Supplementary Material

Facile access to 2-aryl-3-nitro-2*H*-chromenes and 2,3,4-trisubstituted chromanes

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X-ray Crystal Structure Data for Compounds 3i and 4f

1. X-ray crystallographic data for compound 3i

Crystals of compound **3i** suitable for X-ray analysis were obtained by slow evaporation from the solvent of CH_2Cl_2. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC# 920109). Copies of the data can be obtained free of charge on application to the CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

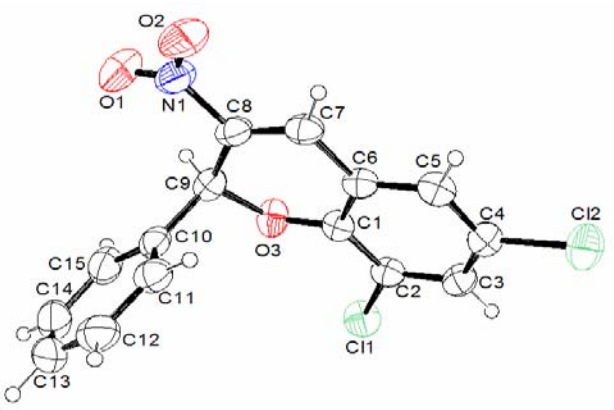

Table S1-1. Crystal data and structure refinement for compound **3i**

Identification code	compound **3i**
Empirical formula	C15 H9 Cl2 N O3
Formula weight	322.13
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 9.0327(12) Å α = 90°.
	B = 9.3313(13) Å β = 93.644(2)°.
	C = 16.806(2) Å γ = 90°.
Volume	1413.7(3) $Å^3$
Z	4
Calculated density	1.514 Mg/m^3
Absorption coefficient	0.467 mm^{-1}
F(000)	656
Crystal size	0.37 x 0.28 x 0.16 mm
Theta range for data collection	3.14 to 25.73°
Limiting indices	-6<=h<=11, -11<=k<=11, -20<=l<=19

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Reflections collected	7237
Independent reflections	2685 [R(int) = 0.0226]
Completeness to theta = 25.73	99.8 %
Absorption correction	constr
Max. and min. transmission	0.9307 and 0.8465
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2685 / 0 / 190
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1264
R indices (all data)	R1 = 0.0503, wR2 = 0.1401
Largest diff. peak and hole	0.247 and -0.298 e.Å^{-3}

Table S1-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for compound **3i**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Cl(1)	926(1)	3896(1)	11076(1)	68(1)
Cl(2)	3838(1)	8500(1)	10059(1)	77(1)
N(1)	3787(2)	1486(3)	7804(1)	72(1)
O(1)	3555(2)	206(2)	7834(1)	101(1)
O(2)	4384(2)	2063(3)	7261(1)	99(1)
O(3)	2123(2)	2466(2)	9717(1)	59(1)
C(1)	2472(2)	3877(2)	9748(1)	46(1)
C(2)	2016(2)	4681(2)	10384(1)	49(1)
C(3)	2417(2)	6100(2)	10479(1)	53(1)
C(4)	3287(2)	6722(2)	9928(1)	52(1)
C(5)	3760(2)	5964(2)	9295(1)	52(1)
C(6)	3345(2)	4533(2)	9198(1)	48(1)
C(7)	3828(2)	3672(2)	8547(1)	53(1)
C(8)	3309(2)	2355(2)	8455(1)	56(1)
C(9)	2221(2)	1662(2)	8979(1)	54(1)
C(10)	709(2)	1457(2)	8579(1)	52(1)
C(11)	117(2)	2409(2)	8011(1)	60(1)
C(12)	-1287(3)	2187(4)	7662(2)	81(1)
C(13)	-2113(3)	1043(4)	7884(2)	88(1)
C(14)	-1550(3)	96(4)	8441(2)	91(1)
C(15)	-139(3)	287(3)	8794(2)	70(1)

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2. X-ray crystallographic data for compound 4f

Crystals of compound **4f** suitable for X-ray analysis were obtained by slow evaporation from the solvent of CH_2Cl_2. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC# 920110). Copies of the data can be obtained free of charge on application to the CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

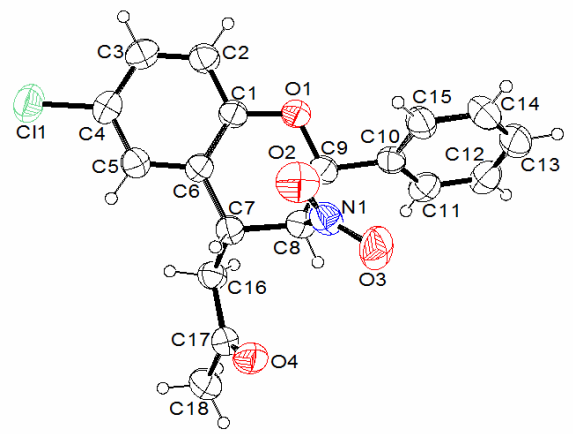

Table S2-1. Crystal data and structure refinement for compound **4f**

Identification code	compound **4f**
Empirical formula	C18 H16 Cl N O4
Formula weight	345.77
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 14.189(4) Å α = 90°. B = 12.900(3) Å β = 90°. C = 18.037(5) Å γ = 90°.
Volume	3301.5(15) $Å^3$
Z	8
Calculated density	1.391 Mg/m^3
Absorption coefficient	0.253 mm^{-1}
F(000)	1440
Crystal size	0.36 x 0.27 x 0.14 mm
Theta range for data collection	2.41 to 25.10 deg.
Limiting indices	-12<=h<=16, -15<=k<=15, -21<=l<=21
Reflections collected	15655

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Independent reflections	2940 [R(int) = 0.1246]
Completeness to theta = 25.10	99.9 %
Absorption correction	constr
Max. and min. transmission	0.9664 and 0.9135
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2940 / 0 / 219
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0601, wR2 = 0.1358
R indices (all data)	R1 = 0.1398, wR2 = 0.1761
Largest diff. peak and hole	0.260 and -0.255 e.Å^{-3}

Table S2-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for compound **4f**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Cl(1)	11632(1)	9805(1)	4044(1)	93(1)
N(1)	6724(3)	11011(2)	3744(2)	70(1)
O(1)	7597(2)	8954(2)	4005(1)	66(1)
O(2)	7129(2)	11172(2)	4325(2)	95(1)
O(3)	5924(2)	11304(2)	3610(2)	100(1)
O(4)	7612(2)	12162(2)	2100(2)	80(1)
C(1)	8535(3)	9199(3)	4000(2)	57(1)
C(2)	9117(3)	8630(3)	4456(2)	65(1)
C(3)	10060(3)	8813(3)	4487(2)	67(1)
C(4)	10432(3)	9602(3)	4046(2)	64(1)
C(5)	9849(3)	10191(3)	3608(2)	62(1)
C(6)	8886(3)	10014(3)	3576(2)	53(1)
C(7)	8255(3)	10682(3)	3098(2)	55(1)
C(8)	7220(3)	10375(3)	3166(2)	56(1)
C(9)	7096(3)	9213(3)	3347(2)	59(1)
C(10)	6090(3)	8870(3)	3460(2)	59(1)
C(11)	5576(3)	8482(3)	2869(2)	69(1)
C(12)	4655(3)	8147(3)	2974(3)	80(1)
C(13)	4256(3)	8213(3)	3663(3)	87(1)
C(14)	4755(4)	8610(4)	4246(3)	86(1)
C(15)	5668(3)	8928(3)	4141(2)	75(1)
C(16)	8552(3)	10672(3)	2285(2)	62(1)
C(17)	8157(3)	11536(4)	1829(2)	66(1)
C(18)	8477(3)	11591(4)	1045(2)	92(2)

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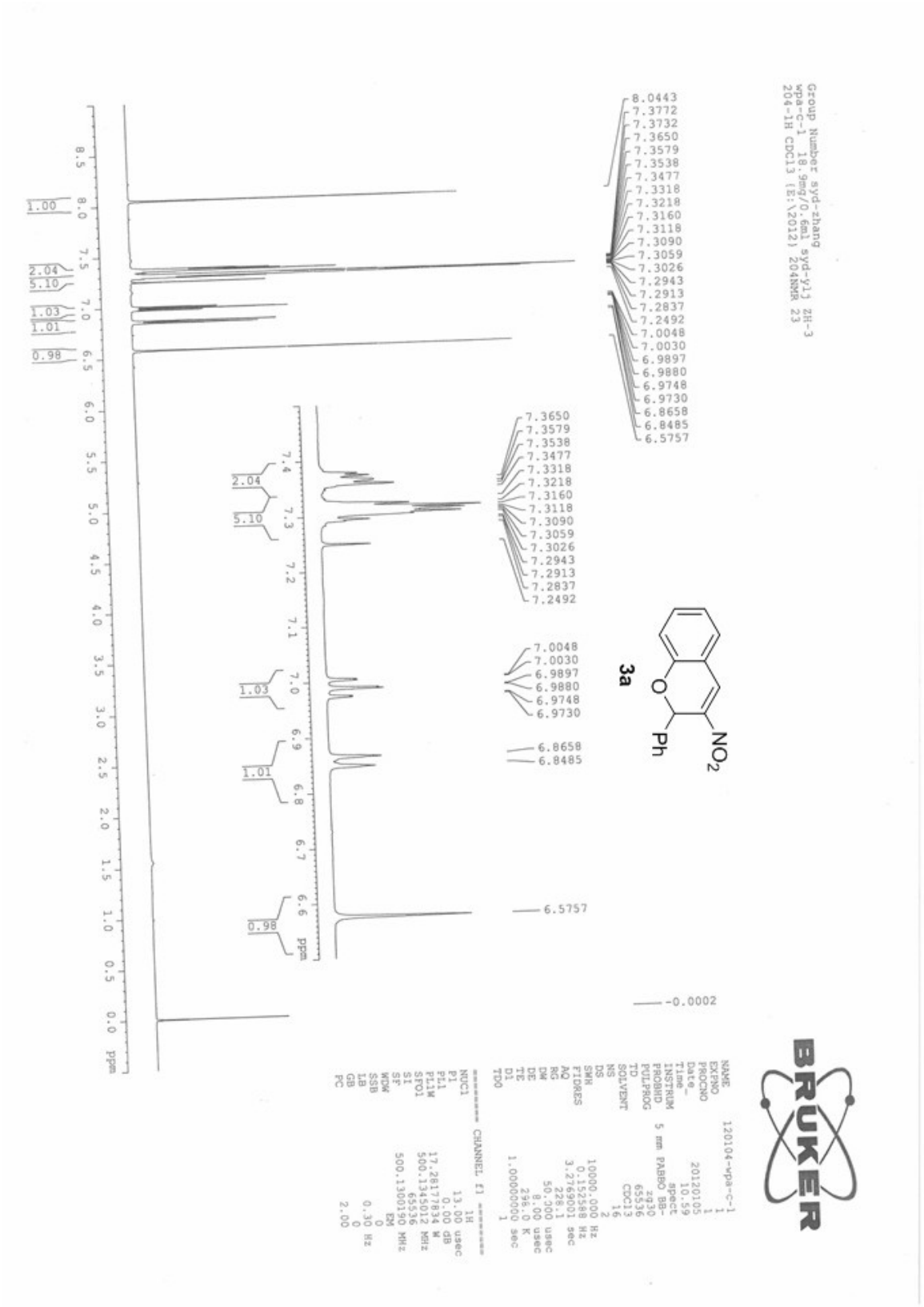

