Supporting Information

Use of Selenium Bound Resin for the Solid Phase Synthesis of Substituted Isoxazolyl-Substituted (*E*)-Olefins

Xian Huang* and Wei-Ming Xu

Department of Chemistry, Zhejiang University (Campus Xixi), Hangzhou, 310028, P. R. China
Laboratory of Organometallic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, P. R. China
huangx@mail.hz.zj.cn

Contents:

1. Experimental section

The melting points were uncorrected. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker Avance 400 spectrometer in $CDCl_3$ with TMS as the internal standard; chemical shifts were quoted in ppm and *J* values were given in Hz. IR spectra were recorded on a Bruker Vector 22 spectrometer. EIMS were run on a HP 5989B mass spectrometer. Elemental analysis was run on Thermofinnigan Flash EA 1112. HPLC were run on a Shimadzu LC-6A. X-ray was run on a Rigaku RAXIS-RAPID diffractometer.

Chromatographic conditions(HPLC)

Column: ODS 5μ 250X4 mm. Mobile phase: THF/MeOH/H_2O=51/17/32 (V/V).

Flow rate: 0.8mL/min. Detector: UV287nm.

Typical procedure for the preparation of isoxazole supported selenium resin 3:

To a suspension of the swellen polystyrene-supported selenenyl bromide (Br: 0.99mmol/g) resin **1** (2.5 g) in dry THF /DMF (V/V=5:1) (30 mL) was added $NaBH_4$ (5 mmol) under nitrogen atmosphere at 40^oC. After stirring for 8 h at 40^oC, propargyl bromide (5.5 mmol) was added dropwise under nitrogen atmosphere, and stirring for another 12 h. The resin **2** was collected by filtration, washed with THF (20 mL×2), MeOH (20 mL×2) and CH_2Cl_2 (20 mL×2) and dried in vacuum. To a suspension of the swellen resin **2** (2.5g) in CH_2Cl_2 was added a mixture of hydroximoyl halide (7.5 mmol) in 10 mL CH_2Cl_2 (prepared from 7.5 mmol of aldoxime and 7.5 mmol of NCS stirring at r.t. for about 3 hours when use). A mixture of Et_3N (15 mmol) in 15 mL CH_2Cl_2 was slowly dropwised in 3 portions every 8 hours (each time 5 mmol in 5 mL dry CH_2Cl_2 was added). After stirring for 24 h at r.t., The resin **3** was collected by filtration, washed with THF (20 mL×2), ether (20 mL×2), THF/H_2O (3:1) (20 mL×2), H_2O (20 mL×2), THF (20 mL×2), benzene (20 mL×2), MeOH (20 mL×2), and CH_2Cl_2 (20 mL×2), and dried in vacuum.

Typical procedure for the preparation of 3-aryl-5-*E*-substituted-ethenyl isoxazoles (products 5a-5g):

To a suspension of the swellen resin **3** (0.5 g) in dry THF, cooled to –60^oC, was added dropwise LDA (2M in THF/hexane, 0.3 mL) under nitrogen. After stirring for 1.5 h at –60^oC, a solution of allyl bromide (2 mmol) in 1 mL of dry THF was added. The suspension was stirred for another 0.5 h at –60^oC. Slowly warm up to –40^oC in 0.5 h then quenched with 1 mL H_2O. The resin **4** was collected by filtration and washed with THF (10 mL×2), THF/H_2O (3:1) (10 mL×2), H_2O (10 mL×2), THF (10 mL×2), and CH_2Cl_2 (10 mL×2). The washed resin was suspended in THF (15 mL), to the mixture was added 30% (aq.) H_2O_2 (0.5 mL) and stirred for 1 h at 0^oC followed by 20 minutes at room temperature. The mixture was filtered and the resin was washed with CH_2Cl_2 (15 mL×2). The filtrate was washed with H_2O (30 mL×2), dried over $MgSO_4$, and evaporated to dryness in vacuum.

Typical procedure for the preparation of Isoxazolyl and Isoxazolinyl substituted (*E*)-olefins (products 8a-8k):

To a suspension of the swellen resin **6** (0.5 g) in CH_2Cl_2 was added a mixture of hydroximoyl halide (1.5 mmol) in 10 mL CH_2Cl_2 (prepared from 1.5 mmol of aldoxime

and 1.5 mmol of NCS stirring at r.t. for about 3 hours when use). A mixture of Et_3N (3 mmol) in 15 mL CH_2Cl_2 was slowly dropwised in 3 portions every 8 hours (each time 1 mmol in 5 mL dry CH_2Cl_2 was added). After stirring for 24 h at r.t., The resin **7** was collected by filtration, washed with THF (10 mL×2), ether (10 mL×2), THF/H_2O (3:1) (10 mL×2), H_2O (10 mL×2), THF (10 mL×2), benzene (10 mL×2), MeOH (10 mL×2), and CH_2Cl_2 (10 mL×2), and dried in vacuum. The washed resin was suspended in THF (15 mL), to the mixture was added 30% (aq.) H_2O_2 (0.5 mL) and stirred for 1 h at 0^oC followed by 20 minutes at room temperature. The mixture was filtered and the resin was washed with CH_2Cl_2 (15 mL×2). The filtrate was washed with H_2O (30 mL×2), dried over $MgSO_4$, and evaporated to dryness in vacuum.

2. Characterization data of key compounds.

Purity and yield are determined by the crude product and NMR MS, FTIR and EA are determined by the purified product.

^1H NMR (400 MHz), ^{13}C NMR (100 M Hz), MS, FTIR and EA of the products **5b, 5c, 5f, 8c, 8d, 8j, 8k.**

5b: 82.3mg, yellow low pointing solid; ^1H NMR ($CDCl_3$) δ 7.72 (2H, d, J = 8.2 Hz), 7.28 (2H, d, J = 8.2 Hz), 7.02 (1H, dd, J_1 = 10.4 Hz, J_2 = 15.6 Hz), 6.53-6.47 (3H, m), 5.53 (1H, d, J = 16.8 Hz), 5.17 (1H, d, J = 10.4 Hz), 2.43 (3H, s); ^{13}C NMR ($CDCl_3$) δ 168.9, 163.0, 140.5, 136.2, 135.8, 130.0, 127.1, 126.6, 122.4, 117.4, 99.9, 21.8; MS *m/z* 158(100), 211(M^+); IR ν_{max} (cm^{-1}) 3405, 3027, 1624, 1493, 1449, 967, 753, 692. Elemental analysis Calcd. for $C_{14}H_{13}NO$, C 79.59 %; H 6.20 %; N 6.63% Found C 79.38 %; H 6.29 %; N 6.72%.

5c: 81.4mg, pale yellow solid, mp. 143-145^oC; ^1H NMR ($CDCl_3$) δ 7.72 (2H, d, J = 7.6 Hz), 7.55 (1H, d, J = 16.0 Hz), 7.30 (2H, d, J = 7.6 Hz), 6.76 (1H, s), 6.68 (1H, d, J = 16.0 Hz), 3.86 (3H, s), 2.43 (3H, s); ^{13}C NMR ($CDCl_3$) δ 166.6, 166.3, 163.3, 141.0, 130.1, 128.1, 127.1, 125.9, 123.7, 104.5, 52.5, 21.8; MS *m/z* 158(100), 243(M^+); IR ν_{max} (cm^{-1}) 1711.8, 1651.1, 1560.4, 1528.8, 1429.6, 1385.3, 1312.4, 1262.2, 1173.4, 972.8, 816.9. Elemental analysis Calcd. for $C_{14}H_{13}NO_3$, C 69.12 %; H 5.39 %; N 5.76% Found C 68.98

%; H 5.52 %; N 5.89%.

5f: 100.3mg, pale yellow solid, mp.76-78^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.69 (2H, d, J = 6.8 Hz), 7.30 (2H, d, J = 6.8 Hz), 6.65-6.59 (1H, m), 6.38 (1H, d, J = 16.0 Hz), 6.36 (1H, s), 1.97 (1H, d, J = 7.2 Hz); ^{13}C NMR ($CDCl_3$) δ 169.8, 162.0, 134.5, 132.5, 128.7, 128.6, 124.5, 117.4, 97.9, 19.1; MS *m/z* 69(100), 264(97, M^+), 266(94, M^++2); IR ν_{max} (cm^{-1}) 1666.5, 1593.9, 155.9, 1501.8, 1424.2, 1376.0, 961.8, 846.8, 813.8, 774.1, 505.2. Elemental analysis Calcd. for $C_{12}H_{10}BrNO$, C 54.57 %; H 3.82 %; N 5.30% Found C 54.70 %; H 3.70 %; N 5.42%.

8c: 147.1mg, yellow solid, mp. 177-179^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.68 (2H, d, J = 8.4 Hz), 7.59 (4H, dd, J_1 = 6.0 Hz, J_2 = 8.4 Hz), 7.23 (2H, d, J = 8.4 Hz), 6.73 (1H, d, J = 16.0 Hz), 7.02 (1H, dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz), 6.50 (1H, s), 5.39-5.36 (1H, m), 3.63 (1H, dd, J_1 = 10.8 Hz, J_2 = 16.4 Hz), 3.25 (1H, dd, J_1 = 7.2 Hz, J_2 = 16.4 Hz), 2.40 (3H, s); ^{13}C NMR ($CDCl_3$) δ 168.3, 162.2, 156.7, 141.1, 134.8, 132.6, 130.0, 128.7, 128.2, 127.1, 126.7, 124.8, 117.3, 100.5, 80.3, 41.5, 21.9; MS *m/z* 131(100), 408(M^+-1), 410(M^++1); IR ν_{max} (cm^{-1}) 2916.7, 1608.2, 1596.1, 1561.4, 1430.4, 1366.2, 967.9, 899.1, 819.0, 803.8. Elemental analysis Calcd. for $C_{21}H_{17}BrN_2O_2$, C 61.63 %; H 4.19 %; N 6.84% Found C 61.77 %; H 4.07 %; N 6.72%.

8d: 118.2mg, yellow solid, mp. 133-134^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.78 (2H, m), 7.57 (2H, d, J = 8.0 Hz), 7.22 (2H, d, J = 8.0 Hz), 7.14 (2H, t, J = 8.4 Hz), 6.72 (1H, d, J =16.0 Hz), 6.61 (1H, dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz), 6.47 (1H, s), 5.39-5.33 (1H, m), 3.63 (1H, dd, J_1 = 11.2 Hz, J_2 = 16.4 Hz), 3.24 (1H, dd, J_1 = 8.0 Hz, J_2 = 16.4 Hz), 2.38 (3H, s); ^{13}C NMR ($CDCl_3$) δ 167.7, 163.7(J = 248.6 Hz), 161.8, 156.3, 140.7, 134.2, 129.5, 128.7(J = 8.1 Hz), 126.7, 126.3, 125.1(J = 2.4 Hz), 117.0, 116.0(J = 21.4 Hz), 110.1, 79.9, 41.0, 21.4; MS *m/z* 162(100), 348(M^+); IR ν_{max} (cm^{-1}) 2962.1, 1608.2, 1560.3, 1430.2, 1366.3, 966.9, 898.6, 831.2, 797.6. Elemental analysis Calcd. for $C_{21}H_{17}FN_2O_2$, C 72.40 %; H 4.92 %; N 8.04% Found C 72.20 %; H 4.80 %; N 8.14%.

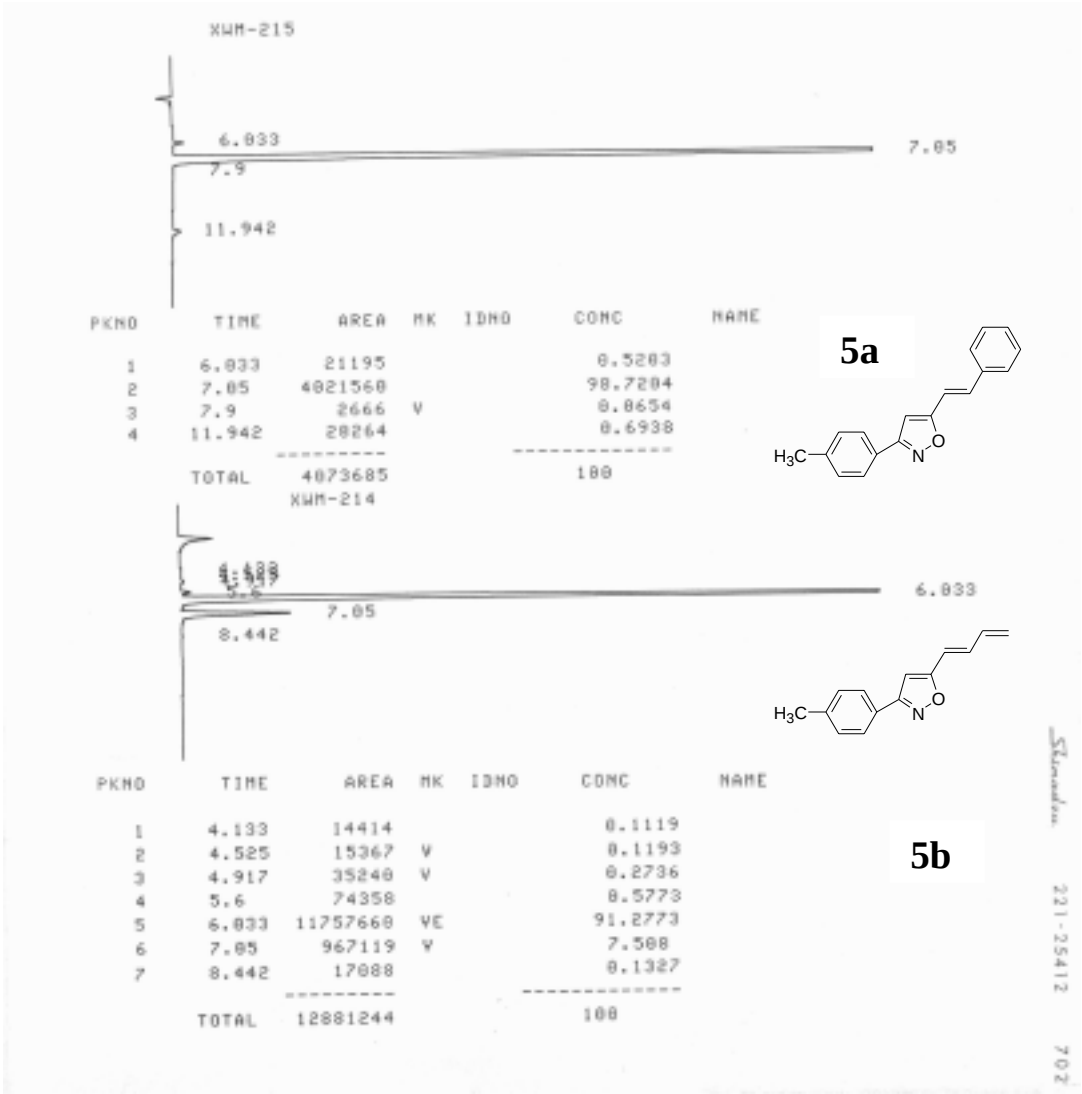
8j: 108.5mg, pale yellow solid, mp. 138-139^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.78 (2H, m), 7.54

