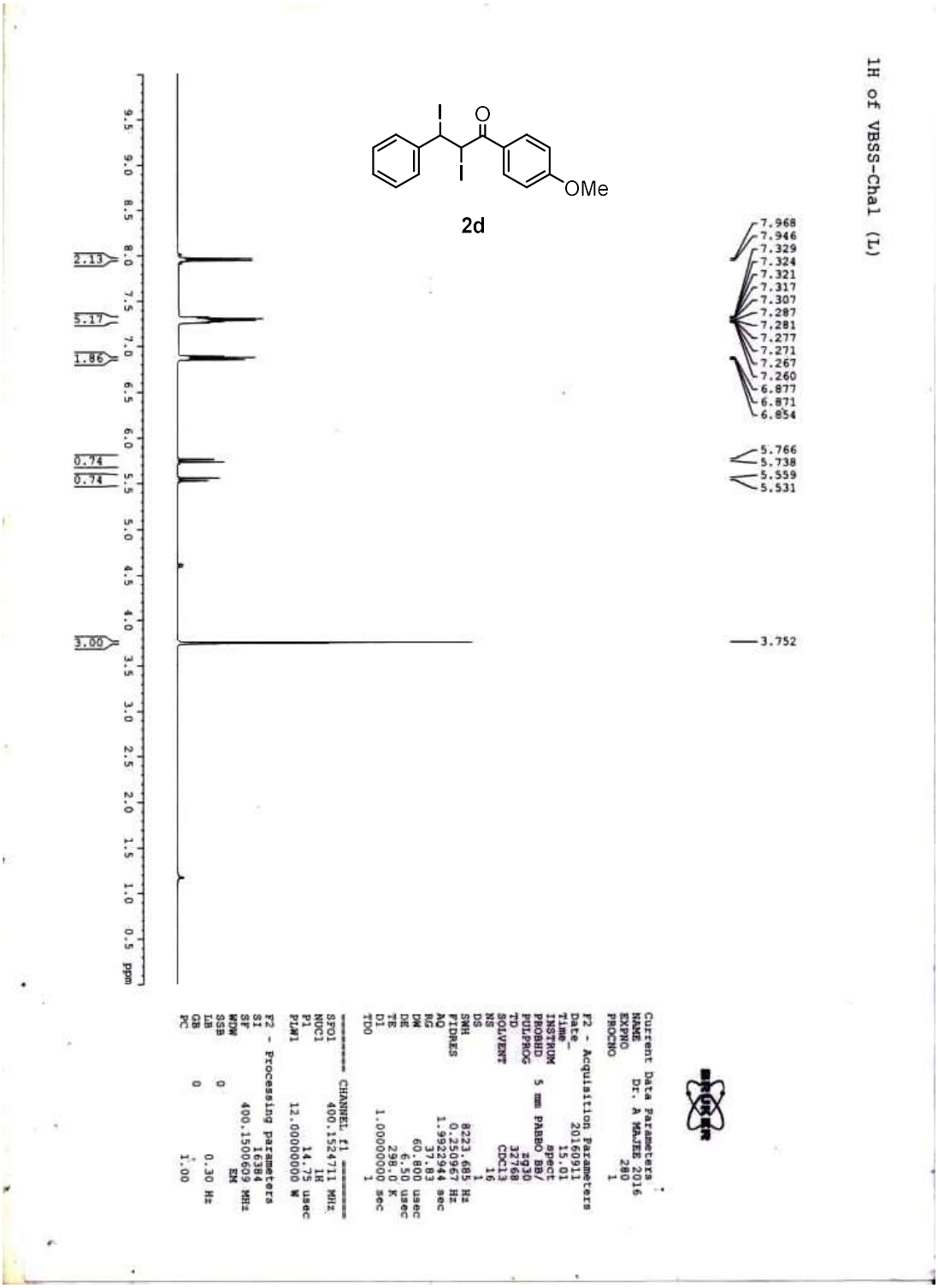

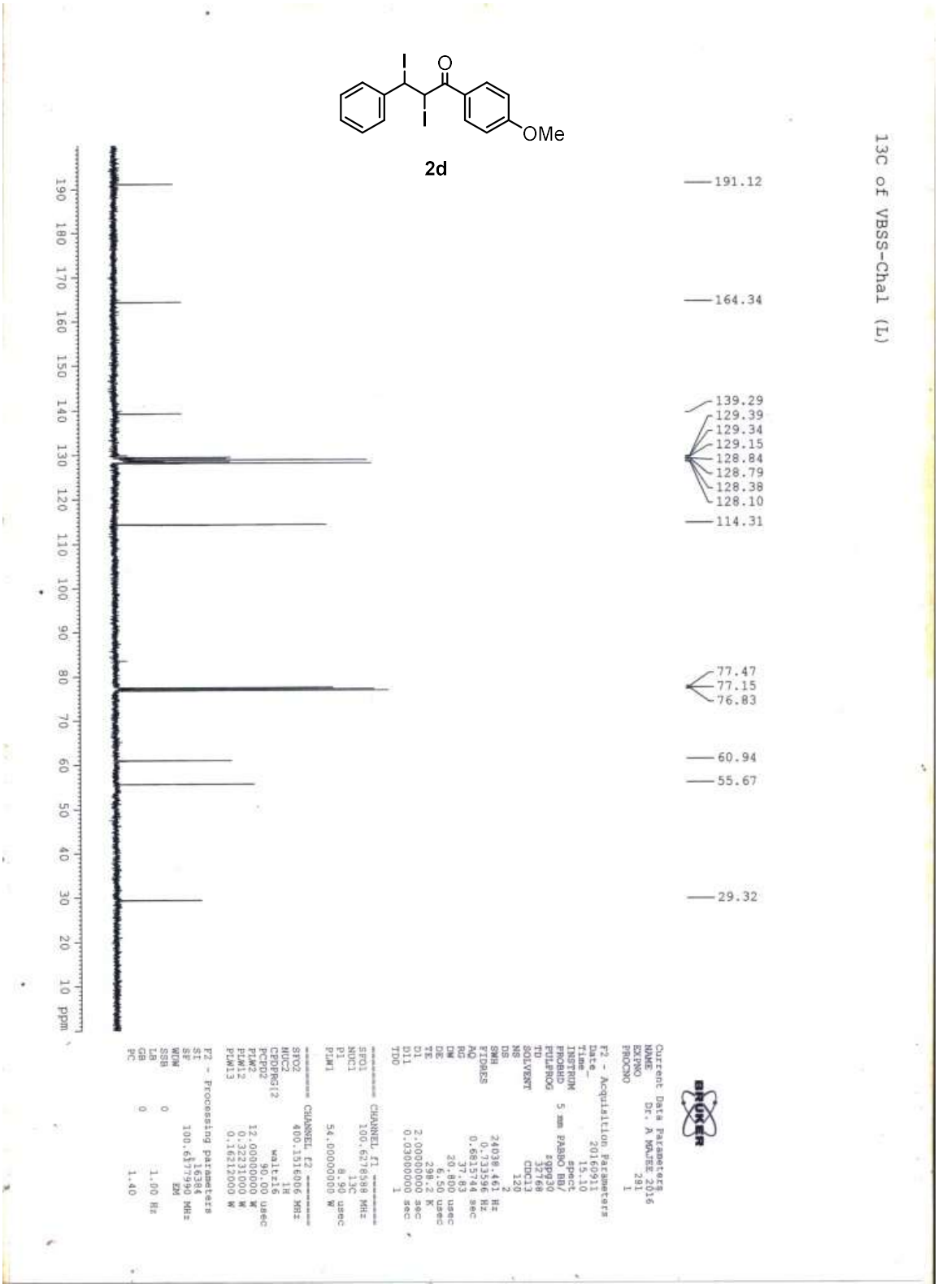