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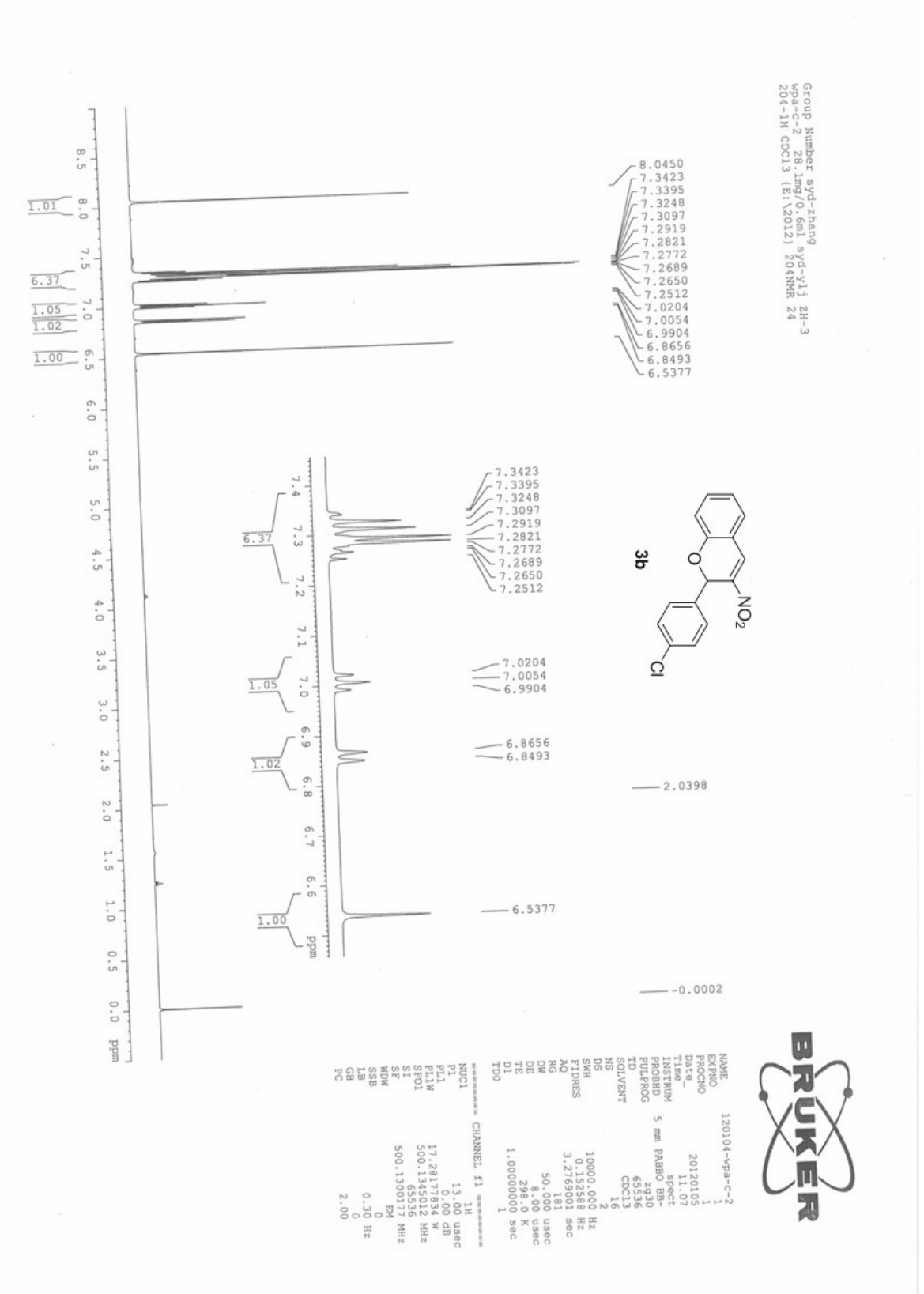

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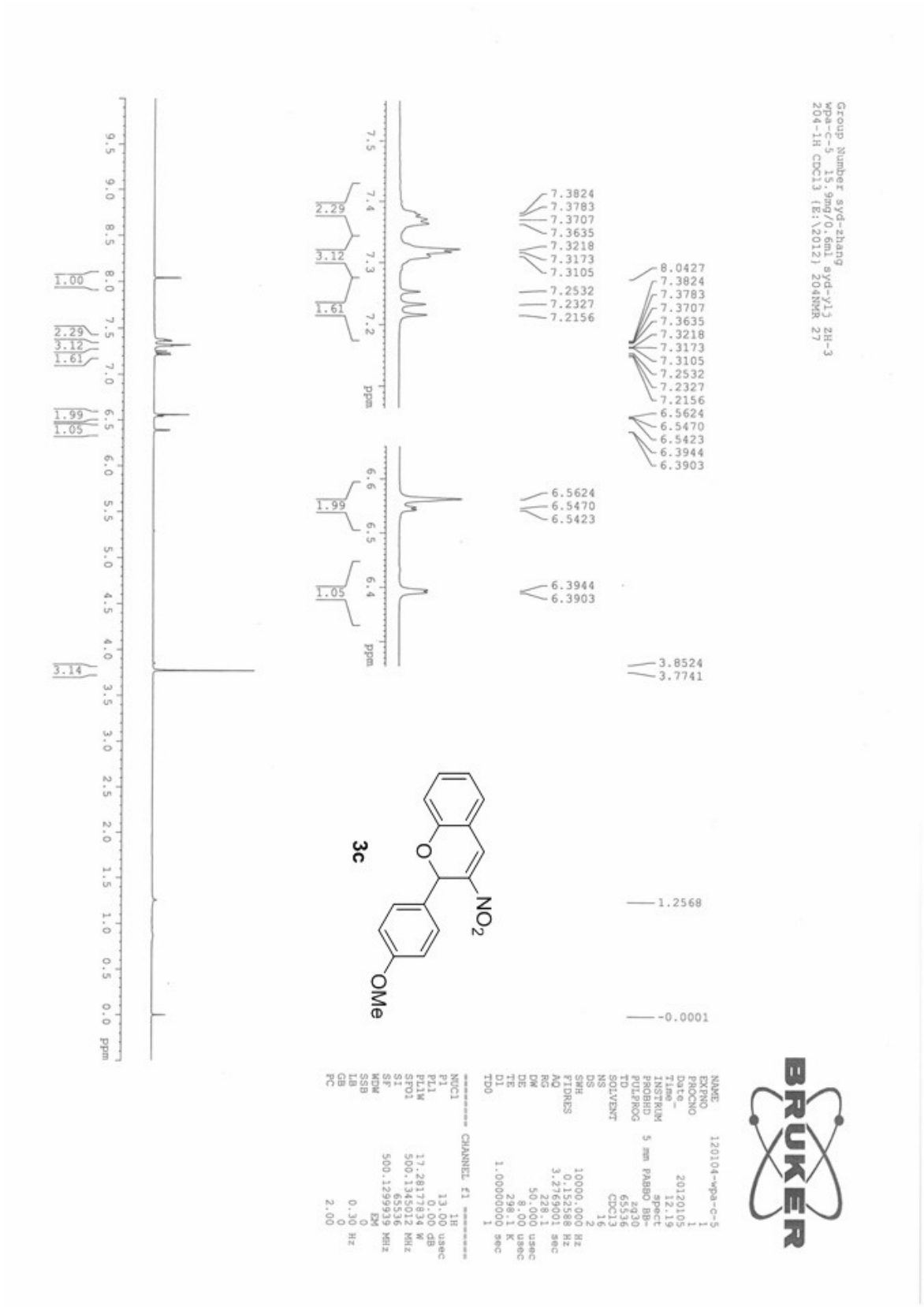

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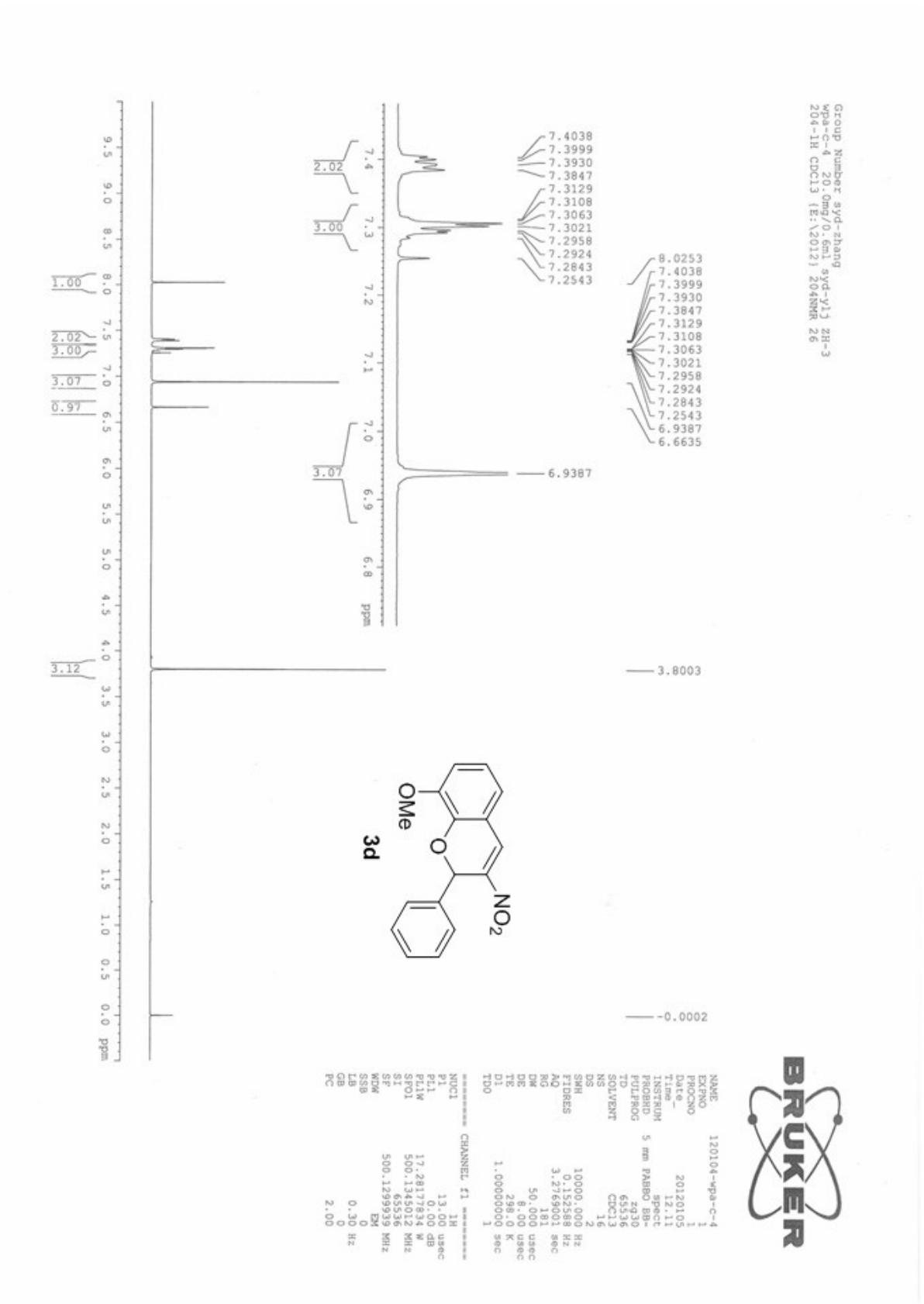

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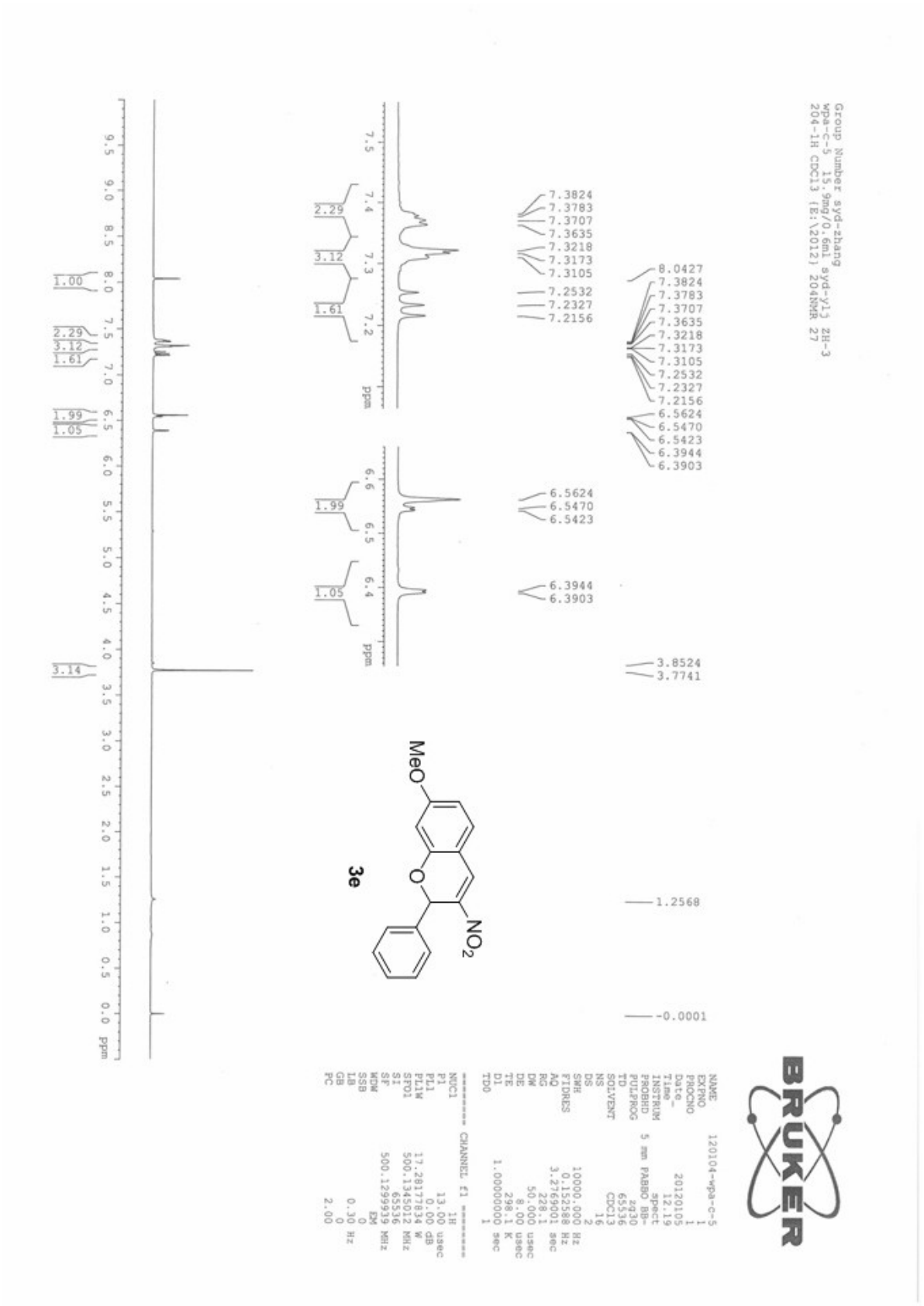