(2H, d, *J* = 8.2 Hz), 7.20 (2H, d, *J* = 8.2 Hz), 7.13 (2H, t, *J* = 8.4 Hz), 6.70 (1H, d, *J* =16.0 Hz), 6.67 (1H, d, *J* =16.0 Hz), 6.43 (1H, s), 3.36 (1H, d, *J* =16.4 Hz), 3.27 (1H, d, *J* =16.4 Hz), 2.37 (3H, s), 1.68 (3H, s); ^{13}C NMR ($CDCl_3$) δ 168.0, 163.7(*J* = 249.1 Hz), 161.8, 156.2, 140.5, 138.6, 129.4, 128.7(*J* = 8.2 Hz), 126.7, 126.5, 125.2(*J* = 3.6 Hz), 116.0(*J* = 22.0 Hz), 114.2, 100.0, 85.5, 46.7, 25.4, 21.4; MS *m/z* 162(100), 362(M^+); IR ν_{max} (cm^{-1}) 2924.2, 1607.4, 1560.7, 1429.6, 1378.4, 1365.1, 964.7, 896.8, 832.0, 796.0; Elemental analysis Calcd. for $C_{22}H_{19}FN_2O_2$, C 72.91 %; H 5.28 %; N 7.73 % Found C 72.70 %; H 5.39 %; N 7.82%.

8k: 137.9mg, pale yellow solid, mp. 115-116^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.79-7.77 (2H, m), 7.59-7.54 (4H, m), 7.46-7.40 (6H, m), 7.21 (2H, d, *J* = 8.4 Hz), 6.92 (1H, d, *J* = 16.0 Hz), 6.69 (1H, d, *J* = 16.0 Hz), 6.48 (1H, s), 3.76 (2H, s), 2.38 (3H, s); ^{13}C NMR ($CDCl_3$) δ 167.7, 162.7, 156.2, 141.7, 140.7, 137.8, 130.0, 129.5, 129.4, 128.9, 128.1, 126.7, 126.6, 126.4, 125.6, 115.2, 100.5, 89.2, 47.8, 21.4; MS *m/z* 143(100), 406(M^+); IR ν_{max} (cm^{-1})3024.1, 2924.2, 1599.1, 1560.3, 1430.7, 1366.6, 968.8, 900.4, 831.0, 801.8. Elemental analysis Calcd. for $C_{27}H_{22}N_2O_2$, C 79.78 %; H 5.46 %; N 6.89 % Found C 79.97 %; H 5.31 %; N 6.76 %.

HPLC copys of **5a-b**, **8b-e**, **8g-h** (page 6-9).
^{1}H, ^{13}C NMR copys of **5a-c**, **8a**, **8c-f**, **8j-k** (page 10-29).

HPLC copys of **5a and 5b**



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4	11.942	28264			0.6938	
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5a

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1	4.133	14414			0.1119	
2	4.525	15367	V		0.1193	
3	4.917	35240	V		0.2736	
4	5.6	74358			0.5773	
5	6.033	11757660	VE		91.2773	
6	7.05	967119	V		7.508	
7	8.442	17088			0.1327	
	TOTAL	12881244			100	

5b

HPLC copys of **8h and 8e**

H

PKNO	TIME	AREA	MK	IDNO	CONC	NAME
1	4.058	2798			0.0998	
2	4.192	12859	V		0.4586	
3	4.475	4758	V		0.1697	
4	4.683	11844	V		0.4224	
5	5.033	26232	V		0.9354	
6	5.225	13416	V		0.4784	
7	5.908	51861			1.8494	
8	6.267	2631	V		0.0938	
9	6.525	79398	V		2.8314	
10	7.058	2467937	V		88.0079	
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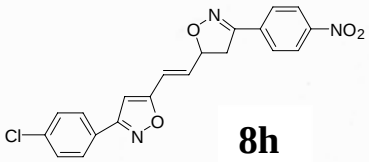

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1	4.05	3165			0.0618	
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4	4.767	6604	V		0.1384	
5	5.208	7609			0.1485	
6	5.958	115869			2.2611	
7	6.367	11797	V		0.2302	
8	6.992	31661			0.6178	
9	7.842	4759766	V		92.8834	
10	8.717	88689	V		1.7307	
11	9.917	15887			0.31	
12	11.9	8629			0.1684	
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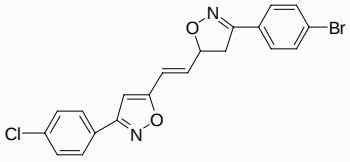
8e



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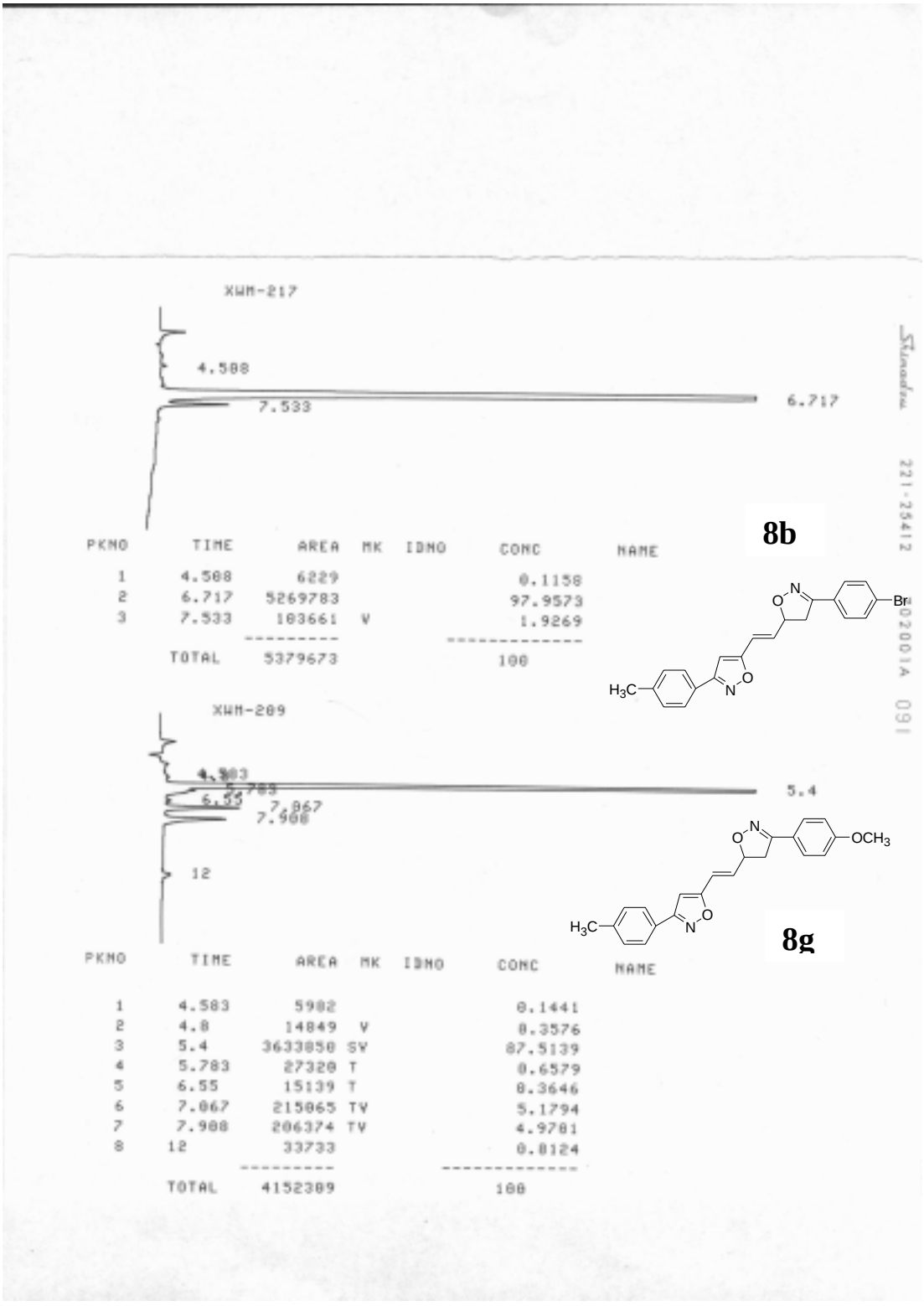

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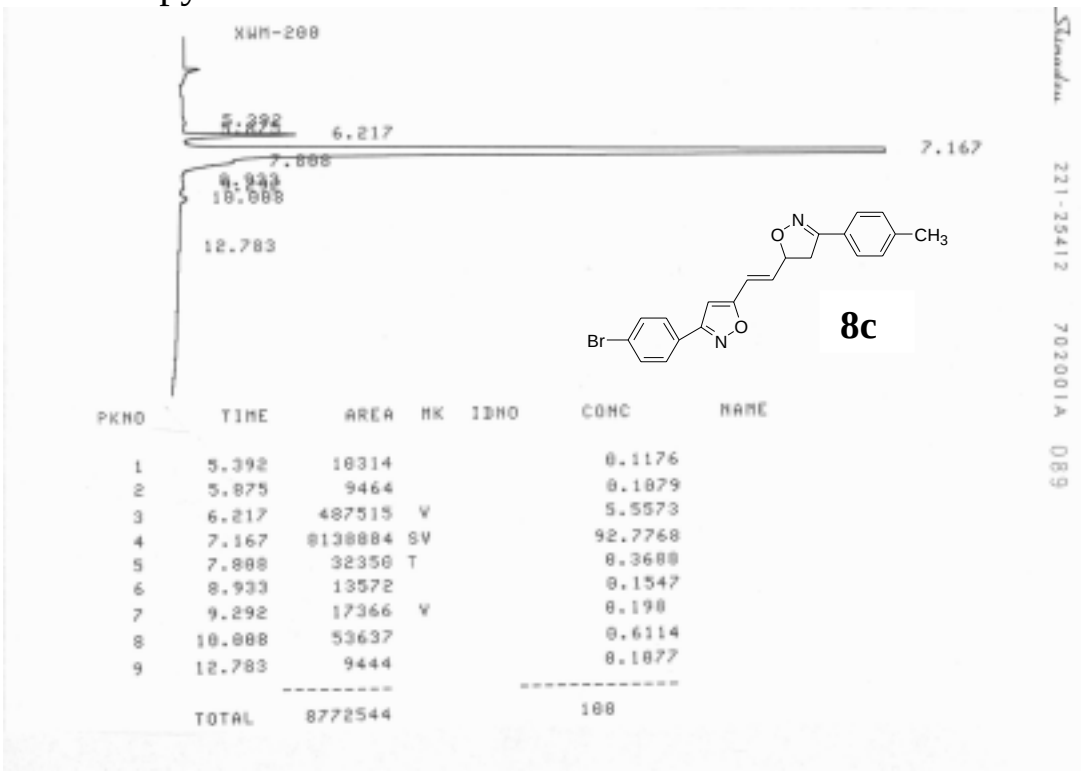

