

Supplemental Information

Facile Protocol for the Synthesis of Electron-rich Benzimidazole Derivatives

Robert D. Pike^a and Brian E. Love^{b*}

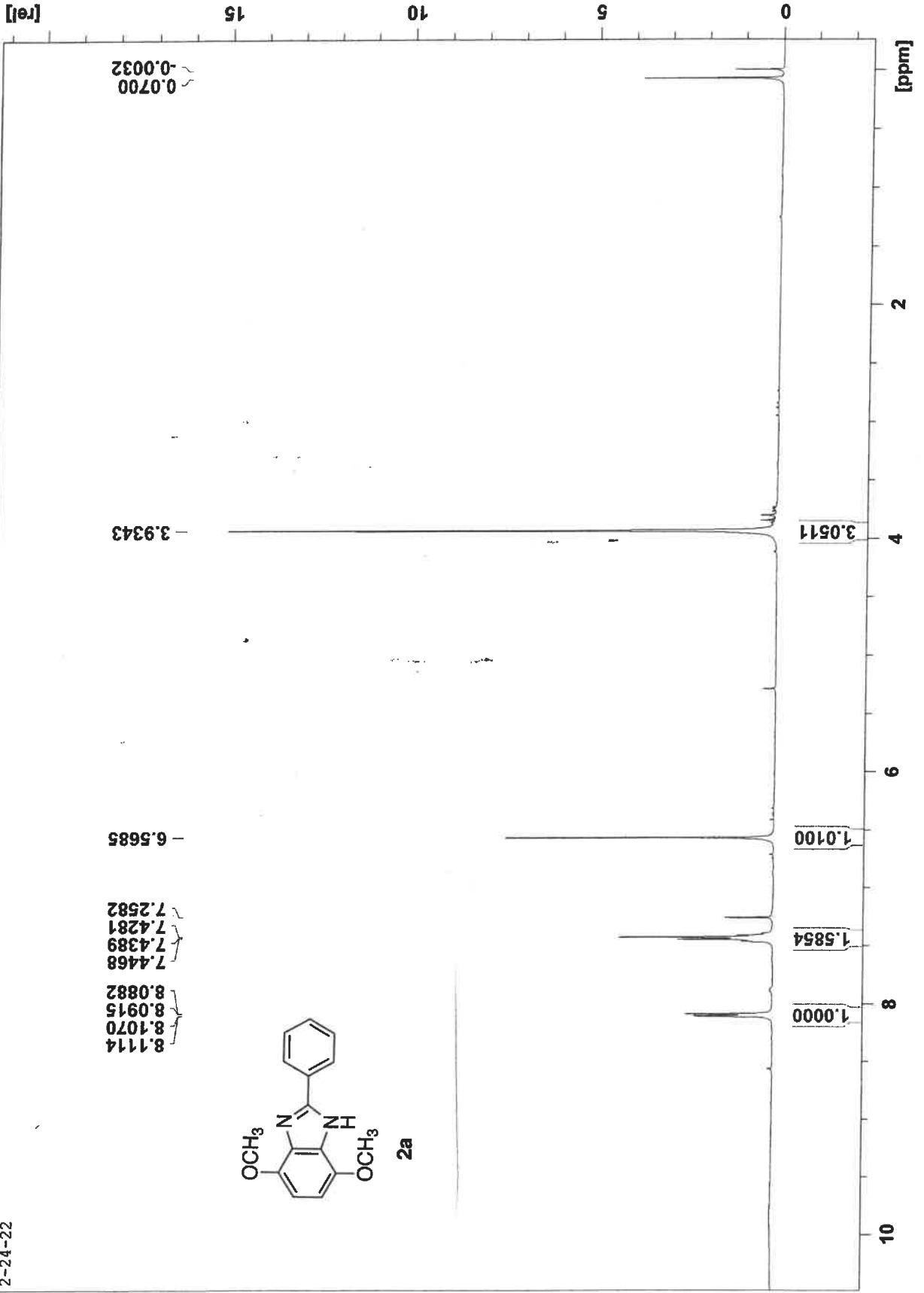
^aDepartment of Chemistry, William and Mary, Williamsburg, VA, 23187. Email: rdpike@wm.edu

^bDepartment of Chemistry, East Carolina University, Greenville, NC, 27858. Email: loveb@ecu.edu

1. ¹H and ¹³C NMR spectra of compounds **2**, **4** and **8**
2. X-ray crystal structure data for compound **2f**

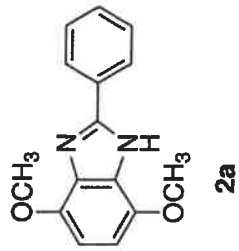
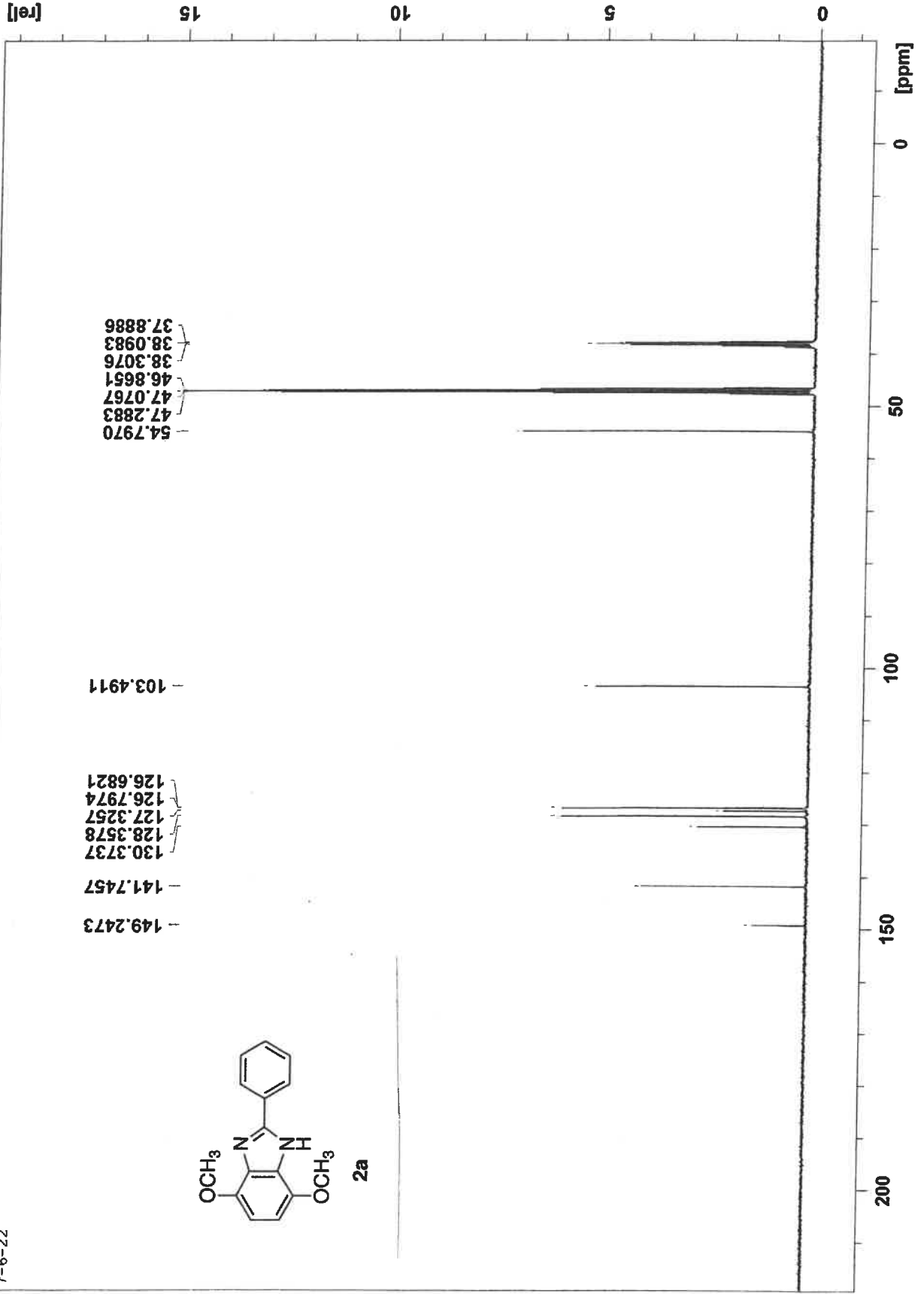
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2-24-22



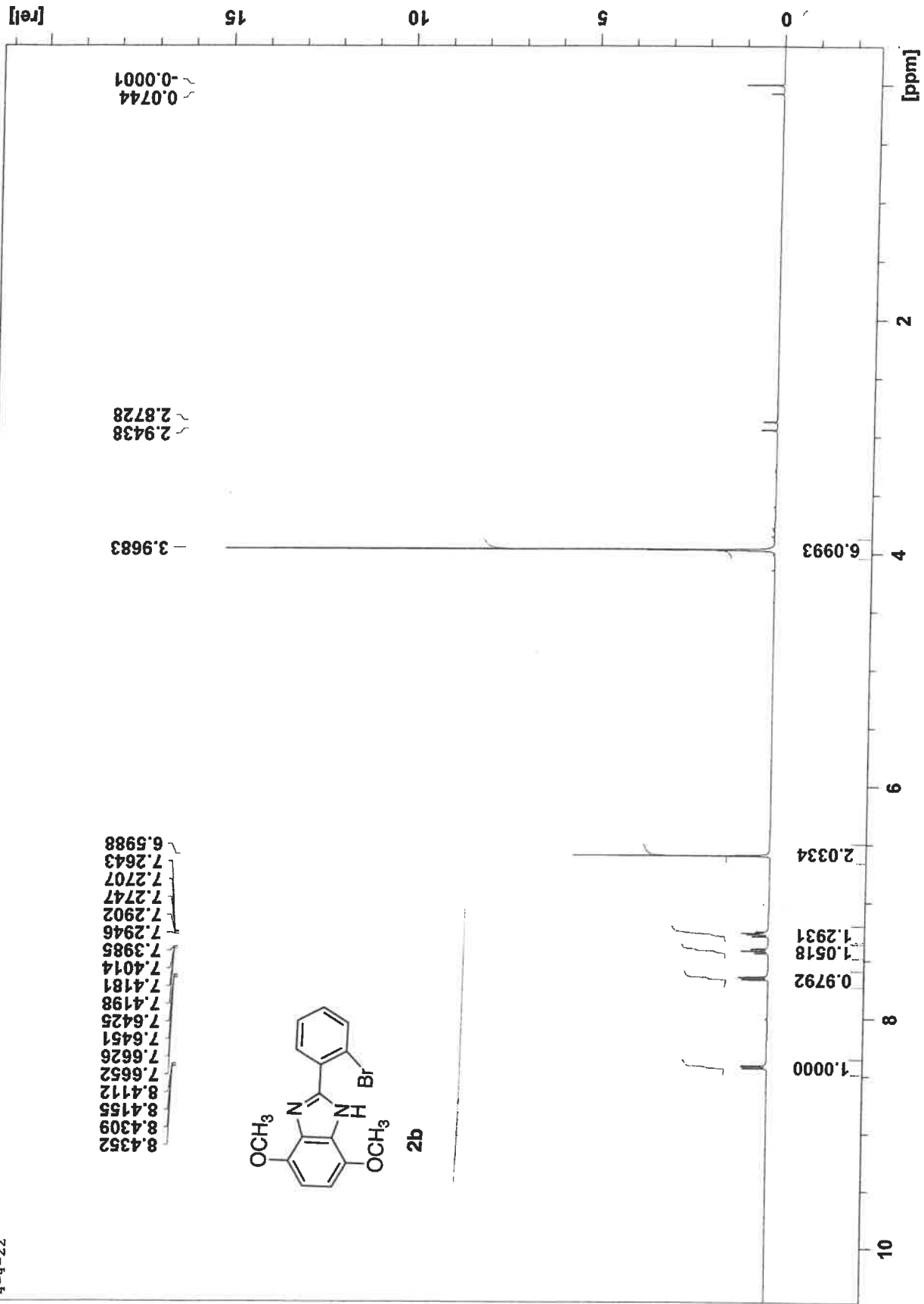
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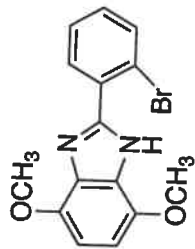
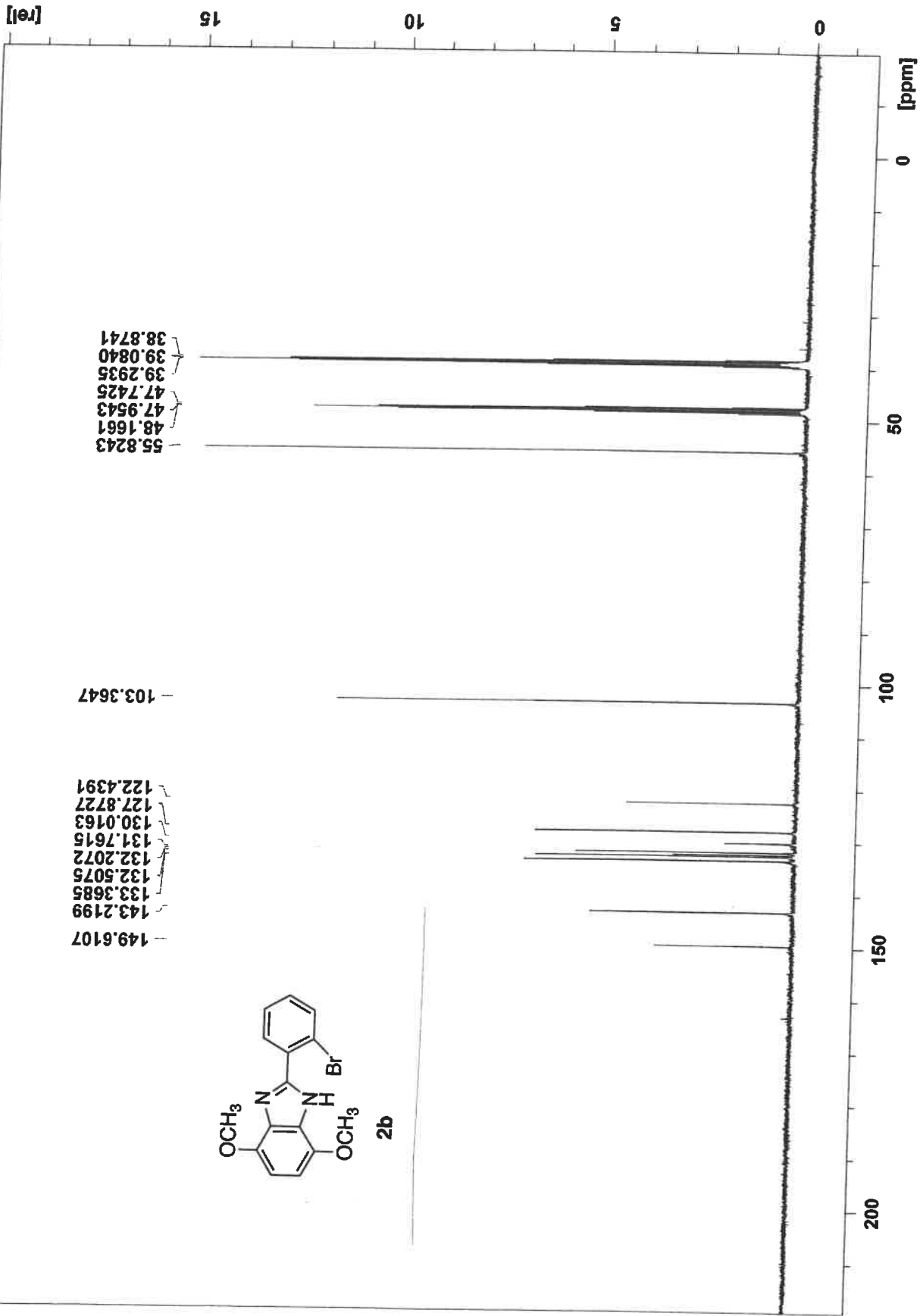
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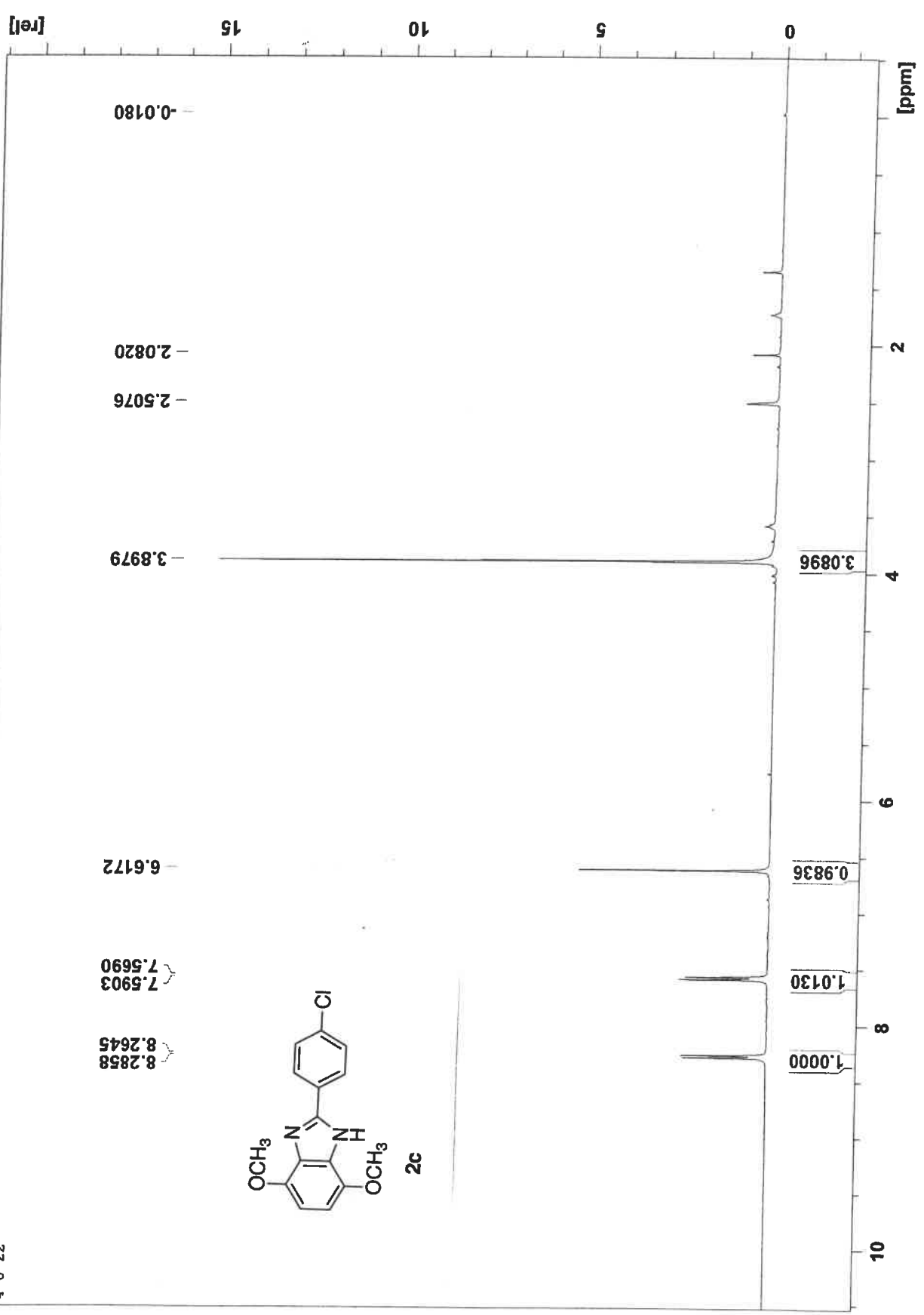
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2b

