Supporting Information for

One-Pot Synthesis of Functionalized Spirobenzofuranones via MCR involving 3-Cyano-Chromones.

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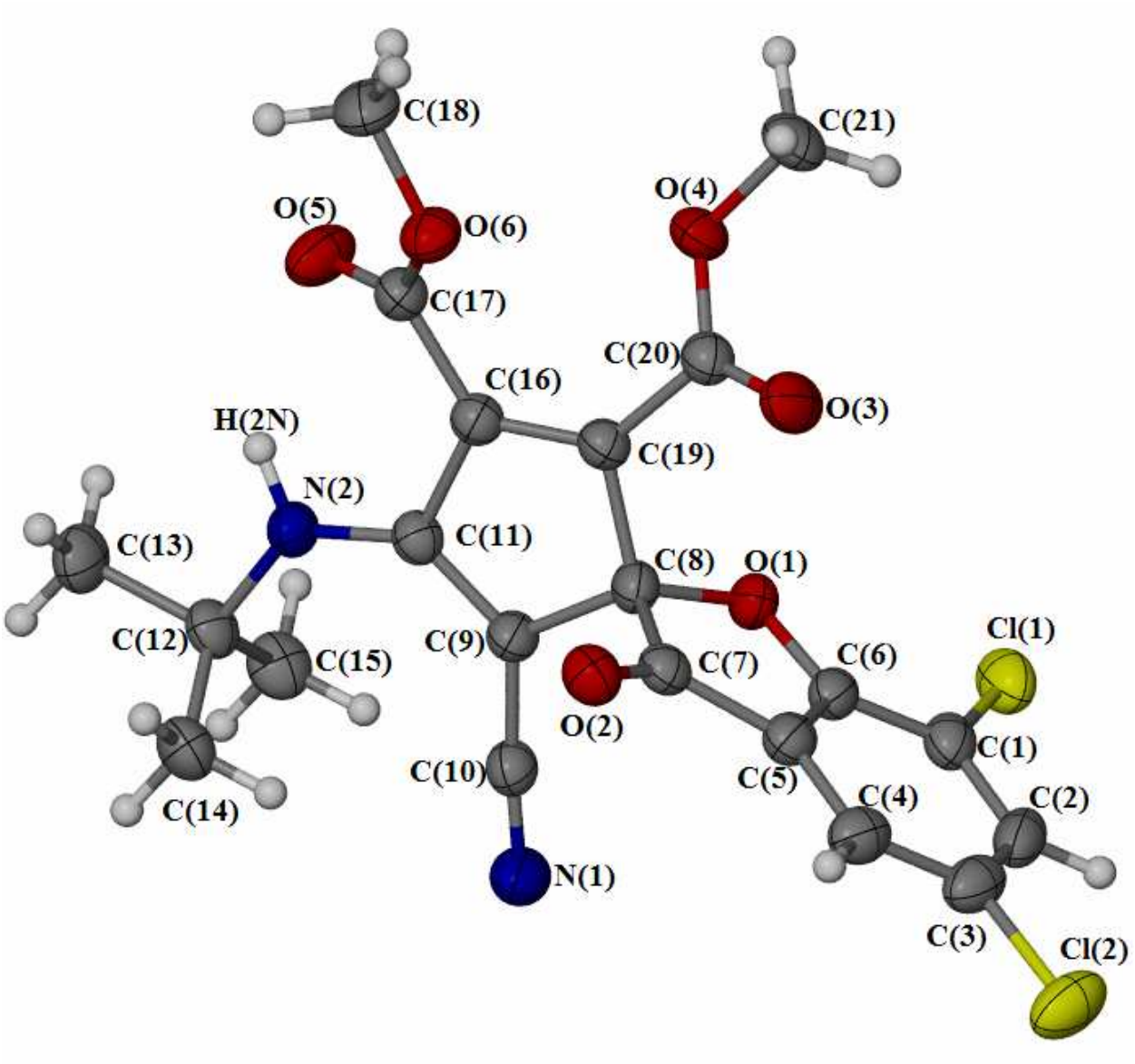

ORTEP diagram of the molecular structure of spirocyclic benzofuranone 4e as determined by single crystal XRD (atoms ellipsoid probability 50%).

Table S1. Crystallographic Data and Structure Refinement for Compound 4e.

Formula	$C_{21}H_{18}Cl_2N_2O_6$	Z	2
Mr	465.27	ρ_{calcd} [g cm^{-3}]	1.422
Cryst size[mm]	0.20 × 0.18 × 0.12	μ(Mo Kα) [mm^{-1}]	0.34
color	orange	F(000)	480
Cryst Syst	Triclinic	reflns collected	8081
Space group	*P-1*	unique reflns	4577
T[K]	180(2)	R_{int}	0.0214
a [Å]	8.8907 (13)	reflns with $I > 2\sigma(I)$	3262
b [Å]	9.4940 (14)	parameters/restraints	283/1
c [Å]	14.442 (2)	GOF on F^2	0.979
α [deg]	72.405 (11)	R1 [$I > 2\sigma(I)$]	0.0364
β [deg]	81.083 (12)	wR2 (all data)	0.0904
γ [deg]	69.498 (11)	Larg differ peak/hole [e Å^{-3}]	0.194 /-0.286
V [Å^3]	1086.7 (3)	CCDC number	824795

Table S2 Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **4e**

Atom	x	y	z	U(eq) [Ang^2]
Cl1	-0.10678	1.08809	0.16154	0.0533
Cl2	-0.37890	1.07250	-0.14229	0.0681
O1	-0.02462	0.73422	0.21017	0.0377
O2	-0.07022	0.45506	0.10840	0.0448
O3	0.27096	0.55928	0.08590	0.0543
O4	0.42785	0.45378	0.21333	0.0436
O5	0.30940	0.15519	0.44893	0.0580
O6	0.39624	0.15535	0.29476	0.0440
N1	-0.40597	0.66556	0.32014	0.0506
N2	-0.02983	0.27516	0.45327	0.0386
C1	-0.15328	0.98327	0.09747	0.0417
C2	-0.23808	1.05711	0.01368	0.0488
C3	-0.27254	0.97074	-0.03805	0.0498
C4	-0.22268	0.80933	-0.00945	0.0459

C5	-0.13823	0.73655	0.07503	0.0389
C6	-0.10536	0.82156	0.12781	0.0371
C7	-0.07226	0.57136	0.12724	0.0362
C8	-0.01012	0.57245	0.22241	0.0353
C9	-0.10587	0.51099	0.31111	0.0358
C10	-0.27197	0.59224	0.31989	0.0389
C11	-0.00705	0.37654	0.36936	0.0345
C12	-0.17772	0.27745	0.51724	0.0403
C13	-0.12537	0.13472	0.60440	0.0538
C14	-0.30281	0.25994	0.46429	0.0490
C15	-0.23900	0.42446	0.55294	0.0501
C16	0.15801	0.34837	0.32102	0.0346
C17	0.29587	0.21022	0.36278	0.0386
C18	0.53966	0.02556	0.32876	0.0544
C19	0.15850	0.46528	0.24076	0.0347
C20	0.29164	0.49650	0.17091	0.0372
C21	0.56557	0.47487	0.14929	0.0524

Table S3 Selected bond length (Å) and bond angles (°) of compound **4e**

Cl1—C1	1.727 (2)	C3—C4	1.383 (3)
Cl2—C3	1.7367 (19)	C4—C5	1.393 (2)
O1—C6	1.3672 (19)	C5—C6	1.387 (3)
O1—C8	1.453 (2)	C5—C7	1.466 (2)
O2—C7	1.208 (2)	C7—C8	1.563 (2)
O3—C20	1.203 (2)	C8—C19	1.498 (2)
O4—C20	1.320 (2)	C8—C9	1.505 (2)
O4—C21	1.450 (2)	C9—C11	1.380 (2)
O5—C17	1.202 (2)	C9—C10	1.412 (2)
O6—C17	1.321 (2)	C11—C16	1.494 (2)
O6—C18	1.454 (2)	C12—C14	1.523 (3)
N2—C11	1.338 (2)	C12—C15	1.525 (3)
N2—C12	1.483 (2)	C12—C13	1.532 (3)

N1—C10	1.150 (2)	C16—C19	1.341 (2)
C1—C2	1.387 (3)	C16—C17	1.487 (2)
C1—C6	1.387 (2)	C19—C20	1.484 (2)
C2—C3	1.393 (3)		
C6—O1—C8	107.57 (12)	C9—C8—C7	111.41 (14)
C20—O4—C21	116.00 (14)	C11—C9—C10	132.08 (15)
C17—O6—C18	116.01 (14)	C11—C9—C8	109.60 (14)
C11—N2—C12	129.79 (15)	C10—C9—C8	118.30 (14)
C2—C1—C6	117.70 (17)	N1—C10—C9	174.83 (19)
C2—C1—Cl1	121.43 (15)	N2—C11—C9	134.35 (16)
C6—C1—Cl1	120.87 (14)	N2—C11—C16	118.65 (15)
C1—C2—C3	120.74 (17)	C9—C11—C16	107.00 (14)
C4—C3—C2	122.02 (17)	N2—C12—C14	109.81 (14)
C4—C3—Cl2	120.24 (17)	N2—C12—C15	110.35 (15)
C2—C3—Cl2	117.73 (15)	C14—C12—C15	112.94 (16)
C3—C4—C5	116.71 (19)	N2—C12—C13	105.03 (14)
C6—C5—C4	121.71 (17)	C14—C12—C13	109.44 (16)
C6—C5—C7	106.81 (14)	C15—C12—C13	108.96 (15)
C4—C5—C7	131.47 (17)	C19—C16—C17	128.17 (15)
O1—C6—C5	115.05 (15)	C19—C16—C11	109.96 (14)
O1—C6—C1	123.83 (16)	C17—C16—C11	121.84 (14)
C5—C6—C1	121.11 (15)	O5—C17—O6	125.19 (16)
O2—C7—C5	130.68 (16)	O5—C17—C16	122.58 (16)
O2—C7—C8	124.46 (15)	O6—C17—C16	112.21 (14)
C5—C7—C8	104.74 (14)	C16—C19—C20	131.10 (15)
O1—C8—C19	112.11 (14)	C16—C19—C8	109.55 (14)
O1—C8—C9	112.05 (13)	C20—C19—C8	119.29 (14)
C19—C8—C9	103.44 (13)	O3—C20—O4	125.62 (16)
O1—C8—C7	105.15 (12)	O3—C20—C19	121.68 (15)
C19—C8—C7	112.89 (13)	O4—C20—C19	112.65 (14)

CARTESIAN COORDINATES

For the optimized structures in the gas phase at 298 K.