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4	7.167	8138884	SV		92.7768	
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6	8.933	13572			0.1547	
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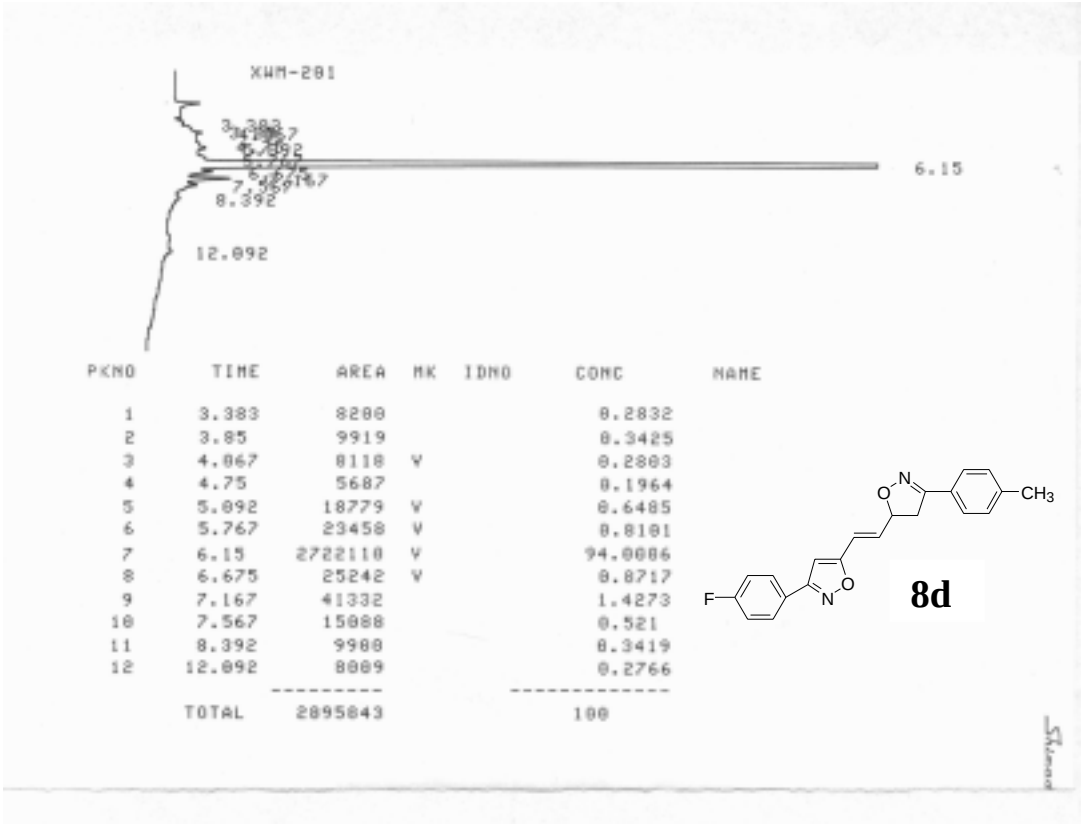