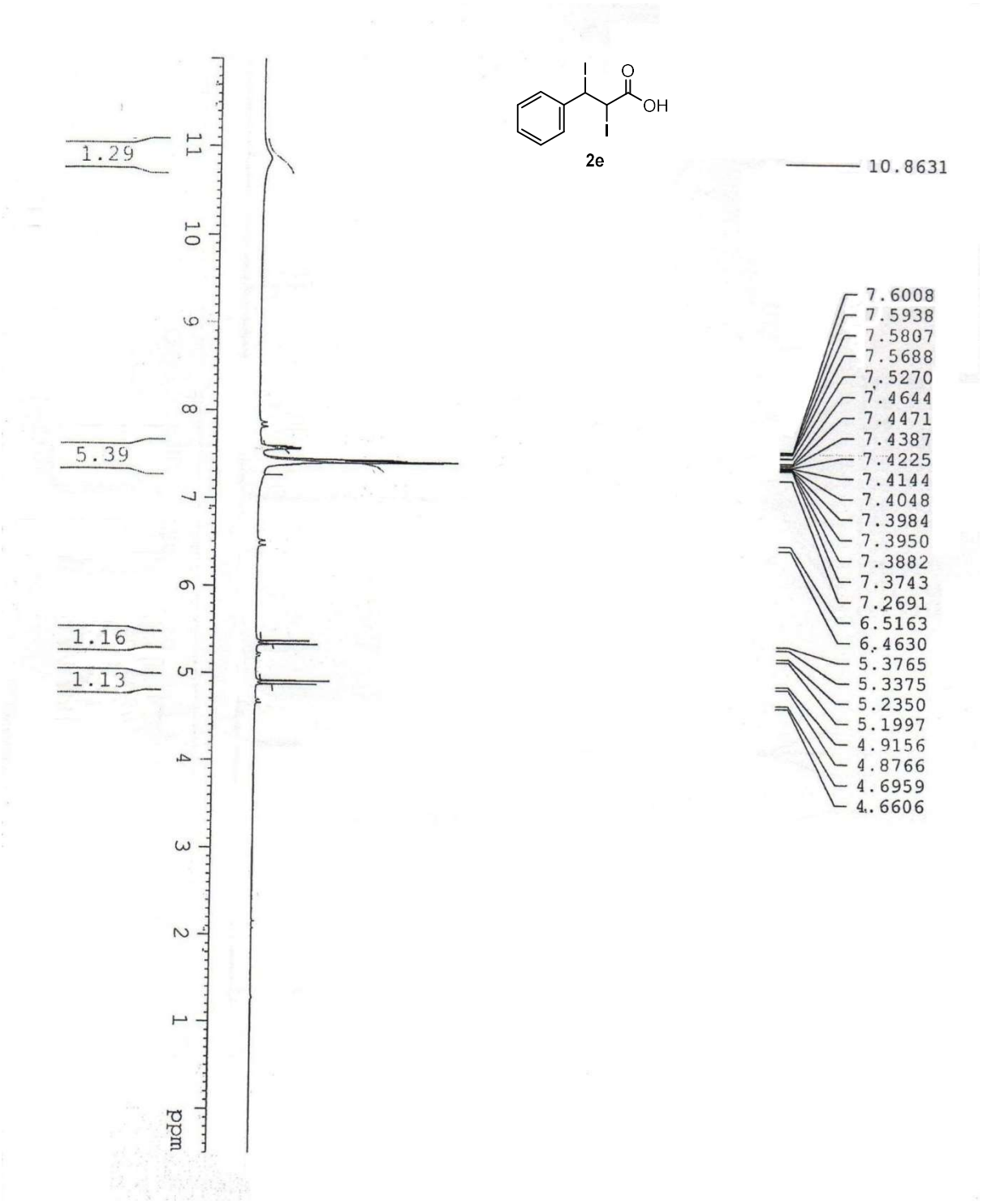

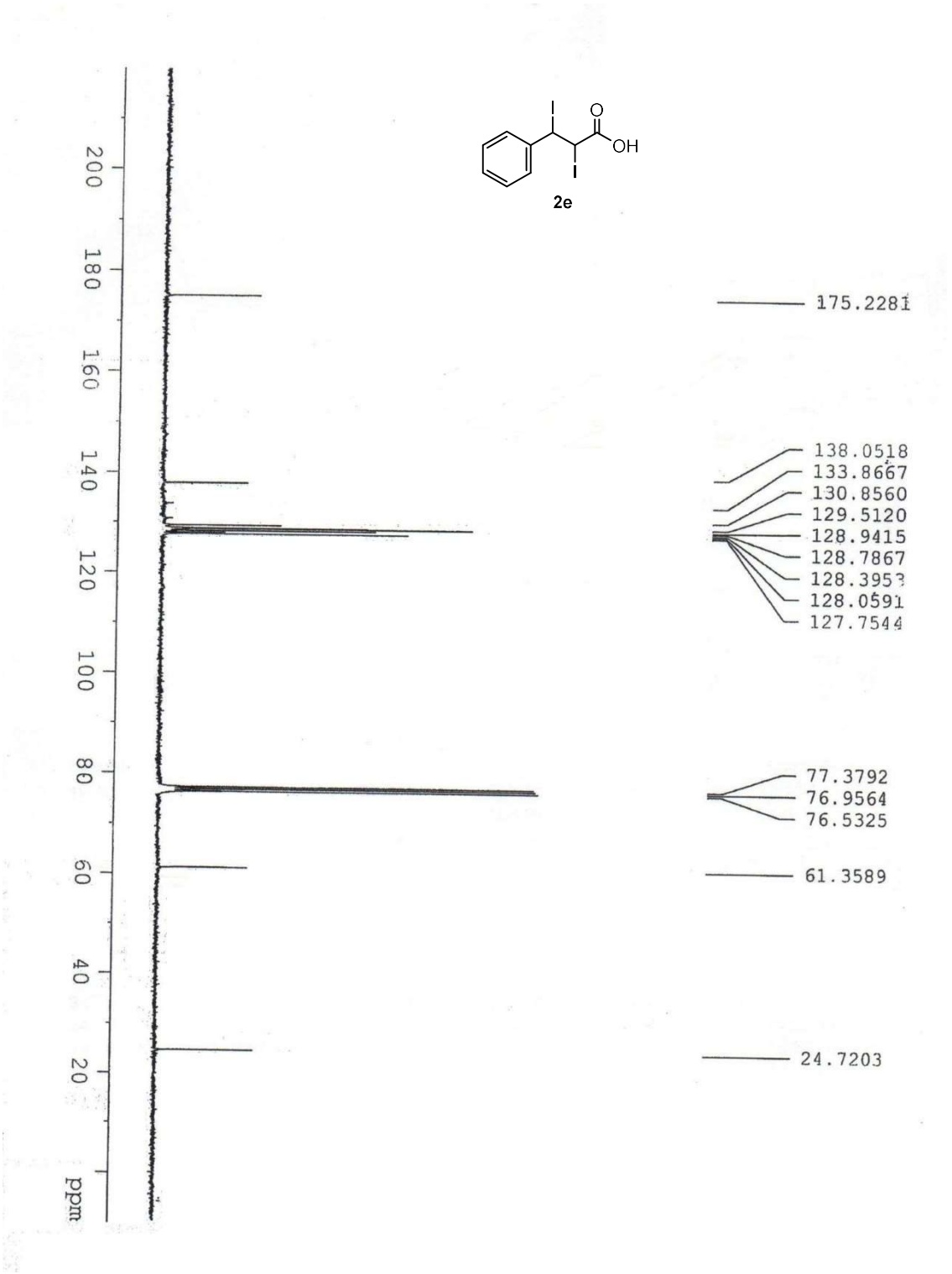

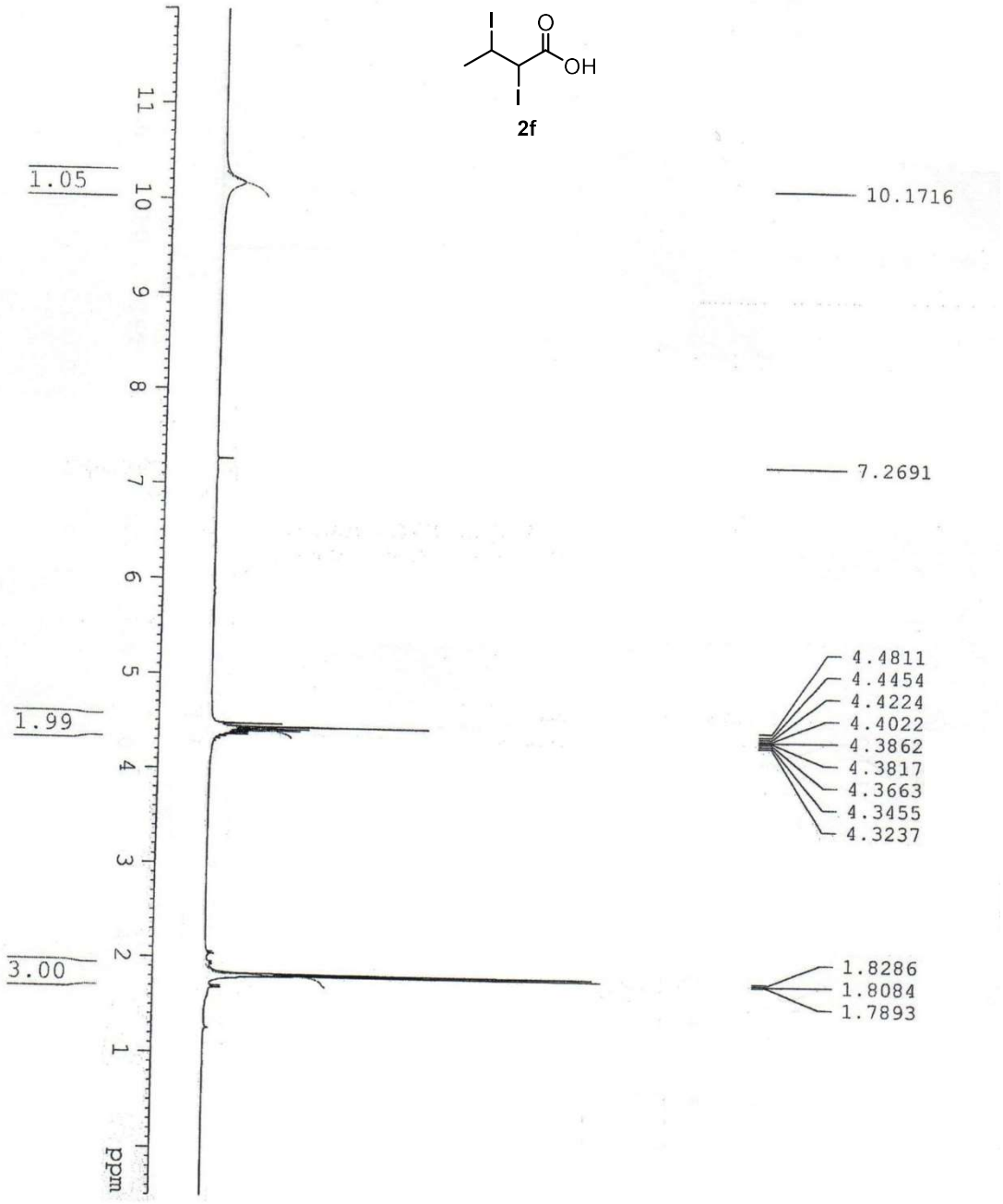