Anion Intermediate **9a**

E_{total} = – 1372.156652 au

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O,0,0.3867411177,-2.3288973362,-0.6373276151
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C,0,0.0353386899,-4.4348512813,0.366462017
C,0,-1.6594055753,-3.2691962759,2.2646896041
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Anion Intermediate **10a**

E_{total} = – 1372.121265 au

Imaginary frequency –309.39 cm^{-1}

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C,0,-1.0049134285,-4.5859269571,1.1372281704
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C,0,-1.2826949381,-2.7337308859,2.6612867589
C,0,-0.9380403464,-1.8513294712,1.6305850936
C,0,-0.8491148774,-0.3925660925,1.7651205951
C,0,-0.481957828,-0.128660424,-0.3505733739
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O,0,-1.2948891285,0.3306037964,2.6051724875
C,0,1.798574776,0.0079912748,0.8047519191
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C,0,0.0874606489,-4.8280863189,-0.5163995488
C,0,-0.2864541902,-4.9449719163,0.8348785681
C,0,-0.4635562906,-3.7983987186,1.6062327347
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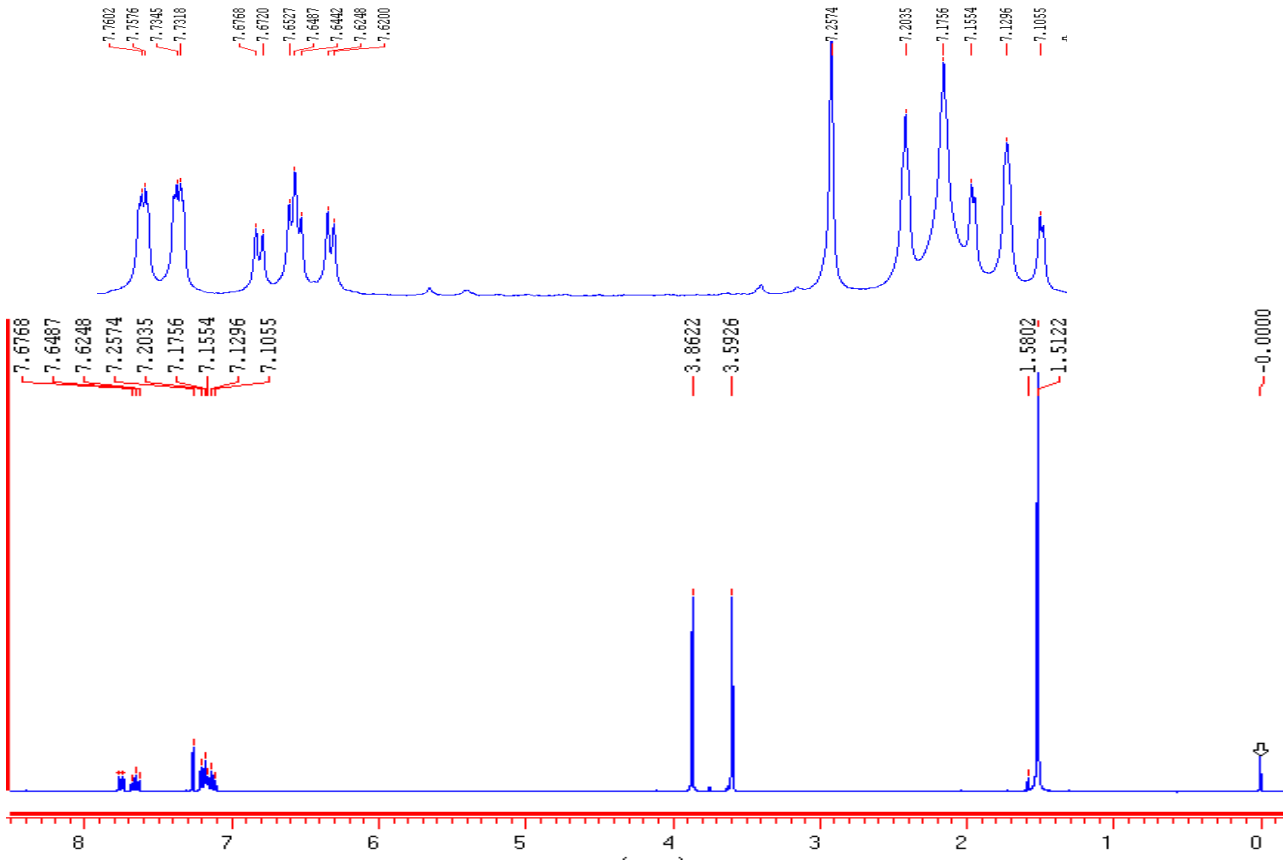
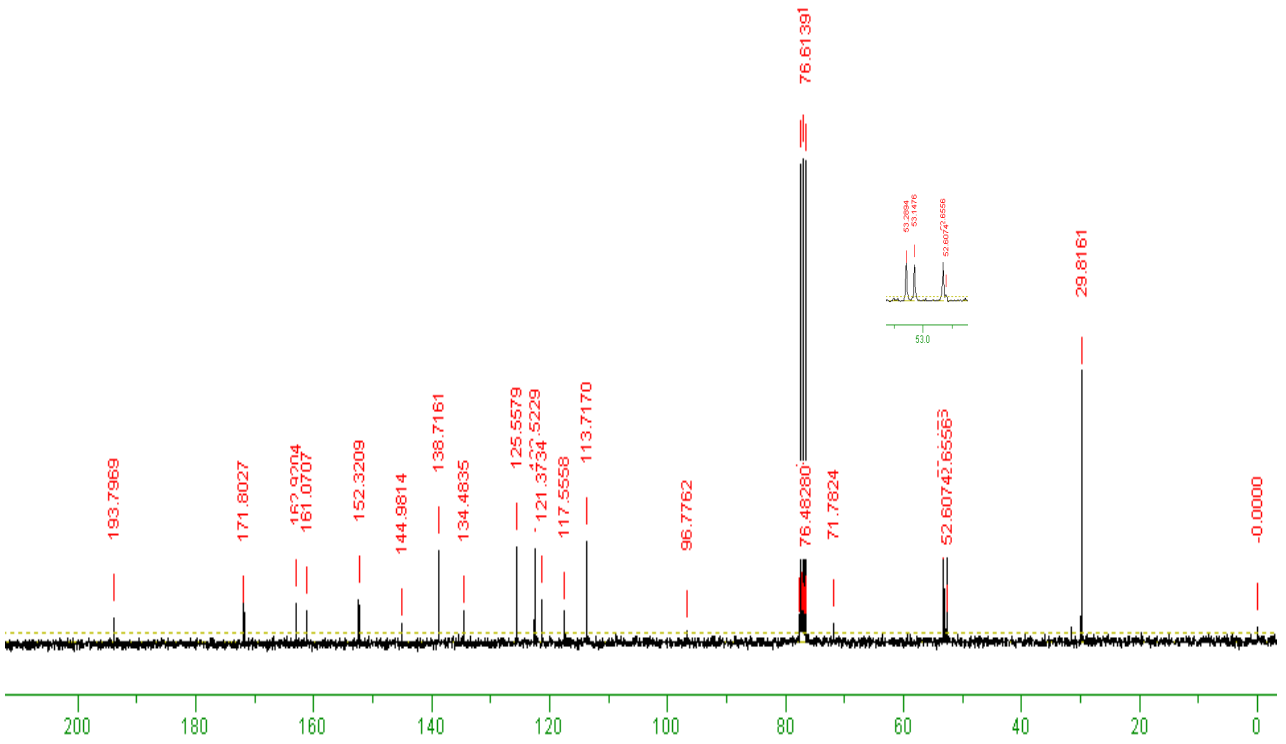
Copies of ^{1}H and ^{13}C Spectra