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4	4.75	5687			0.1964	
5	5.092	18779	V		0.6485	
6	5.767	23458	V		0.8101	
7	6.15	2722110	V		94.0086	
8	6.675	25242	V		0.8717	
9	7.167	41332			1.4273	
10	7.567	15088			0.521	
11	8.392	9988			0.3419	
12	12.092	8009			0.2766	
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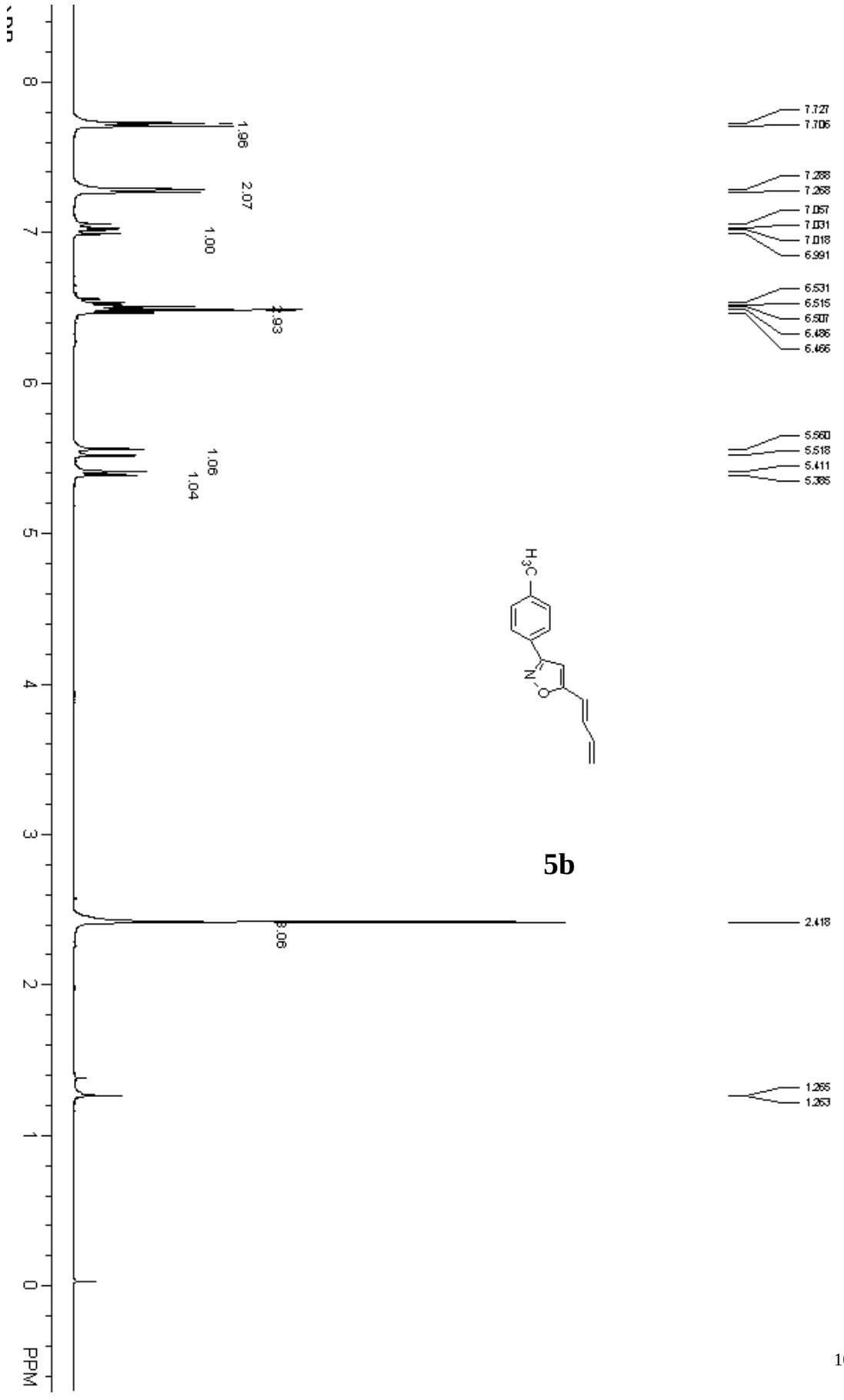
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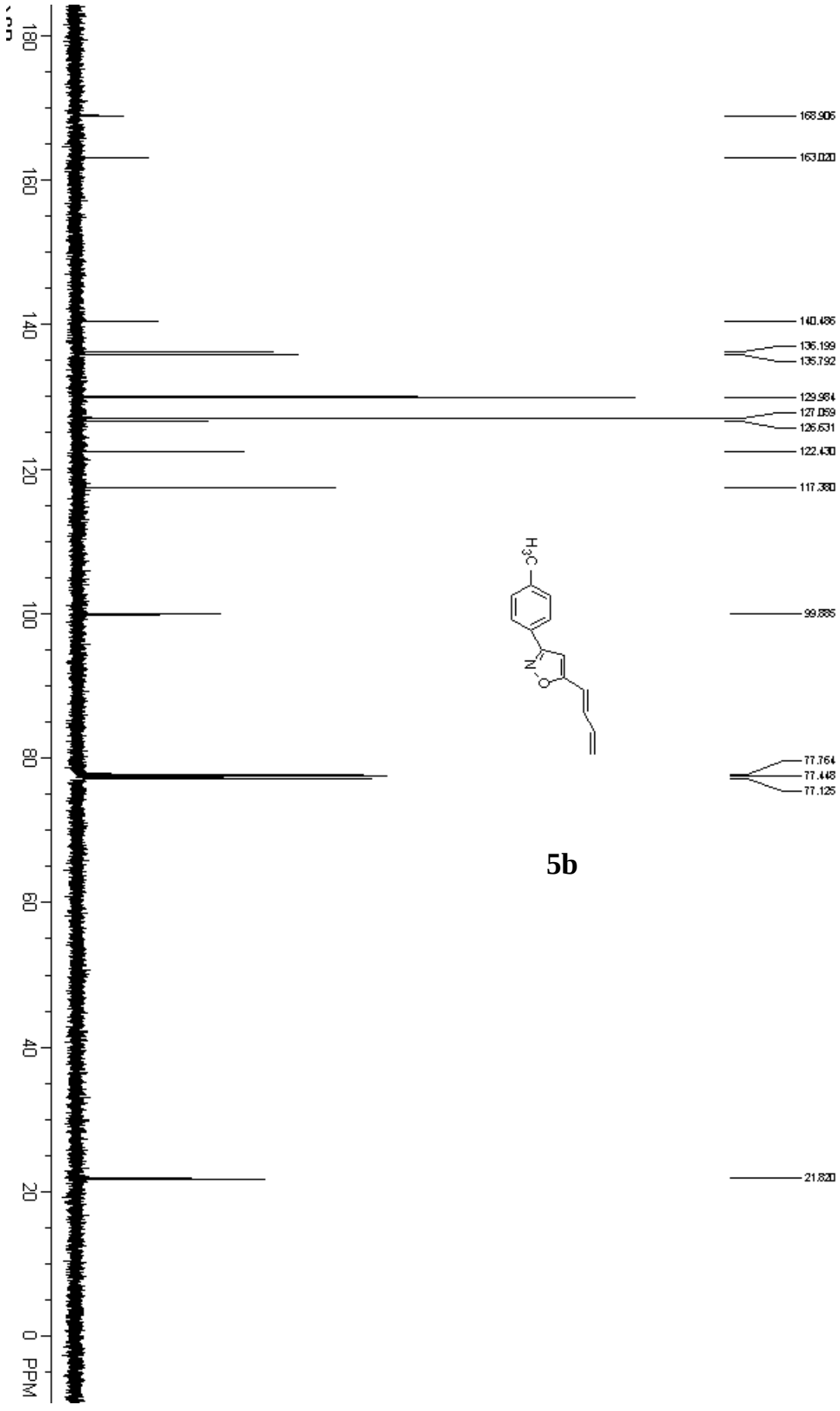
5b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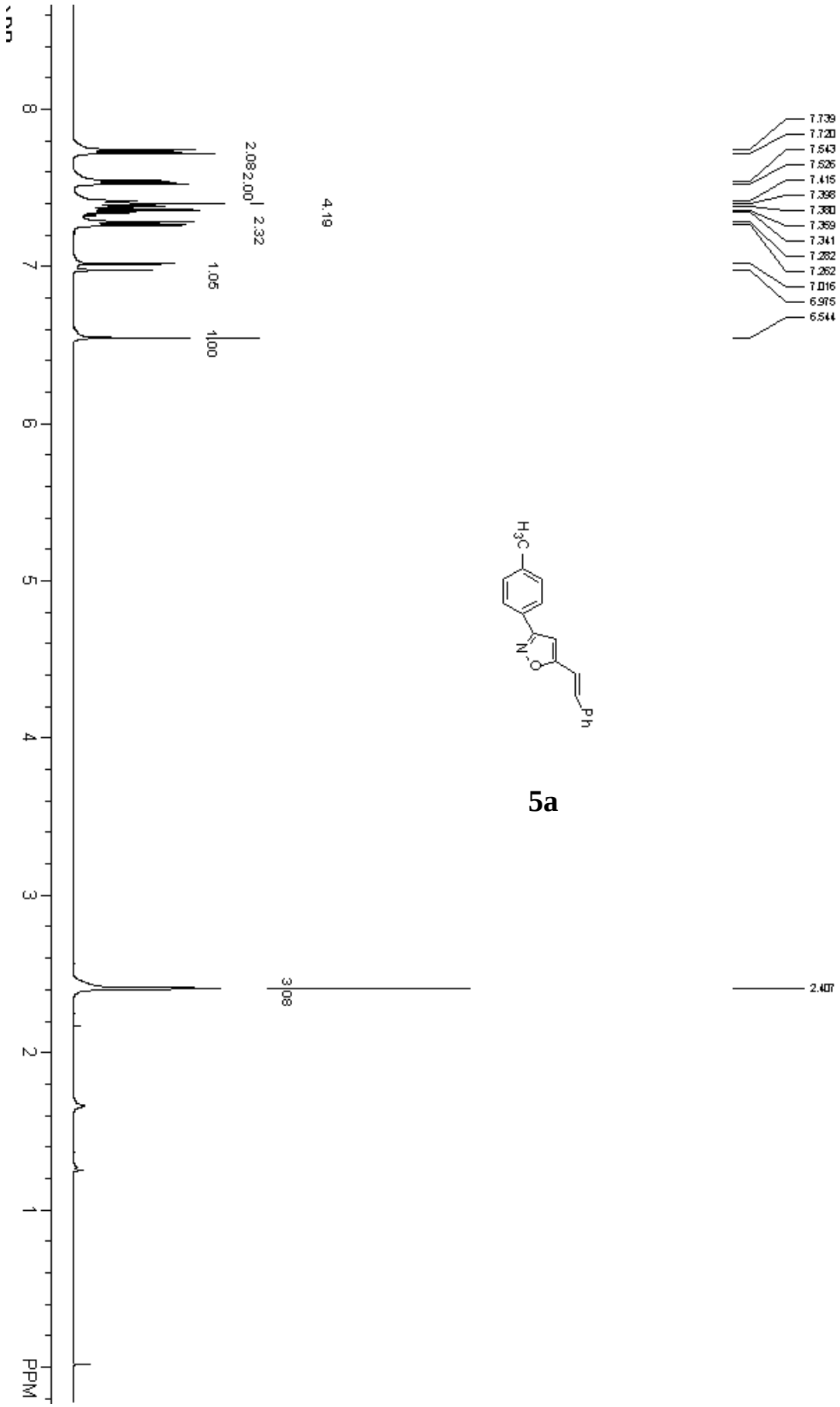
5b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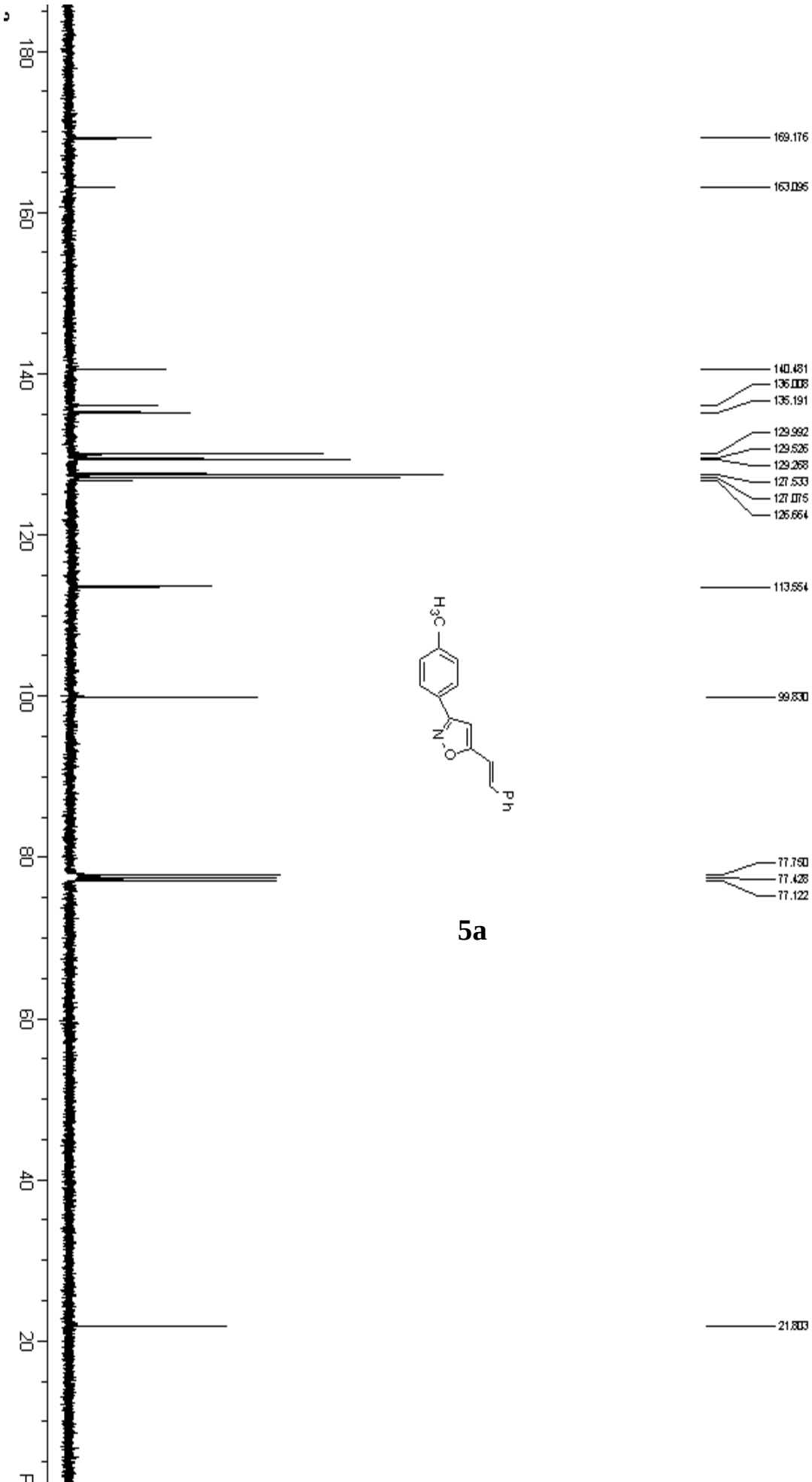
5a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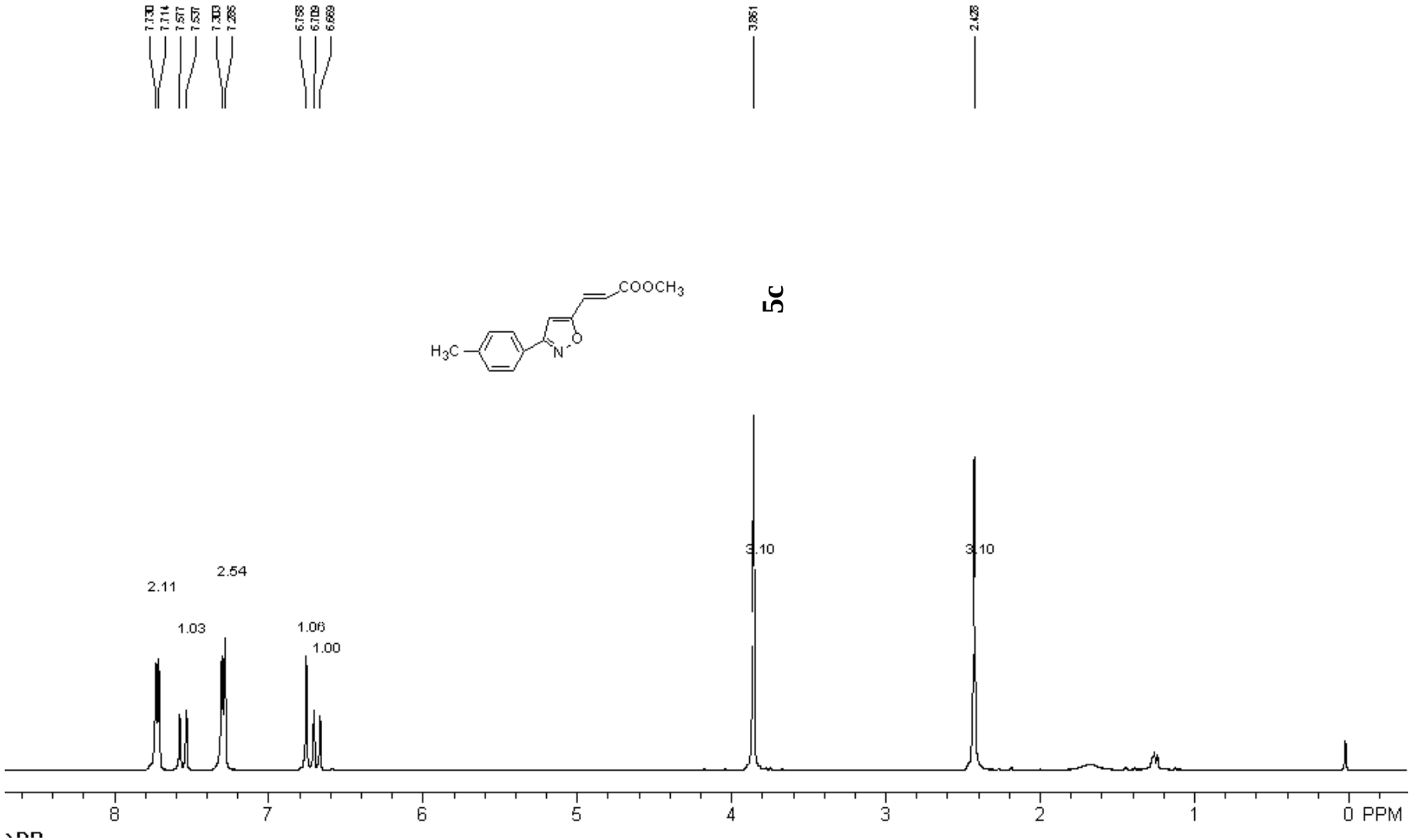
5a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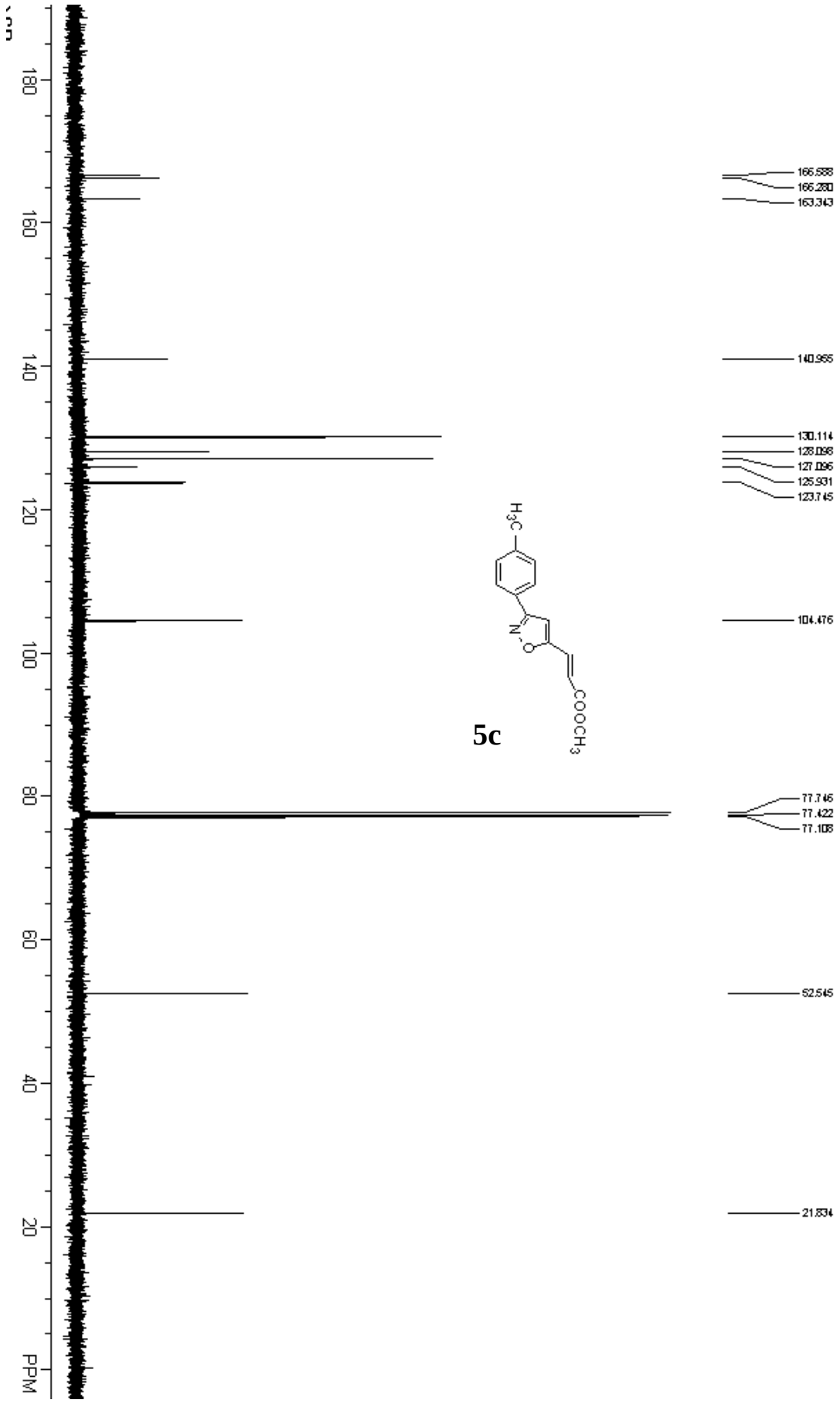
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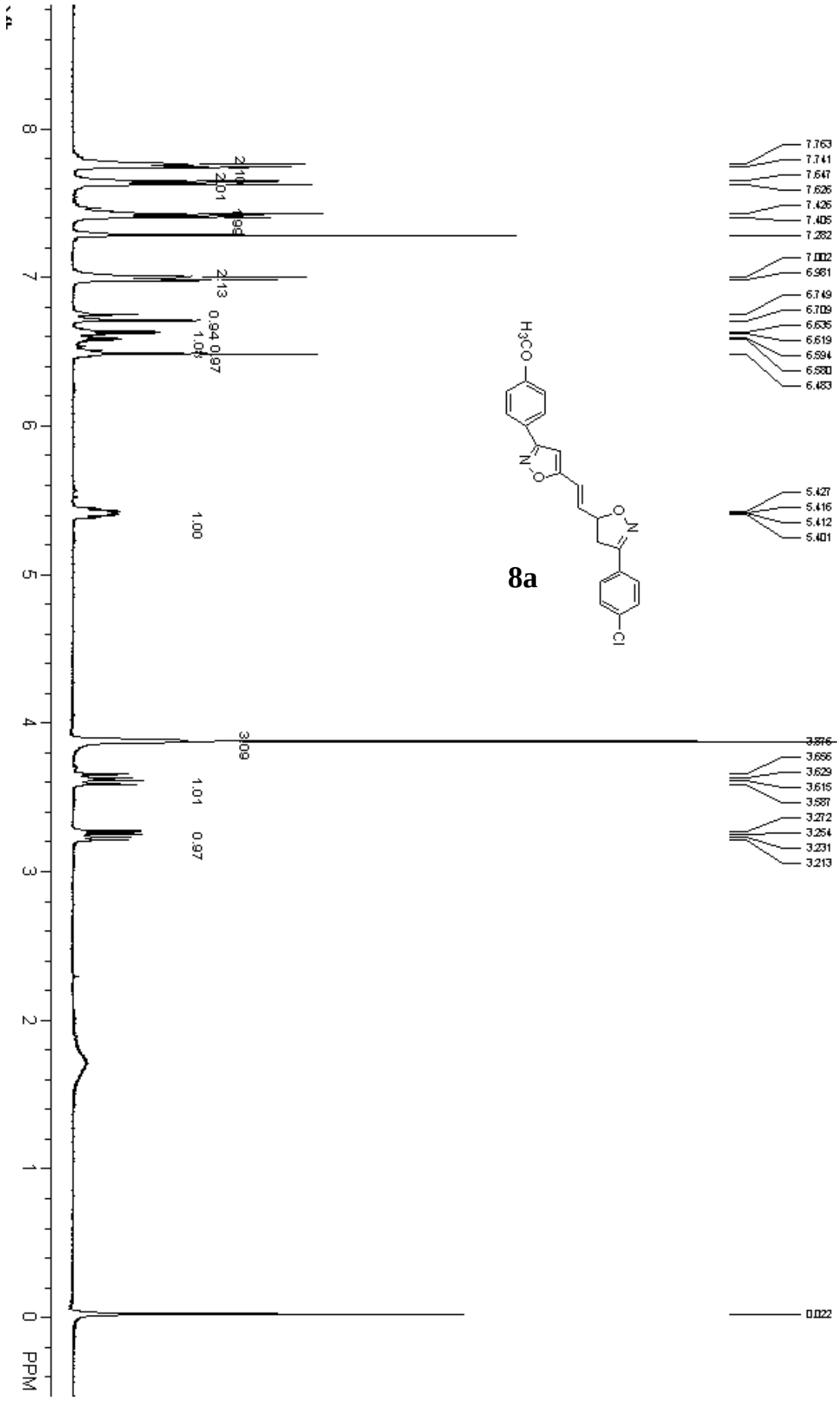
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6.594
6.580
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5.401
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3.587
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3.231
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2.13
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0.97
1.05
1.00
3.09
1.01
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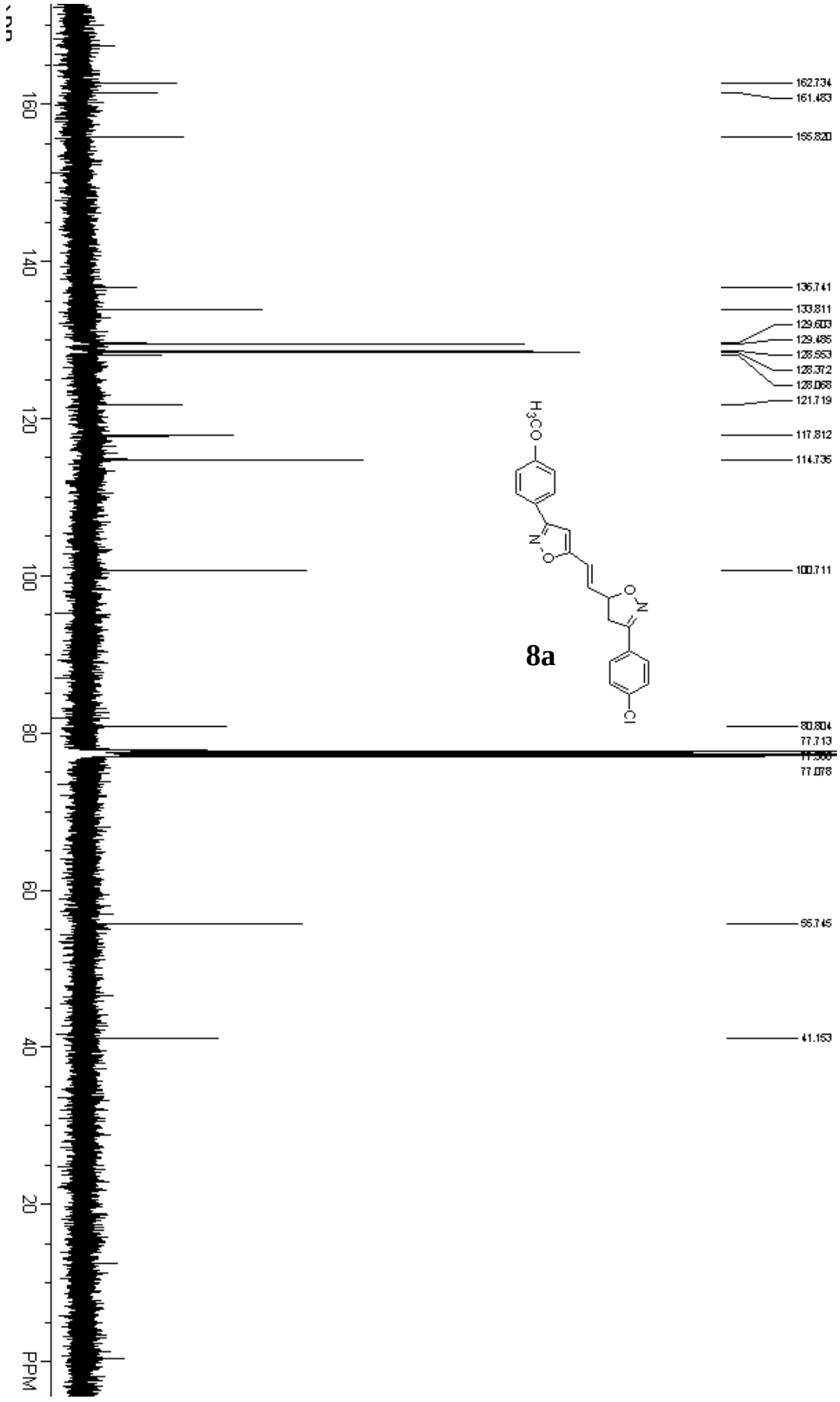
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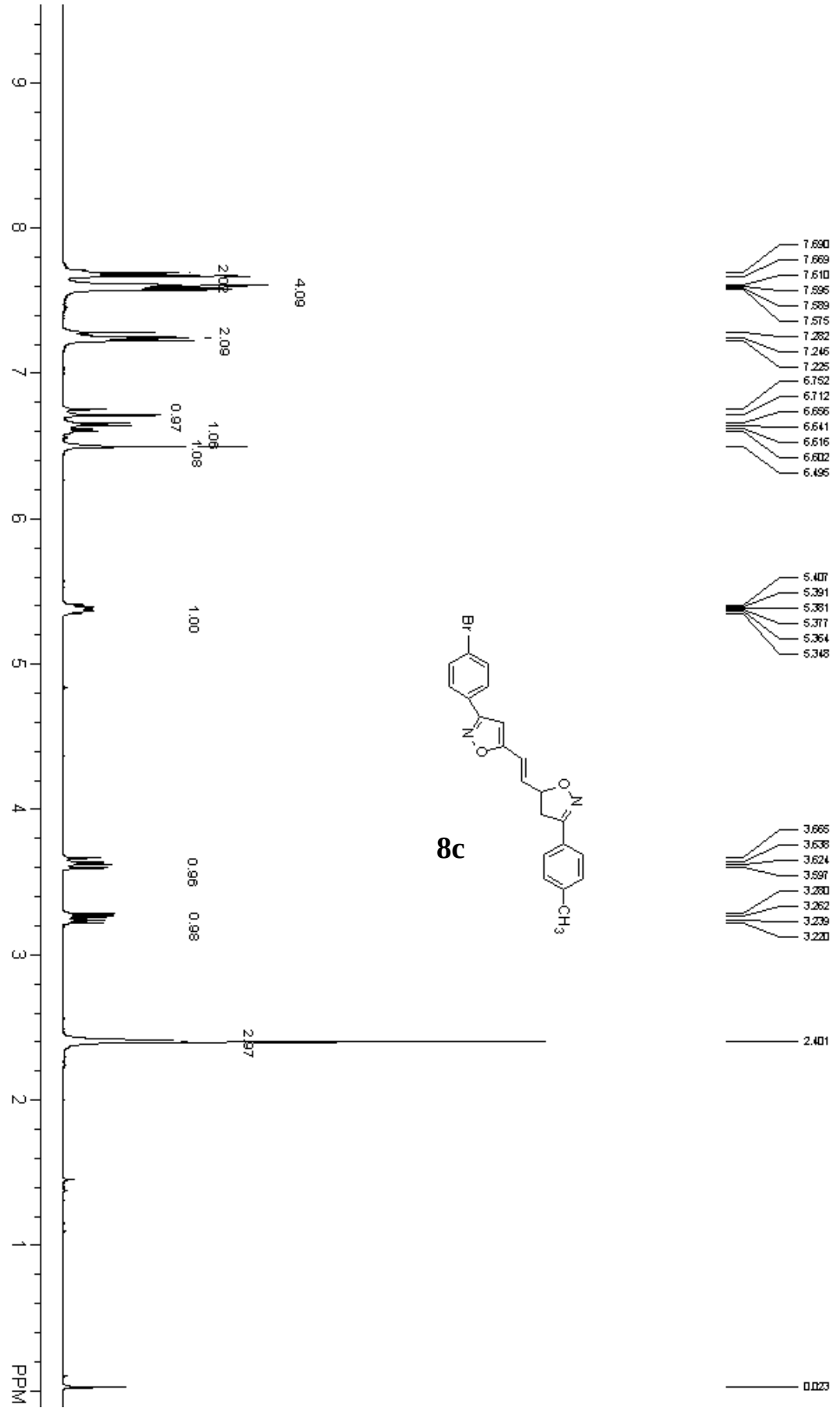
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5.391
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5.364
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3.624
3.597
3.280
3.262
3.239
3.220
2.401
0.023
4.09
2.09
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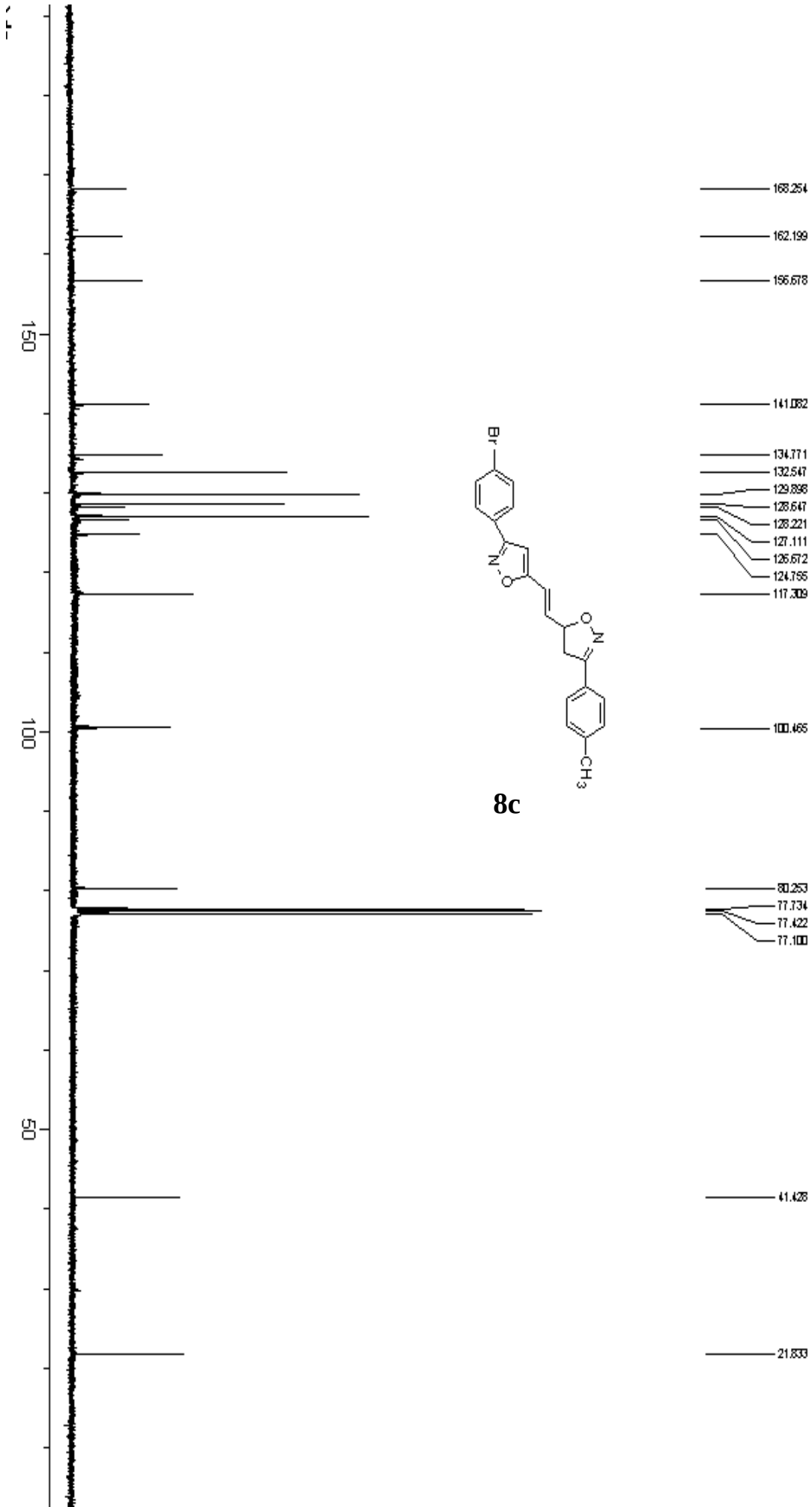
N
CH3
8c
PPM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124.755
117.309
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77.100
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100
50
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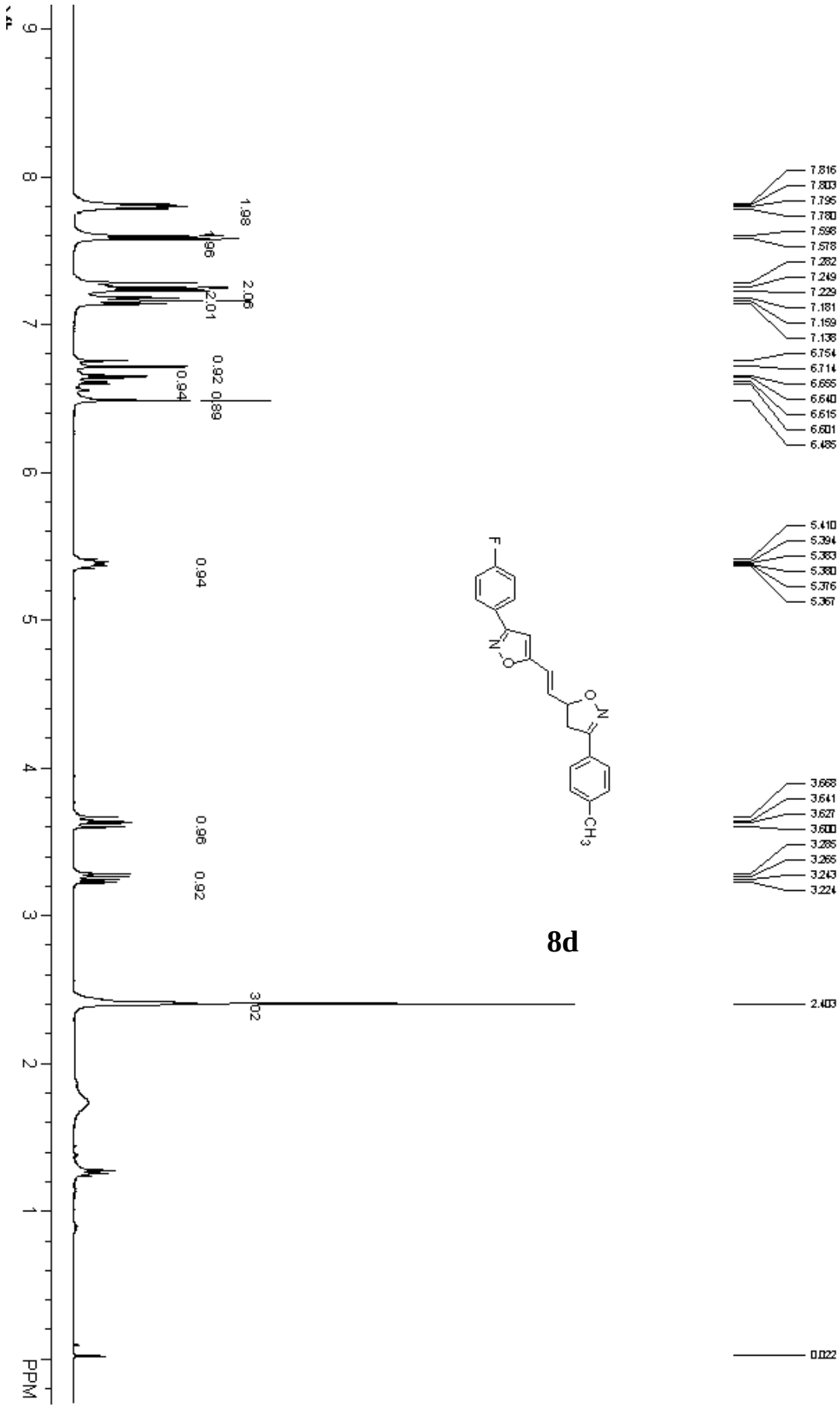
N
CH3