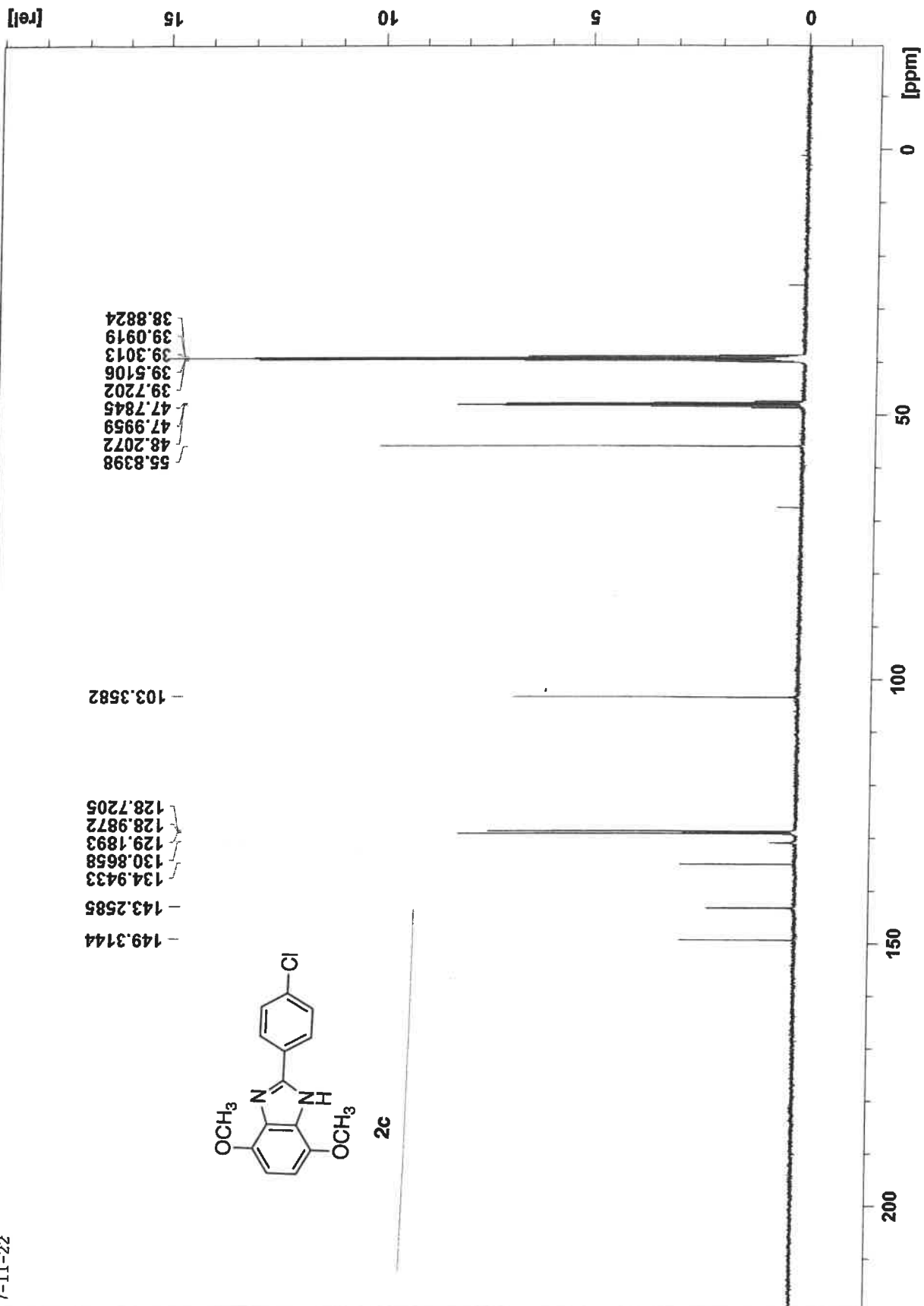
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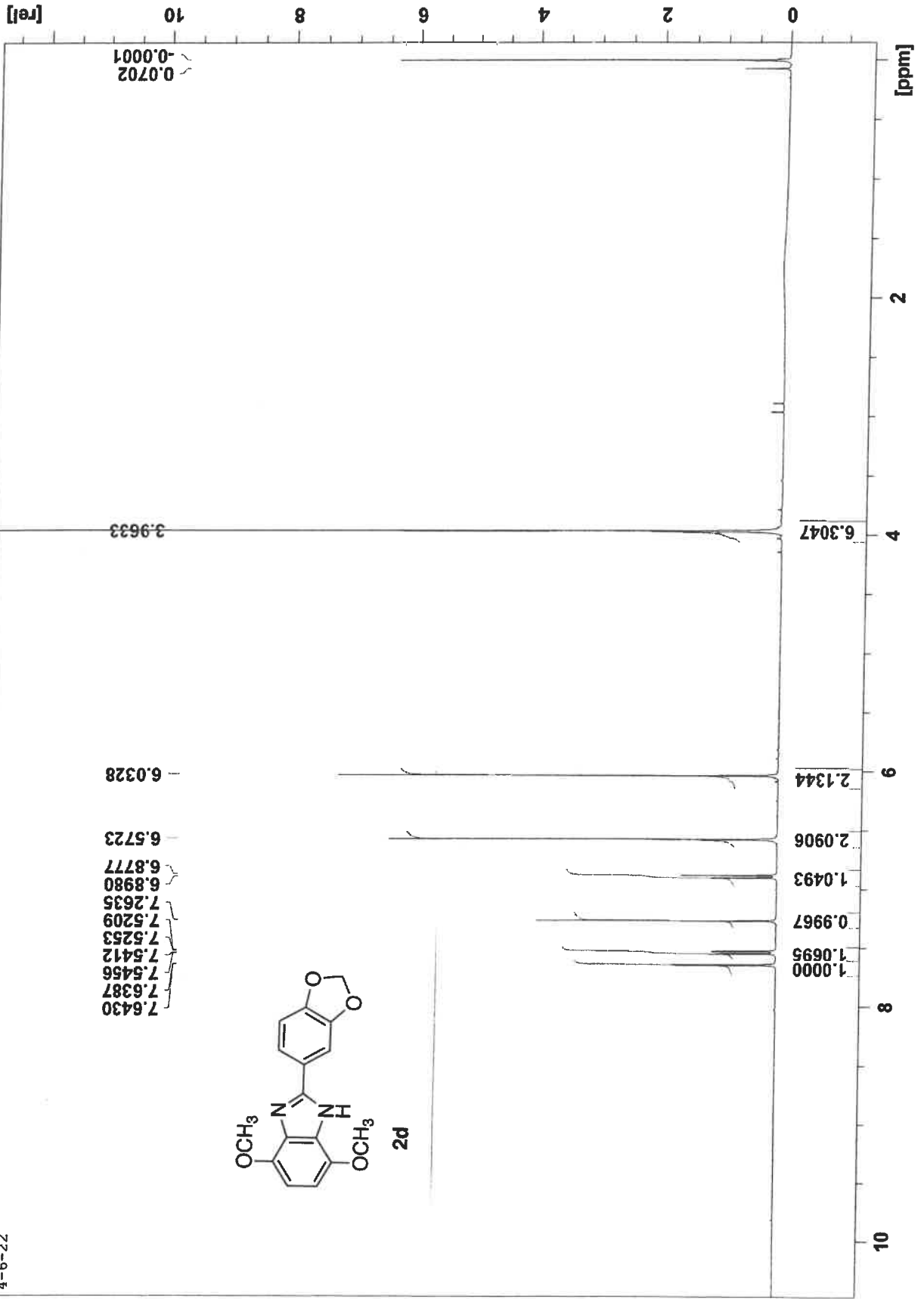
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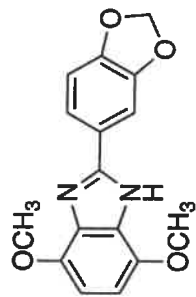
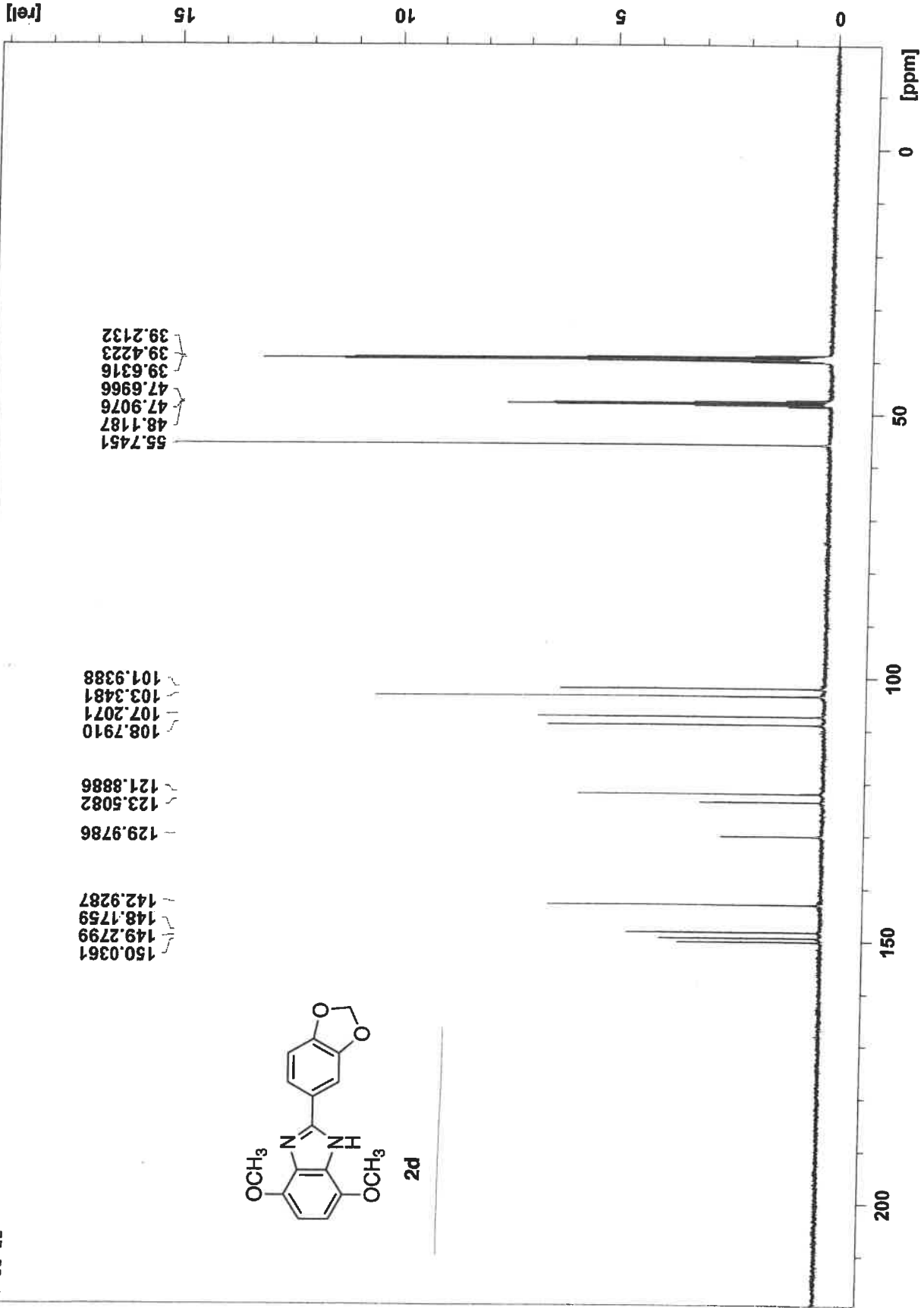
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4-6-9-22