4a





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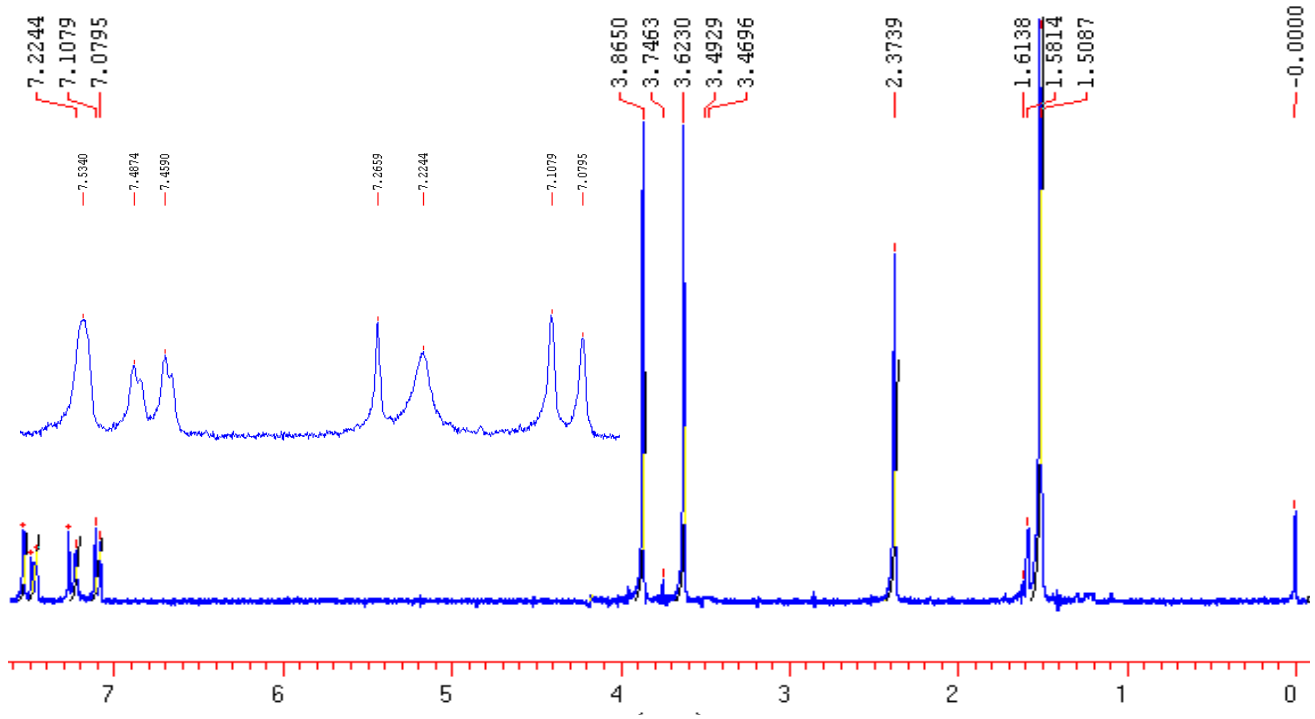
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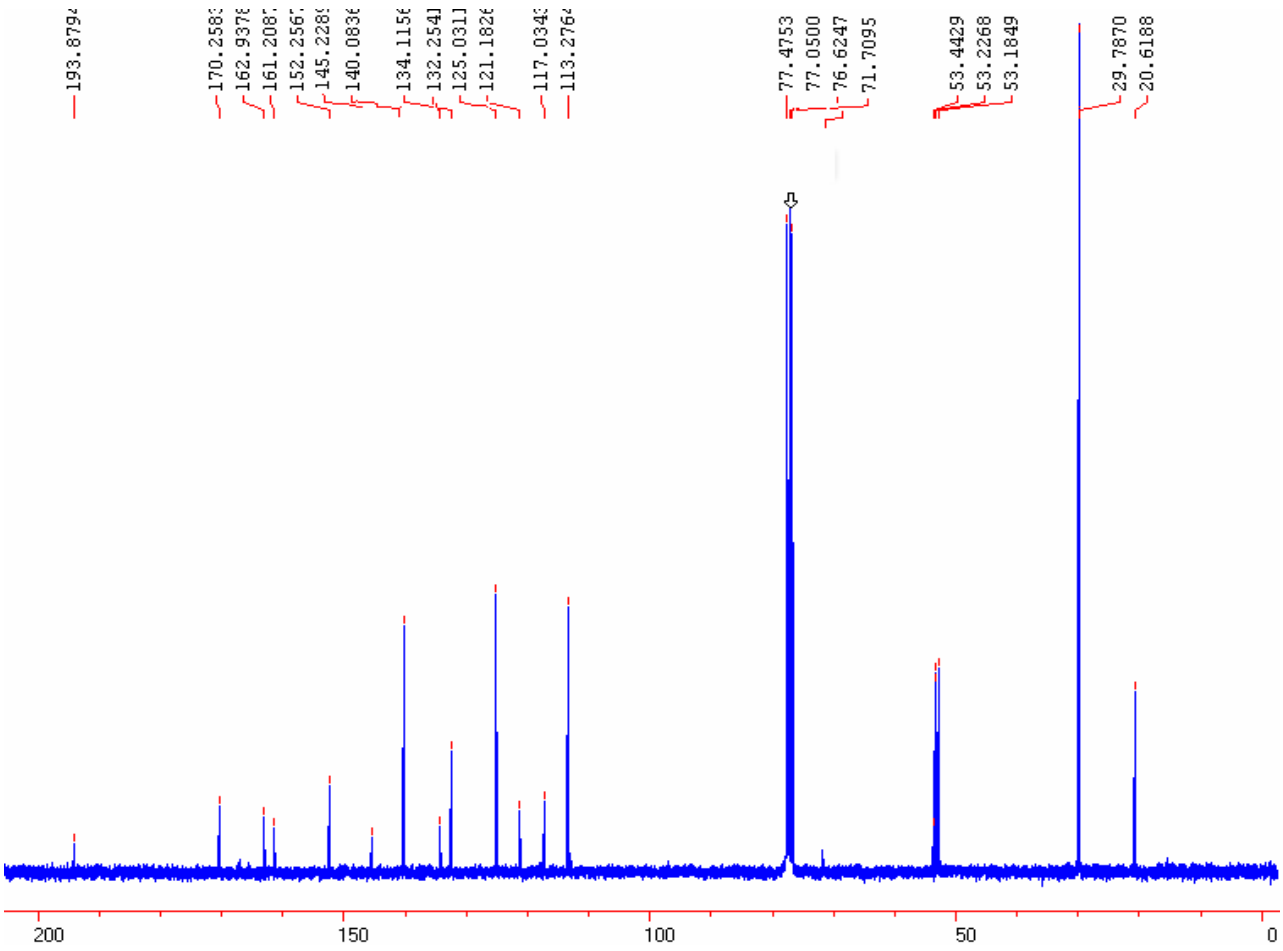
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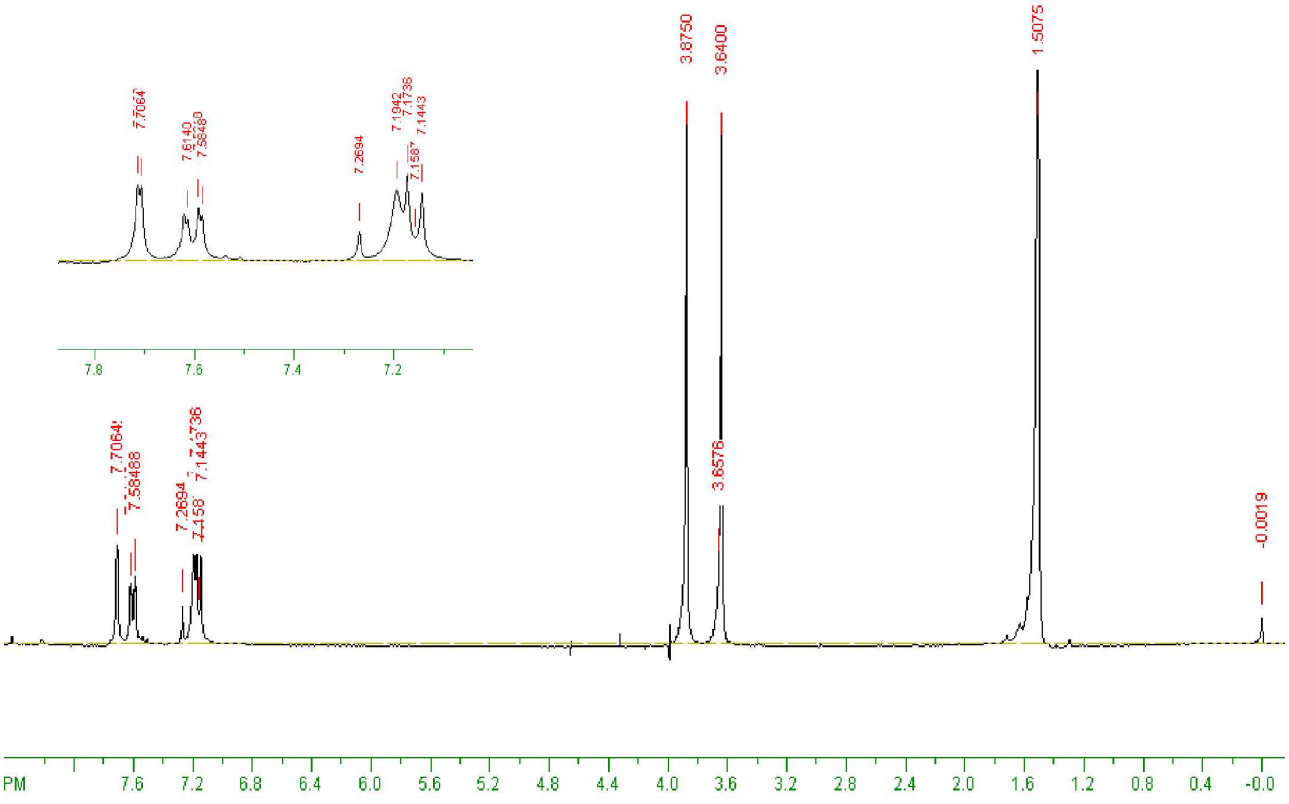
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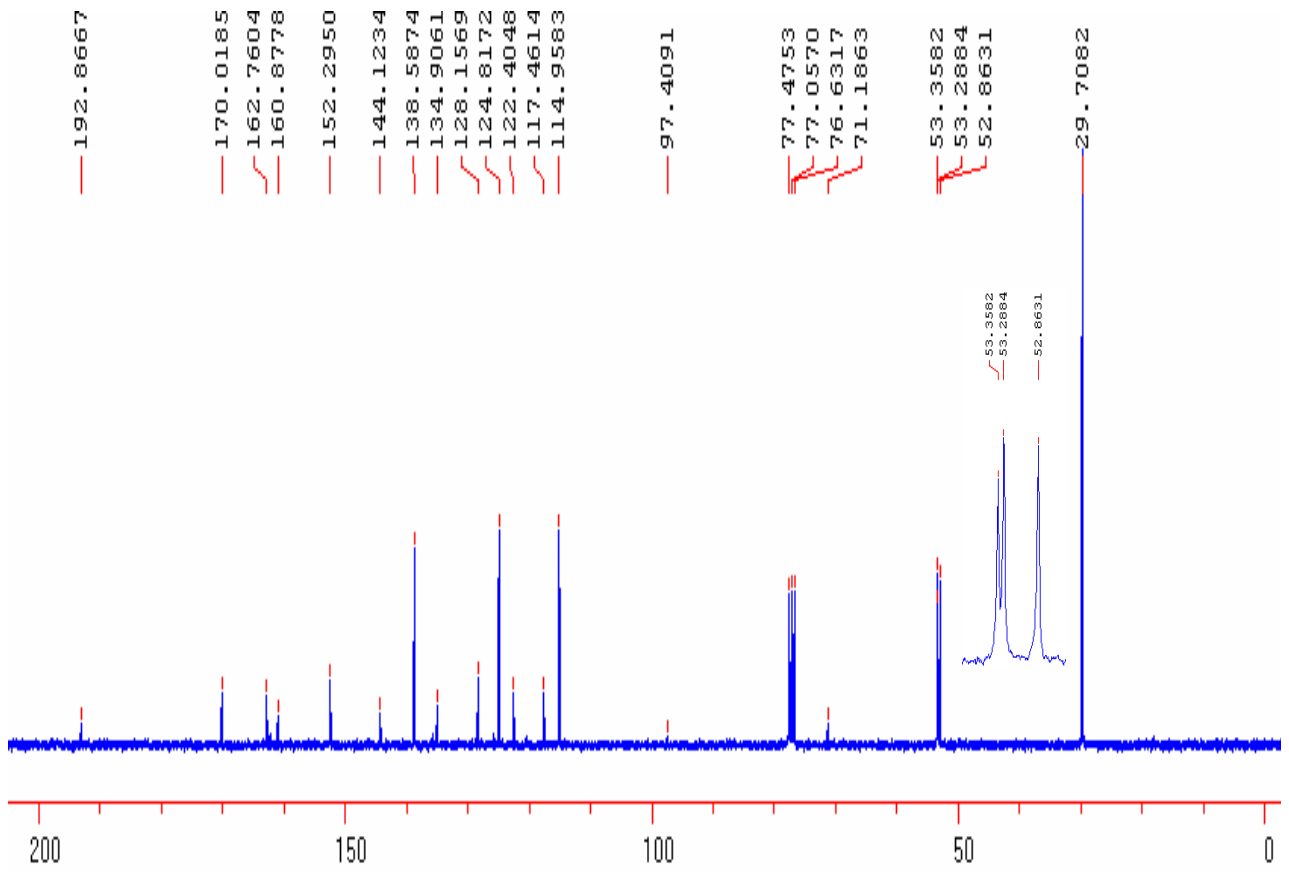
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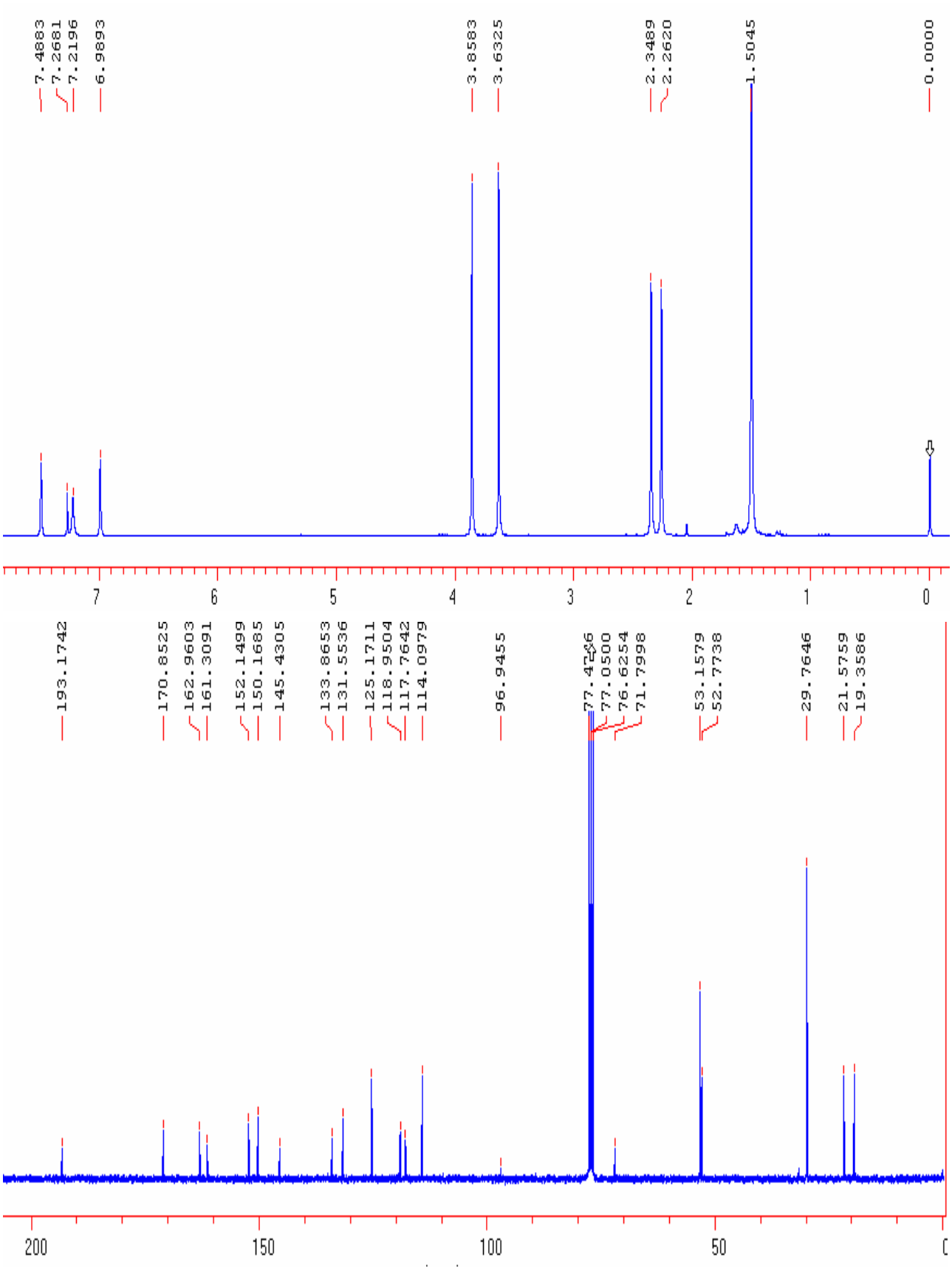
4d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4
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2
1
0
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162.9603