8c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3.285
3.265
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3.224
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1.98
1.96
2.06
2.01
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0.92
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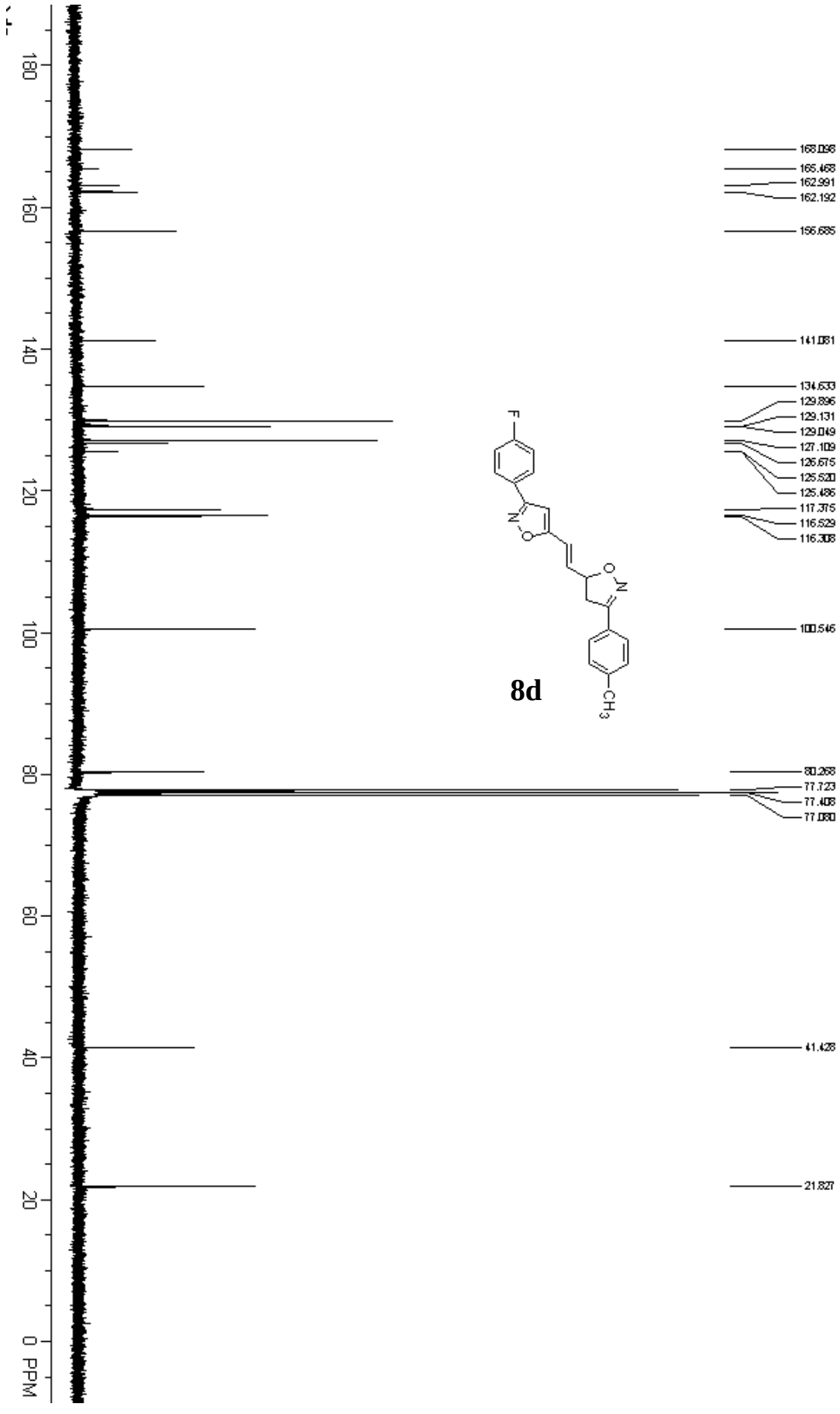
CH3
PPM