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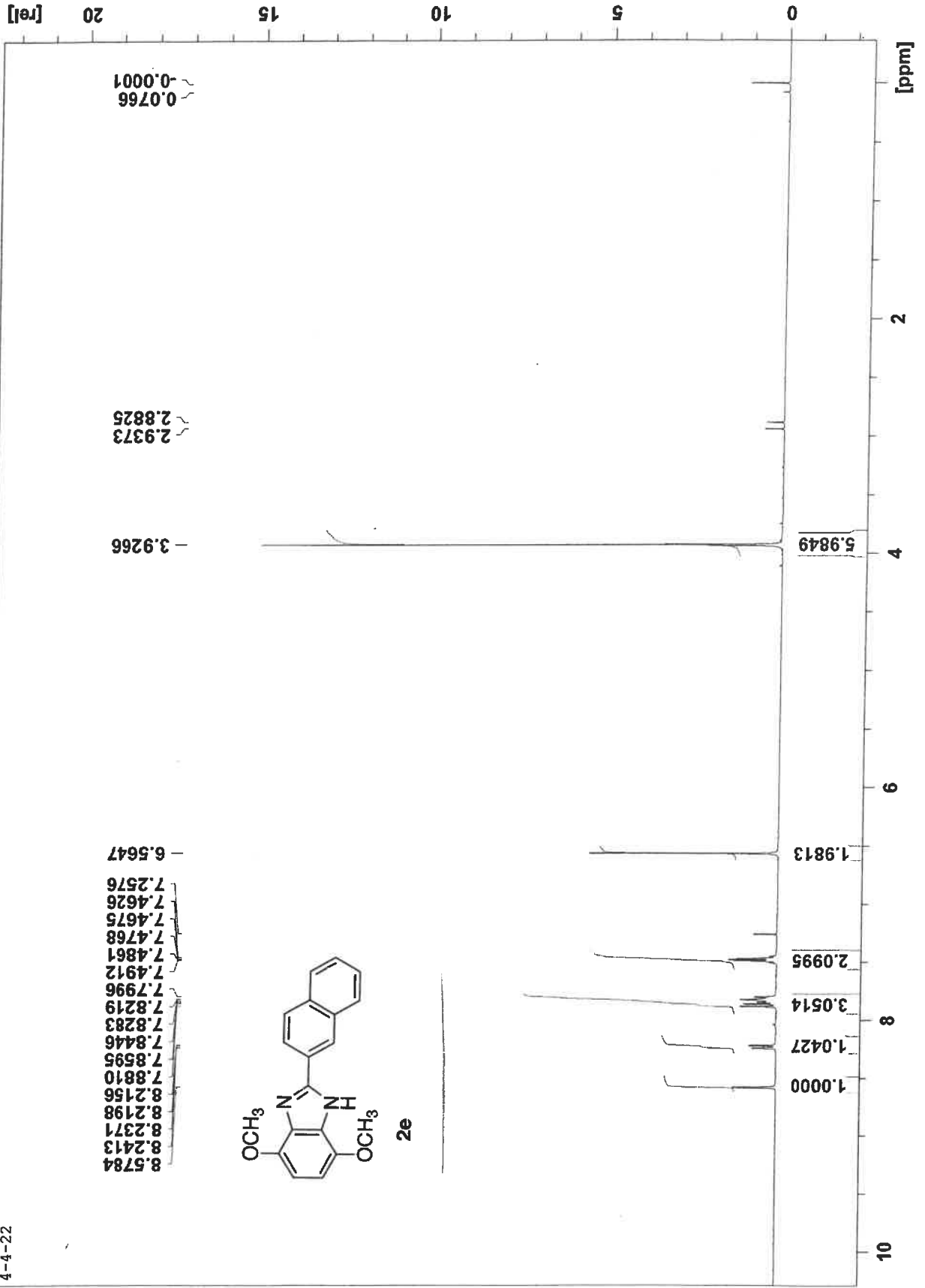
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2d