161.3091
152.1499
150.1685
145.4305
133.8653
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125.1711
118.9504
117.7642
114.0979
96.9455
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77.0500
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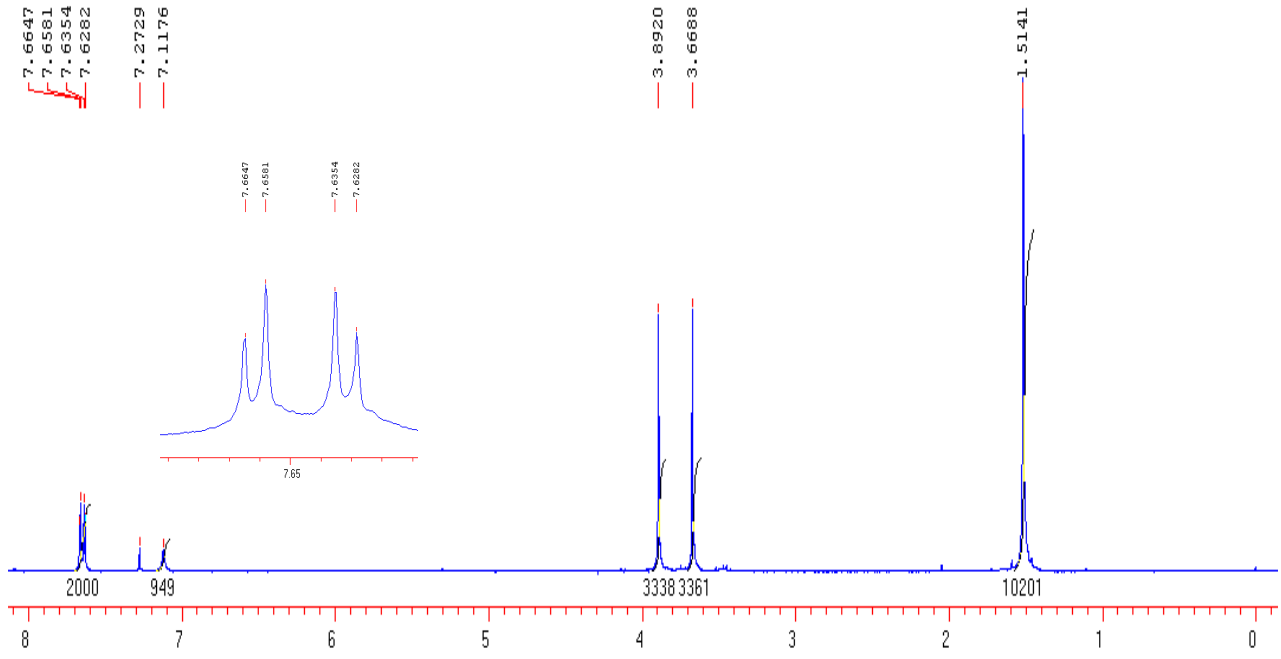
4e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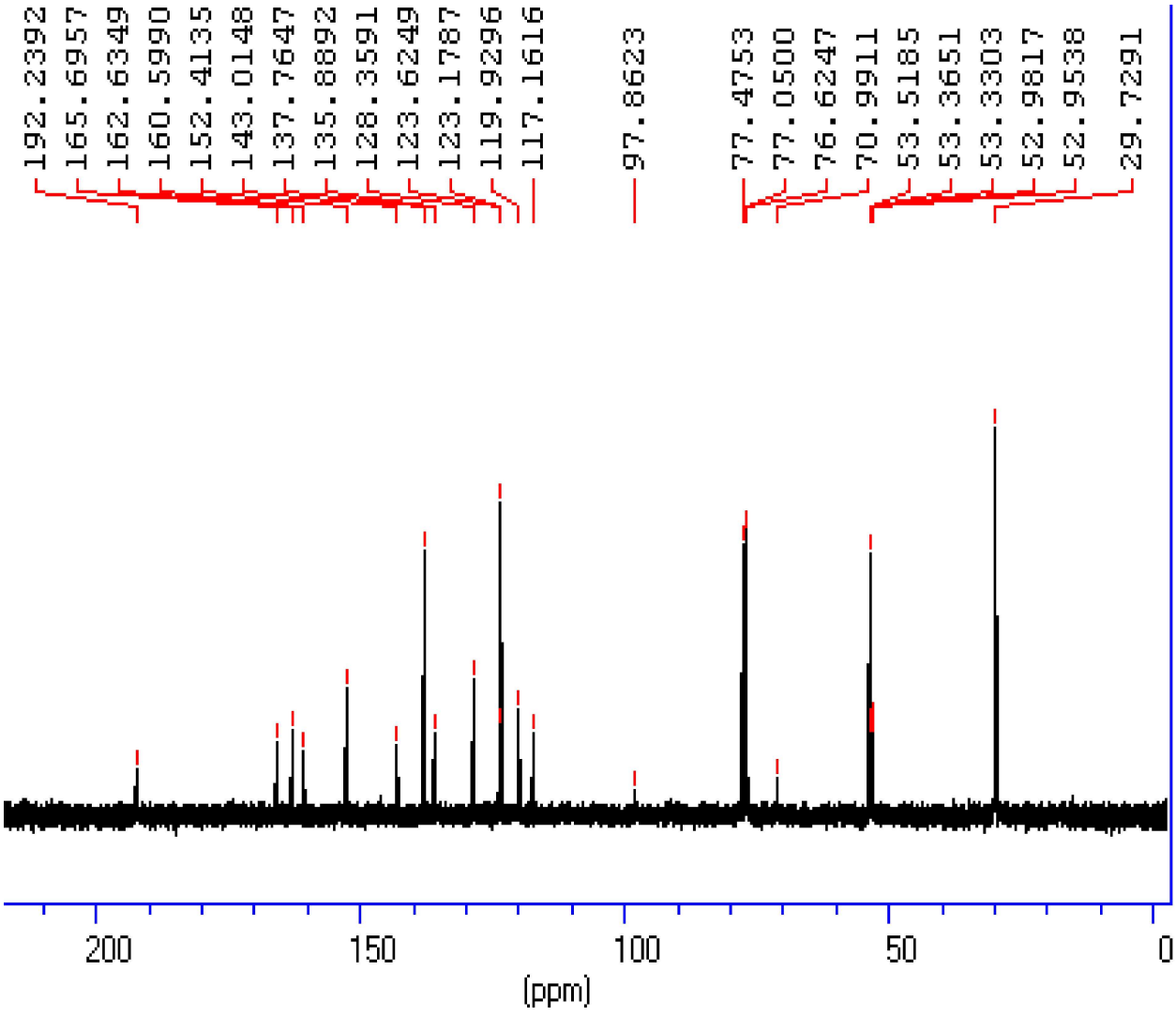
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119.9296
117.1616
97.8623
77.4753
77.0500
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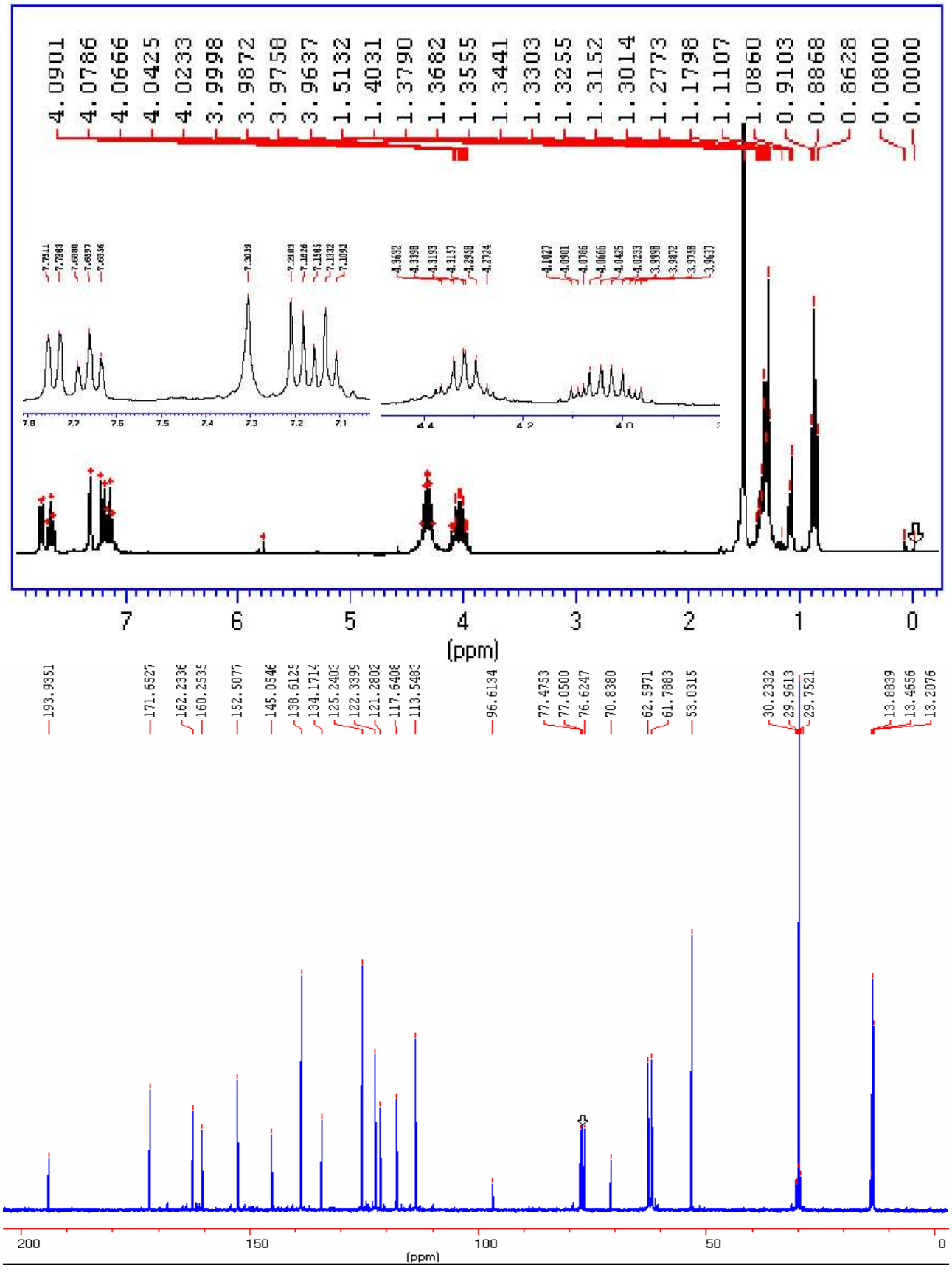
53.3303
52.9817
52.9538
29.7291
(ppm)