8d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116.529
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77.723
77.408
77.080
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120
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O
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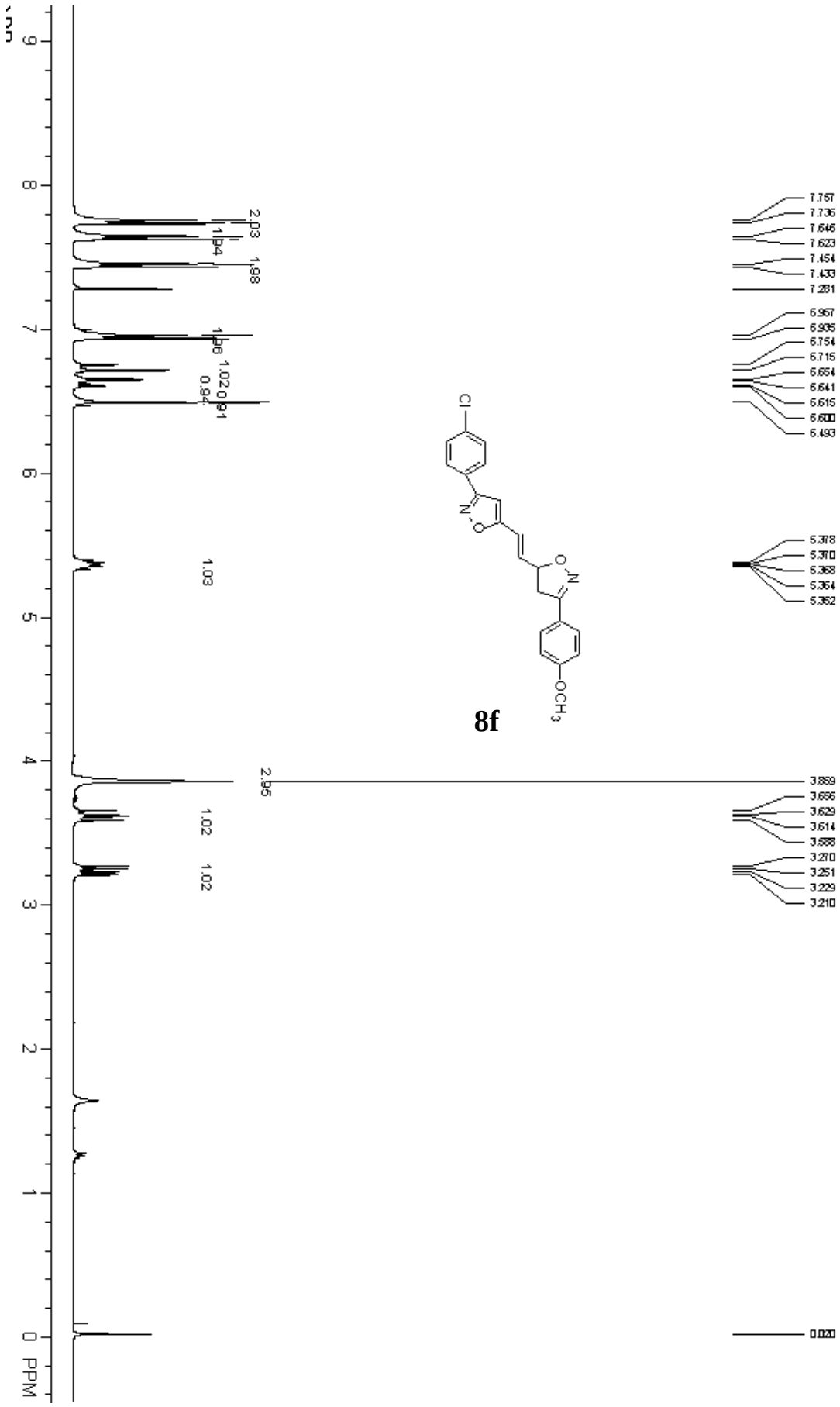
CH3