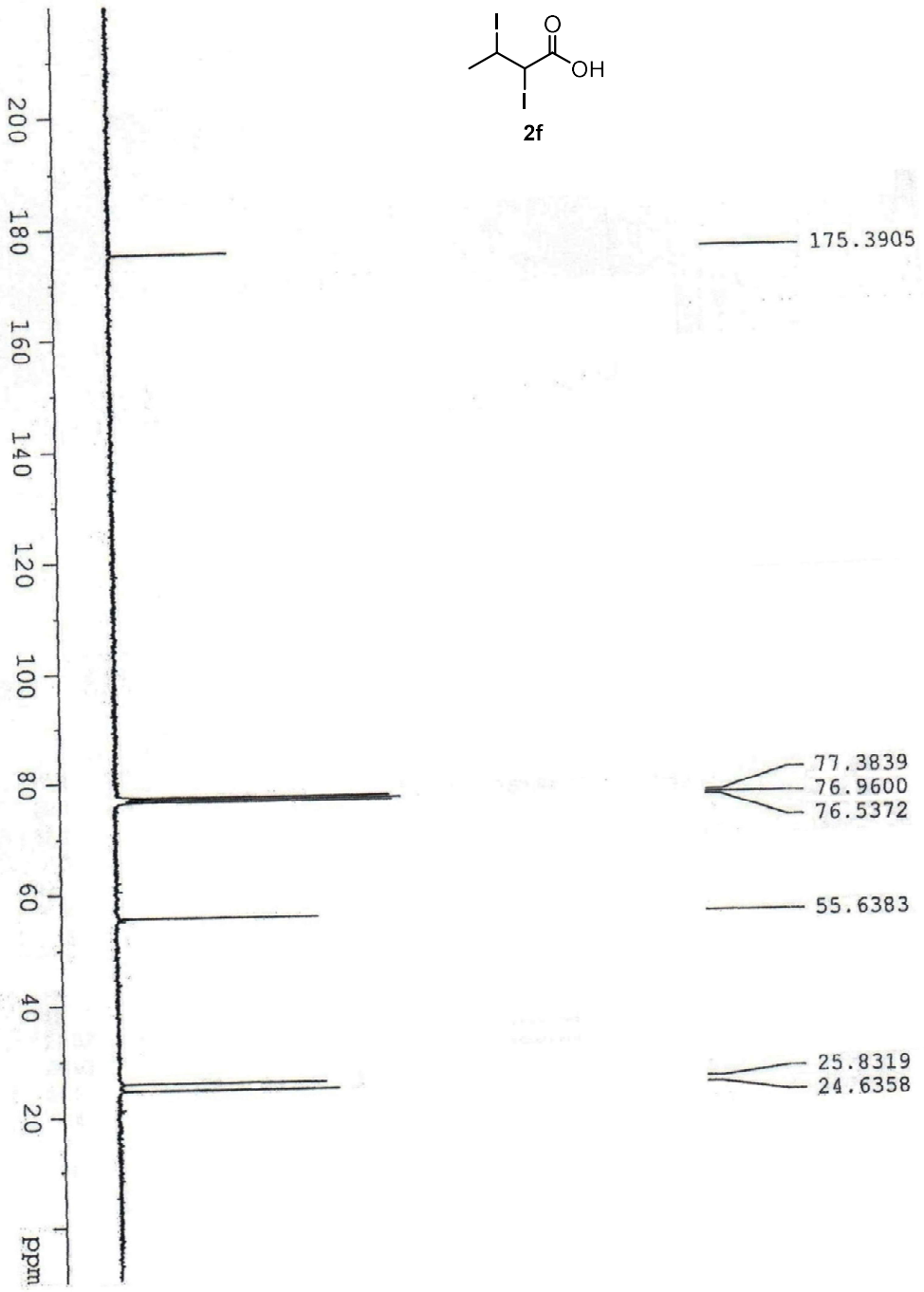

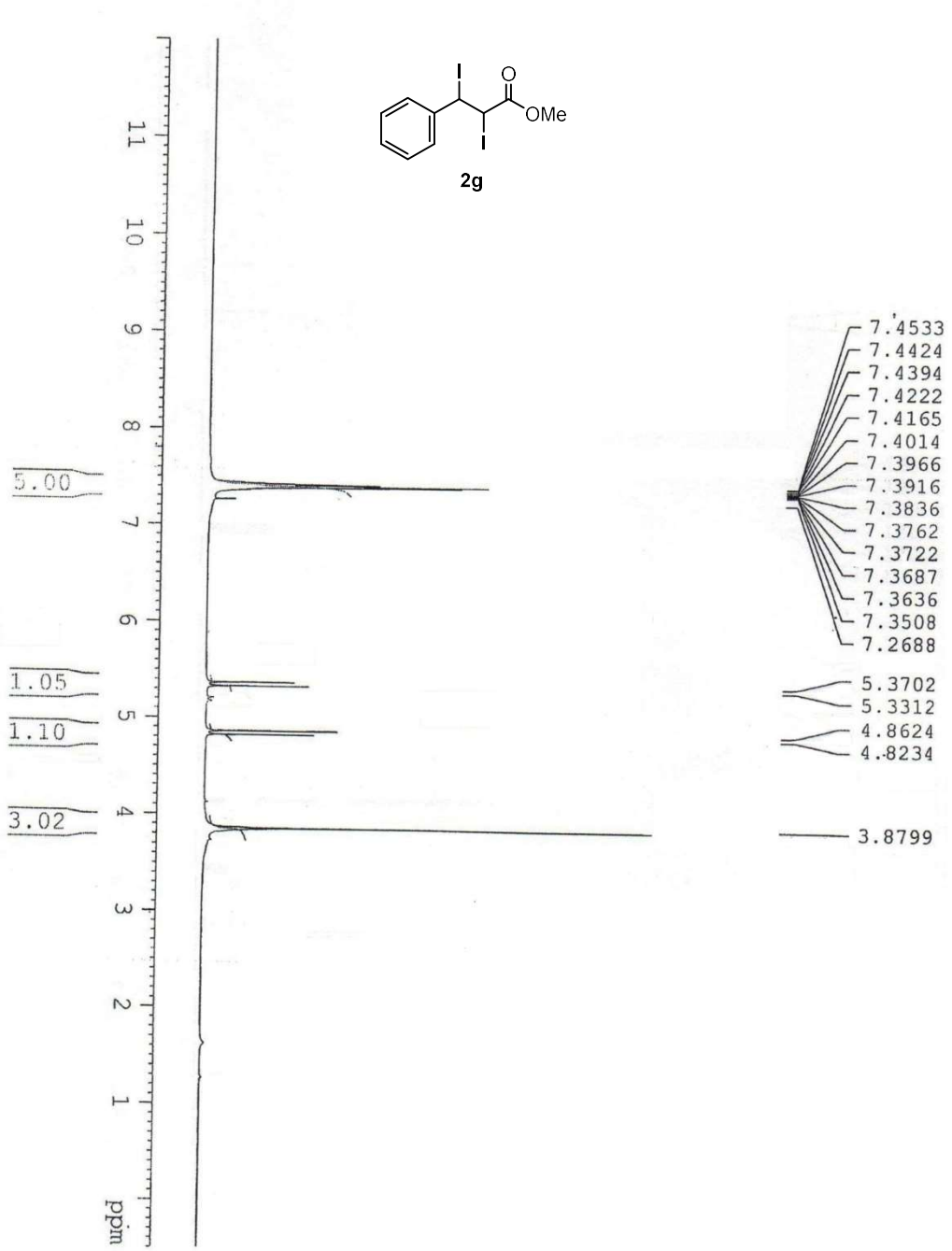