4f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1.3152
1.3014
1.2773
1.1798
1.1107
1.0860
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(ppm)
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171.6527
162.2336
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138.6125
134.1714
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122.3395
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117.6408
113.5485
96.6134
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77.0500
76.6247
70.8380
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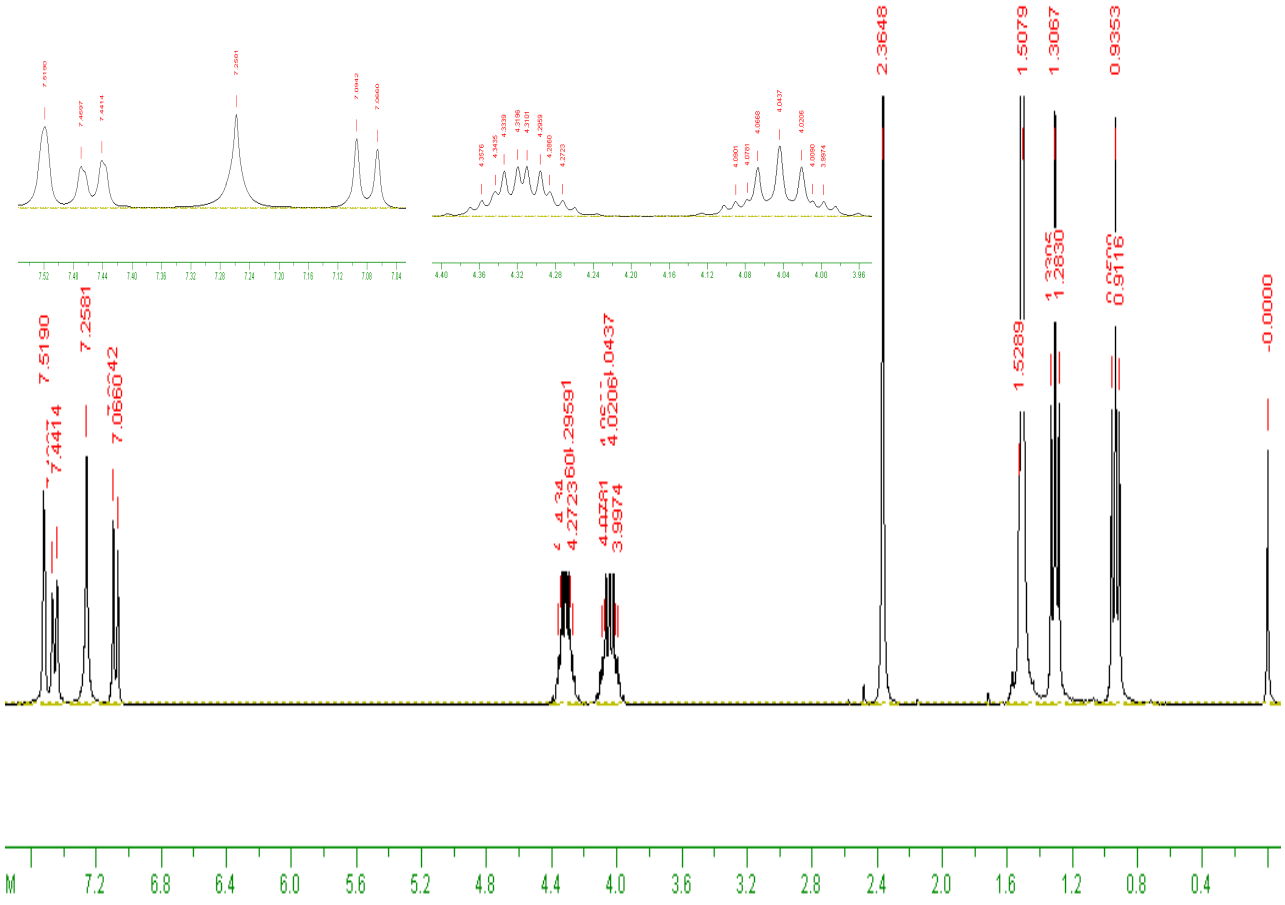
(ppm)