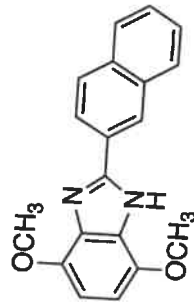
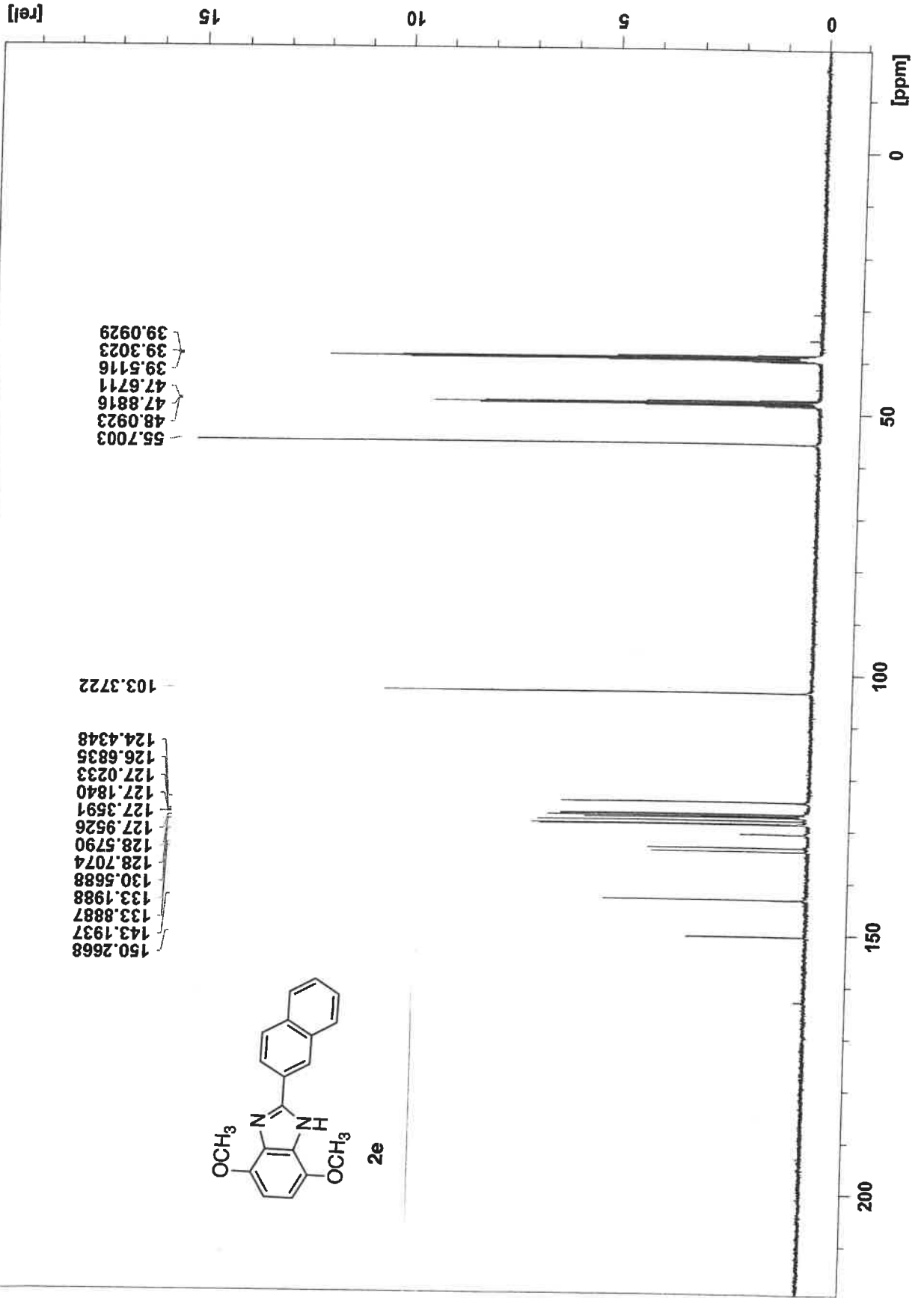
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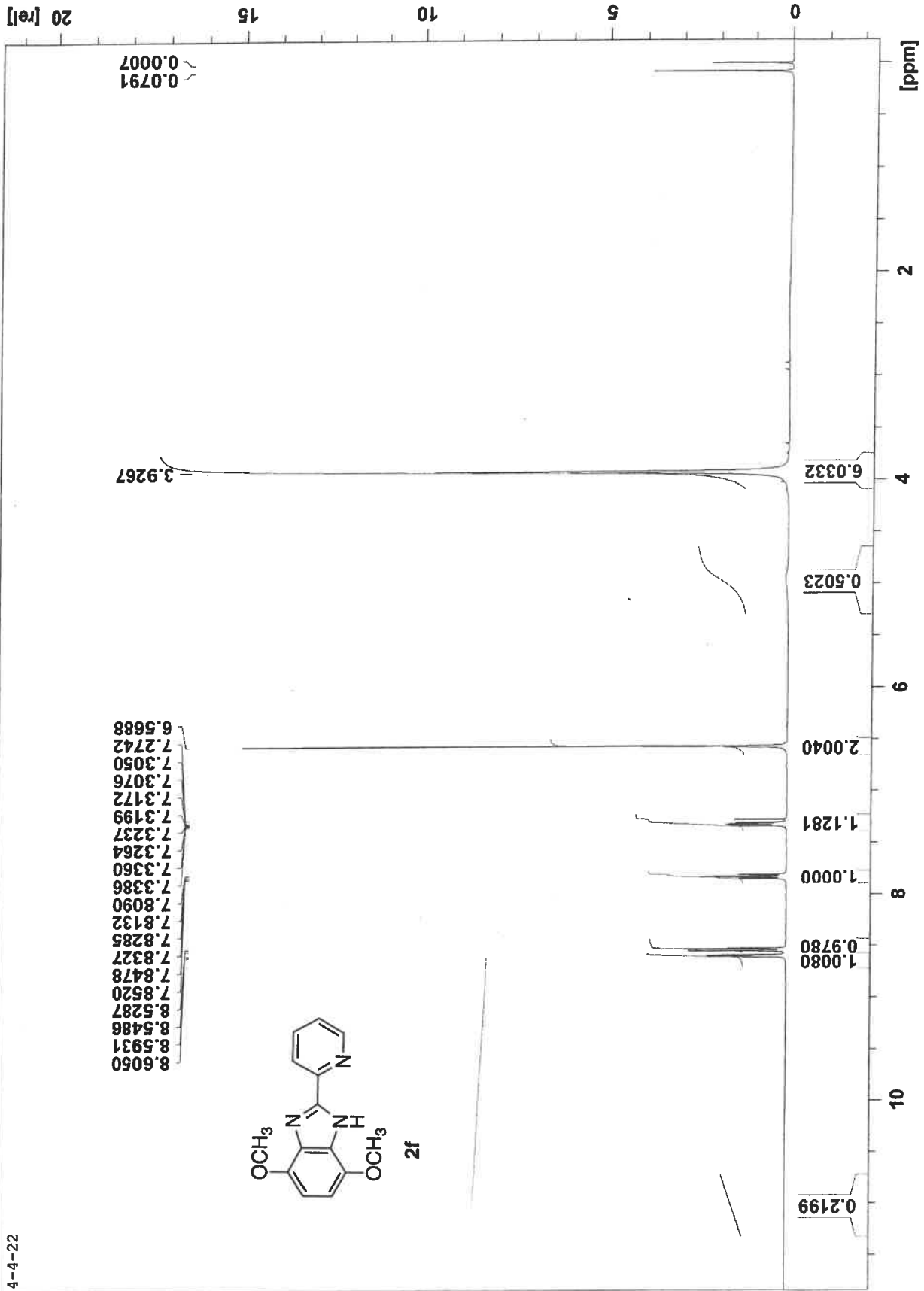
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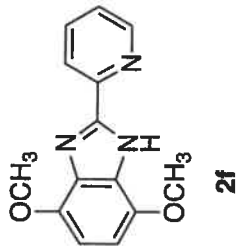
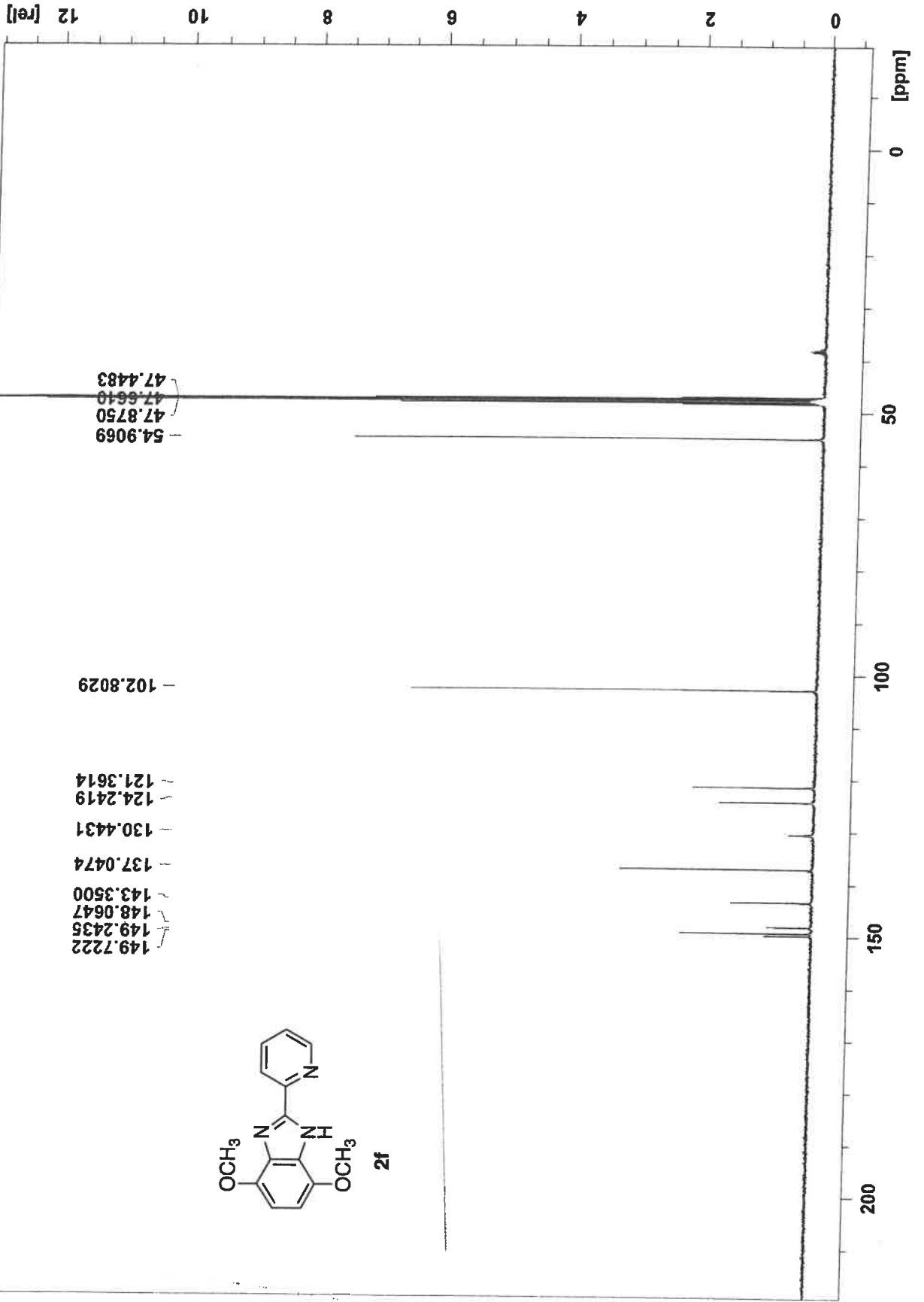
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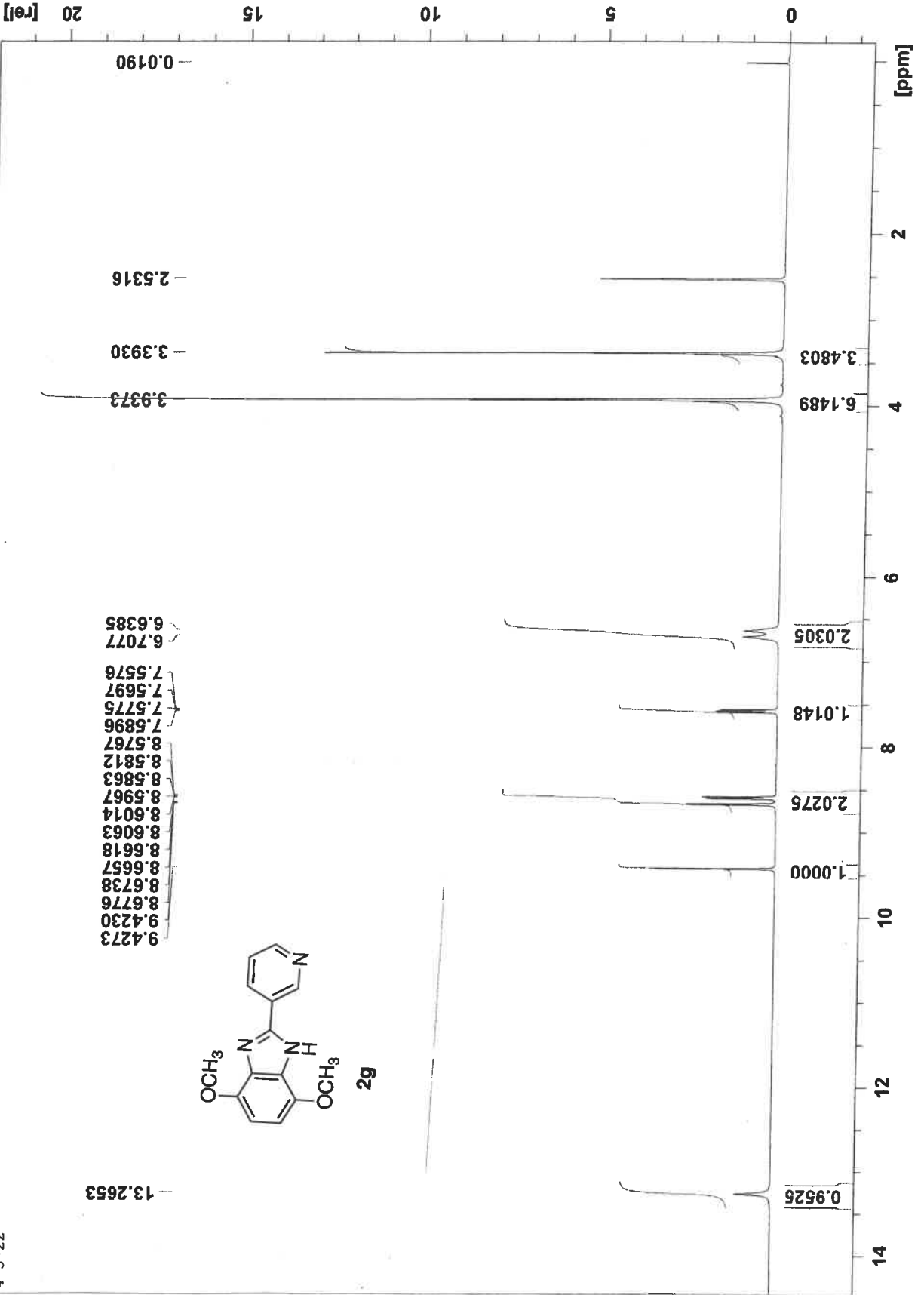


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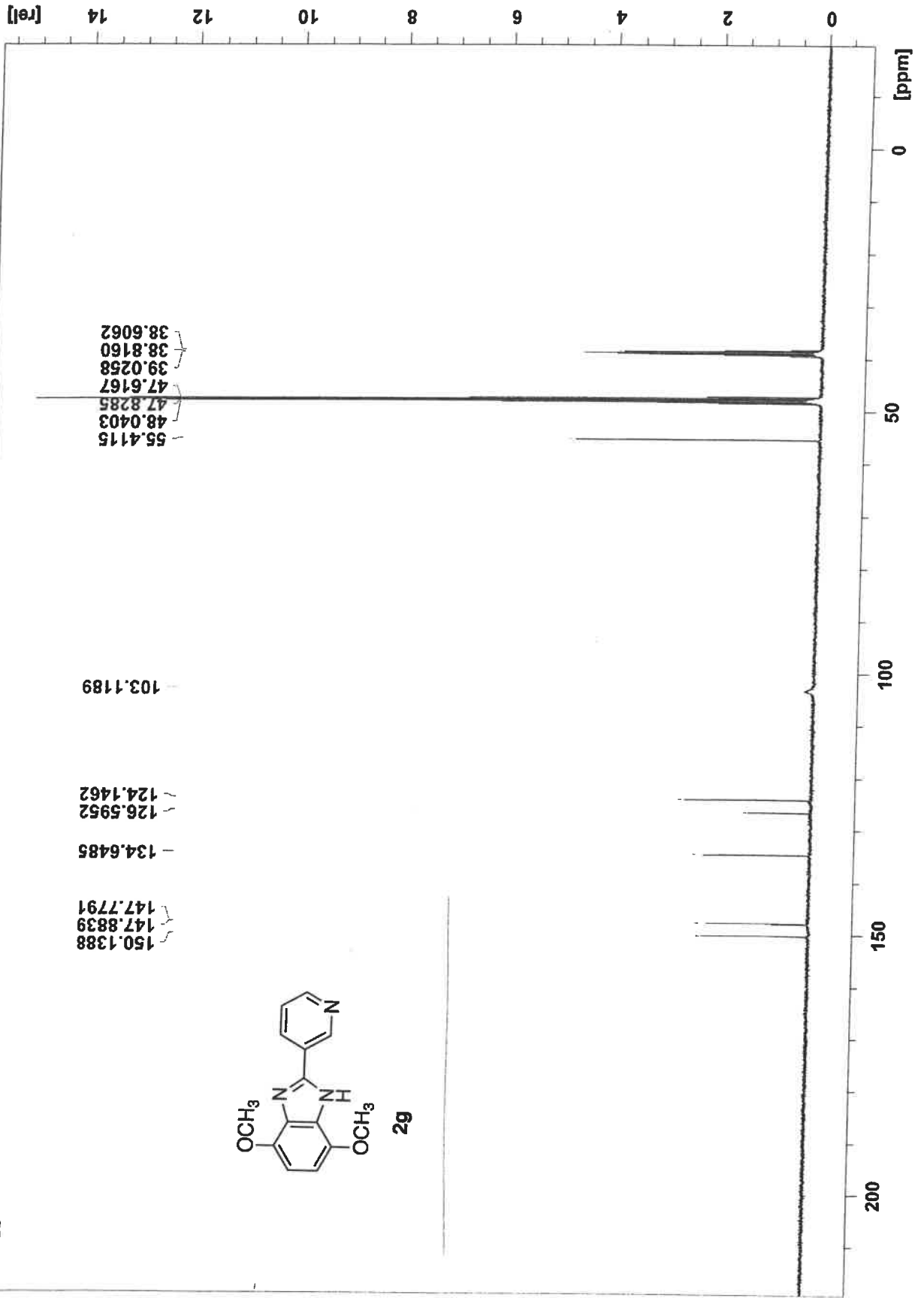