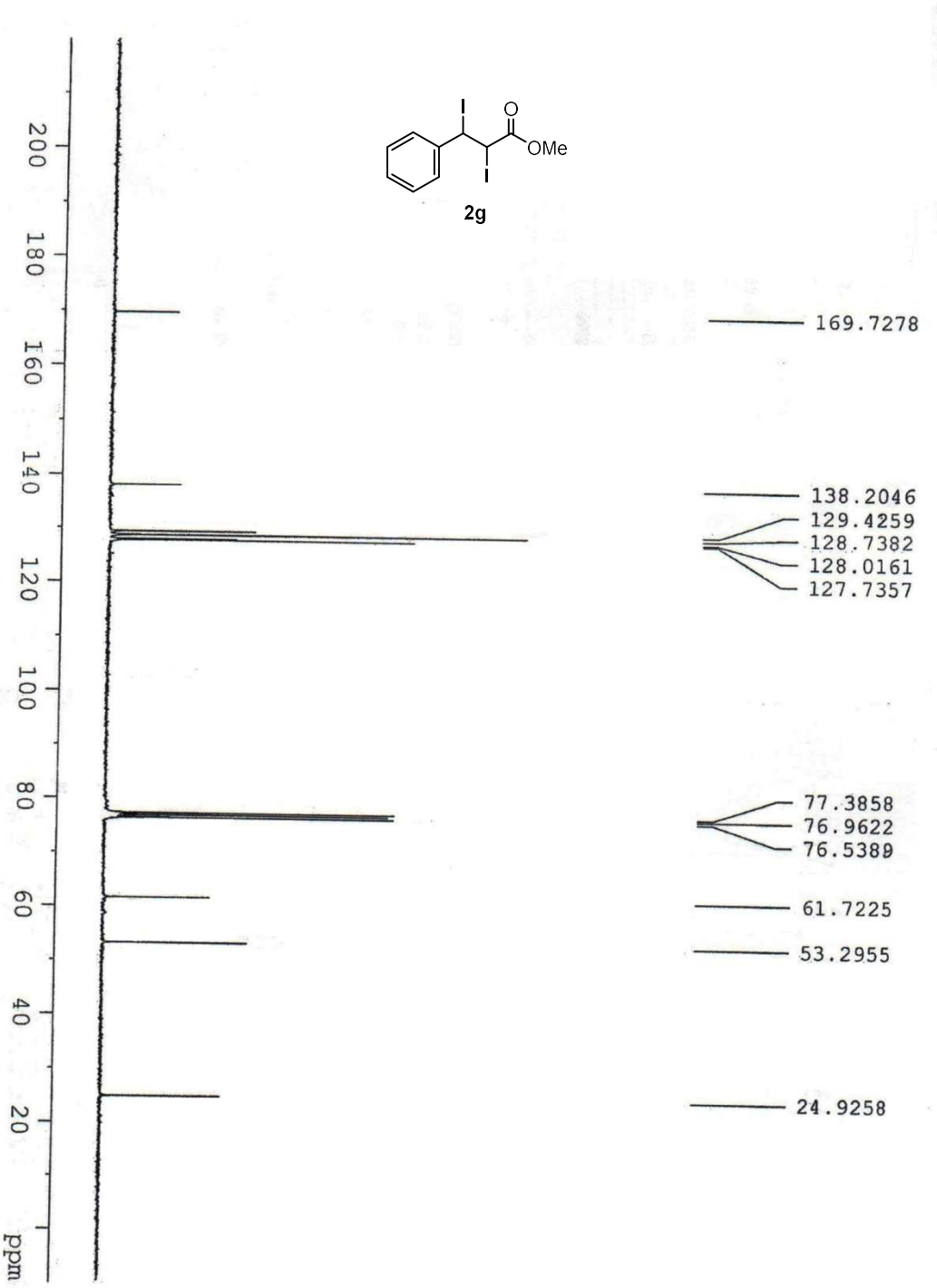

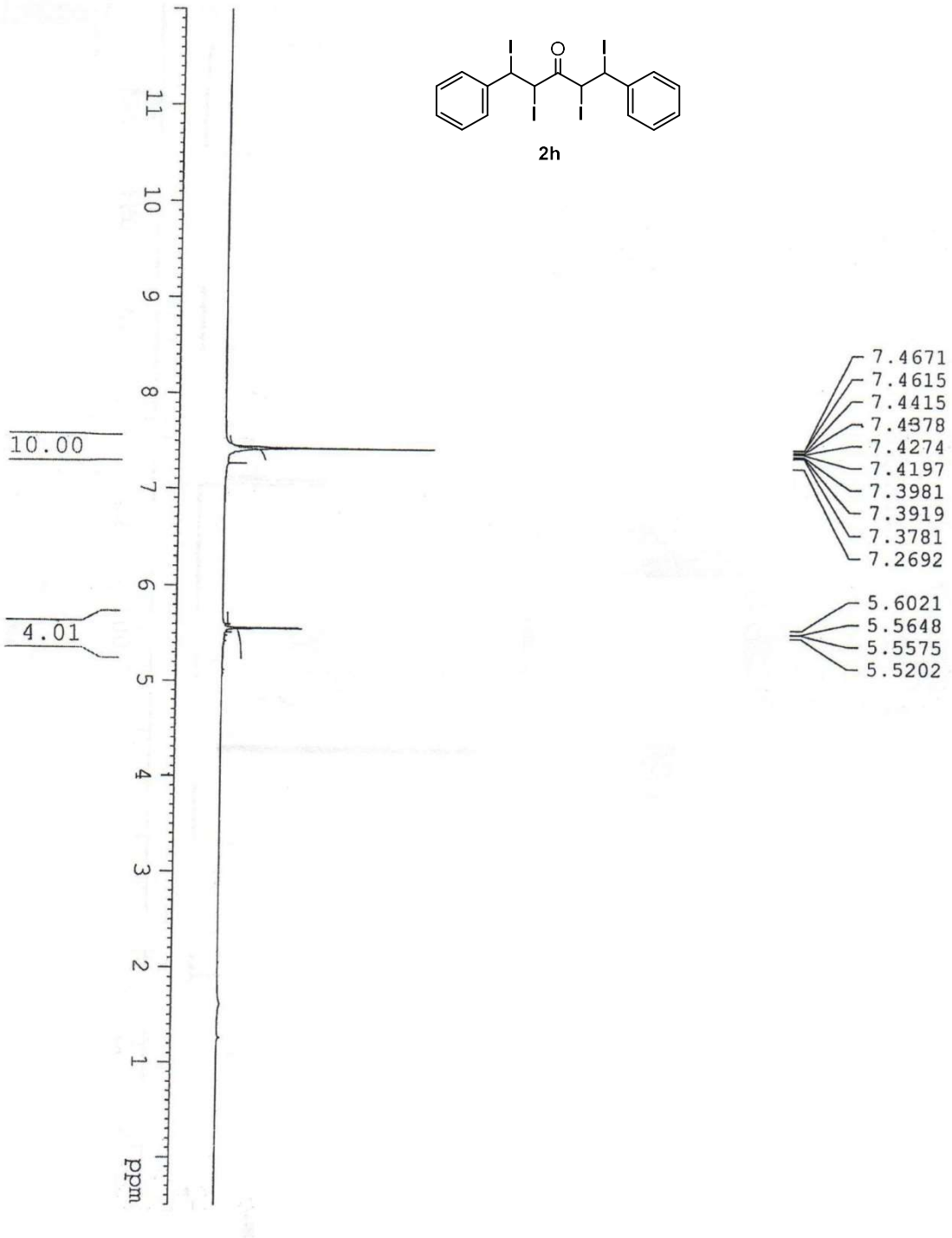