4g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M
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6.8
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6.0
5.6
5.2
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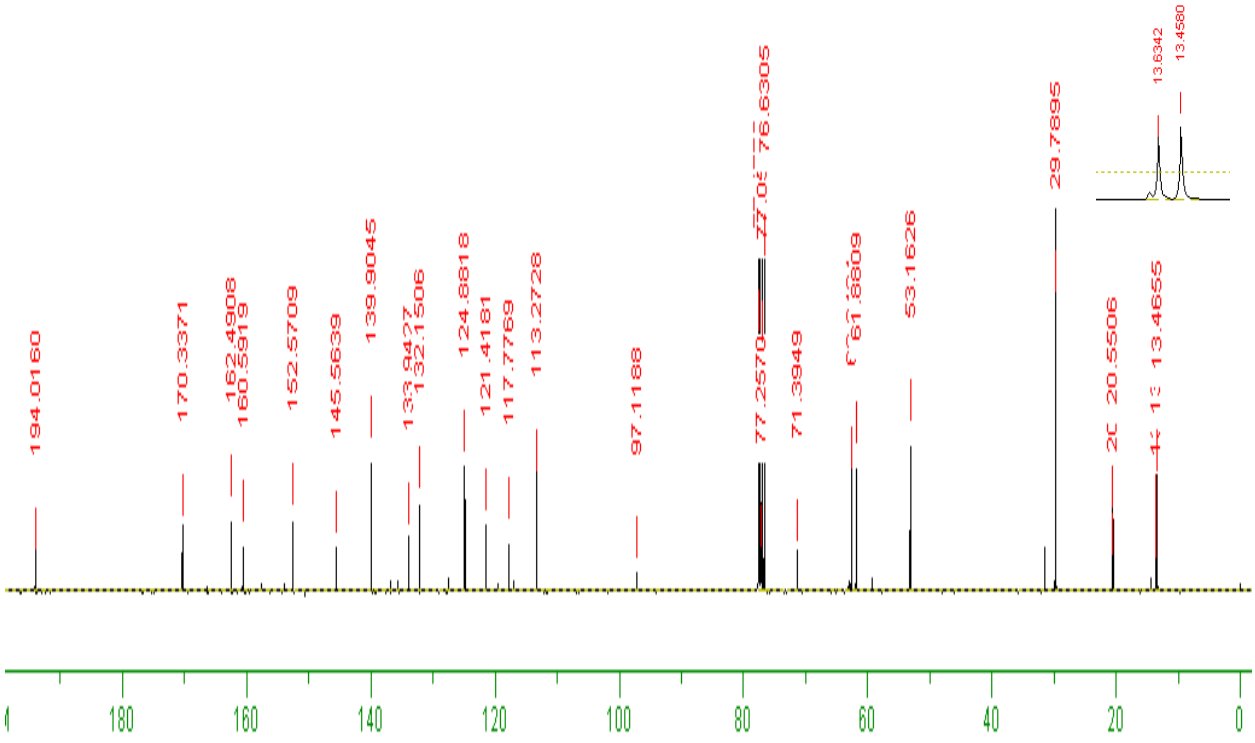
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77.0376
76.6305
71.3949
61.8809
53.1626
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13.4580
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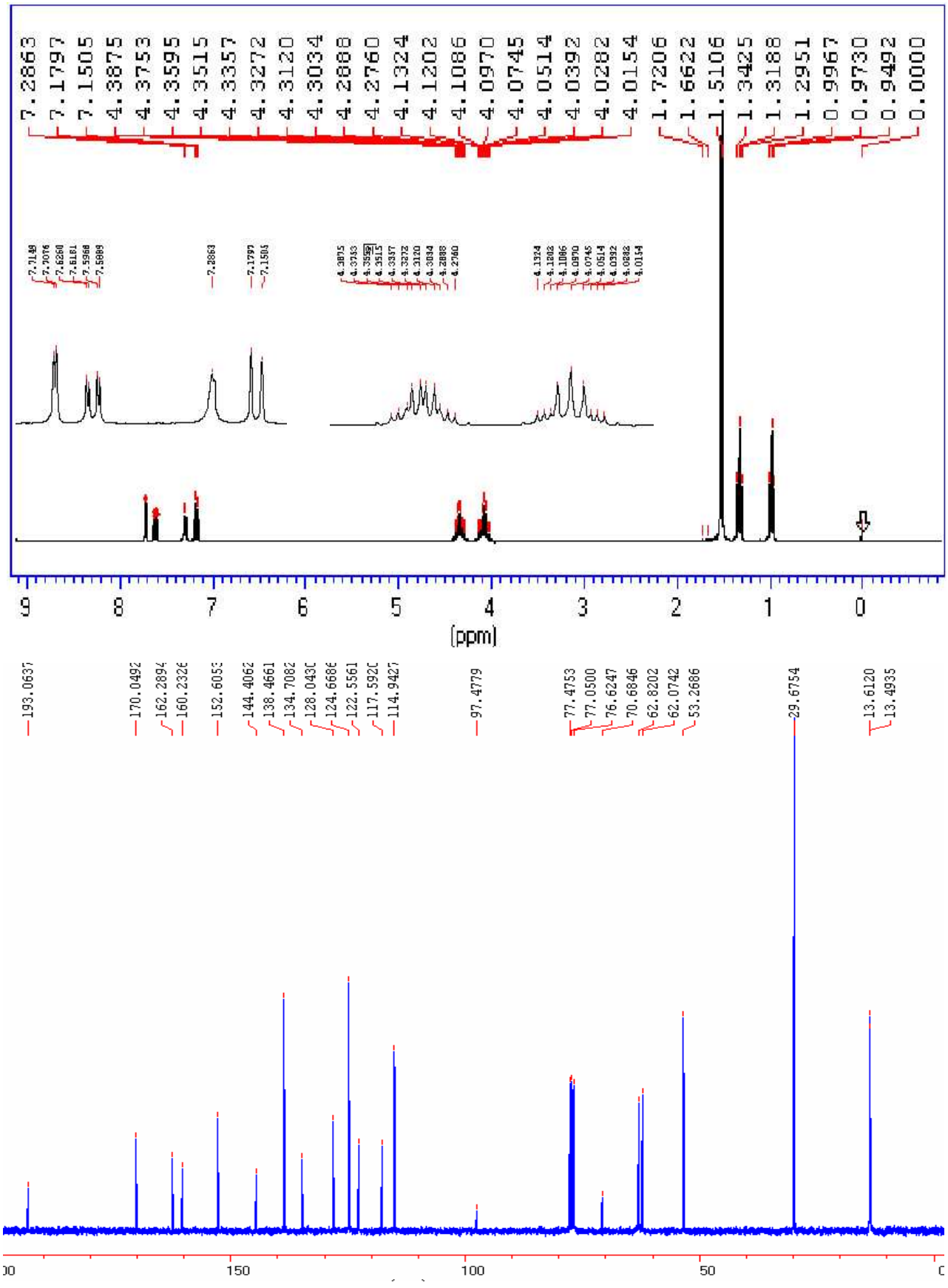
140
120
100
80
60
40
20
0