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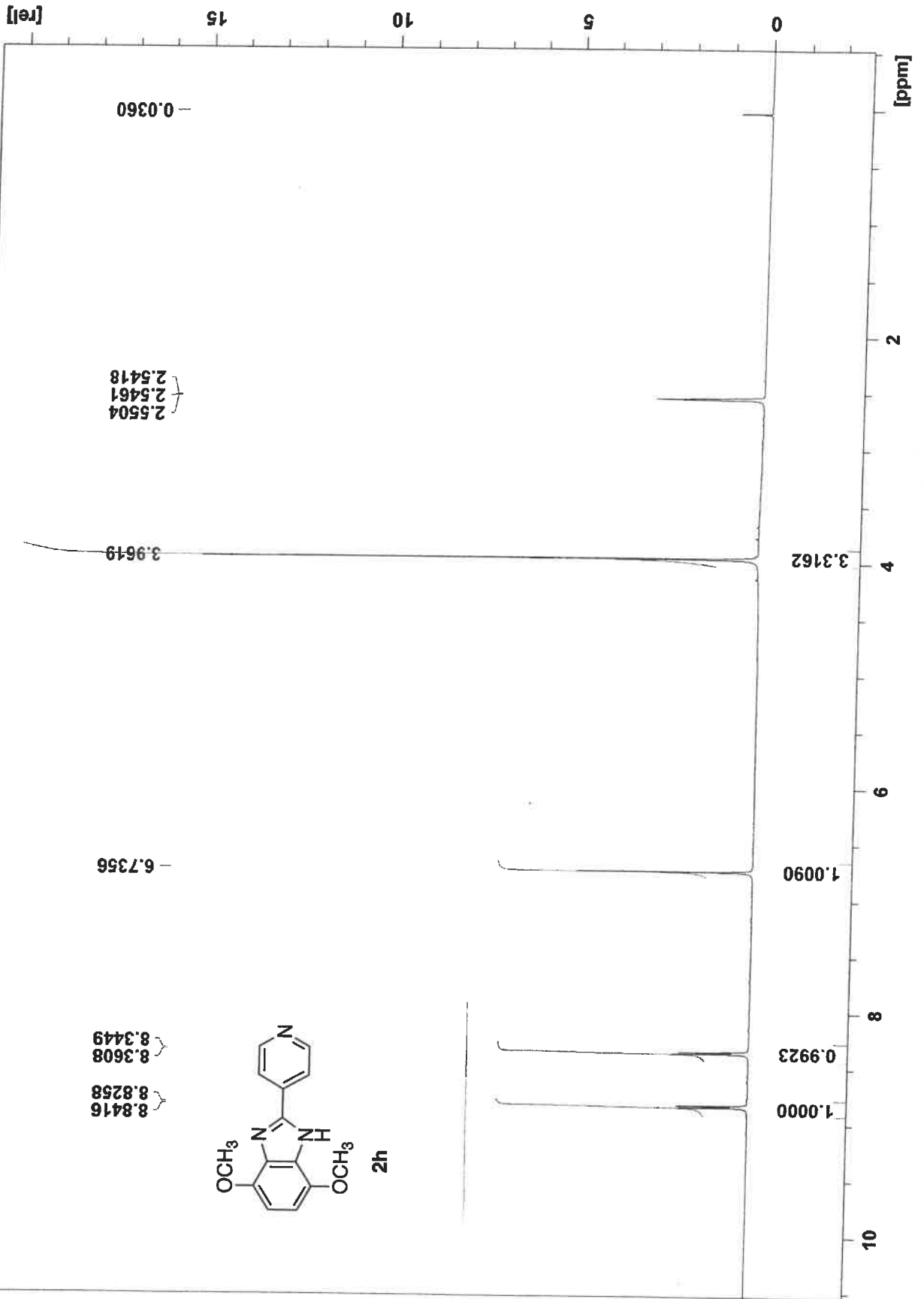
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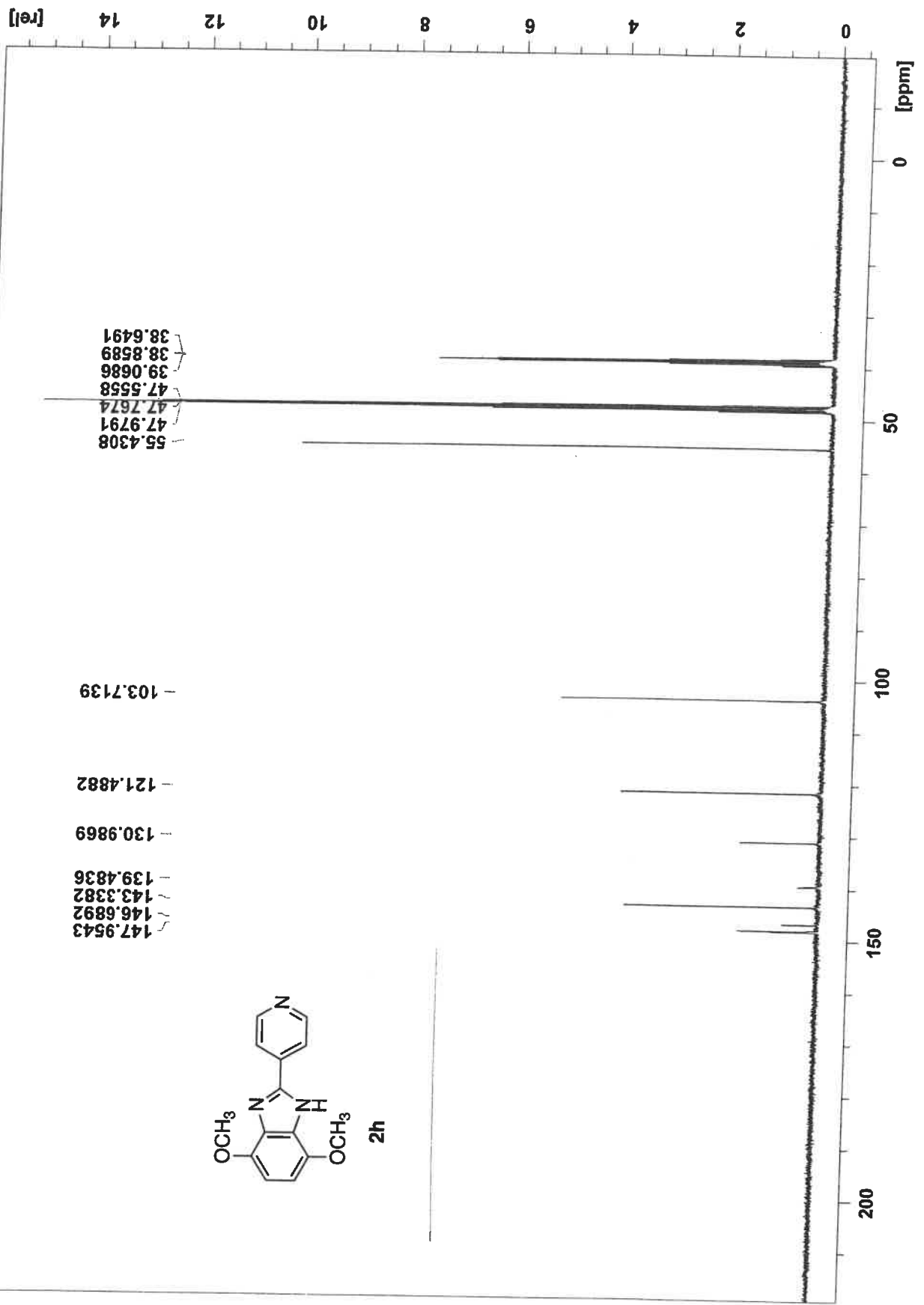
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7-11-22



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4-5-22



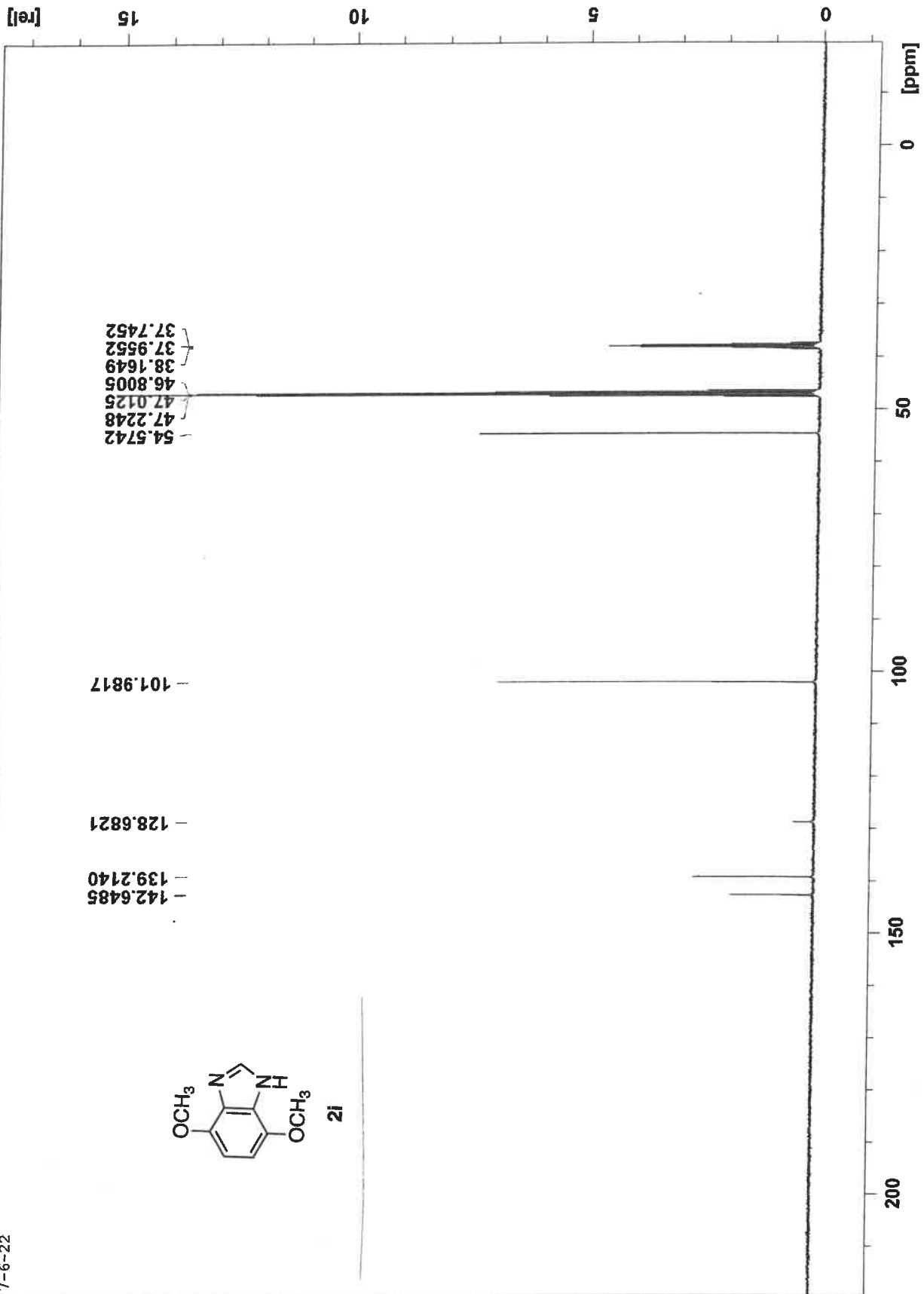
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(JMSO/MeOH)

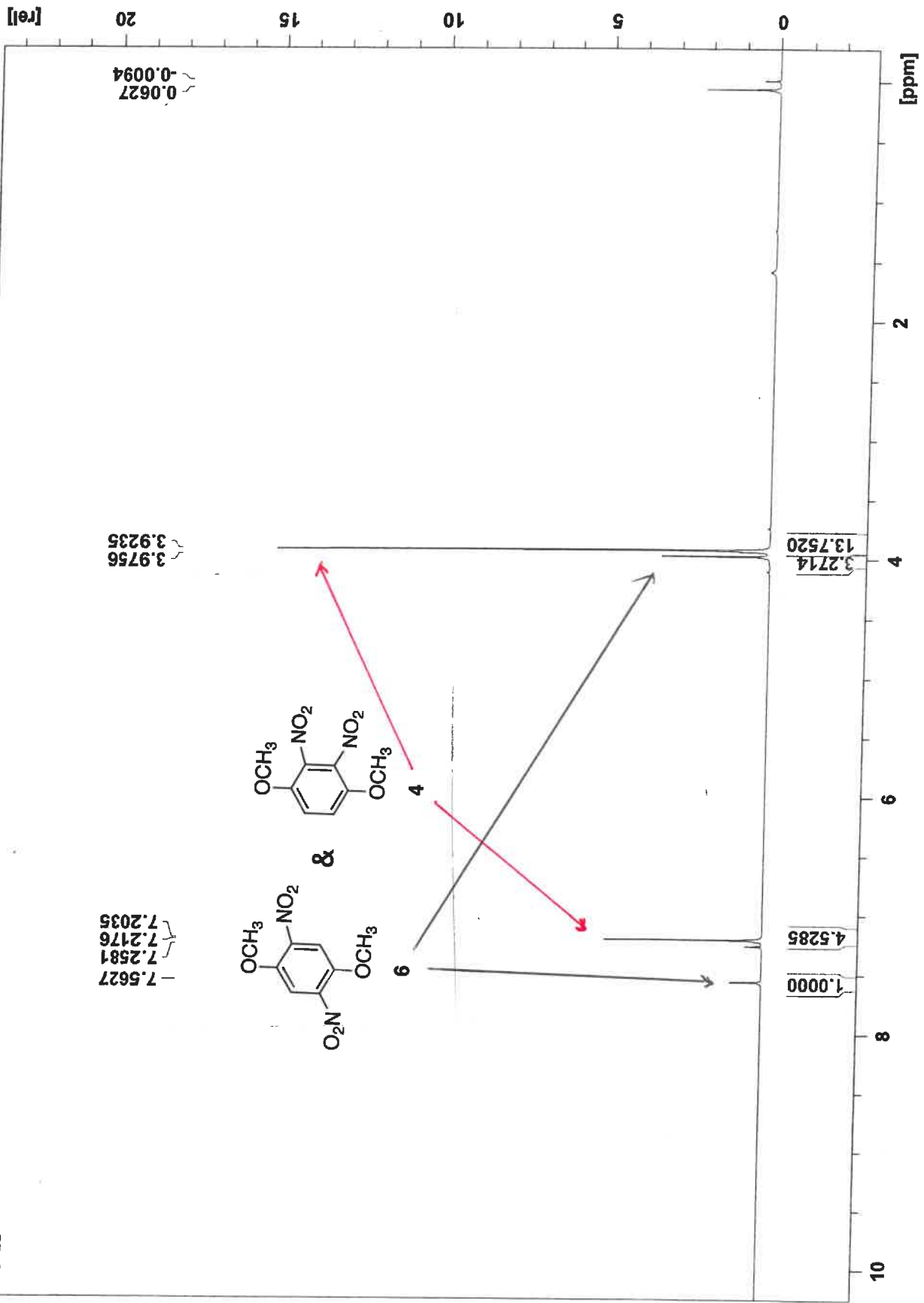
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7-6-22