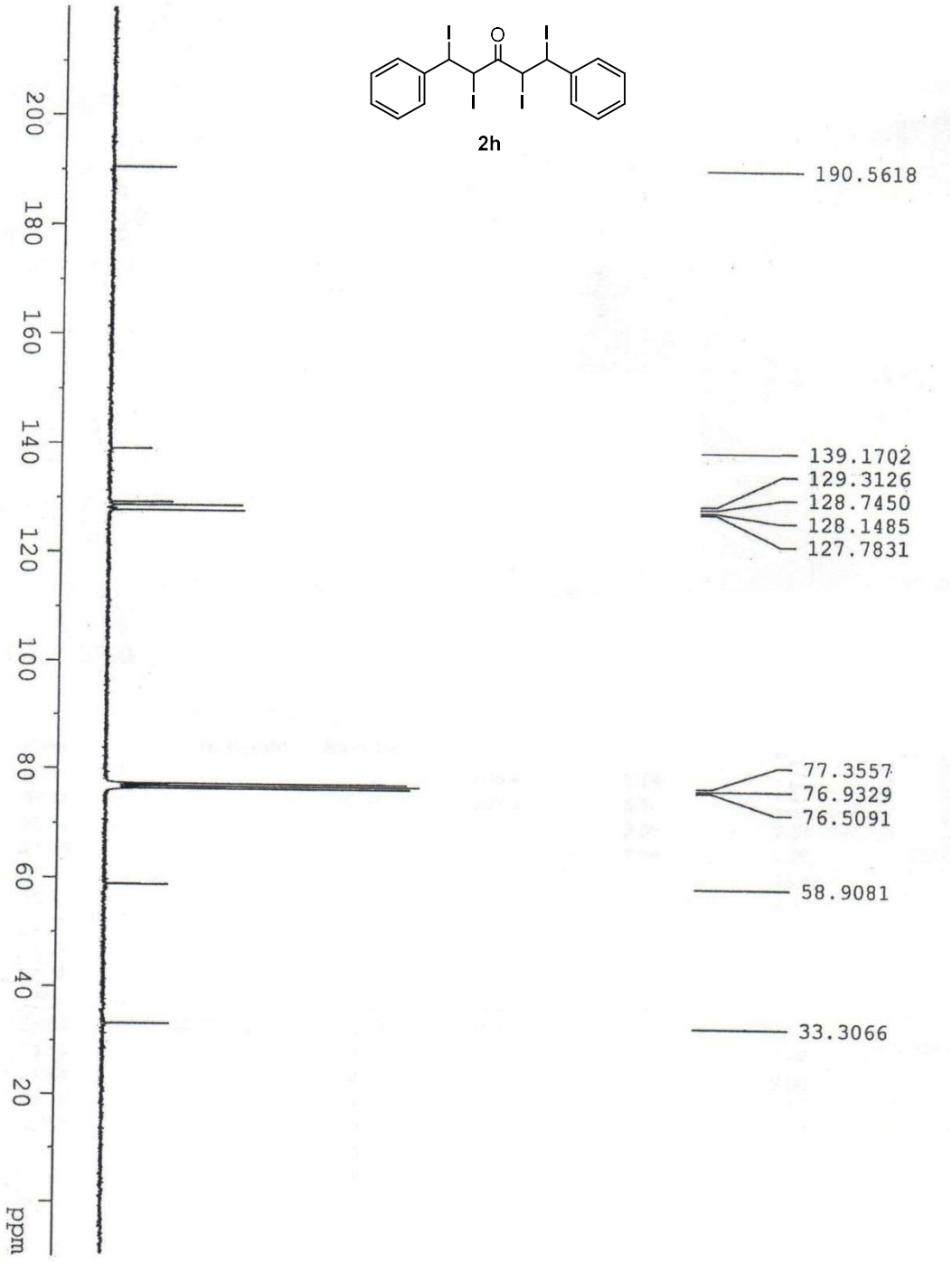

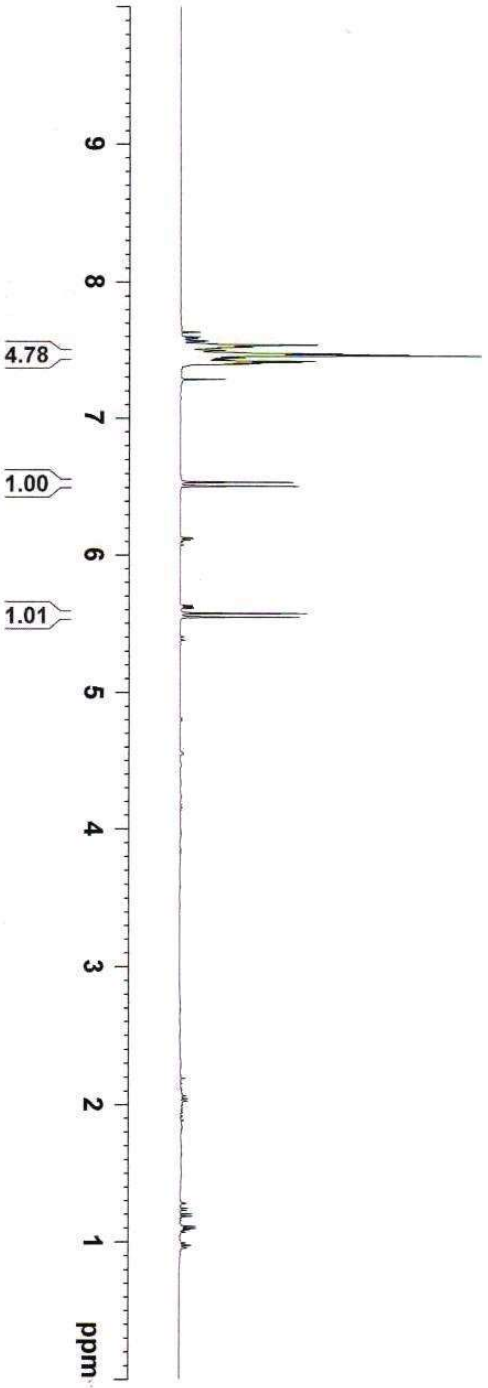

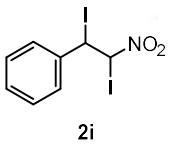