4h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4.3515
4.3357
4.3272
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4.2888
4.2760
4.1324
4.1202
4.1086
4.0970
4.0745
4.0514
4.0392
4.0282
4.0154
1.7206
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(ppm)
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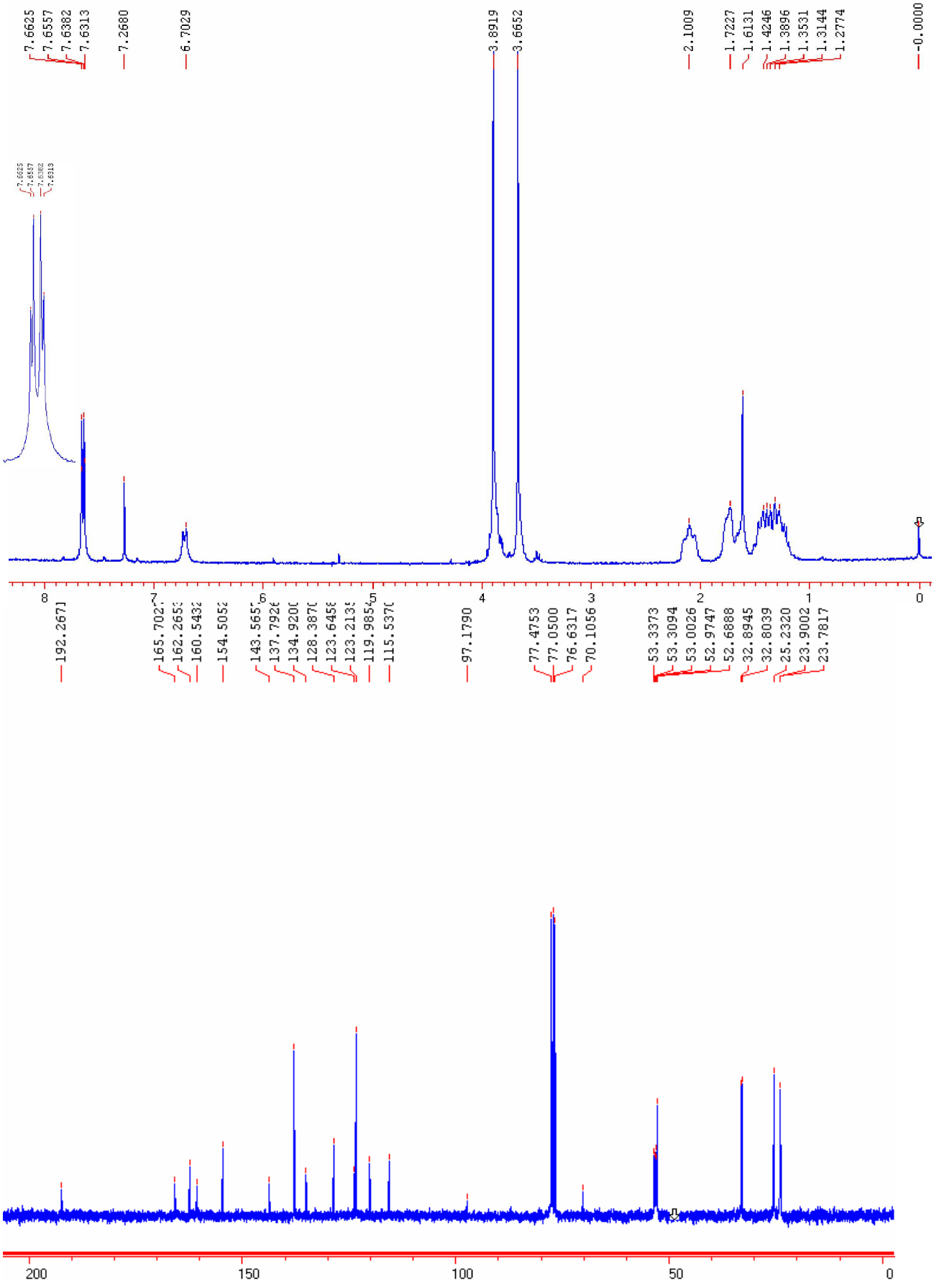
4i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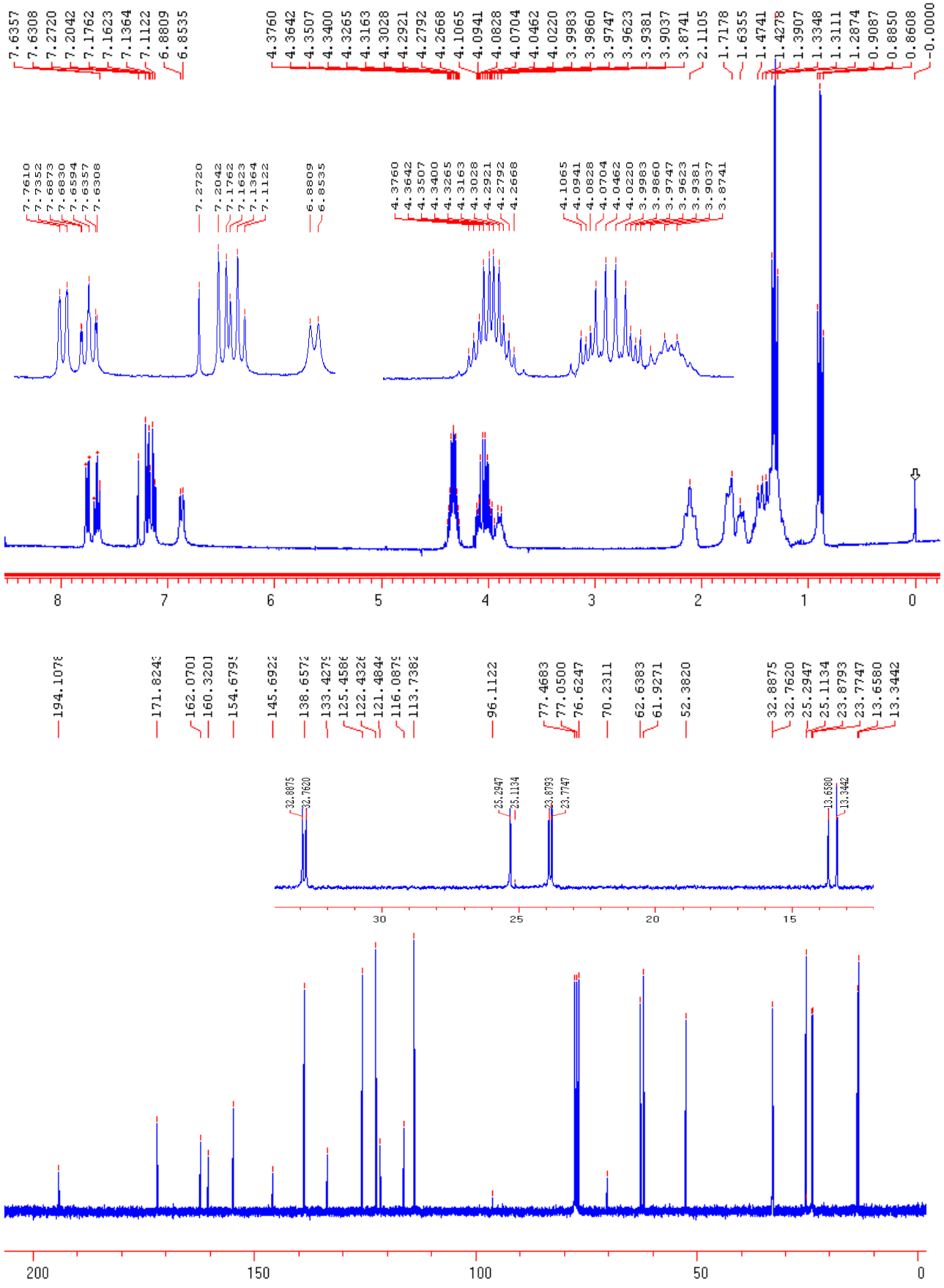
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4.3642
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4.3028
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4.1065
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4.0828
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4.0462
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3.9860
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2.1105
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1.3111
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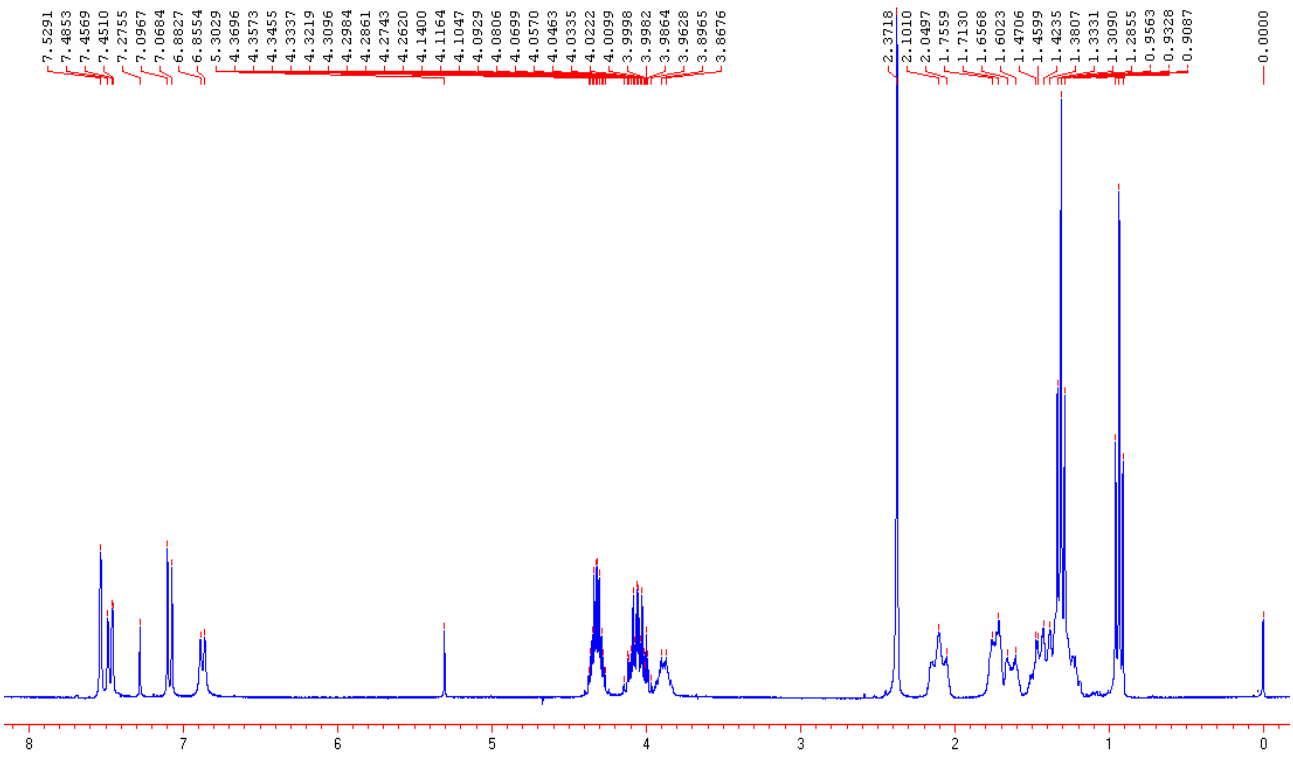
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4.0099
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3.9982
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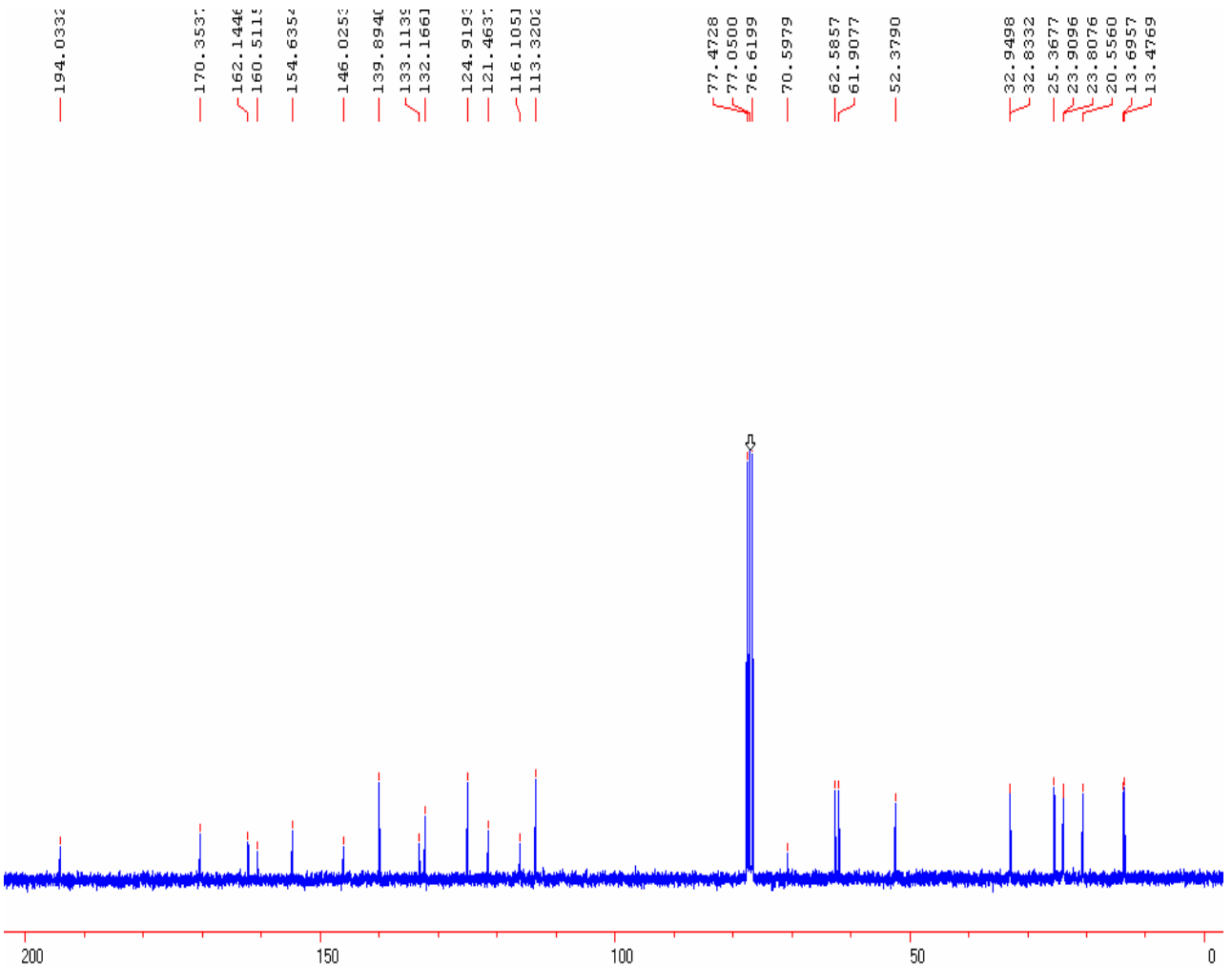
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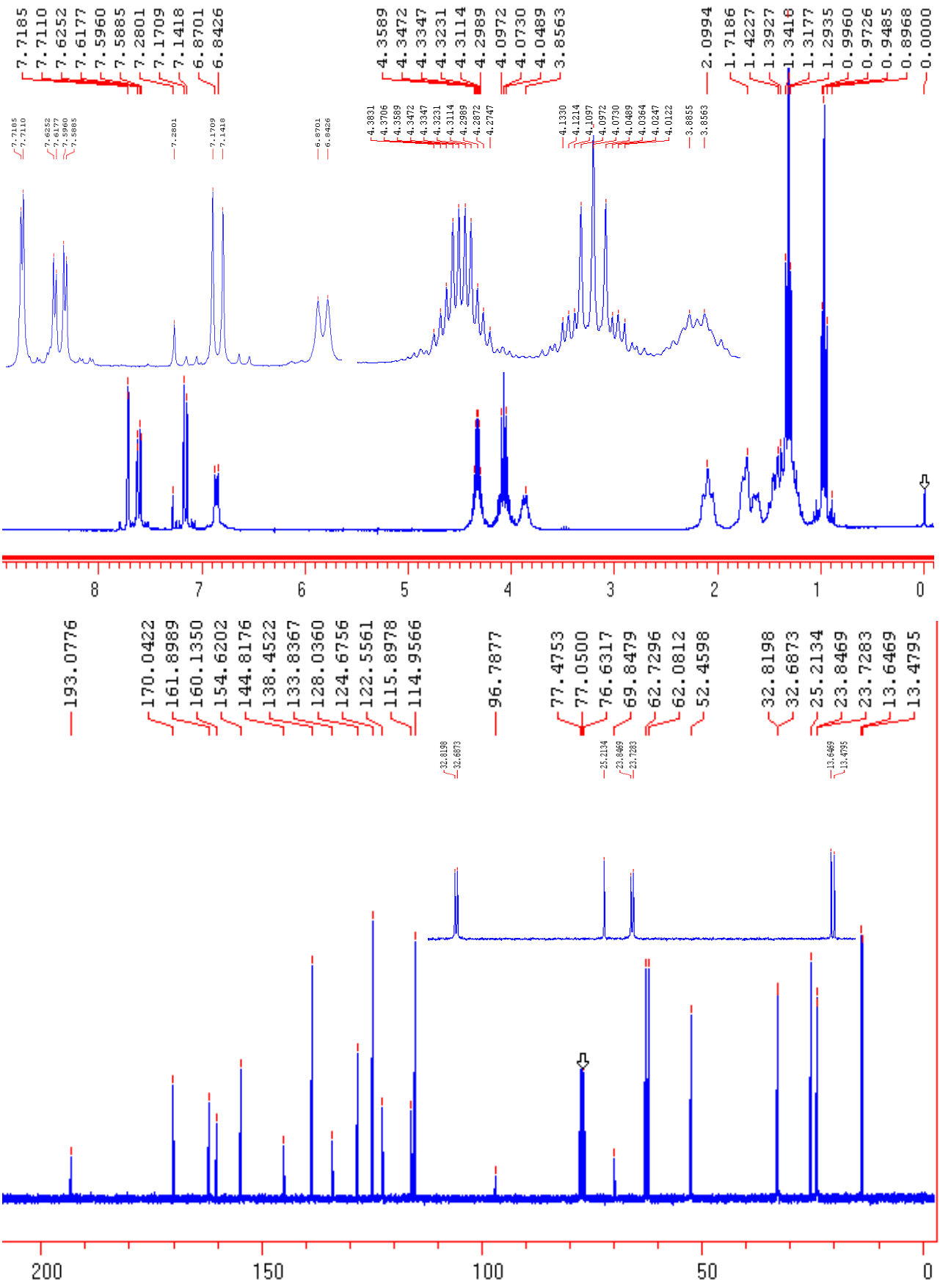
100
50
0