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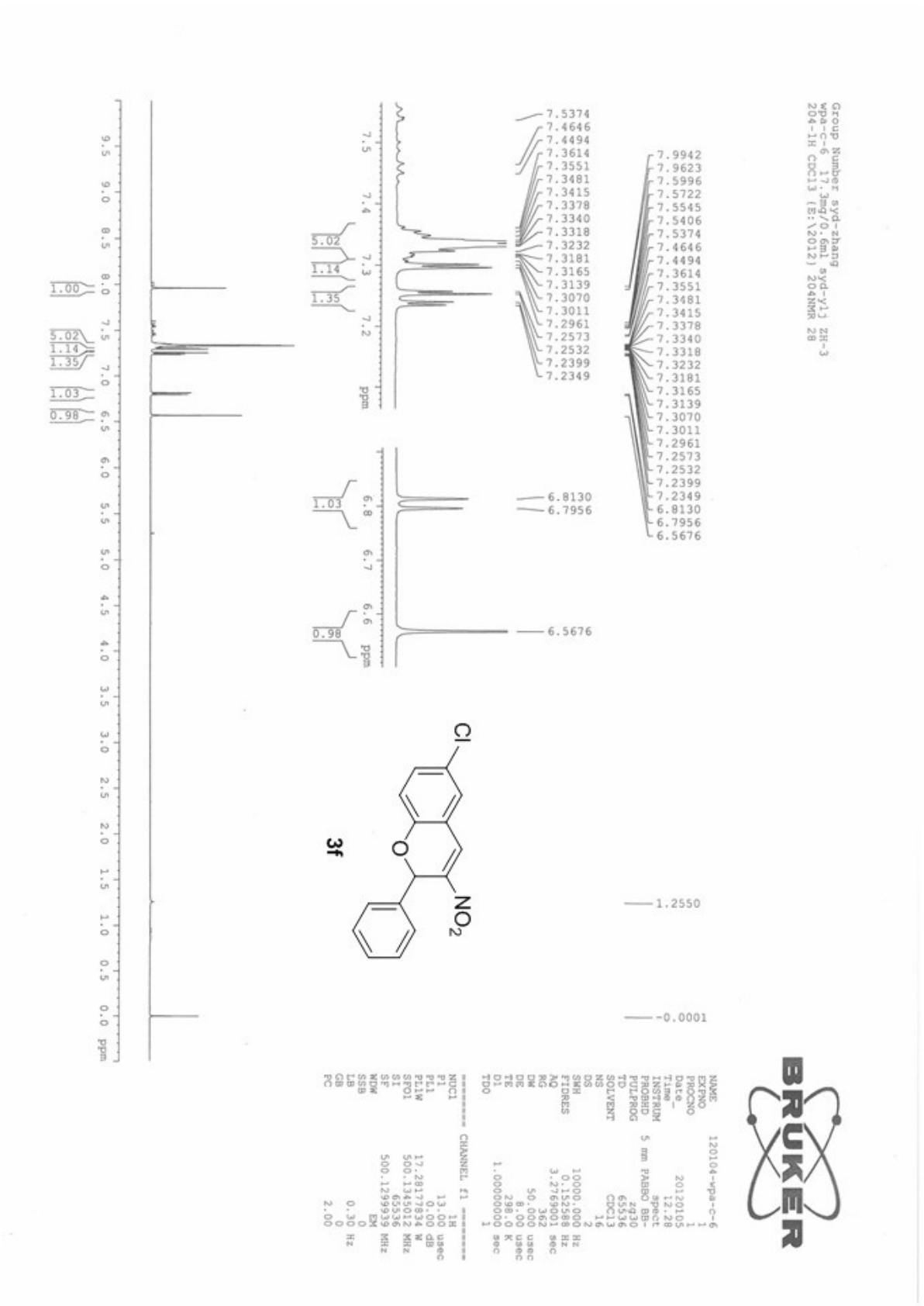

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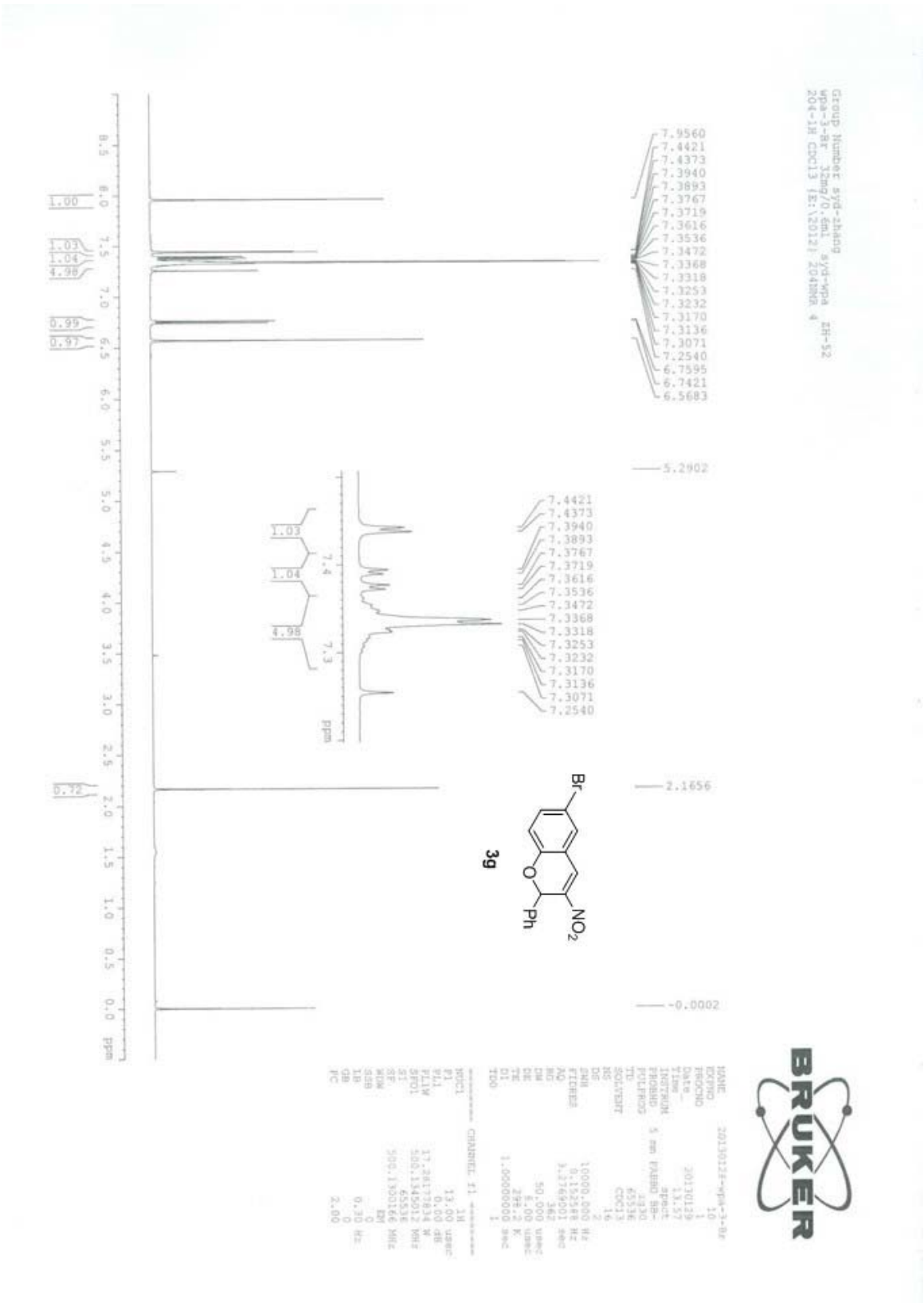

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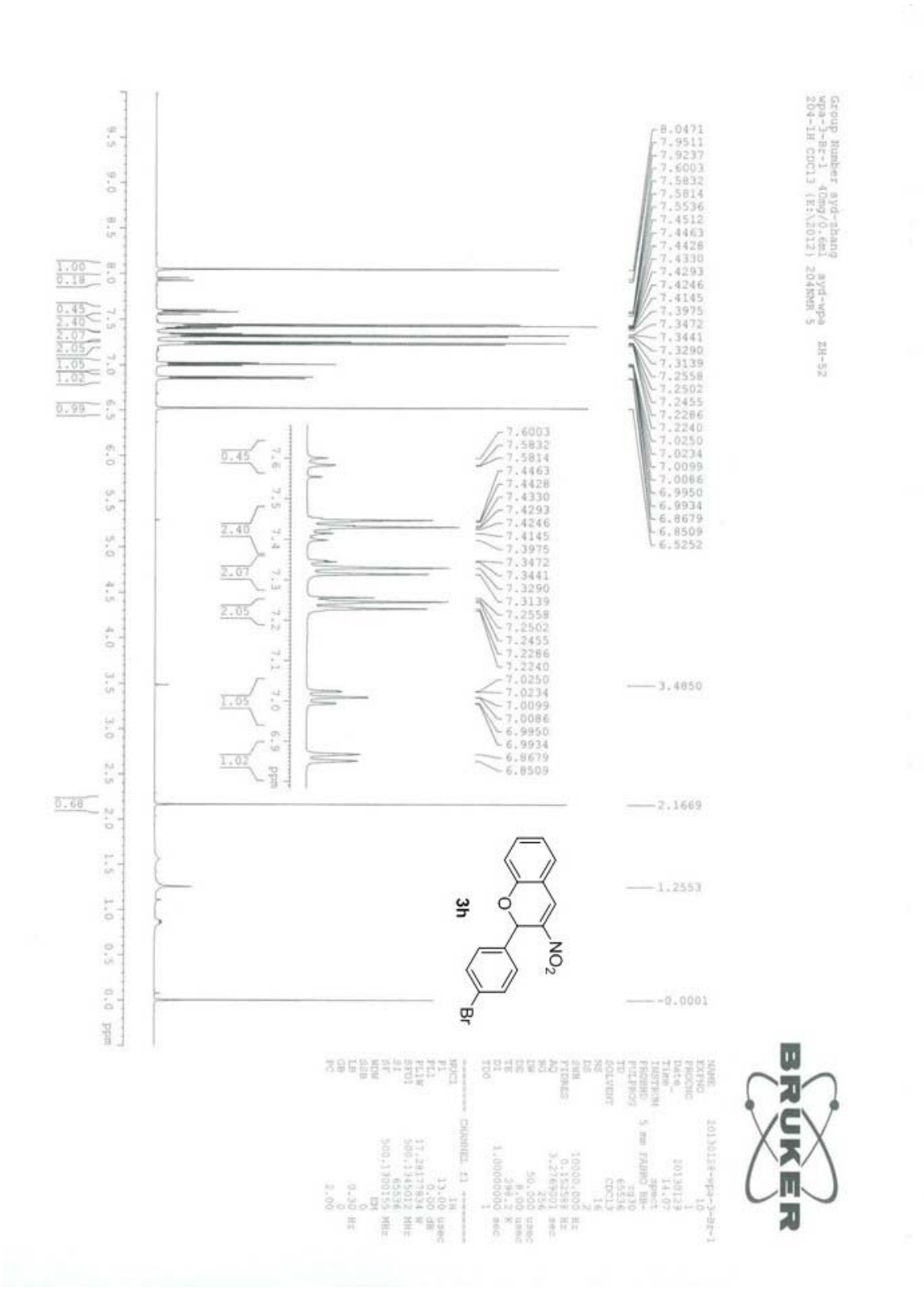