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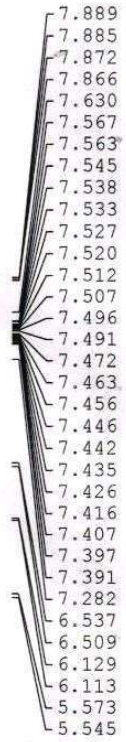
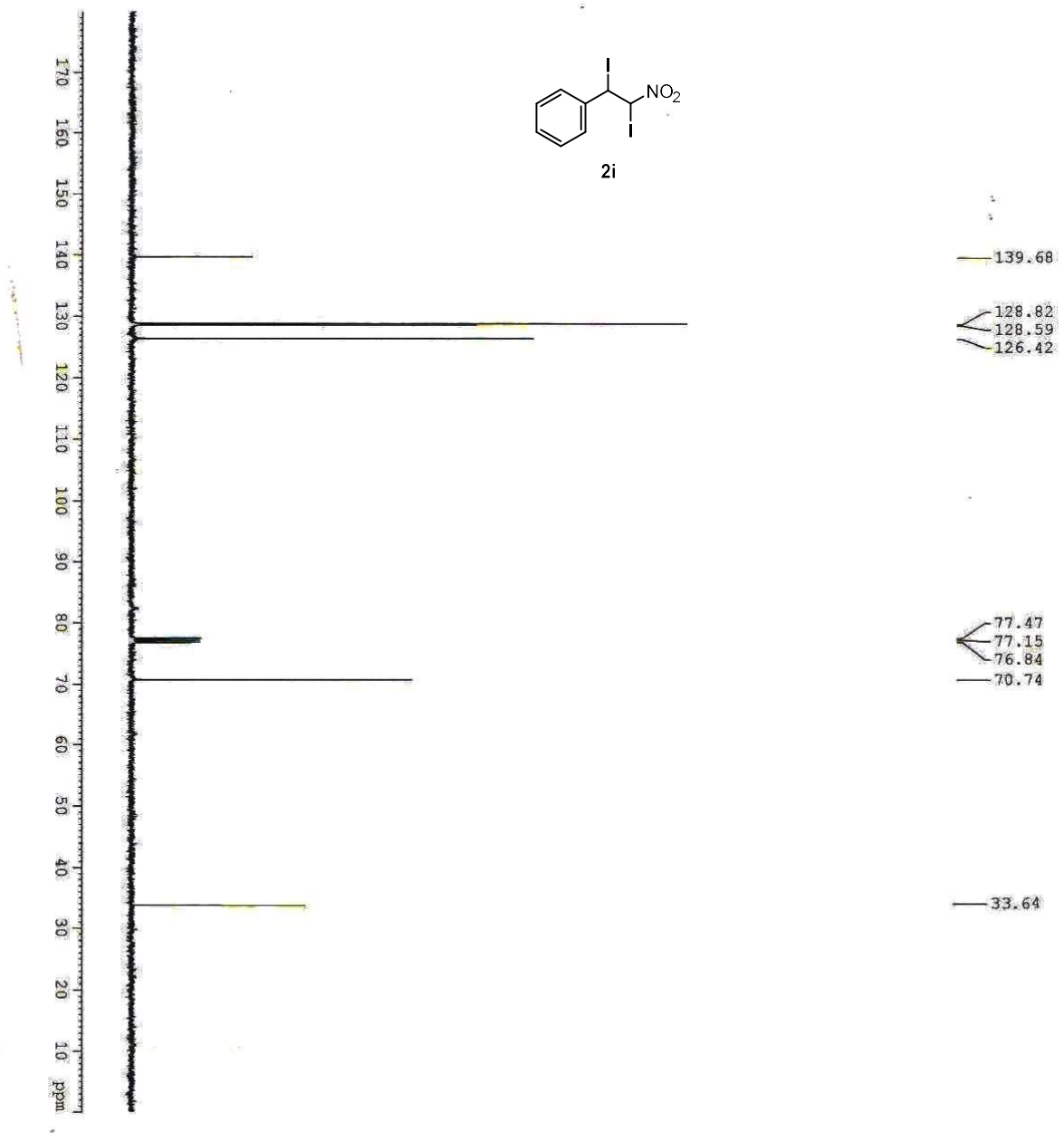
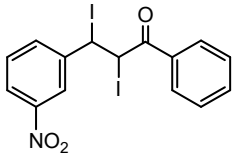