4l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7.1418
6.8701
6.8426
4.3589
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3.8563
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1.7186
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6
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4
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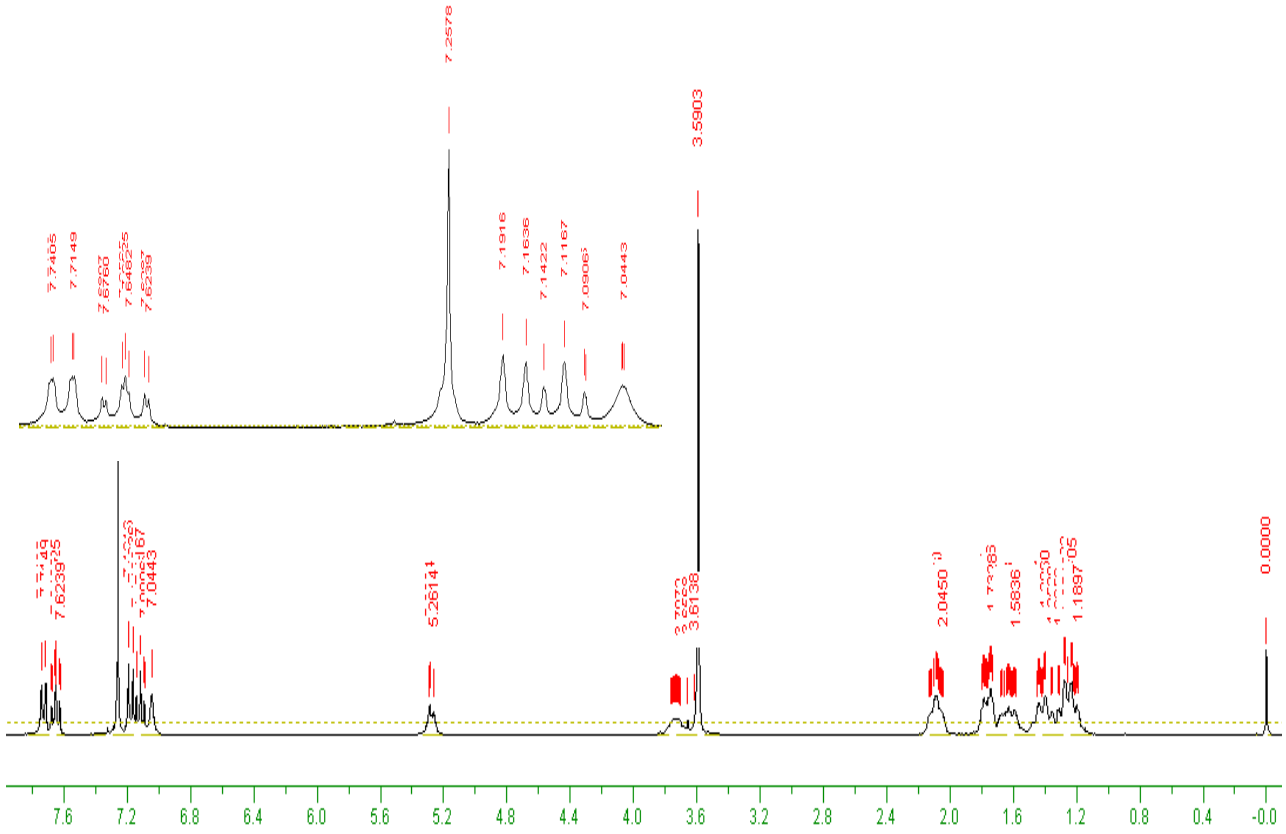
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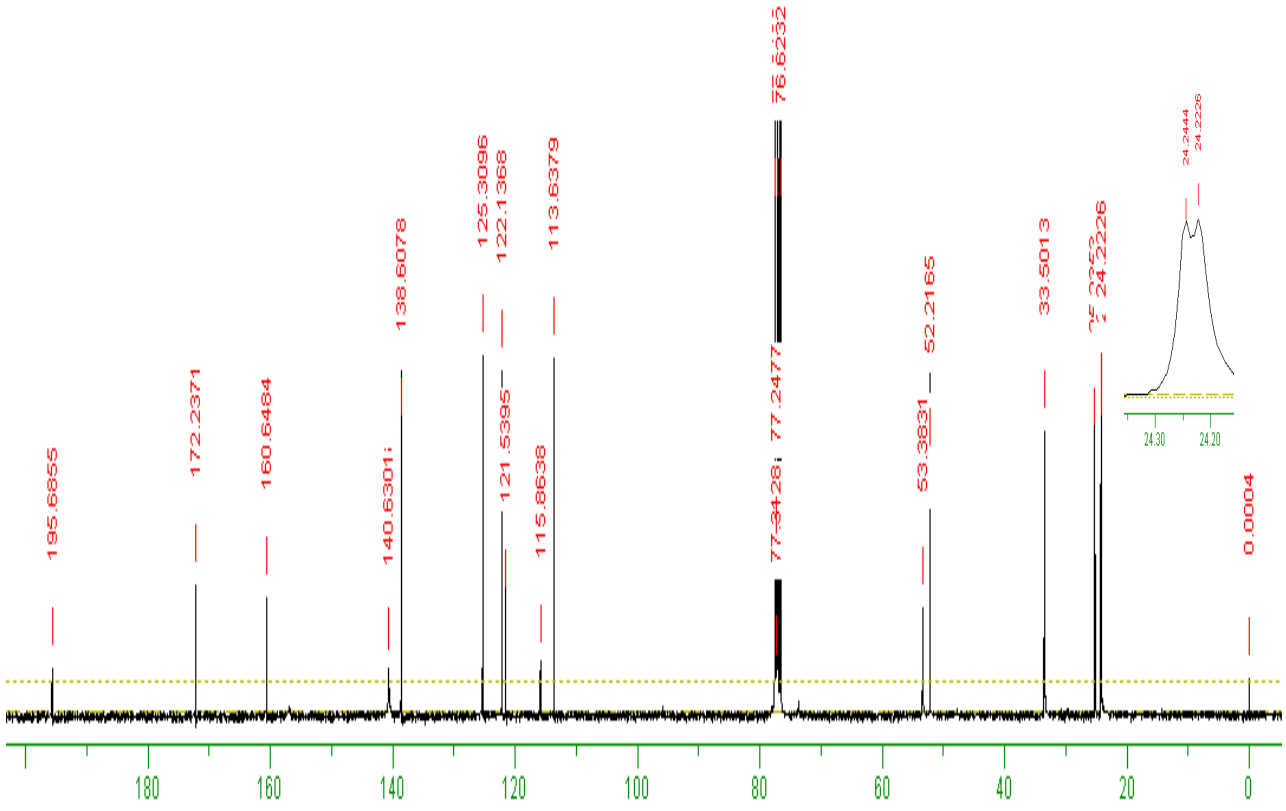
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