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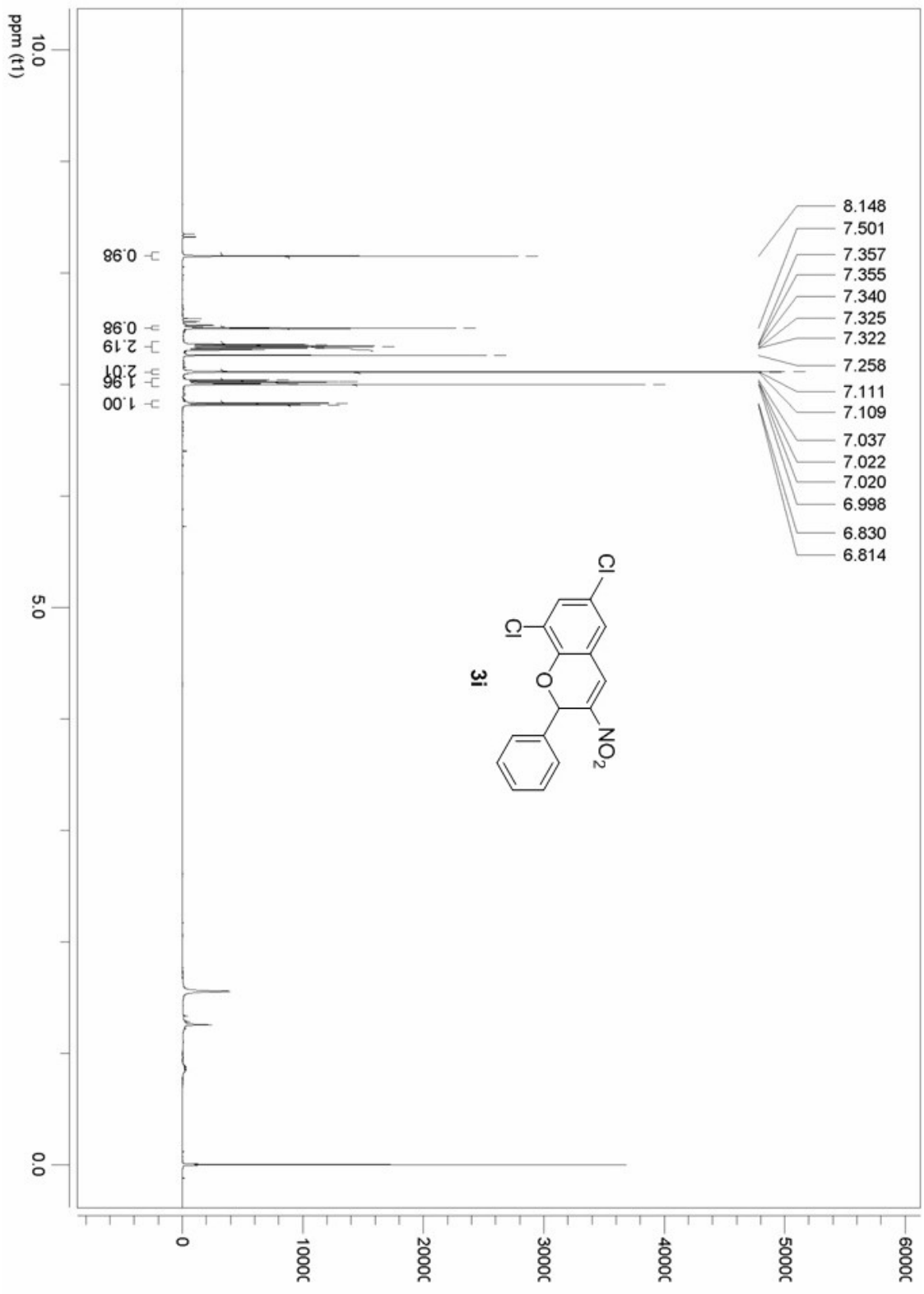

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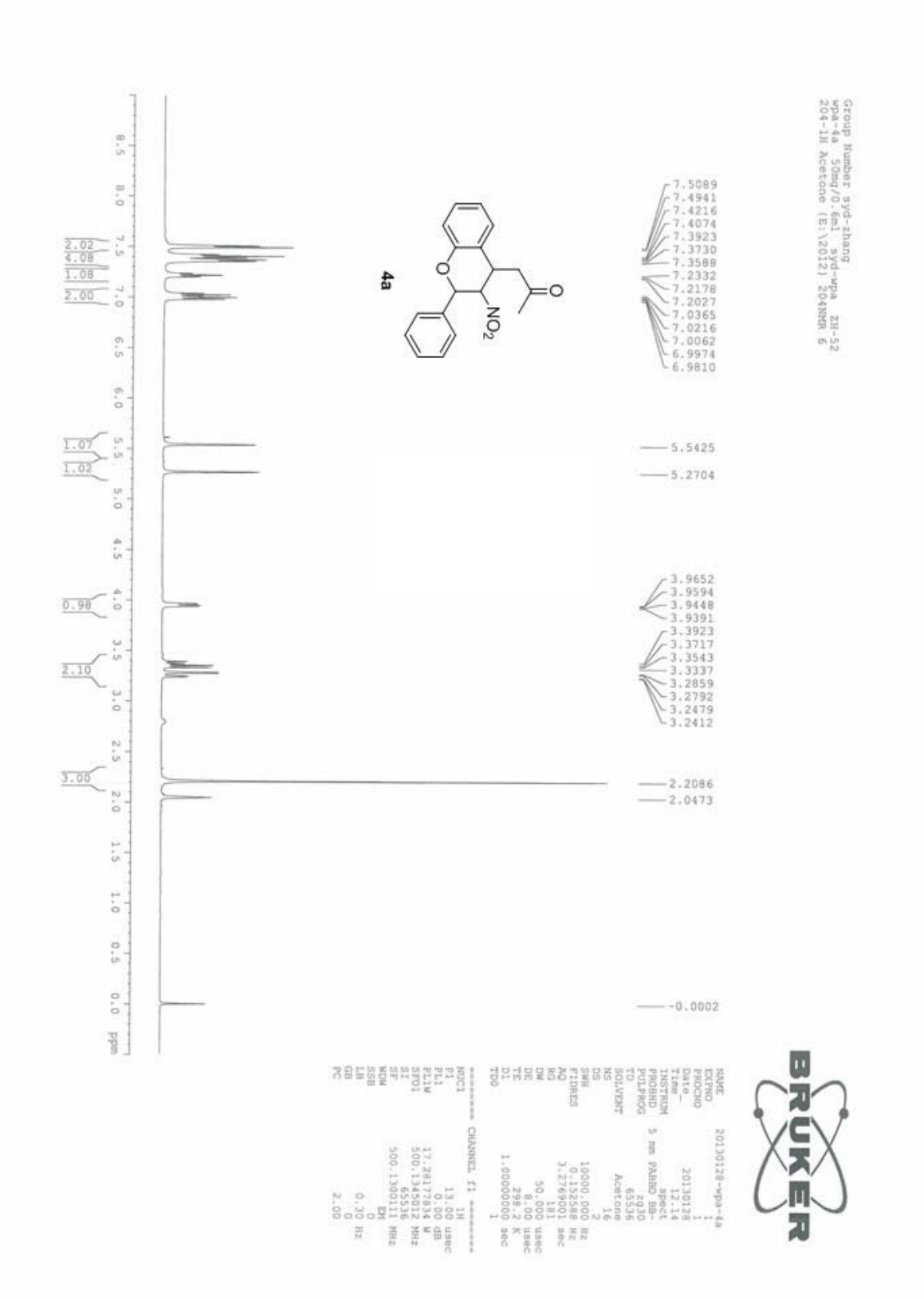

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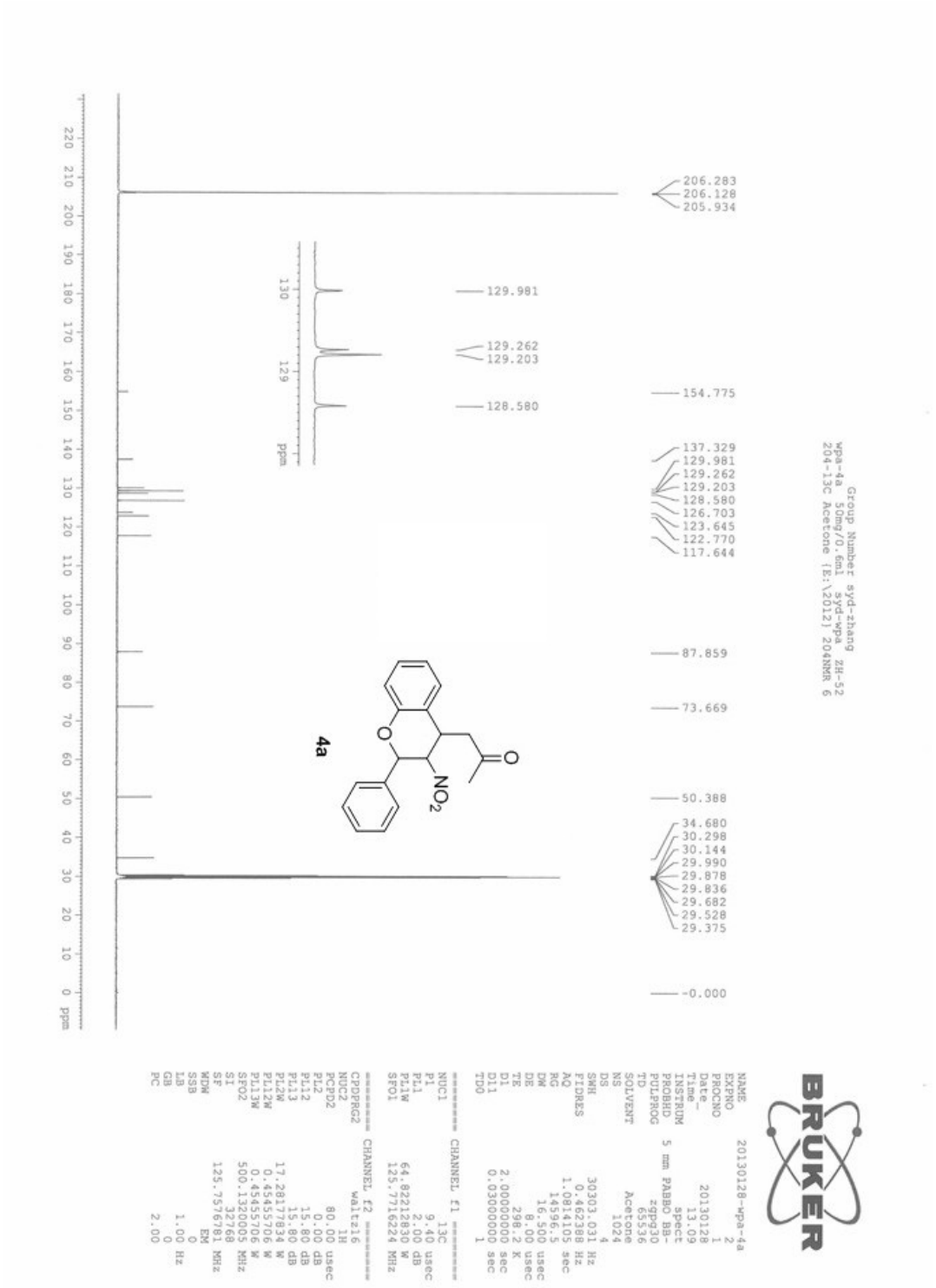