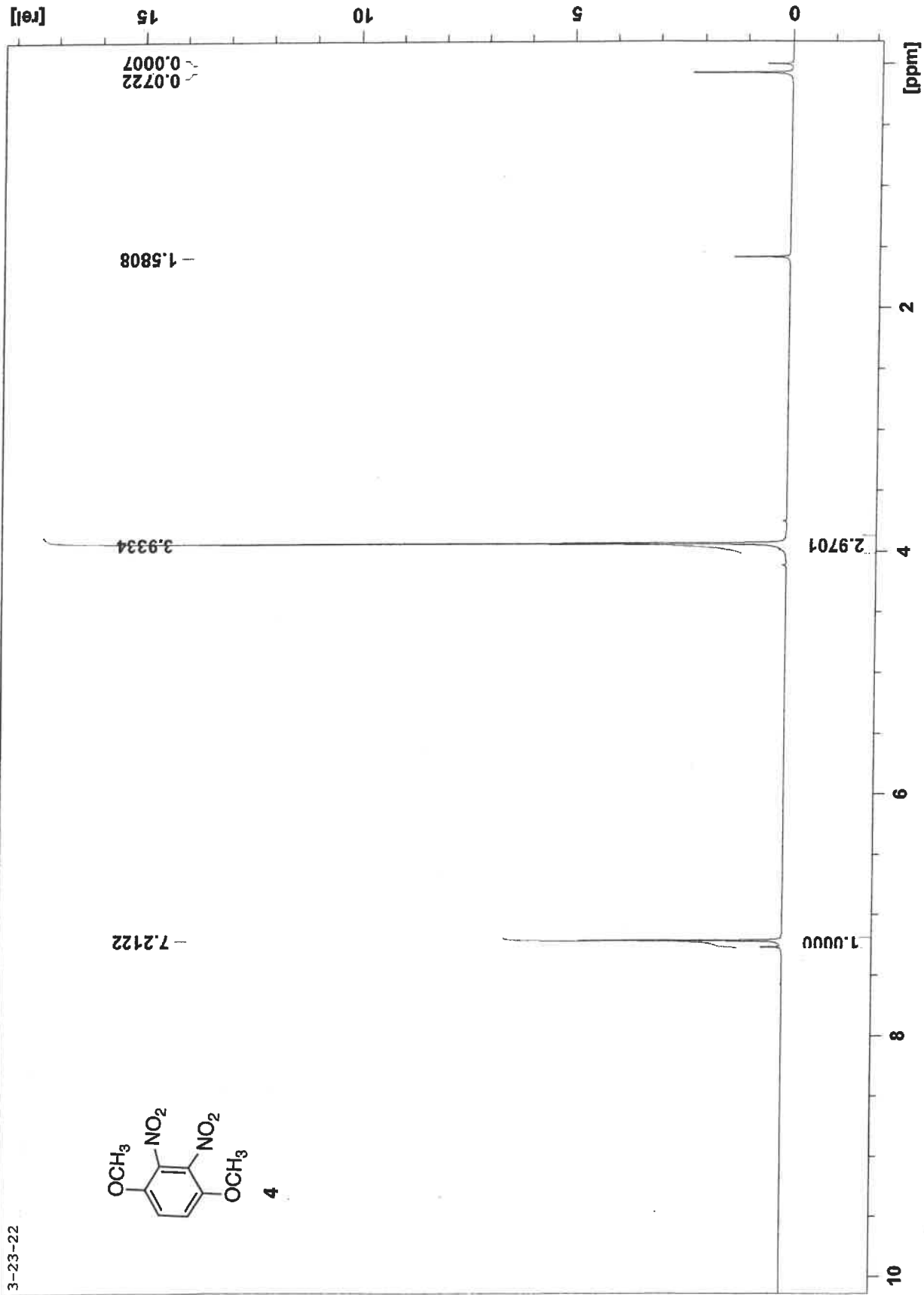
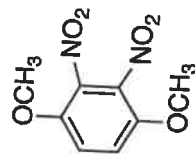
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3-3-22



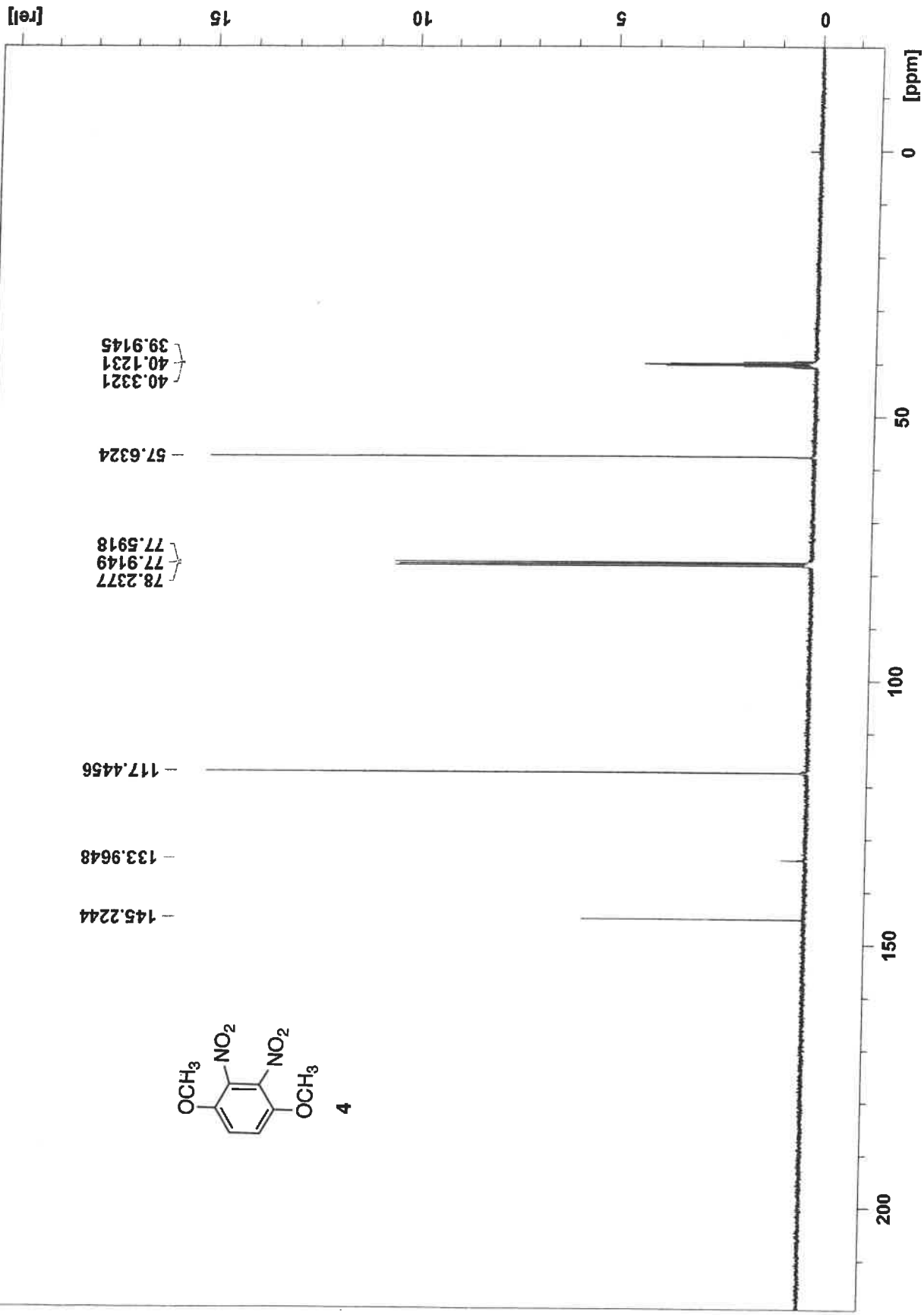
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3-23-22