8d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3.629
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3.270
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3.229
3.210
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1.98
1.96
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2.95
1.02
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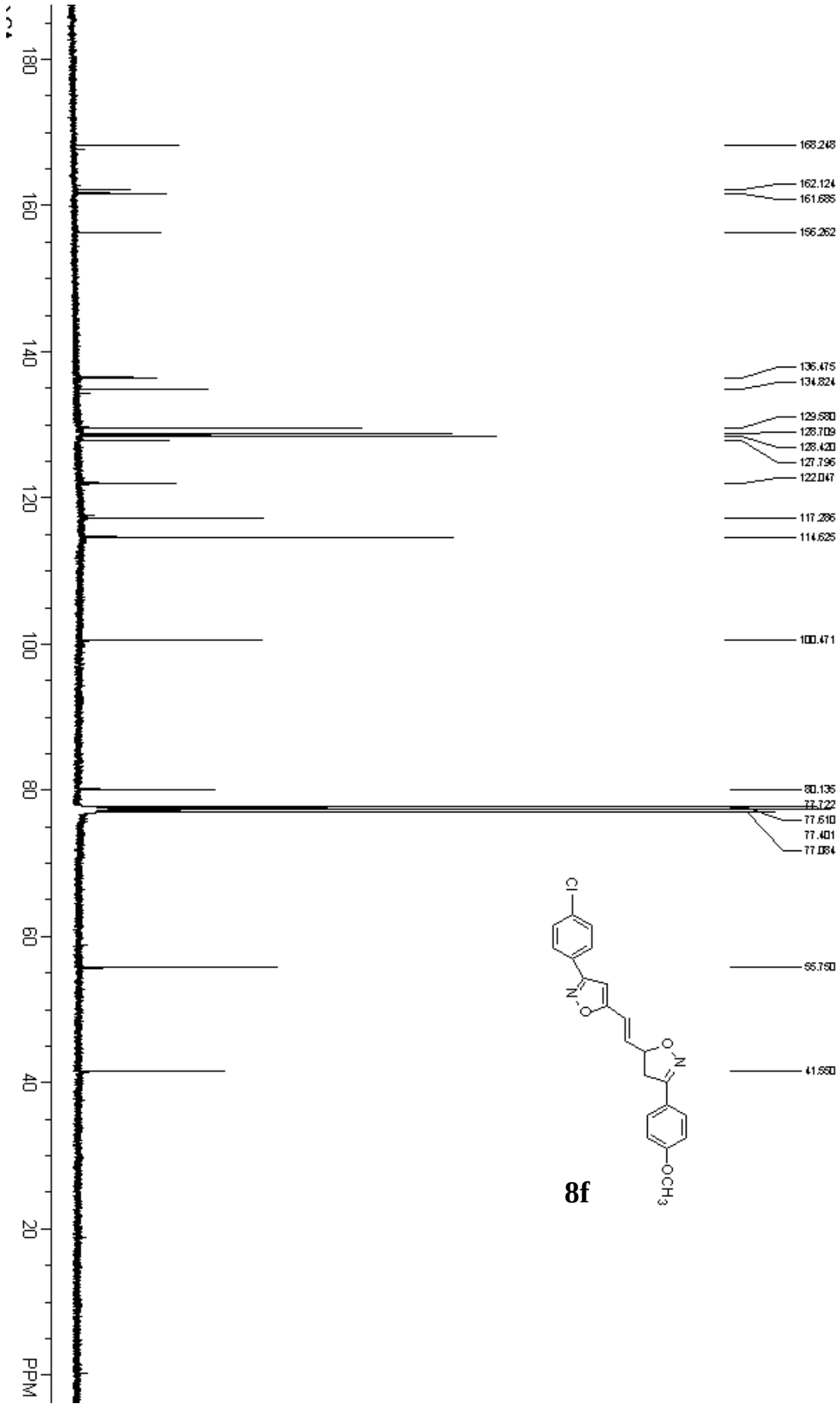
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OCH3
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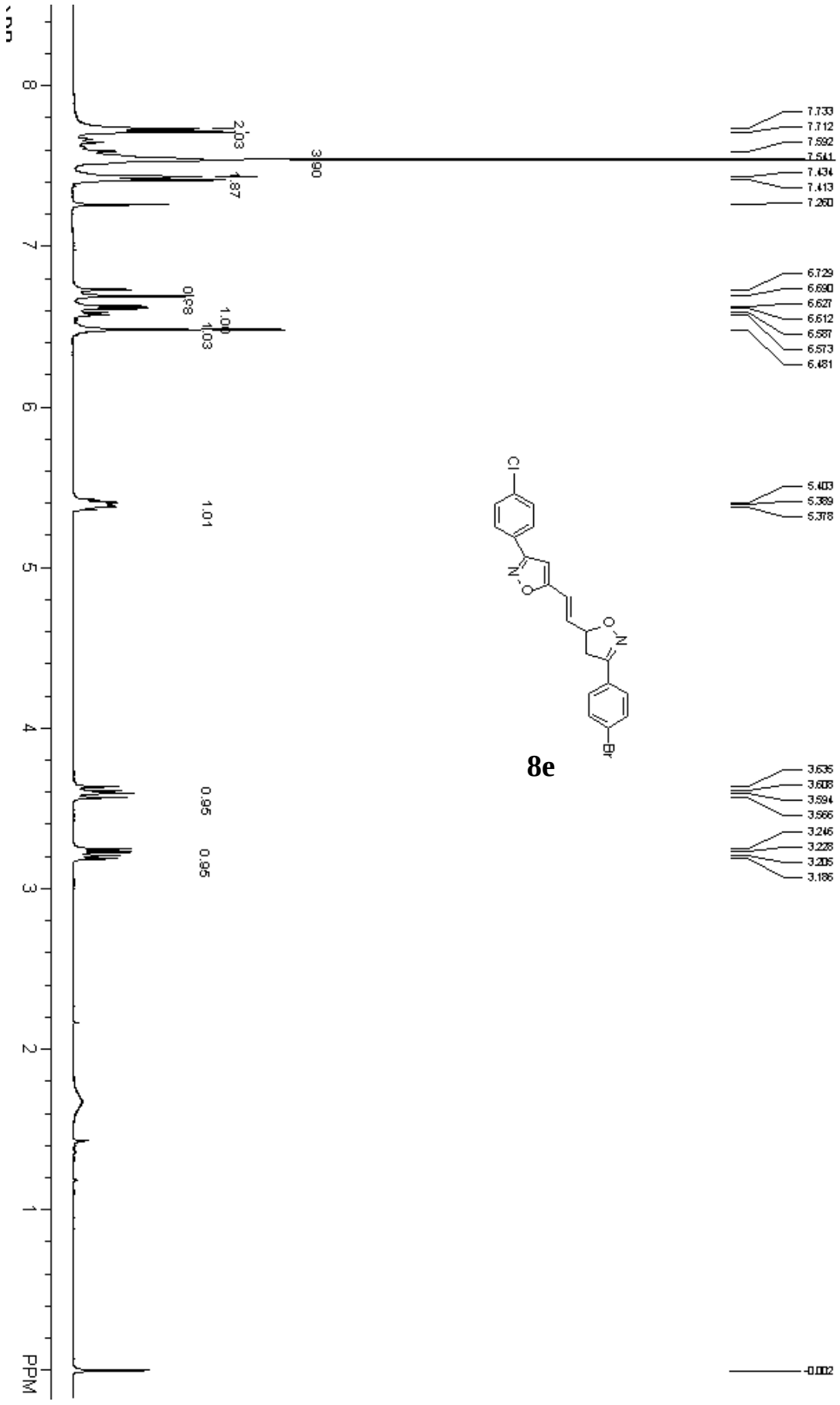
8f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6.729
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6.627
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6.573
6.481
5.403
5.389
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3.608
3.594
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3.246
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3.205
3.186
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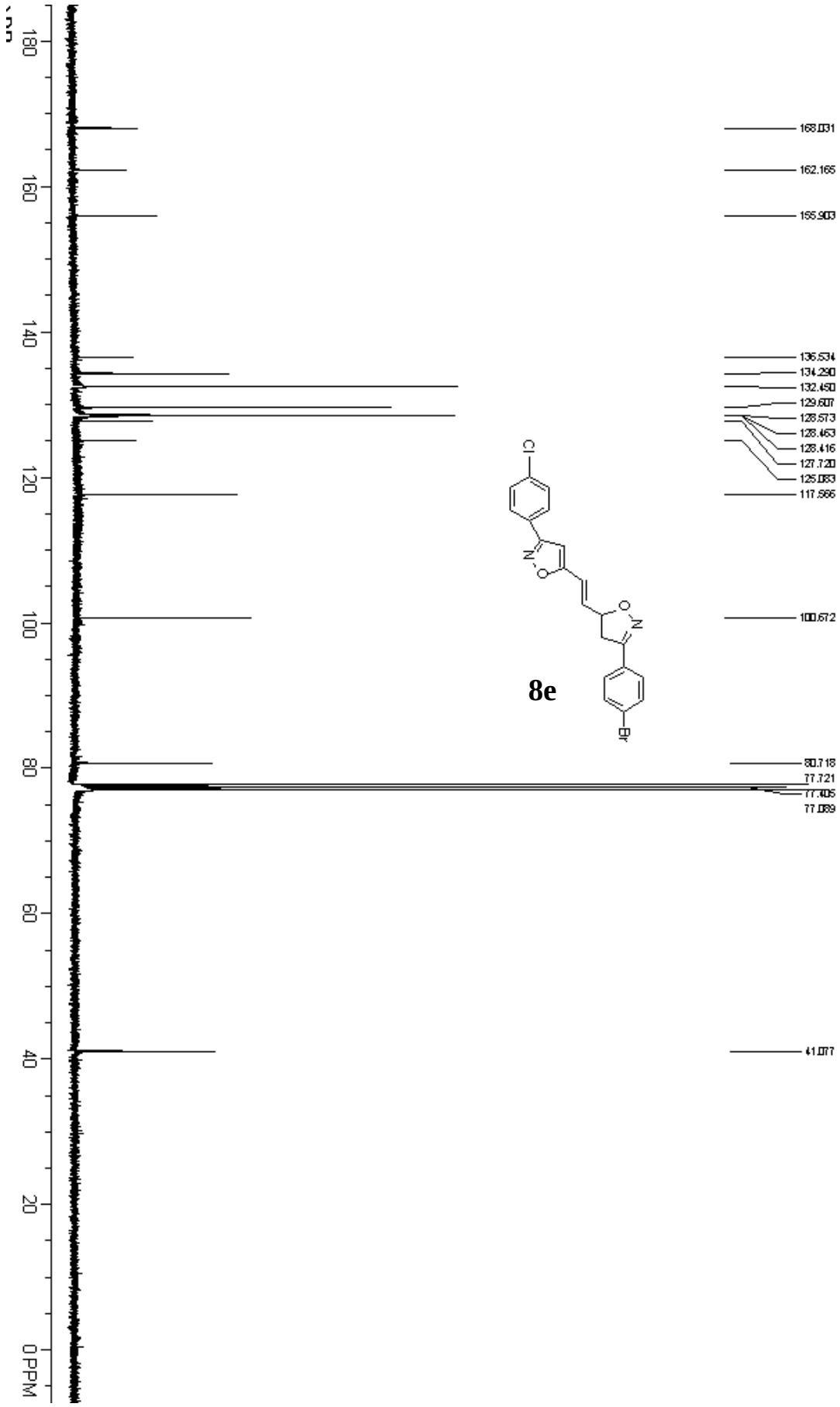
N
O
Br
PPM

8e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77.405
77.089
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80
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40
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Br