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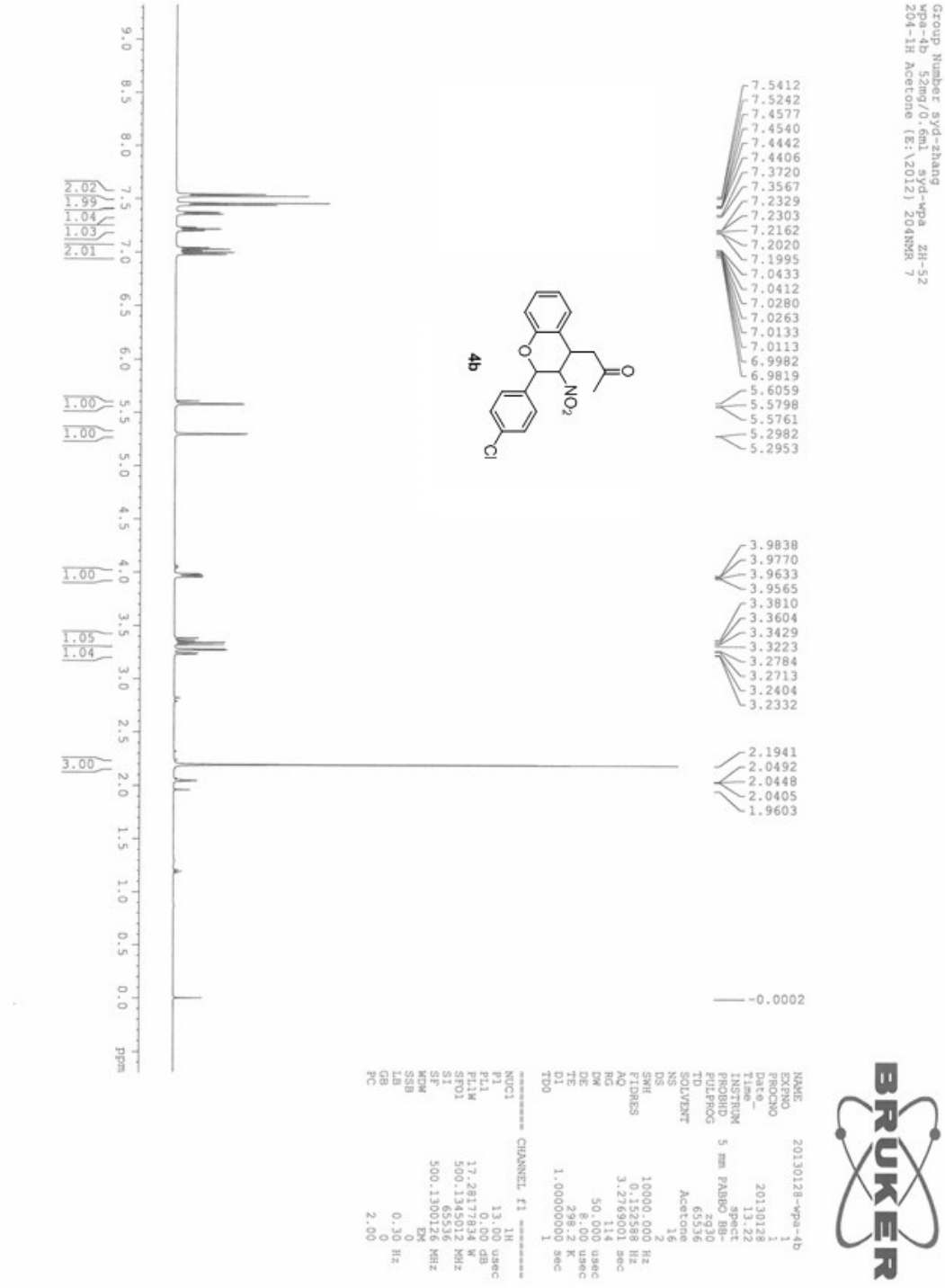

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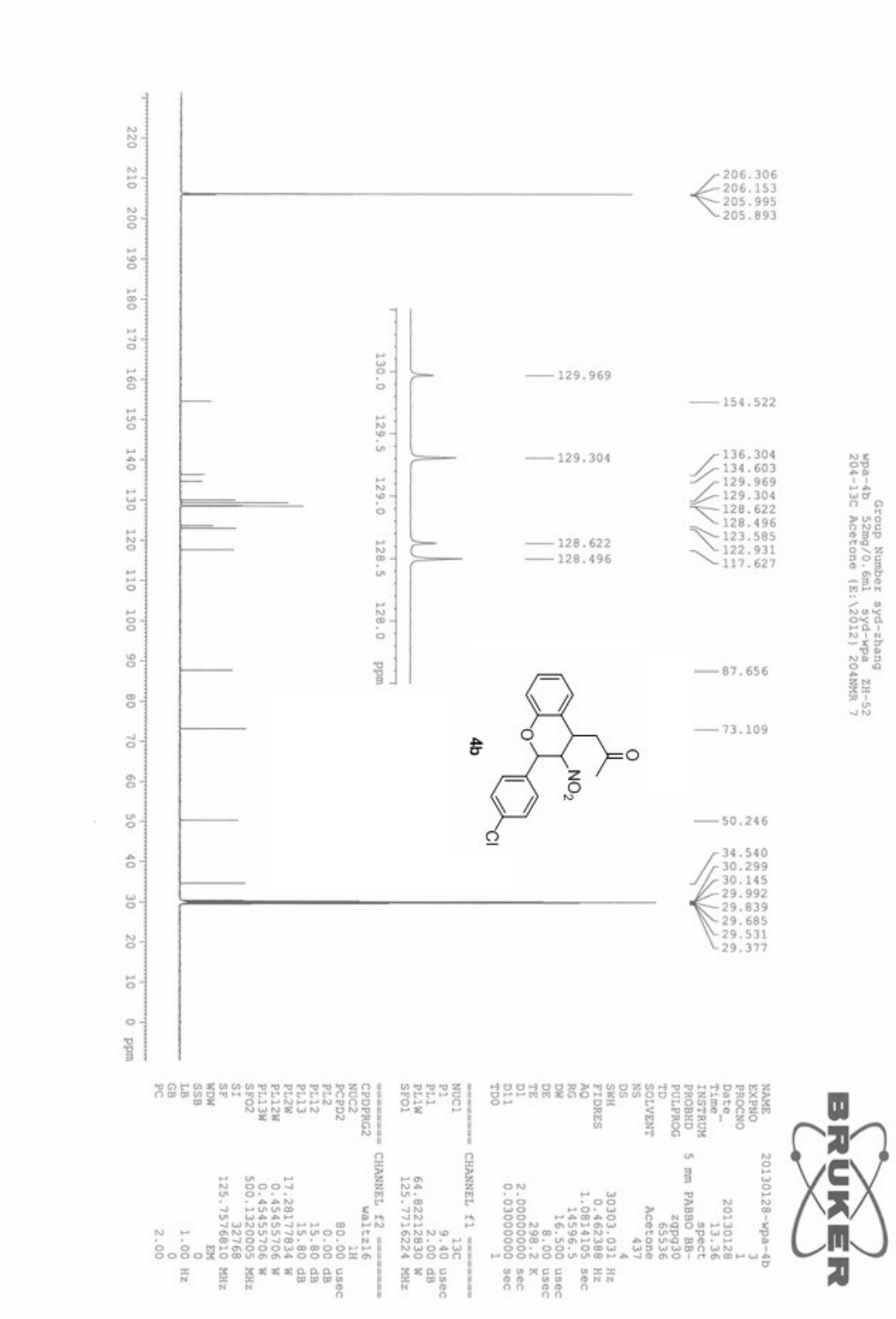

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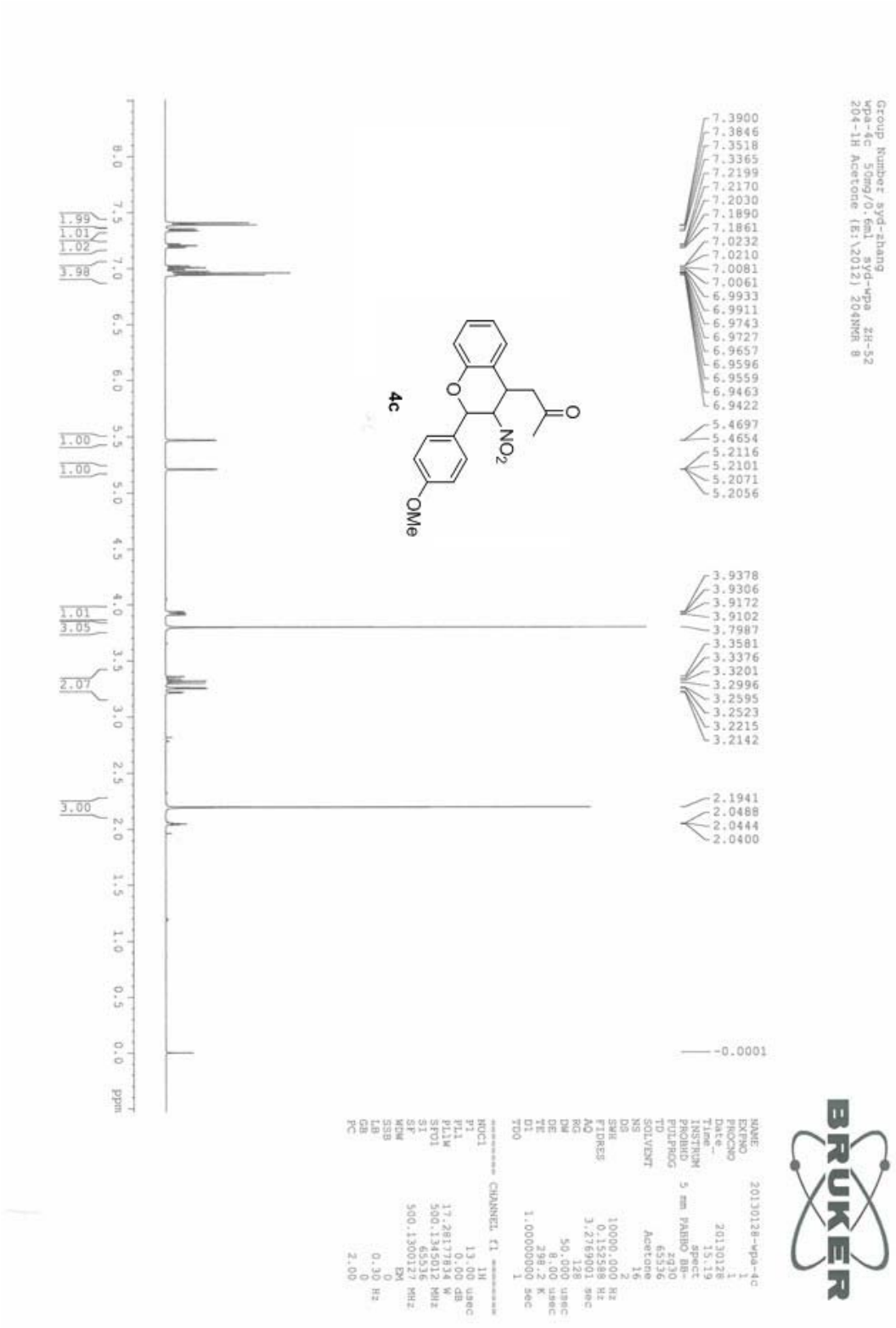

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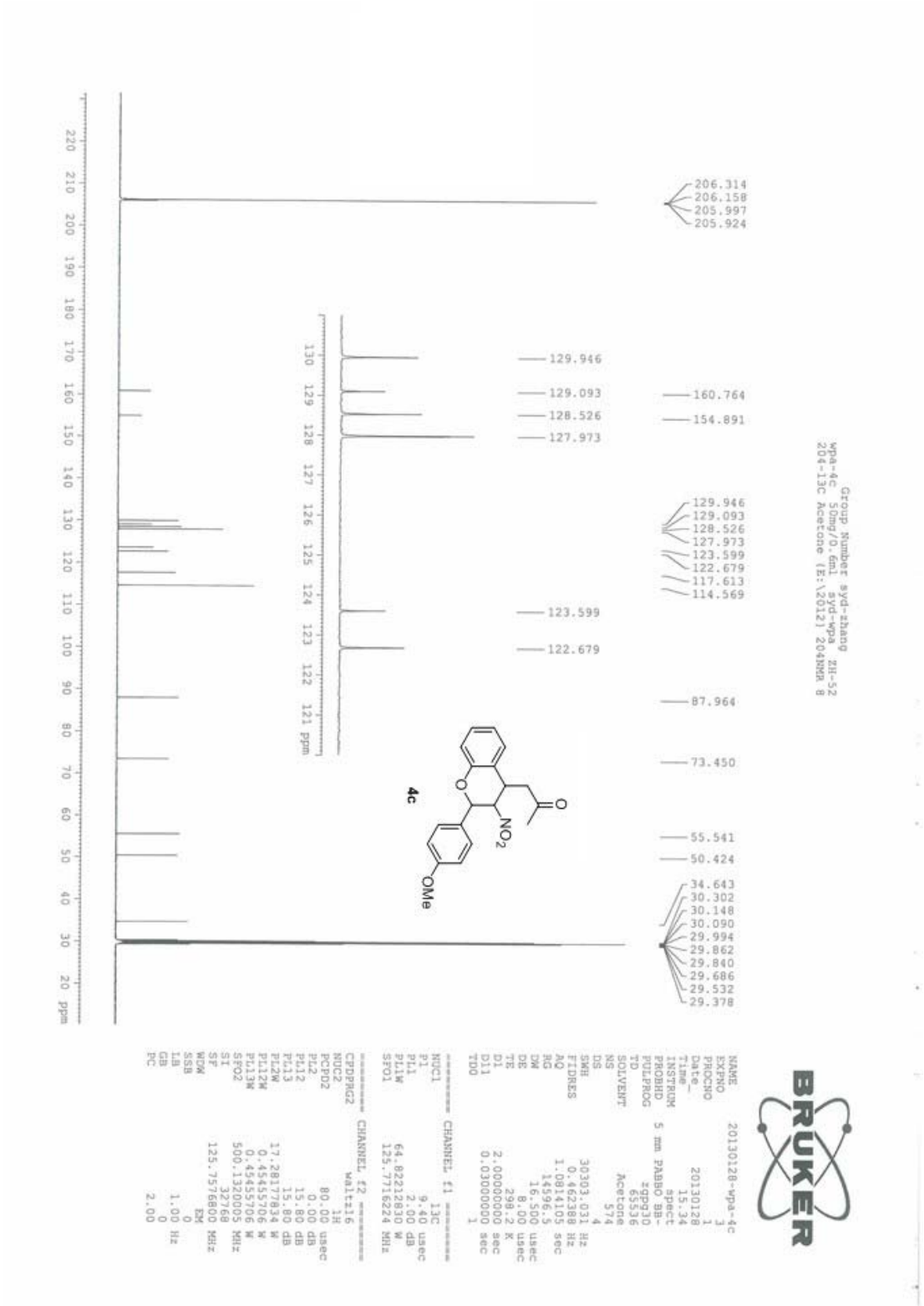