Structure Determination of compound 2,3-diiodo-3-(3-nitro-phenyl)-1-phenyl-propan-1-one (2c):



Single crystal suitable for X-ray diffraction of 2,3-diiodo-3-(3-nitro-phenyl)-1-phenyl-propan-1-one was grown from pet ether/EtOAc.

Molecular Formula: $C_{15}H_{11}I_2NO_3$; Mol. Wt.: 507.06

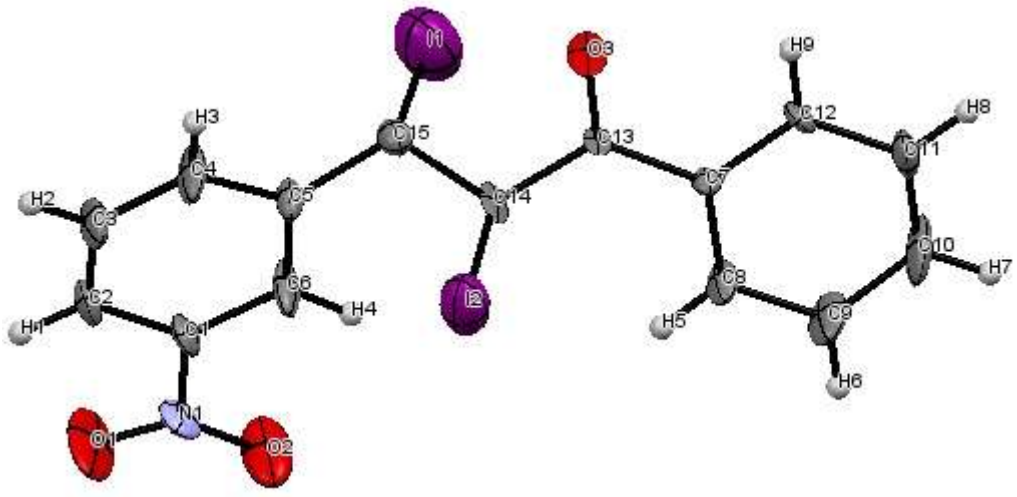
A specimen of $C_{15}H_{11}I_2NO_3$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The total exposure time was 5.55 hours. The frames were integrated with the Bruker SAINT Software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 25807 reflections to a maximum θ angle of 30.04° (0.71 Å resolution), of which 4207 were independent (average redundancy 6.134, completeness = 94.5%, R_{int} = 20.19%, R_{sig} = 8.23%) and 3405(80.94%) were greater than $2\sigma(F^2)$. The final cell constants of $\underline{a}$ = 9.1267(9) Å, $\underline{b}$ = 9.2452(10) Å, $\underline{c}$ = 10.5181(10) Å, α = 89.390(5)°, β = 68.455(4)°, γ = 68.534(4)°, volume = 760.34(14) $Å^3$, are based upon the refinement of the XYZ-centroids of 9860 reflections above 20 σ(I) with 4.783° < 2θ < 59.09°. Data were corrected for absorption effects using the multi-scan method (SADABS).

The final anisotropic full-matrix least-squares refinement on F^2 with 190 variables converged at R1 = 16.53%, for the observed data and wR2 = 48.10% for all data. The goodness-of-fit was 3.053. The largest peak in the final difference electron density synthesis was 6.298 $e^-/Å^3$ and the largest hole was -4.469 $e^-/Å^3$ with an RMS deviation of 0.538 $e^-/Å^3$. On the basis of the final model, the calculated density was2.969 g/cm^3 and F(000), 600 e^-.

Identification code	vbchem005

Chemical formula	$C_{15}H_{11}I_2NO_3$	
Formula weight	169.93 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.1267(9) Å	α = 89.390(5)°
	b = 9.2452(10) Å	β = 68.455(4)°
	c = 10.5181(10) Å	γ = 68.534(4)°
Volume	760.34(14) $Å^3$	
Z	8	
Density (calculated)	2.969 g/cm^3	
Absorption coefficient	8.201 mm^{-1}	
F(000)	600	



ORTEP diagram for the structure of 2,3-diiodo-3-(3-nitro-phenyl)-1-phenyl-propan-1-one (**2c**)