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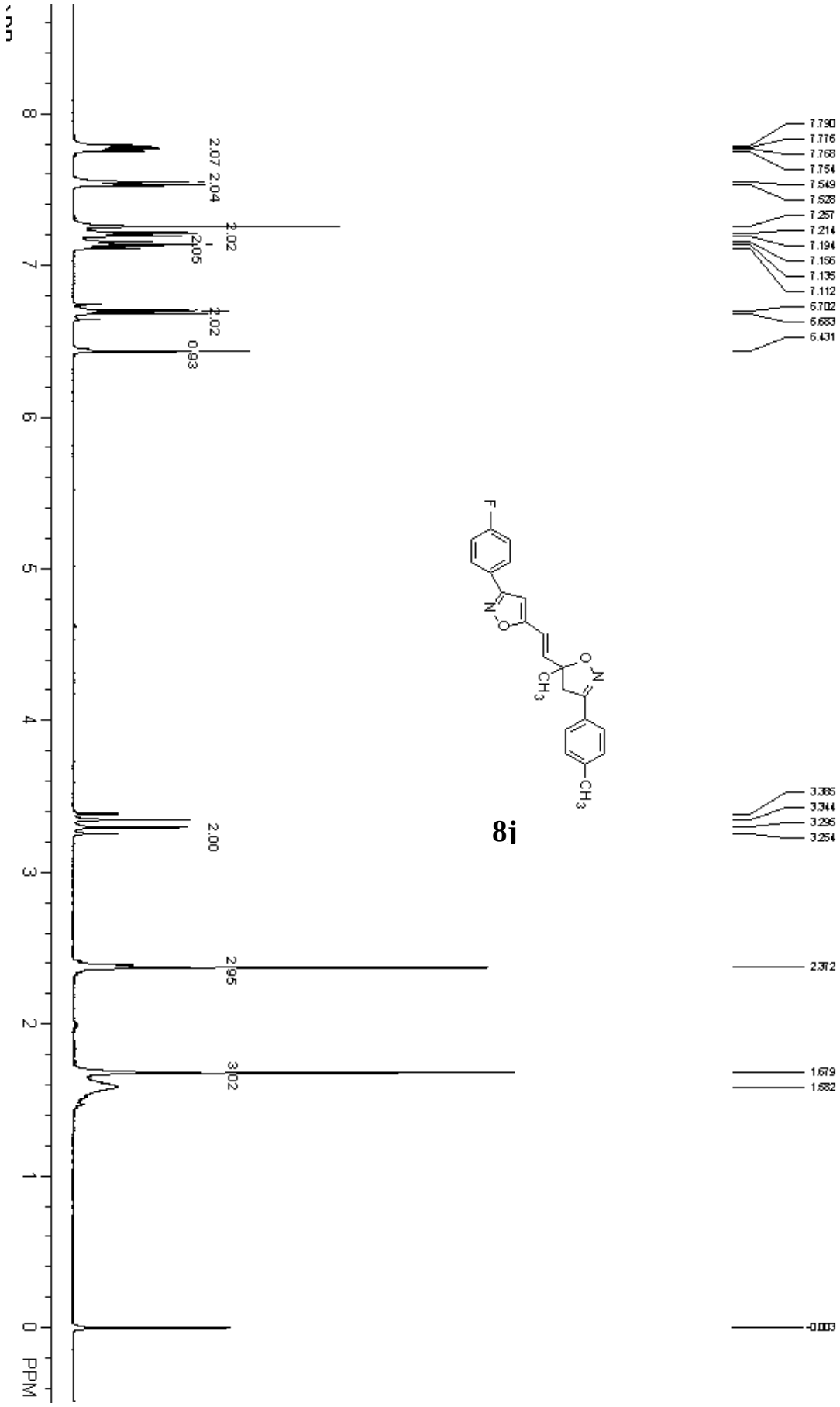
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1.679
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2.04
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3.02
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F
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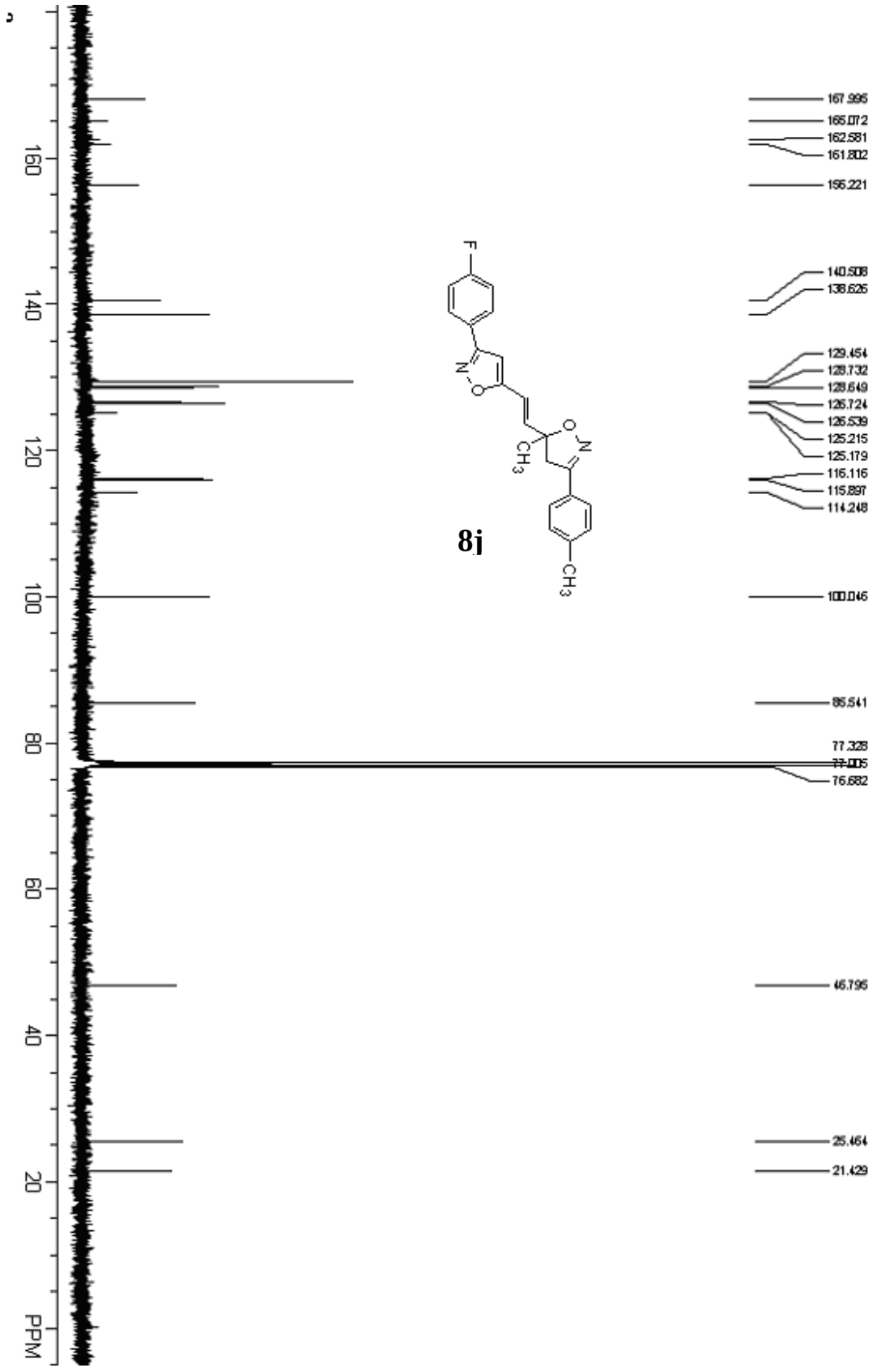
N
CH3
CH3

8j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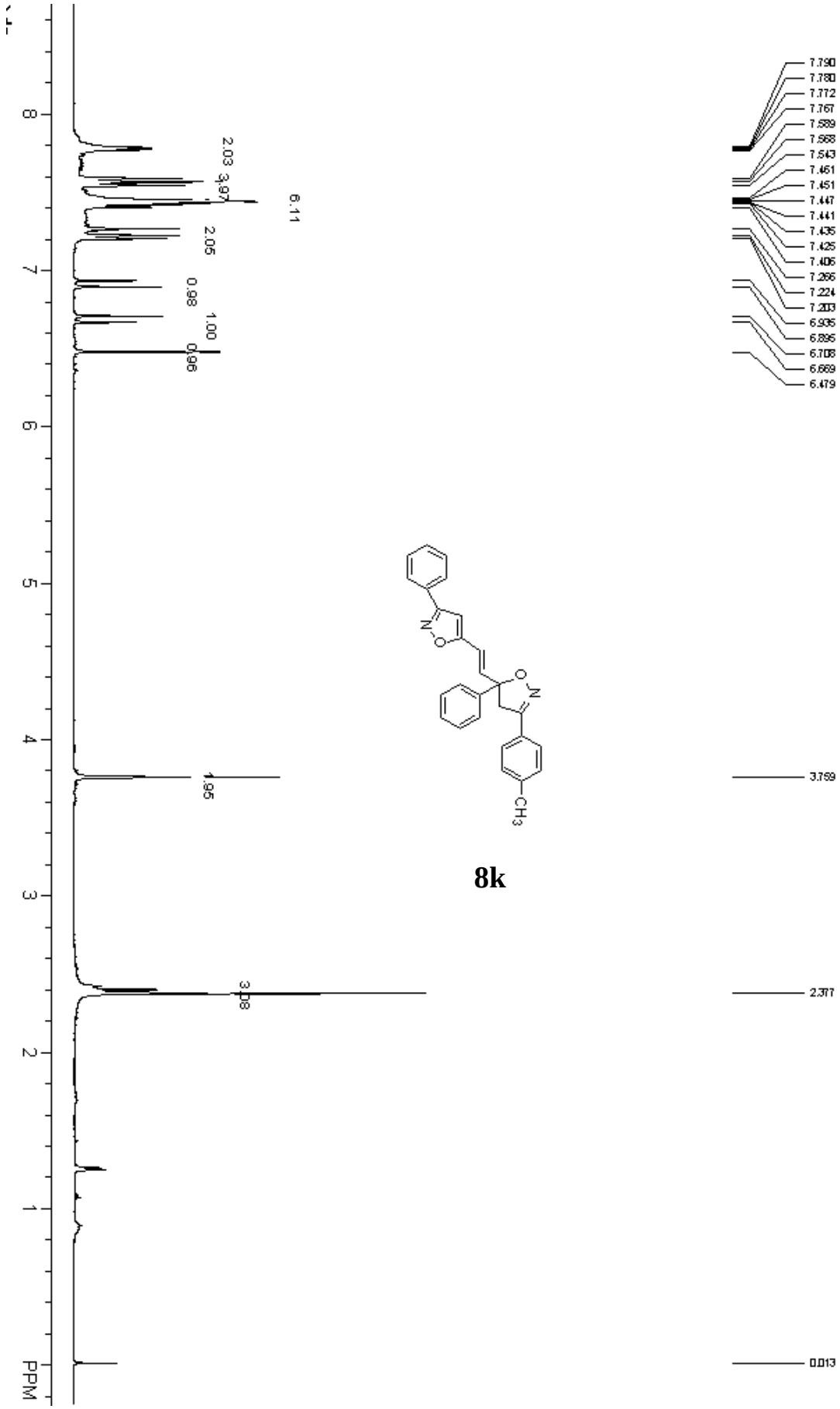
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7.266
7.224
7.203
6.935
6.896
6.708
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6.479
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2.377
0.013
2.03
3.97
6.11
2.05
0.98
1.00
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PPM
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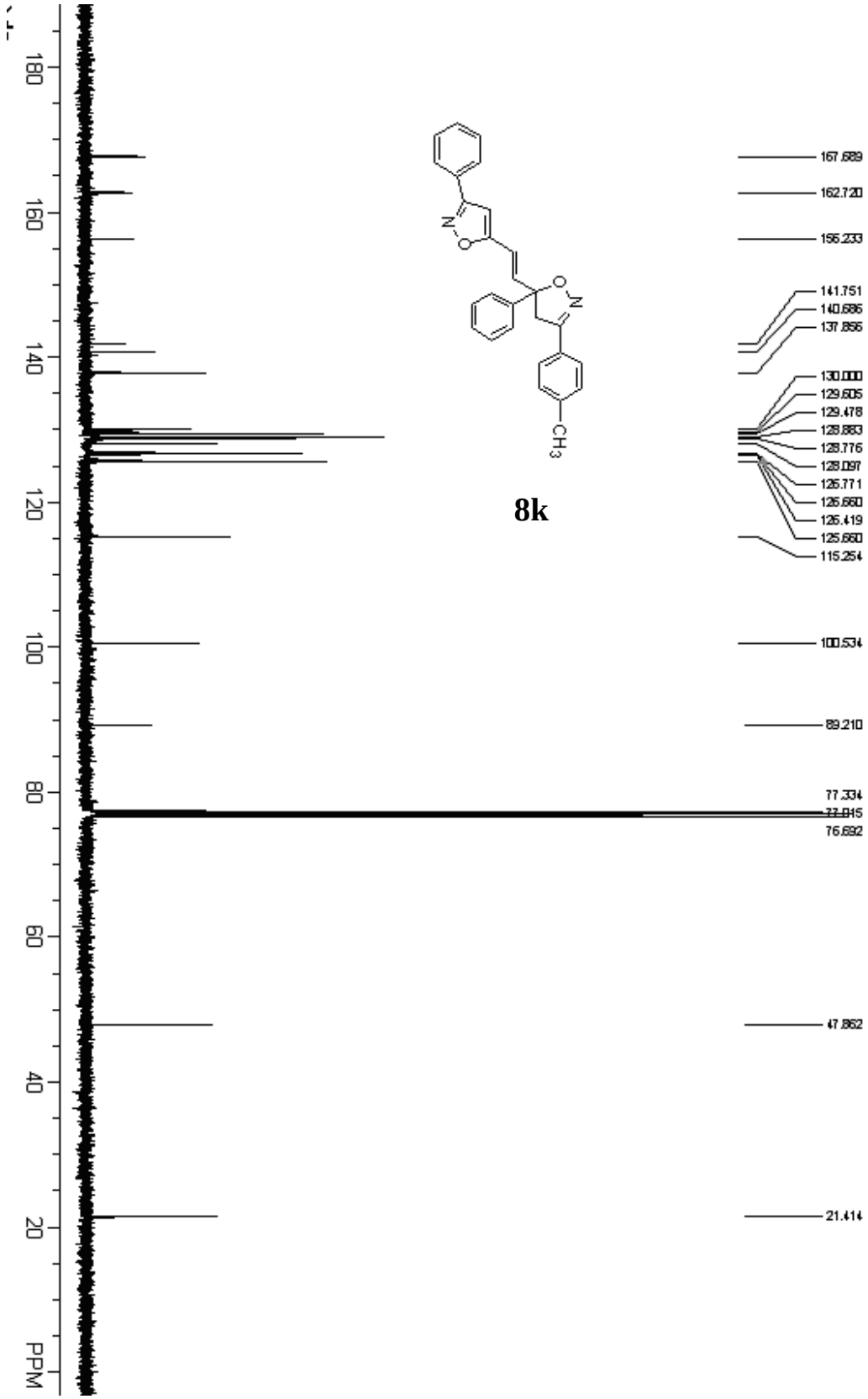
N
CH3

8k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126.660
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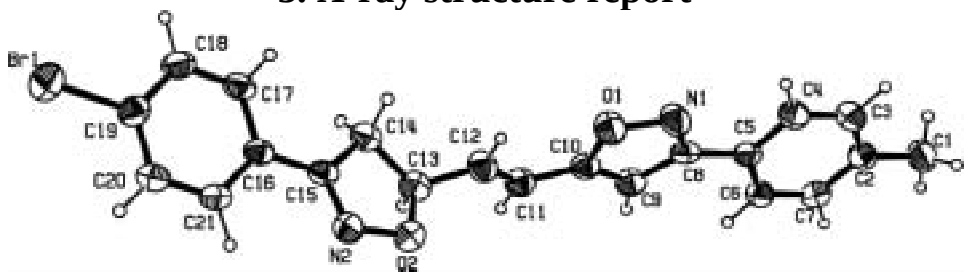
PPM

8k

3. X-ray structure report



Crystal Data

Empirical Formula	$C_{21}H_{17}N_2BrO_2$
Formula Weight	409.28
Crystal Color, Habit	yellow, platelet
Crystal Dimensions	0.45 X 0.25 X 0.16 mm
Crystal System	monoclinic
Lattice Type	Primitive
Detector Position	127.40 mm
Pixel Size	0.100 mm
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.476 g/cm^3
F_{000}	832.00
Diffractometer	Rigaku RAXIS-RAPID