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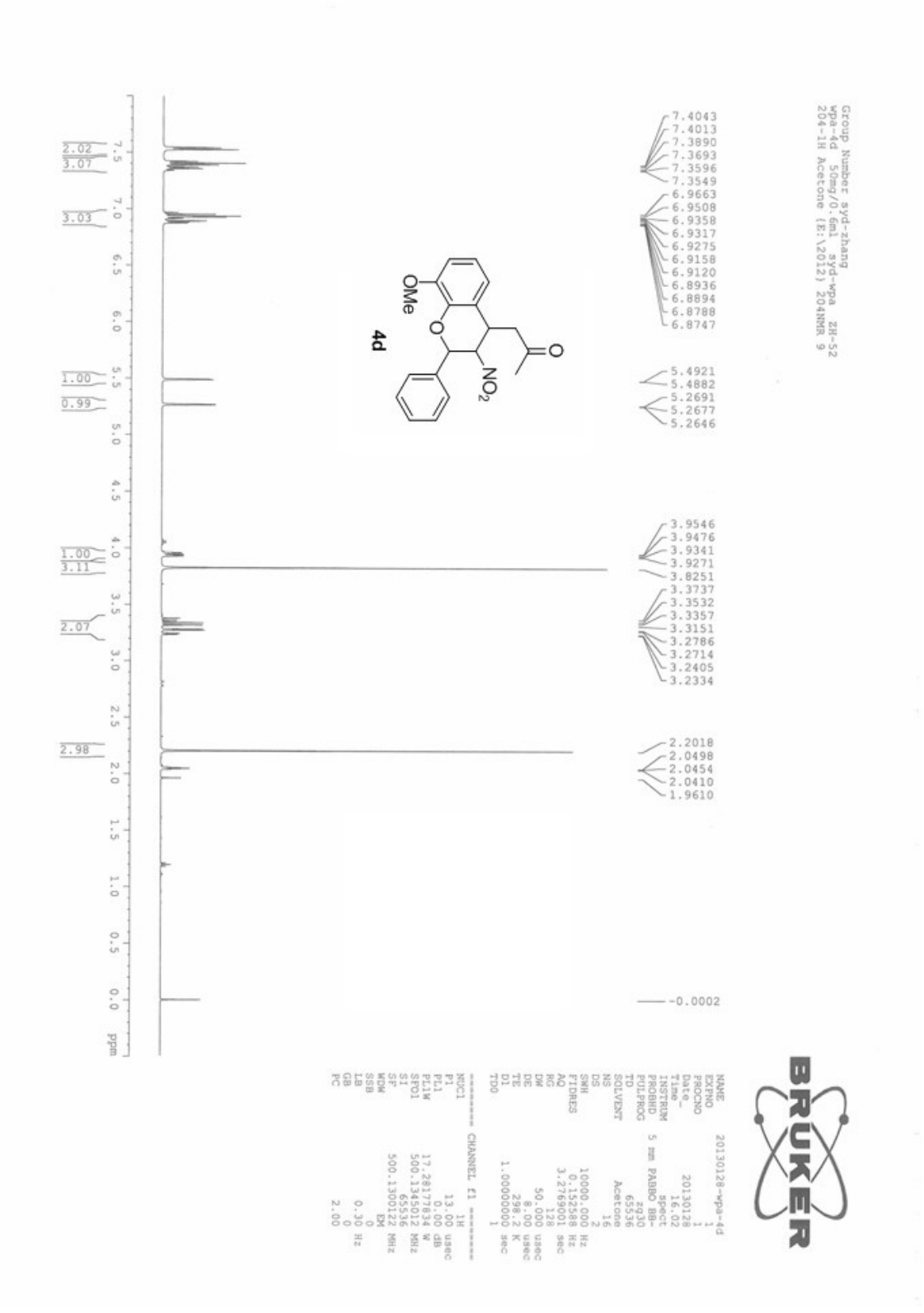

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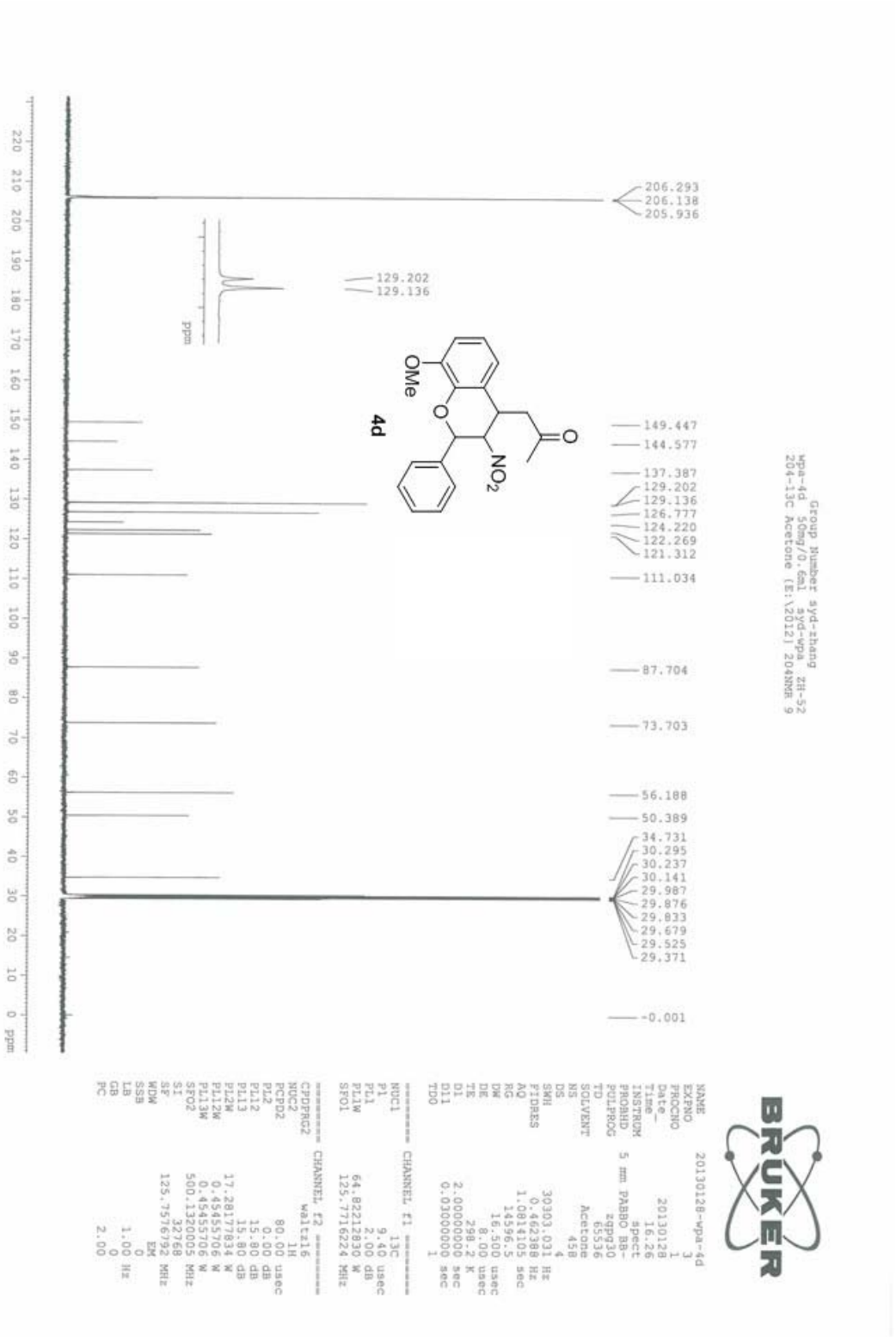

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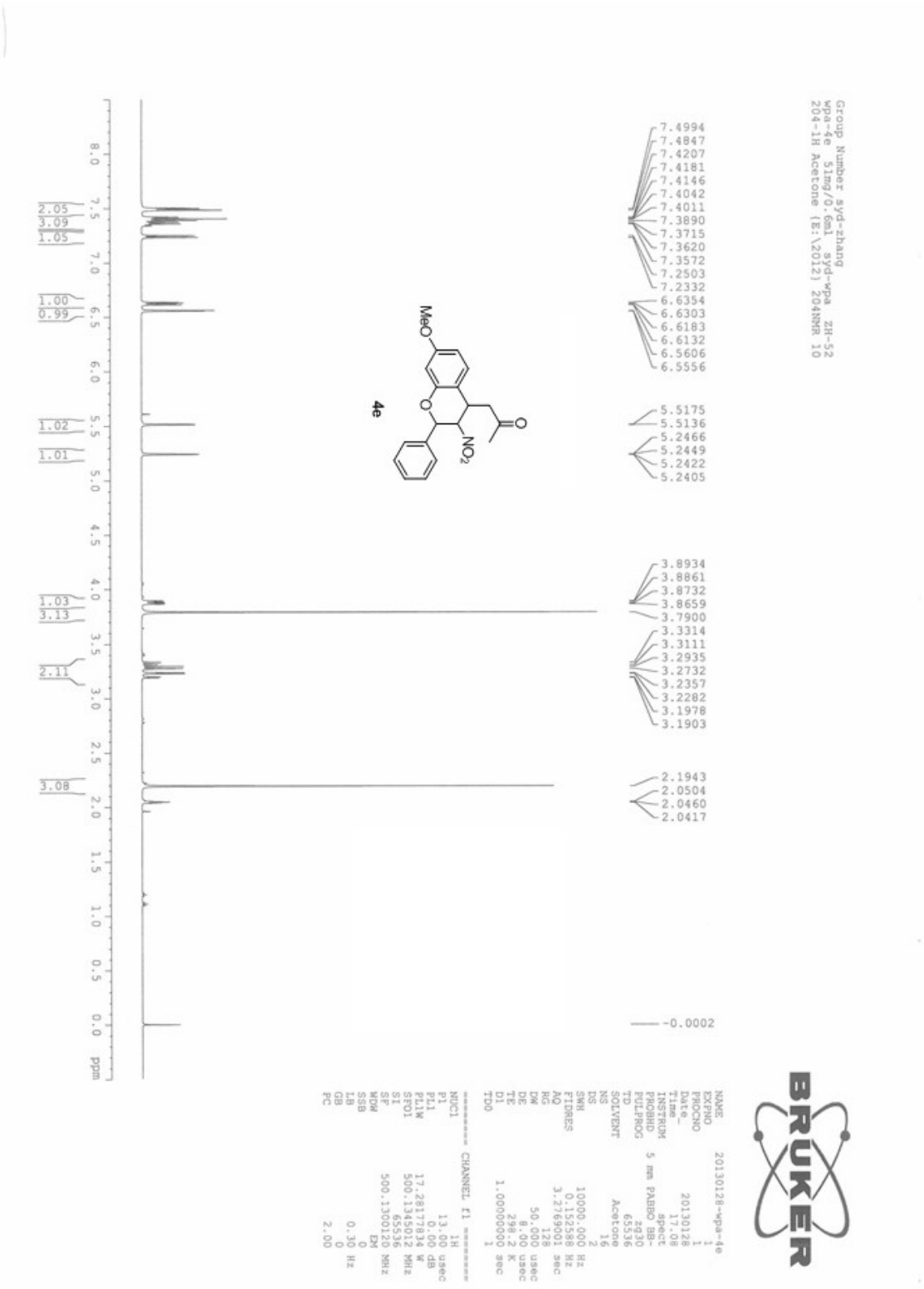