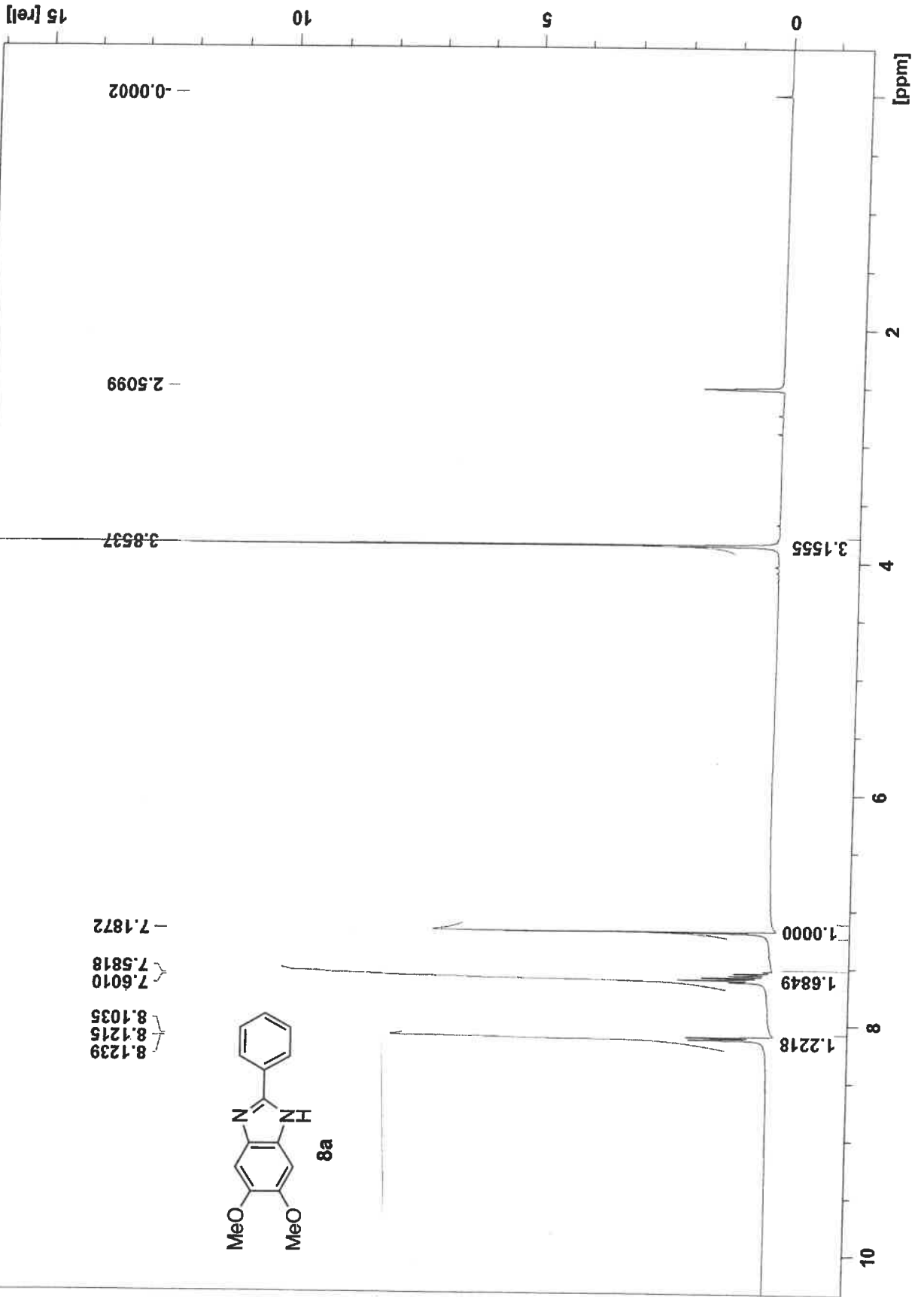


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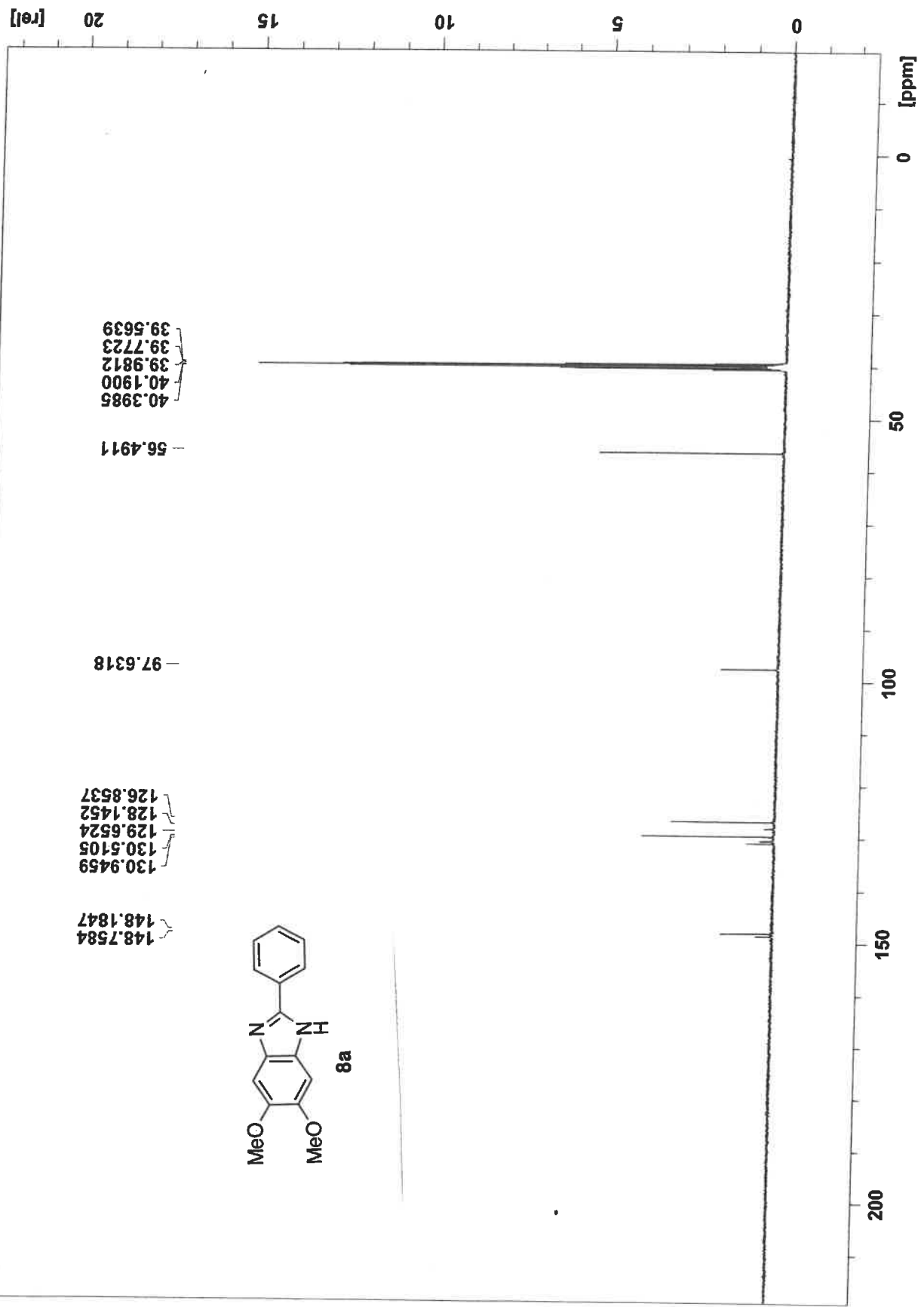
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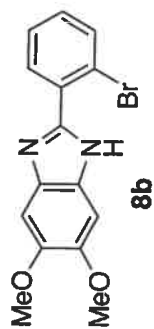
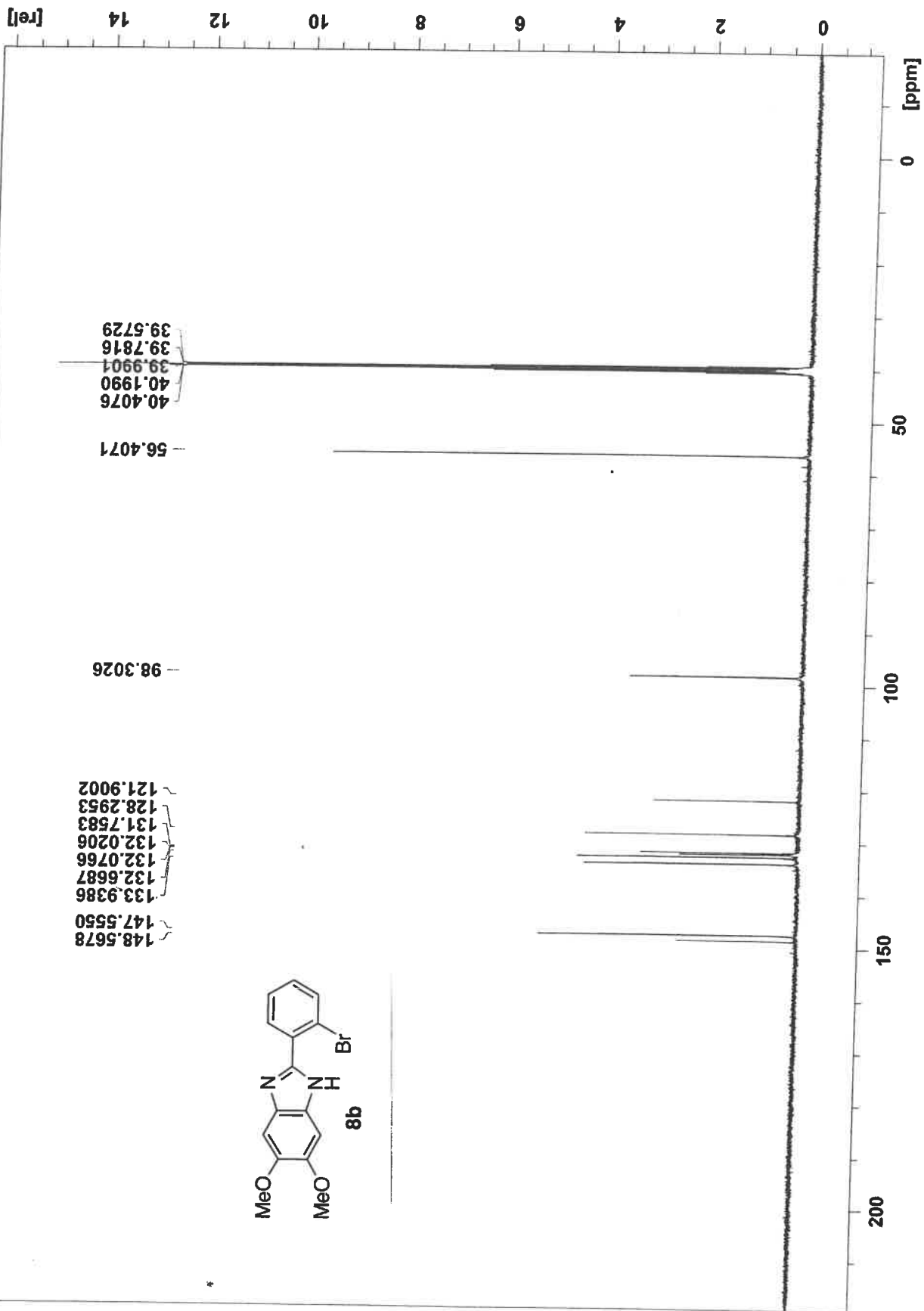
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4-21-22



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4-21-22

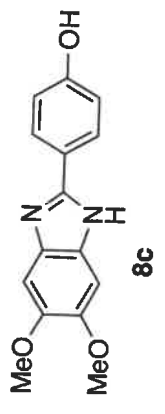
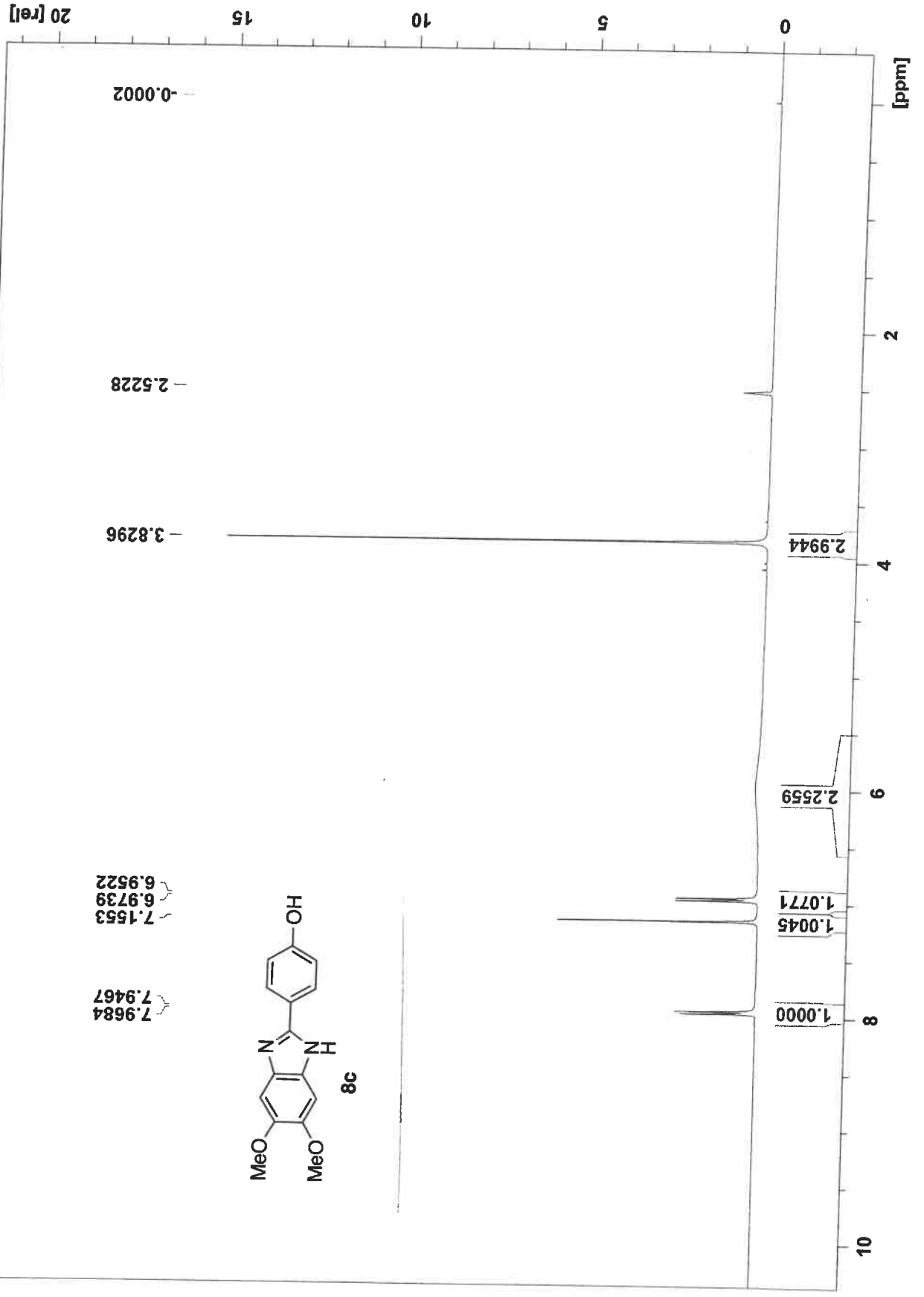


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4-20-22



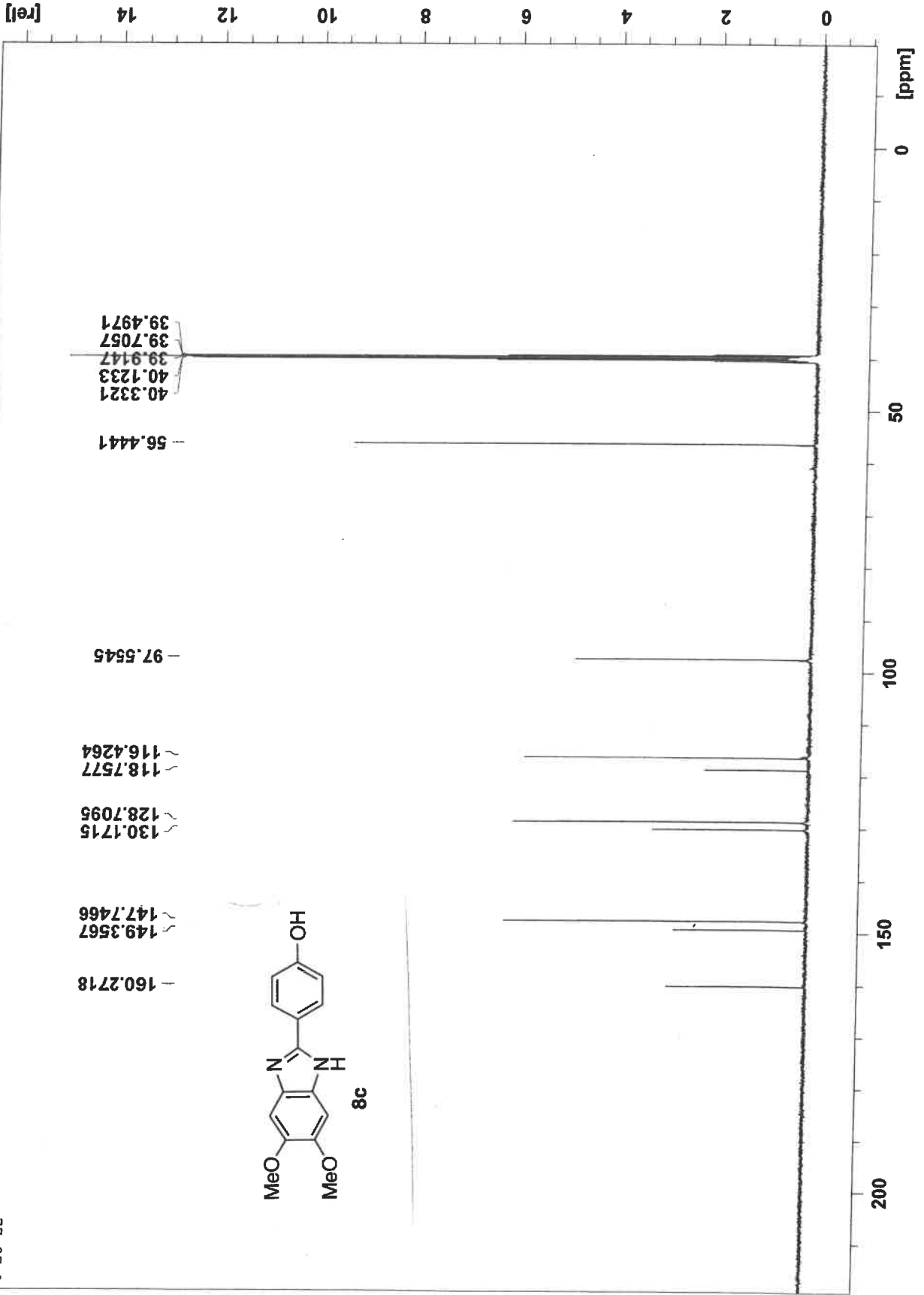
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4-20-22