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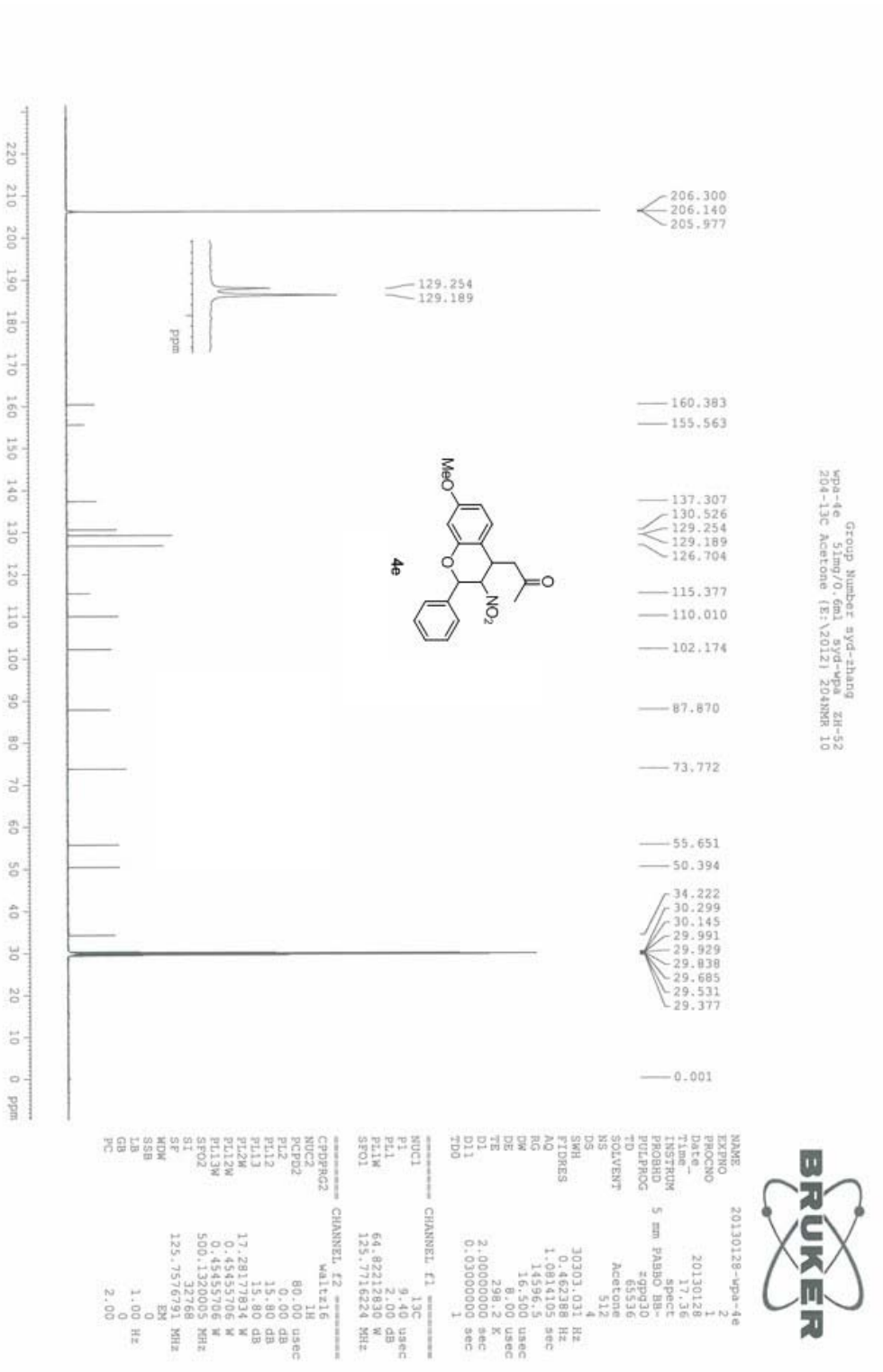

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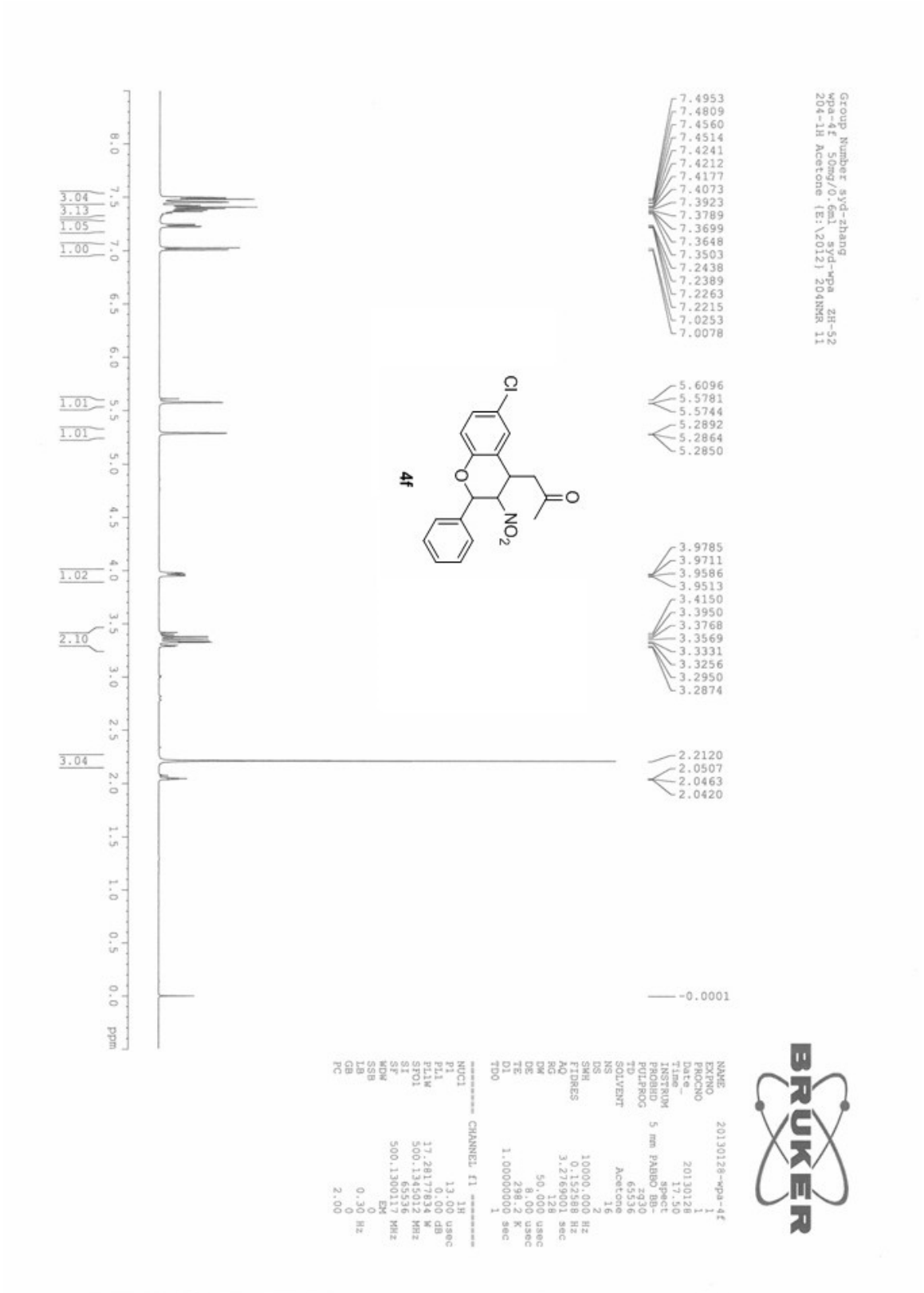

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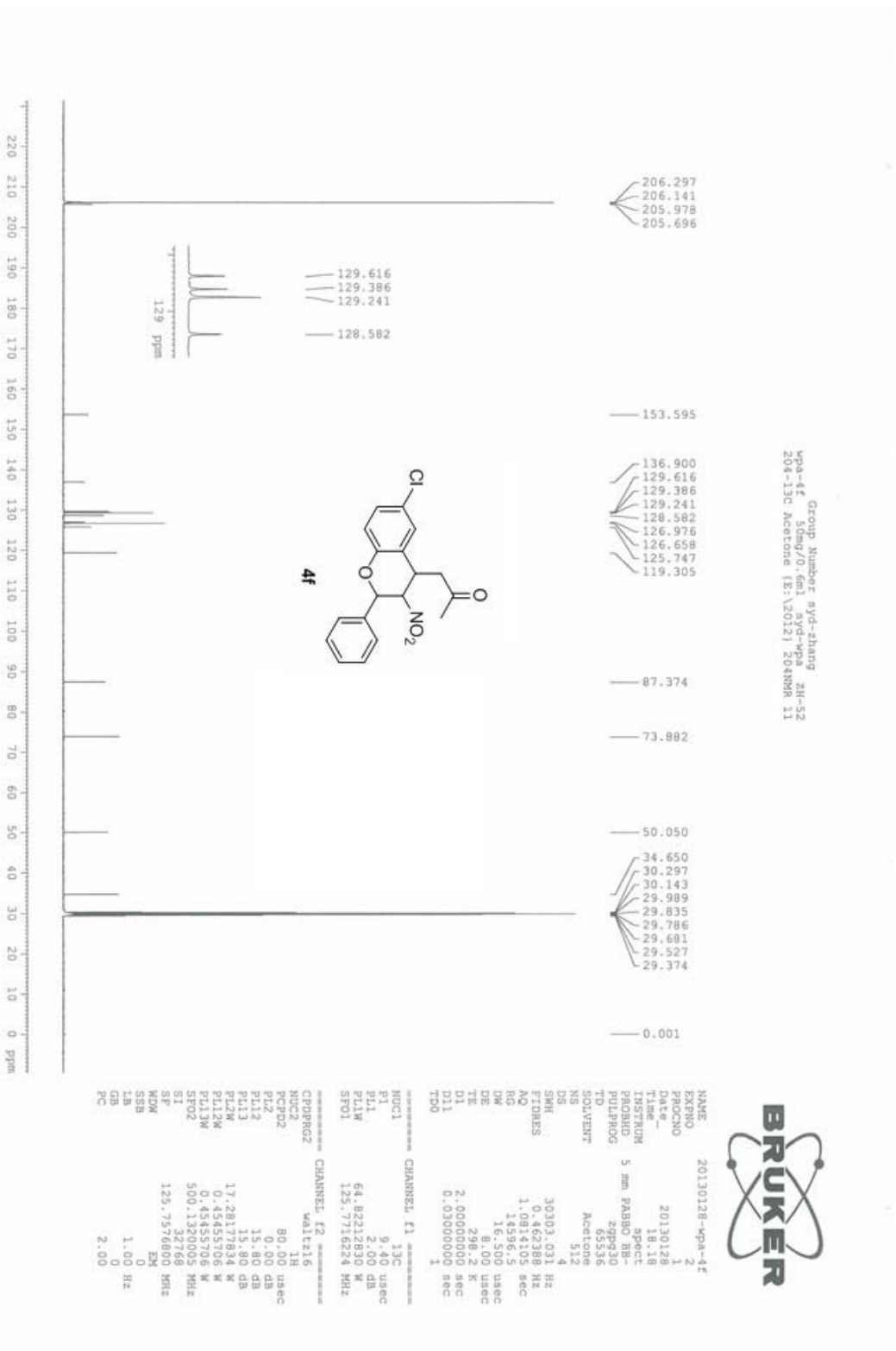

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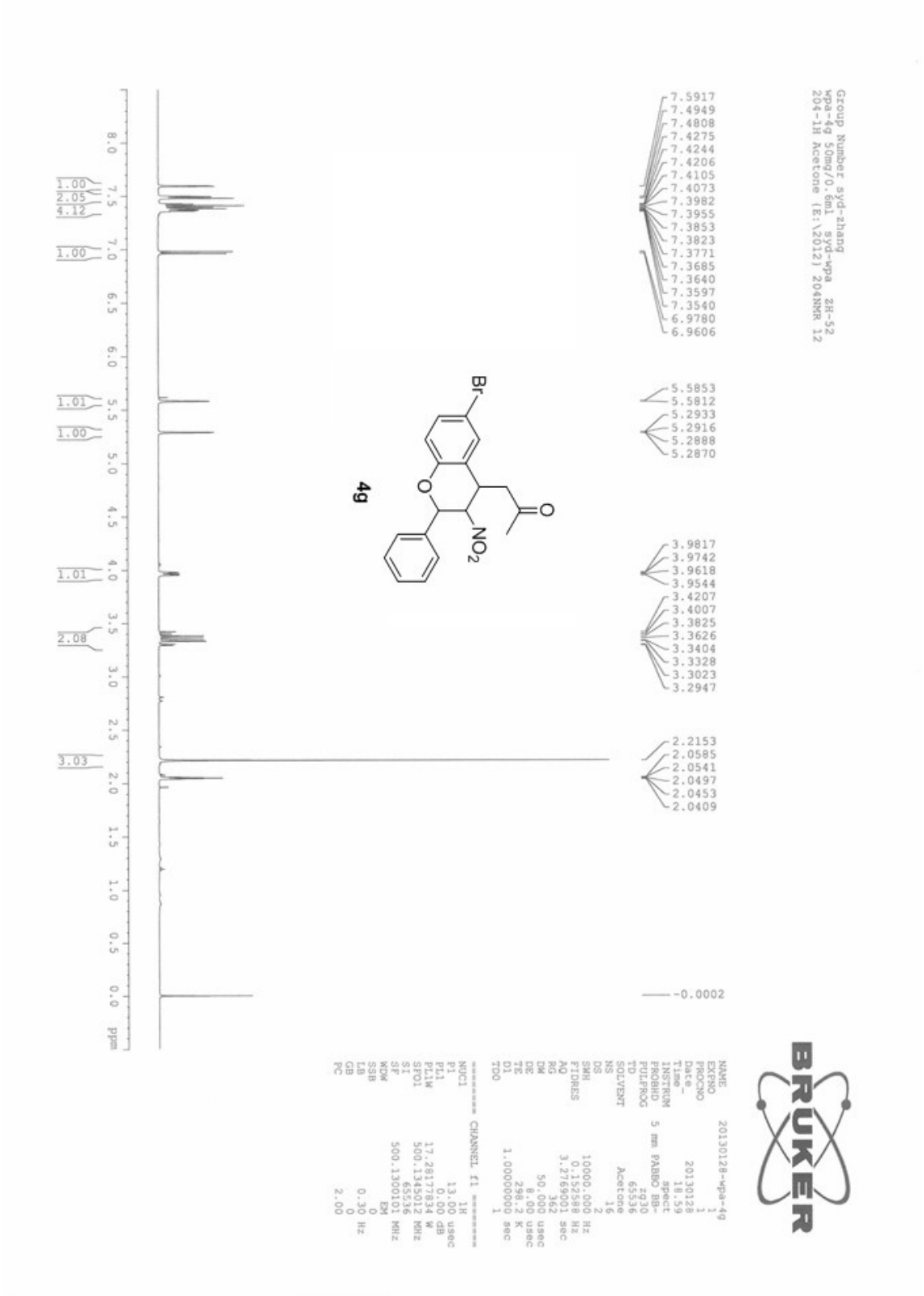

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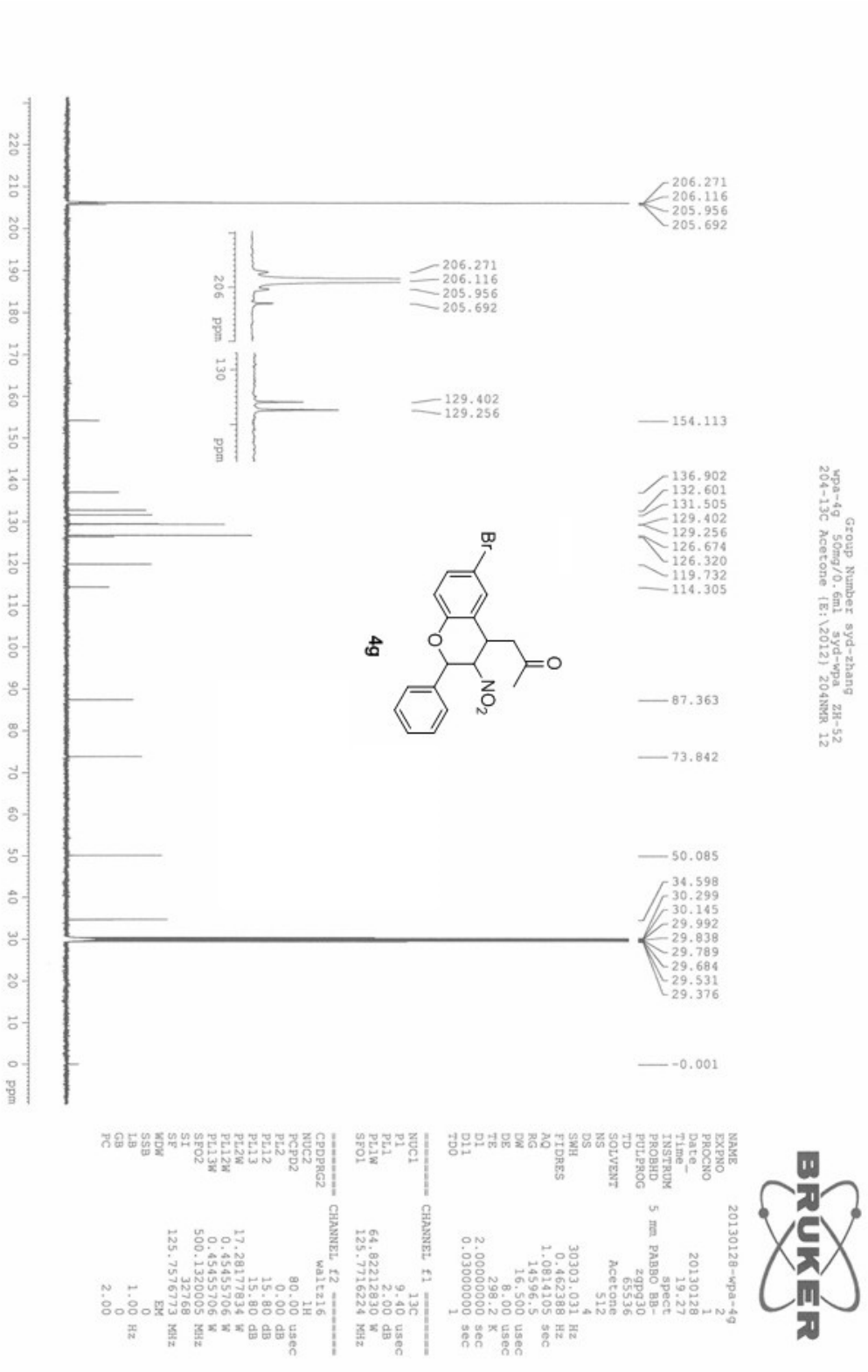

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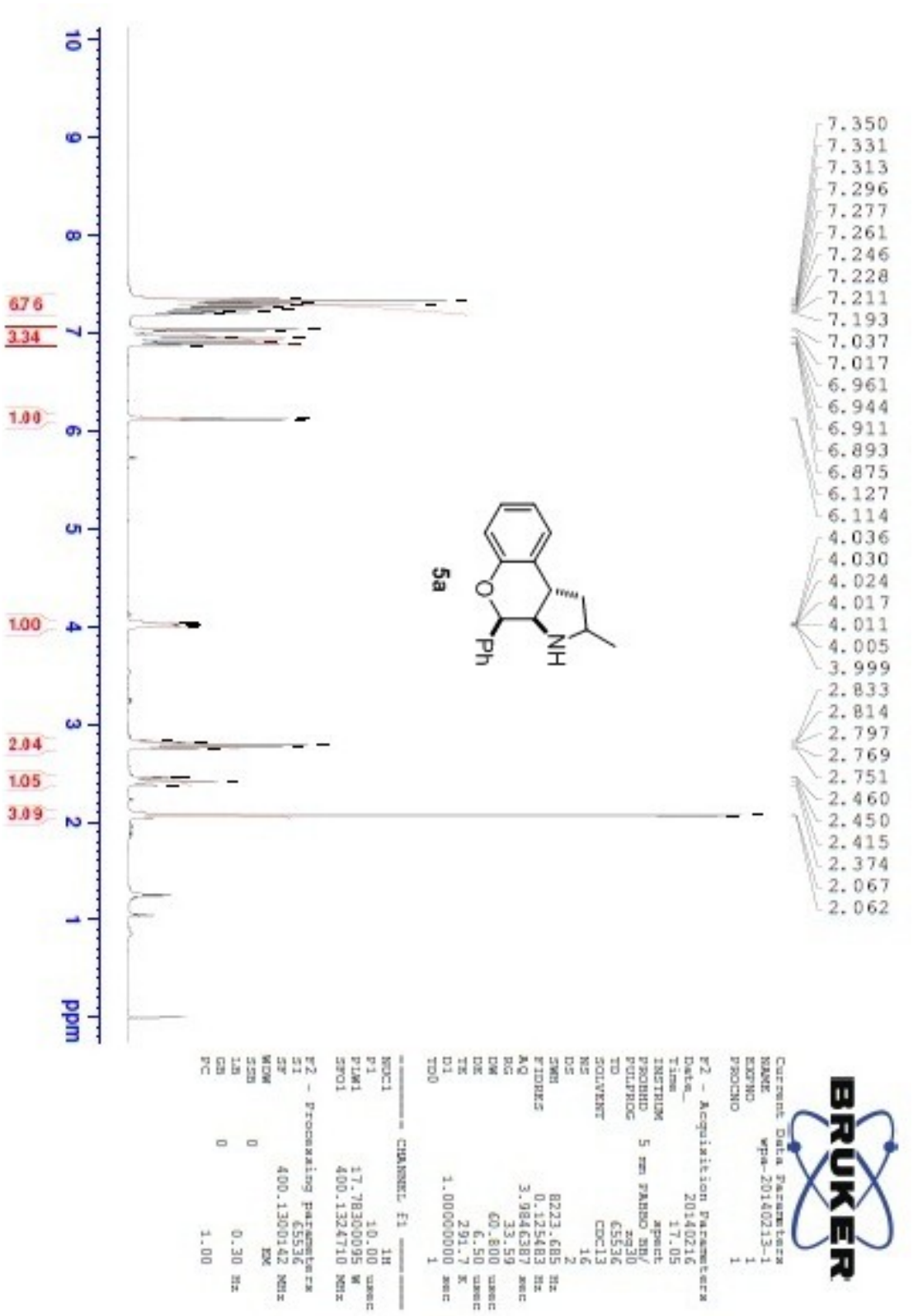

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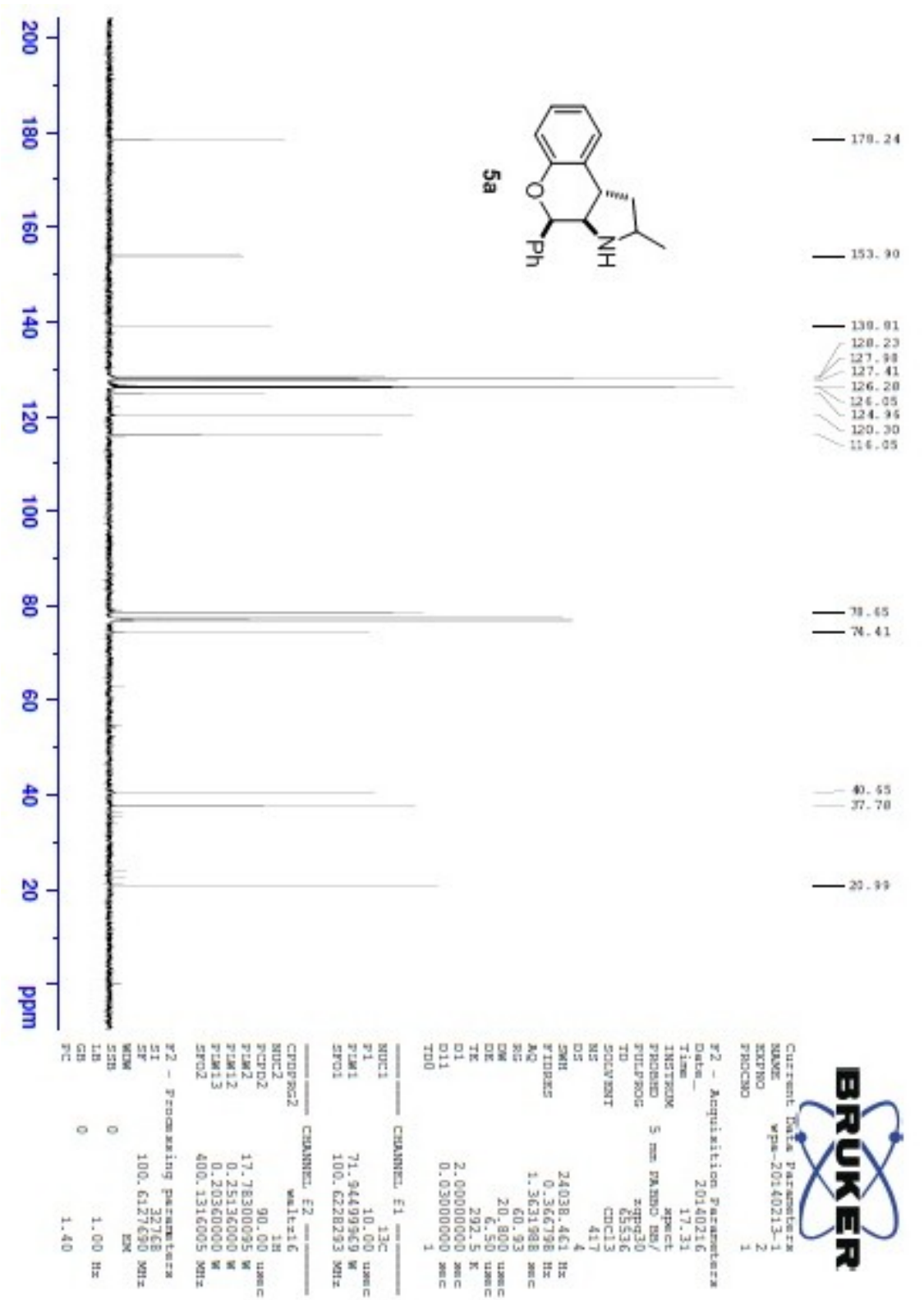

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