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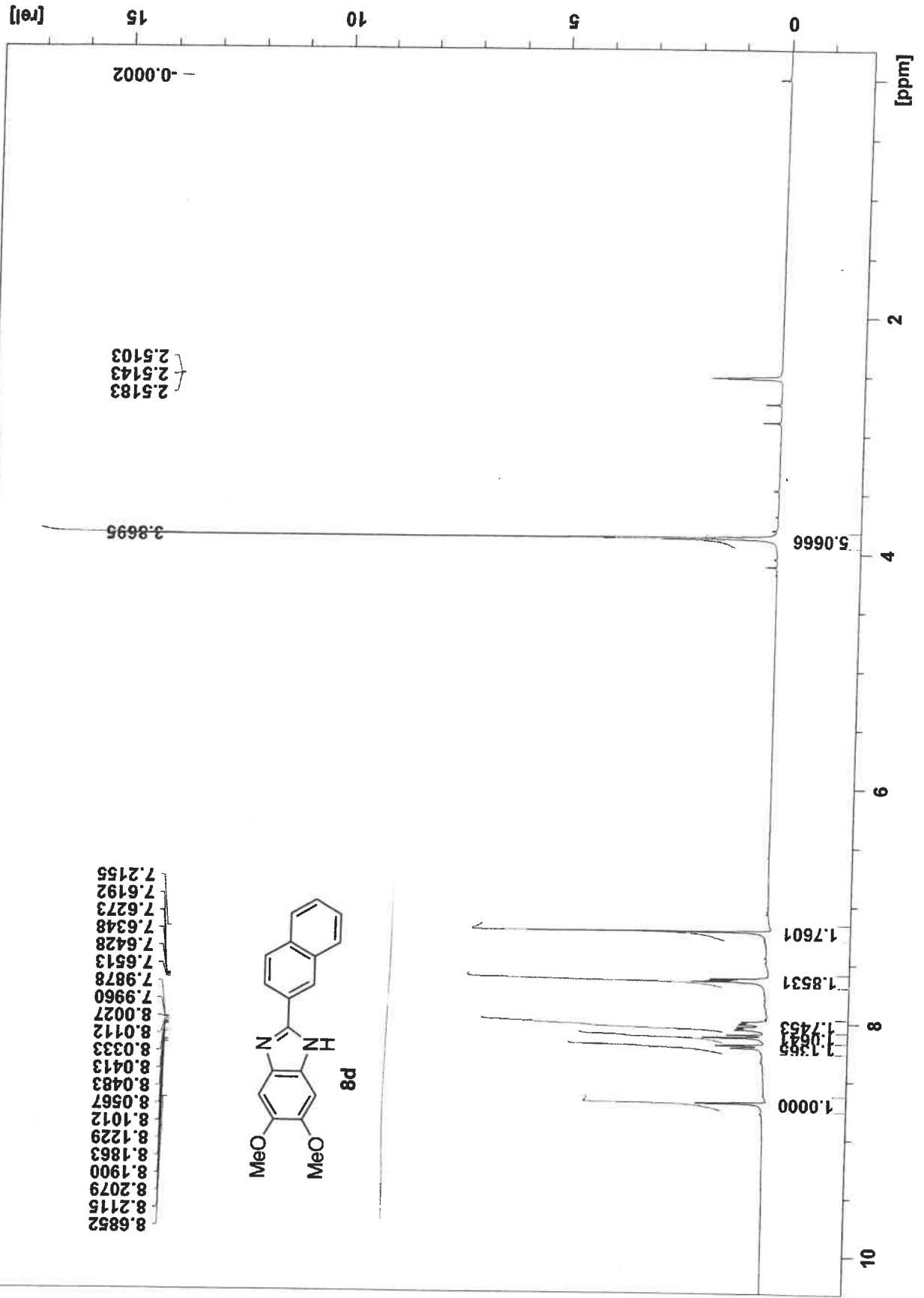
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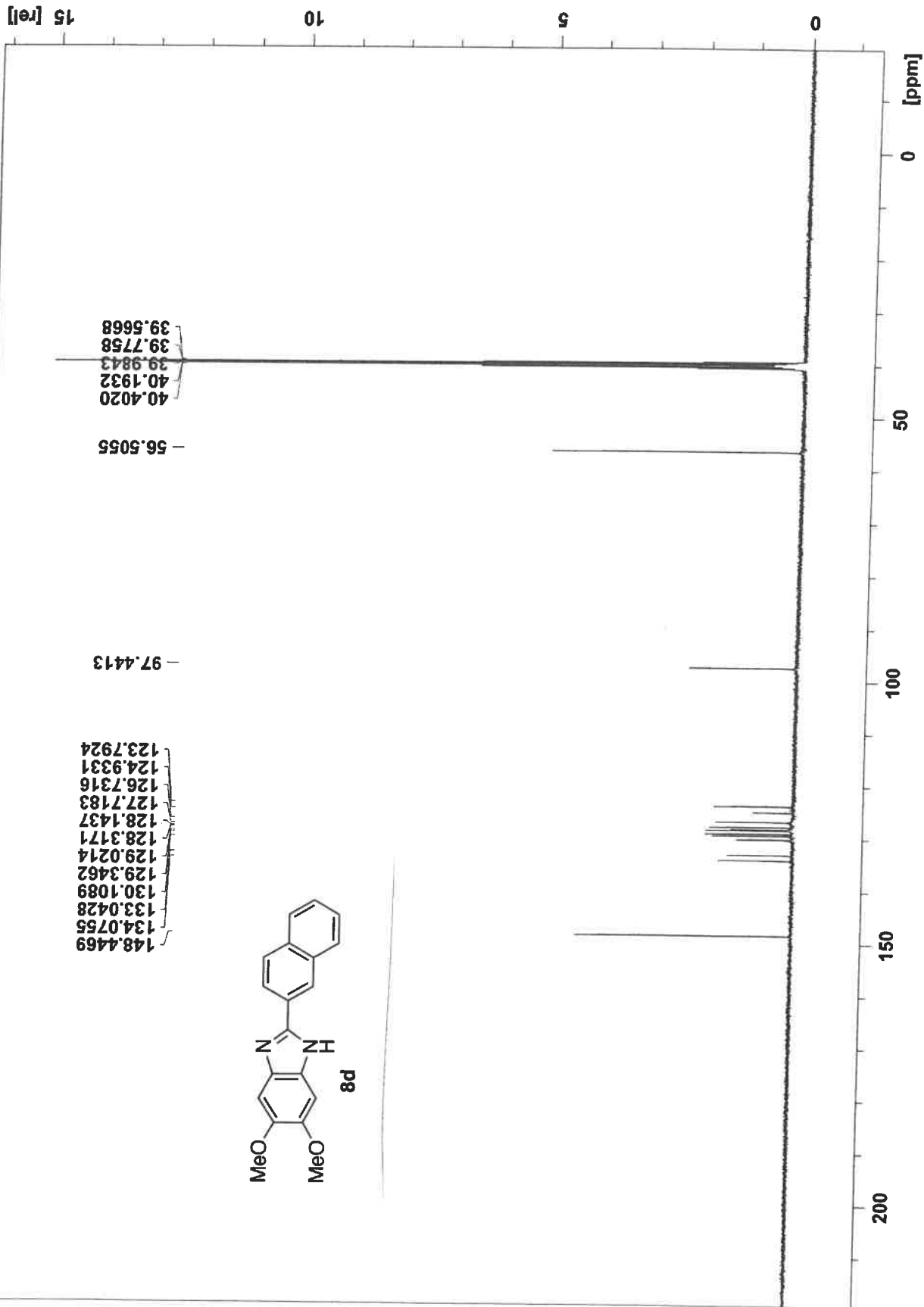
(DMSO)

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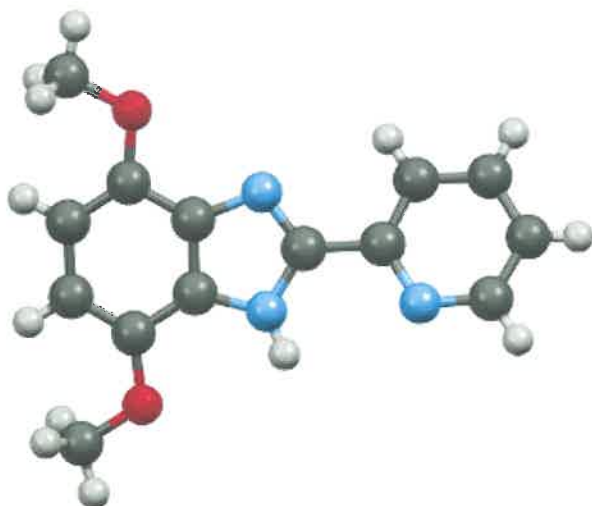
4-21-22



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4-21-22



Structural information for compound **2f** obtained via X-ray crystallography:



Crystals of compound **2f** were obtained via evaporation of a CH₂Cl₂ solution. A crystal was mounted on a glass fiber. All measurements were made using microfocus Cu K α radiation using multilayer optics on a Bruker-AXS DUO three-circle diffractometer, equipped with an Apex II CCD detector. Initial space group determination was based on a matrix consisting of 120 frames. The data were reduced using SAINT+ [1] and empirical absorption correction applied using SADABS [2]. The structure was solved using intrinsic phasing. Least-squares refinement was carried out on F^2 . All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in riding positions and refined isotropically. Structure solution, refinement, and the calculation of derived results were performed using the SHELX_{TL} package of computer programs [3] and ShelXle [4].

- (1) SAINT PLUS: Bruker Analytical X-ray Systems: Madison, WI, 2001.
- (2) SADABS: Bruker Analytical X-ray Systems: Madison, WI, 2001.
- (3) Sheldrick GM (2015) Crystal structure refinement with SHELXL. Acta Crystallogr Sect C 71: 3-8. (<https://doi.org/10.1107/S2053229614024218>)

(4) Hubschle CB, Sheldrick GM, Dittick B (2011) ShelXle: a Qt graphical user interface for SHELXL. *J Appl Cryst* 44:1281-1284.

(<https://doi.org/10.1107/S0021889811043202>)

Data Tables (see labeled figure below)

Table 1. Crystal data and structure refinement for cu_Love003_0m_a.res.

Identification code	cu_Love003_0m_a	
Empirical formula	C ₁₄ H ₁₃ N ₃ O ₂	
Formula weight	255.27	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.6886(5) Å	α = 90°.
	b = 8.9772(2) Å	β = 96.1640(10)°.
	c = 13.6228(4) Å	γ = 90°.
Volume	2515.48(11) Å ³	
Z	8	
Density (calculated)	1.348 Mg/m ³	
Absorption coefficient	0.761 mm ⁻¹	
F(000)	1072	
Crystal size	0.310 x 0.270 x 0.040 mm ³	
Theta range for data collection	4.299 to 69.699°.	
Index ranges	-24 ≤ h ≤ 24, -10 ≤ k ≤ 10, -16 ≤ l ≤ 16	
Reflections collected	14076	
Independent reflections	2329 [R(int) = 0.0439]	
Completeness to theta = 67.679°	98.9 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2329 / 0 / 174	
Goodness-of-fit on F ²	1.053	
Final R indices [I > 2σ(I)]	R1 = 0.0362, wR2 = 0.0957	
R indices (all data)	R1 = 0.0385, wR2 = 0.0979	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.212 and -0.248 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cu_Love003_0m_a.res. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5733(1)	2284(1)	5291(1)	26(1)
O(2)	3265(1)	4768(1)	5379(1)	24(1)
N(1)	4163(1)	590(1)	1875(1)	21(1)
N(2)	4621(1)	1886(1)	3763(1)	18(1)
N(3)	3619(1)	2823(1)	3839(1)	18(1)
C(1)	3924(1)	-257(2)	1113(1)	26(1)
C(2)	3274(1)	-644(2)	920(1)	25(1)
C(3)	2838(1)	-112(1)	1543(1)	23(1)
C(4)	3073(1)	779(1)	2332(1)	20(1)
C(5)	3737(1)	1096(1)	2475(1)	18(1)
C(6)	3989(1)	1973(1)	3342(1)	17(1)
C(7)	4652(1)	2728(1)	4612(1)	18(1)
C(8)	5151(1)	2972(1)	5380(1)	21(1)
C(9)	5004(1)	3851(2)	6149(1)	23(1)
C(10)	4379(1)	4490(2)	6174(1)	23(1)
C(11)	3887(1)	4229(1)	5430(1)	19(1)
C(12)	4029(1)	3313(1)	4642(1)	17(1)
C(13)	6218(1)	2430(2)	6117(1)	34(1)
C(14)	3155(1)	5912(2)	6068(1)	32(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for *cu_Love003_0m_a.res*.

O(1)-C(8)	1.3699(15)
O(1)-C(13)	1.4307(15)
O(2)-C(11)	1.3685(15)
O(2)-C(14)	1.4253(16)
N(1)-C(1)	1.3384(17)
N(1)-C(5)	1.3442(16)
N(2)-C(6)	1.3708(15)
N(2)-C(7)	1.3772(16)
N(2)-H(2)	0.8800
N(3)-C(6)	1.3189(16)
N(3)-C(12)	1.3825(15)
C(1)-C(2)	1.3871(18)
C(1)-H(1)	0.9500
C(2)-C(3)	1.3861(19)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.3861(18)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3959(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4678(16)
C(7)-C(12)	1.3955(17)
C(7)-C(8)	1.4065(17)
C(8)-C(9)	1.3720(19)
C(9)-C(10)	1.4168(18)
C(9)-H(9)	0.9500
C(10)-C(11)	1.3775(17)
C(10)-H(10)	0.9500
C(11)-C(12)	1.4087(17)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

C(8)-O(1)-C(13)	115.95(11)
C(11)-O(2)-C(14)	115.93(10)
C(1)-N(1)-C(5)	116.84(11)
C(6)-N(2)-C(7)	106.04(10)
C(6)-N(2)-H(2)	127.0
C(7)-N(2)-H(2)	127.0
C(6)-N(3)-C(12)	104.40(10)
N(1)-C(1)-C(2)	124.03(12)
N(1)-C(1)-H(1)	118.0
C(2)-C(1)-H(1)	118.0
C(3)-C(2)-C(1)	118.61(12)
C(3)-C(2)-H(2A)	120.7
C(1)-C(2)-H(2A)	120.7
C(4)-C(3)-C(2)	118.48(12)
C(4)-C(3)-H(3)	120.8
C(2)-C(3)-H(3)	120.8
C(3)-C(4)-C(5)	118.92(11)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
N(1)-C(5)-C(4)	123.12(11)
N(1)-C(5)-C(6)	118.07(10)
C(4)-C(5)-C(6)	118.77(11)
N(3)-C(6)-N(2)	113.49(11)
N(3)-C(6)-C(5)	123.15(11)
N(2)-C(6)-C(5)	123.13(11)
N(2)-C(7)-C(12)	105.74(10)
N(2)-C(7)-C(8)	132.38(11)
C(12)-C(7)-C(8)	121.77(11)
O(1)-C(8)-C(9)	126.59(11)
O(1)-C(8)-C(7)	116.57(11)
C(9)-C(8)-C(7)	116.82(11)
C(8)-C(9)-C(10)	121.97(11)
C(8)-C(9)-H(9)	119.0
C(10)-C(9)-H(9)	119.0
C(11)-C(10)-C(9)	121.19(12)

C(11)-C(10)-H(10)	119.4
C(9)-C(10)-H(10)	119.4
O(2)-C(11)-C(10)	126.46(11)
O(2)-C(11)-C(12)	116.10(10)
C(10)-C(11)-C(12)	117.45(11)
N(3)-C(12)-C(7)	110.31(10)
N(3)-C(12)-C(11)	128.91(11)
C(7)-C(12)-C(11)	120.75(11)
O(1)-C(13)-H(13A)	109.5
O(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(2)-C(14)-H(14A)	109.5
O(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5 ^a
O(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

Symmetry transformations used to generate equivalent atoms:

