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Convenient preparation of arylnitromethanes by oxidation of benzaldoximes with urea hydrogen peroxide

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Experimental details.

Materials and Methods. Melting points were measured using a Boetius melting point apparatus and were uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker DRX-500 instrument [working frequencies of 500.13 MHz (^{1}H) and of 125.76 MHz (^{13}C), respectively] and Bruker AVANCE-II [working frequencies of 300.13 MHz (^{1}H), and of 75.47 MHz (^{13}C), respectively]. Chemical shifs are reported in parts per million (ppm) and referenced to the appropriate NMR solvent peaks. Spin–spin coupling constants (*J*) were reported in Hertz (Hz). NMR spectra were prepared using an original software designed at N. D. Zelinsky Institute of Organic Chemistry RAS (Moscow, Russian Federation). Low resolution mass-spectra (m/z) were recorded on a Finnigan MAT/INCOS 50 mass spectrometer at 70 eV using direct probe injection. High resolution mass spectra (HRMS) were measured on a Bruker maXis and micrOTOF II instruments using electrospray ionization (ESI). Elemental analysis was performed on the automated Perkin-Elmer2400 CHN microanalyzer. IR spectra have been measured by Bruker AlphaT instrument. Thin layer chromatography (TLC) analysis was performed using Merck 60 F_{254} plates. Flash chromatography was accomplished using Silica (Acros, 0.035– 0.070 mm, 60 Å). All solvents and reagents were purified according to standard procedures.

General procedure for preparation of oximes

A. Hydroxylamine hydrochloride (0.23 mol) was added portionwise to a stirred solution of sodium hydroxide (0.38 mol) in water (75 ml). Then corresponding aldehyde (0.15 mol) was added dropwise for 10 min and left for 1.5 h. The reaction mixture was acidified with HCl aq until pH=7. The product was extracted with ethyl acetate (3×30 ml), the extracts were combined, dried with $MgSO_4$, and the volatiles were removed *in vacuo* to afford the corresponding oximes of benzaldehydes.

B. Corresponding aldehyde (15 mmol) was added portionwise to a suspension of $(NH_2OH)_2 \times H_2SO_4$ (22.5 mmol) in water (15 ml) at 45 °C. If required, methanol (2 - 5 ml) was added for better dissolution. The reaction mixture was stirred at 45 °C for 2 h and then heated once to achieve transparency (TLC control). The reaction mixture was poured into a saturated solution of $NaHCO_3$, the water layer was extracted with ethyl acetate (2×25 ml), the extracts were combined, dried with $MgSO_4$, the solvents were removed *in vacuo* to afford the corresponding oximes of benzaldehydes.

C. A mixture of aq. HCl (3.67 ml) and *E*-oxime (**1d** or **1f**) (6.62 mmol) was heated stirred under heating until dissolving, then left for 30 min at room temperature and filtrated. The precipitate was washed with hexane and put into a saturated $NaHCO_3$ solution. Neutralization (pH=7) was performed by the addition of aq. HCl, then the product was filtrated and dried to give the corresponding *Z*-oxime.

(E)-Benzaldehyde oxime (*E*-**1a**). Yellowish solid (method A, 91%; method B, 99%) Mp 25 °C; (lit[S1] 32–33 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.24 (s, 1H, OH), 8.15 (s, 1H, CH=N), 7.60 (d, *J* = 7.5 Hz, 2H, H-2,6, Ph), 7.49 – 7.34 (m, 3H, H-3,4,5, Ph).

(E)-4-Bromobenzaldehyde oxime (*E*-**1b**). White crystals (method A, 92%) Mp 110–112 °C, (lit[S2] 113–114 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.36 (s, 1H, OH), 8.14 (s, 1H, CH=N), 7.60 (d, *J* = 8.6 Hz, 2H, H-2,6), 7.54 (d, *J* = 8.6 Hz, 2H, H-3,5).

(E)-3-Nitrobenzaldehyde oxime (*E*-**1c**). White crystals (method A, 86%) Mp 117–118 °C, (lit[S3] 120–122 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.65 (s, 1H, OH), 8.42 (t, *J* = 2.0 Hz, 1H, H-2), 8.33 (s, 1H, CH=N), 8.22 (ddd, *J* = 8.2, 2.4, 1.0 Hz, 1H, H-4), 8.05 (dt, *J* = 7.8, 1.3 Hz, 1H, H-6), 7.70 (t, *J* = 8.0 Hz, 1H, H-5).

(E)-4-Nitrobenzaldehyde oxime (*E*-**1d**). White crystals (method A, 84%) Mp 123–125 °C; (lit[S3] 126–128 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.86 (s, 1H, OH), 8.30 (s, 1H, CH=N), 8.25 (d, *J* = 8.8 Hz, 2H, H-2,6), 7.85 (d, *J* = 8.7 Hz, 2H, H-3,5).

(Z)-4-Nitrobenzaldehyde oxime (*Z*-**1d**). White crystals (method C, 87%) Mp 178–180 °C, (lit[S4] 175–178 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.22 (br.s, 1H, OH), 8.30 (d, *J* = 8.8 Hz, 2H, H-3,5), 8.22 (d, *J* = 8.5 Hz, 2H, H-2,6), 7.66 (s, 1H, HC=N).

(E)-Nicotinaldehyde oxime (*E*-**1e**). White crystals (method A, 74%) Mp (lit[S5] 146–148 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.52 (s, 1H, OH), 8.75 (s, 1H, H-2), 8.55 (d, *J* = 4.9 Hz, 1H, H-6), 8.20 (s, 1H, HC=N), 7.98 (d, *J* = 8.0 Hz, 1H, H-4), 7.45 – 7.40 (dd, *J* = 7.9, 4.9 Hz, 1H, H-5).

(E)-4-Methoxybenzaldehyde oxime (*E*-**1f**). Yellowish crystals (method A, 91%) Mp 63–64 °C; (lit[S3] 63–64 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.95 (s, 1H, OH), 8.06 (s, 1H, HC=N), 7.52 (d, *J* = 8.5 Hz, 2H, H-2,6), 6.96 (d, *J* = 8.7 Hz, 2H, H-3,5), 3.77 (s, 3H, OCH_3).

(Z)-4-Methoxybenzaldehyde oxime (*Z*-**1f**). White crystals (method C, 81%) Mp 127–129 °C; (lit[S4] 128–133 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.37 (br.s, 1H, OH), 7.94 (d, *J* = 8.8 Hz, 2H, H-2,6), 7.31 (s, 1H, HC=N), 6.98 (d, *J* = 8.6 Hz, 2H, H-3,5), 3.79 (s, 3H, OCH_3).

(E)-4-Ethoxybenzaldehyde oxime (*E*-**1g**). Yellow crystals (method A, 87%) Mp 83–86 °C (lit[S6] 72–74 °C), ^{1}H NMR (300.13 MHz, DMSO-d_6) δ 10.94 (1H, s, N-OH), 8.05 (1H, s, HC=N), 7.50 (2H, d, *J* = 8.7 Hz, H-2,6), 6.92 (2H, d, *J* = 8.7 Hz, H-3,5), 4.03 (2H, q, *J* = 6.9 Hz, CH_2), 1.32 (3H, t, *J* = 7.0 Hz, CH_3); ^{13}C NMR (150.9 MHz, $CDCl_3$) δ 161.3, 150.7, 129.3 (2C), 124.9, 115.5 (2C), 65, 15.

(E)-3,4-Dimethoxybenzaldehyde oxime (*E*-**1h**). Pale yellow crystals (method A, 92%) Mp 85–86 °C; (lit[S7] 94–95 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.95 (s, 1H, OH), 8.06 (s, 1H, CH=N), 7.21 (d, *J* = 1.8 Hz, 1H, H-2), 7.10 (dd, *J* = 8.0, 1.7 Hz, 1H, H-6), 6.98 (d, *J* = 8.3 Hz, 1H, H-5), 3.78 (s, 6H, OMe).

(E)-3,4,5-Trimethoxybenzaldehyde oxime (*E*-**1i**). White crystals (method B, 3.33g, 99%) Mp 90–92 °C; (lit[S8] 94–95 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.11 (s, 1H, OH), 8.05 (s, 1H, CH=N), 6.91 (s, 2H, H-2,6), 3.78 (s, 6H, OMe), 3.67 (s, 3H, OMe).

(E)-2,5-Dimethoxy-3,4-methylenedioxybenzaldehyde oxime (*E*-**1j**). White crystals (method B, 3.04g, 90%) Mp 157–158 °C; (lit[S9] 157–158 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.13 (s, 1H, OH), 8.13 (s, 1H, CH=N), 6.90 (s, 1H, H-6), 6.05 (s, 2H, CH_2), 3.83 (s, 3H, OMe), 3.78 (s, 3H, OMe).

(E)-4-Hydroxybenzaldehyde oxime (*E*-**1k**). Off-white crystals (method A, 1,73g, 84%) Mp 106–110 °C; (lit[S3] 93–95 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.80 (br.s, 1H, OH), 8.00 (s, 1H, CH=N), 7.40 (d, 2H, H-3,5), 6.78 (d, 2H, H-2,6).

(E)-4-Methoxy-3-nitrobenzaldehyde oxime (*E*-**1l**). Yellowish crystals (method A, 94%) Mp 160–163 °C, (lit[S10] 166 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.34 (s, 1H, OH), 8.16 (s, 1H, CH=N), 8.06 (d, *J* = 2.2 Hz, 1H, H-2), 7.87 (dd, *J* = 8.8, 2.2 Hz, 1H, H-6), 7.40 (d, *J* = 8.8 Hz, 1H, H-5), 3.94 (s, 3H, OMe).

General procedure for preparation of arylnitromethanes

A. *Oxidation with sodium perborate*. A corresponding oxime (60 mmol) was dissolved in glacial acetic acid (300 ml), and powdered sodium perborate (360 mmol) was added for 30 min under stirring at 60 °C. The reaction mixture was stirred at 60 °C for 6 h then left overnight at room temperature. The resulting suspension was poured into distilled water

(400 ml), extracted with dichloromethane (3×45 ml), the combined organic layers were washed with 1 N NaOH (aq., ~2×45 ml) until pH=8-9 (usually accompanied by color-changing), and then washed with water until pH=7. Crystals of the corresponding benzoic acid were filtered off (if needed), the solution was dried with $MgSO_4$, the solvent was removed *in vacuo* to afford arylnitromethanes. Further purification was performed by column chromatography (benzene-benzene/ethyl acetate 10:1) if required.

B. *Oxidation with urea hydrogen peroxide - boric acid complex (UHP-$B(OH)_3$).* Boric acid (310 mmol) was dissolved in glacial acetic acid (150 ml) when heated up to 100–110 °C, then the mixture was cooled to 60 °C. The corresponding oxime (62 mmol) was dissolved in the prepared suspension,. Powdered UHP (372 mmol) was added portionwise at 60 °C for 40 min. The reaction mixture was stirred at 60 °C for 6 h, then left overnight at room temperature. Work up was the same as described above for the procedure of oxidation with sodium perborate.

(Nitromethyl)benzene (**2a**). Yelowish oil[S11], (method A 46%; method B 8 h, 66%) ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.51-7.43 (m, 5H, Ph), 5.74 (s, 2H, CH_2); ^{13}C NMR (125.76 MHz, DMSO-d_6) δ 130.6, 130.4 (2C), 129.5, 128.8 (2C), 79.2.

1-Bromo-4-(nitromethyl)benzene (**2b**). Yellowish crystals (method A 43%; method B 10 h, 55%) Mp 46 °C, (lit[S12] 46 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.66 (d, J = 8.2 Hz, 2H, H-3,5), 7.47 (d, J = 8.2 Hz, 2H, H-2,6), 5.75 (s, 2H, CH_2); ^{13}C NMR (125.76 MHz, DMSO-d_6) δ 132.8 (2C), 131.8 (2C), 129.8, 123.1, 78.1.

1-Nitro-3-(nitromethyl)benzene (**2c**). Yellowish crystals (method A 40%, 7 h, 6%; method B with further column chromatography (benzene-benzene/ethyl acetate 10:1, 29%) Mp 95–99 °C, (lit[S13] 94–95 °C); ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.46 (t, J = 2.0 Hz, 1H, H-2), 8.31 (dd, J = 7.8, 1.6 Hz, 1H, H-6), 7.98 (dt, J = 7.7, 2.0 Hz, 1H, H-4), 7.77 (t, J = 7.8 Hz, 1H, H-5), 5.95 (s, 2H, CH_2).

1-Nitro-4-(nitromethyl)benzene (**2d**). White crystals (method A 16%; method B 26%) Mp 90–92 °C; (lit[S13] 90–91 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, J = 8.3 Hz, 2H, H-2,6), 7.67 (d, J = 8.3 Hz, 2H, H-3,5), 5.56 (s, 2H, CH_2); ^{13}C NMR (125.76 MHz, $CDCl_3$) δ 148.9, 135.7 , 131.1 (2C), 124.3 (2C), 78.7 ; υ_{max} (KBr) 1561, 1540, 1350, 826, 722.

1-Methoxy-4-(nitromethyl)benzene (**2f**). Yellow oil (method A 55°C, 9 h, 43%; method B 35%) ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.44 (d, J = 8.7 Hz, 2H, H-3,5), 6.99 (d, J = 8.7 Hz, 2H, H-2,6), 5.65 (s, 2H, CH_2), 3.78 (s, 3H, OMe); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.2, 132.0, 122.7, 114.1, 78.7, 55.2; υ_{max} (KBr) 1612; 1551; 1514; 1373; 1252; 1179; 1030; 827.

1-Ethoxy-4-(nitromethyl)benzene (**2g**). Yellowish crystals (method A 50°C, 39%; method B 50°C, 13%) Mp 44–46 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.36 (d, J = 7.8 Hz, 2H, H-3,5), 6.92 (d, J = 7.8 Hz, 2H, H-2,6), 5.36 (s, 2H, CH_2), 4.04 (q, 2H, J = 6.6 Hz, CH_2), 1.42 (t, J = 6.8 Hz 3H, CH_3); ^{13}C NMR (125.76 MHz, DMSO-d_6) δ 160.3, 131.6 (2C), 121.8, 114.9 (2C), 79.6, 63.6, 14.8.

1,2-Dimethoxy-4-(nitromethyl)benzene (**2h**). Yellowish crystals (method B 55°C, 9 h, 17%) Mp 72–75 °C; (lit[S14] 66–67 °C); ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.11 (s, 1H, H-3), 7.05 (d, J = 8.2 Hz, 1H, H-5), 7.00 (d, J = 8.2 Hz, 1H, H-6), 5.63 (s, 2H, CH_2), 3.78 (s, 3H, OMe), 3.77 (s, 3H, OMe); ^{13}C NMR (126 MHz, DMSO-d_6) δ 149.8, 148.7, 126.5, 123.4, 113.9, 111.6, 79.1, 55.6, 55.2.

1,2,3-Trimethoxy-5-(nitromethyl)benzene (**2i**). Yellowish crystals (method B 55°C, 9 h**,** further purification by column chromatography (benzene-benzene/ethyl acetate 10:1), 2%) Mp 83–85 °C; ^{1}H NMR (500 MHz, $CDCl_3$-d) δ 6.67 (s, H-4,6), 5.37 (s, 2H, CH_2), 3.88 (s, 6H, OMe), 3.86 (s, 3H, OMe); ^{13}C NMR (125.76 MHz, $CDCl_3$) δ 153.5 (2C), 139.4, 125.0, 107.1 (2C), 80.3, 60.8, 56.2 (2C); υ_{max} (KBr) 1598, 1548, 1462, 1253, 1122, 1007; HRMS (ESI/QTOF) m/z: $[M+H -HNO_2]^+$ Calcd for $C_{10}H_{13}O_3$ 181.0859; Found 181.0861.

4,7-Dimethoxy-5-(nitromethyl)benzo[d][1,3]dioxole (**2j**). Yellowish crystals (method B 55°C, 9 h, further purification by column chromatography (benzene-benzene/ethyl acetate 10:1), 5%) Mp 82–83 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.78 (s, 1H, H-6), 6.07 (s, 2H, OCH_2O), 5.58 (s, 2H, CH_2), 3.82 (s, 3H, OMe), 3.79 (s, 3H, OMe); ^{13}C NMR (126 MHz, DMSO-d_6) δ 138.5, 138.1, 137.9, 137.0, 115.8, 111.4, 102.2, 74.4, 59.7, 56.7; υ_{max} (KBr) 1548, 1461, 1257, 1148, 1072, 1053; HRMS (ESI/QTOF) m/z: $[M+H -HNO_2]^+$ Calcd for $C_{10}H_{11}O_4$ 195.0652; Found 195.0660.

1-Methoxy-2-nitro-4-(nitromethyl)benzene (**2l**). Yellow crystals (method A 60°C, 10 h, 10%; method B 41%) Mp 79–81 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (d, J = 2.2 Hz, 1H, H-3), 7.82 (dd, J = 8.7, 2.3 Hz, 1H, H-5), 7.45 (d, J = 8.7 Hz, 1H, H-6), 5.78 (s, 2H, CH_2), 3.96 (s, 3H, OMe); ^{13}C NMR (125.76 MHz, DMSO-d_6) δ 152.8, 138.9, 137.2, 127.5, 122.7, 114.7, 77.0,

56.9; υ_{max} (KBr) 1624, 1549, 1533, 1359, 1284, 1018; HRMS (ESI/QTOF) m/z: $[M+NH_4]^+$ Calcd for $C_8H_{12}N_3O_5$ 230.0771; Found 230.0777; $[M+Na]^+$ Calcd for $C_8H_8N_2O_5Na$ 235.0325; Found 235.0333.

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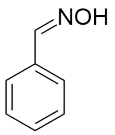

***E*-1a**

The Best Applied NMR!

NMR/29210166

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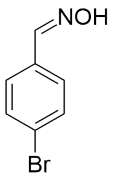

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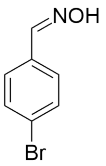

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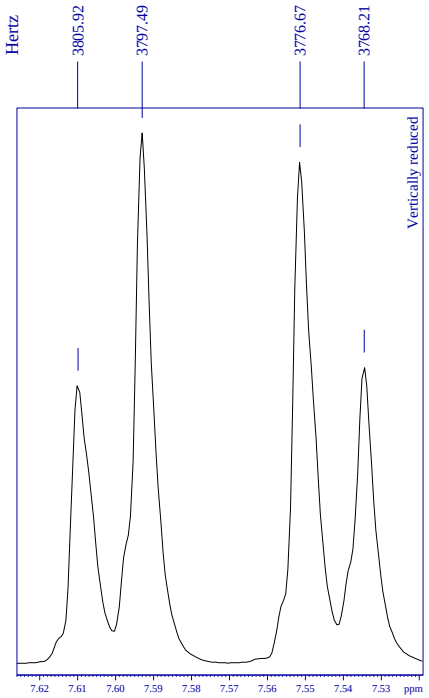

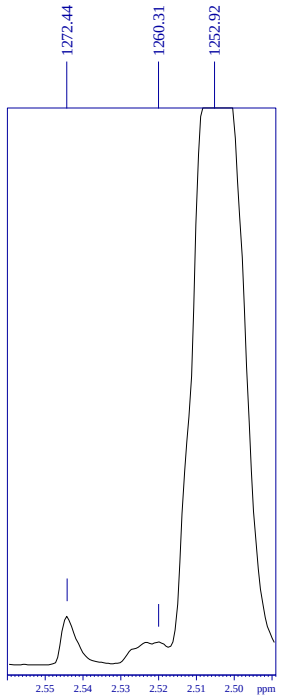

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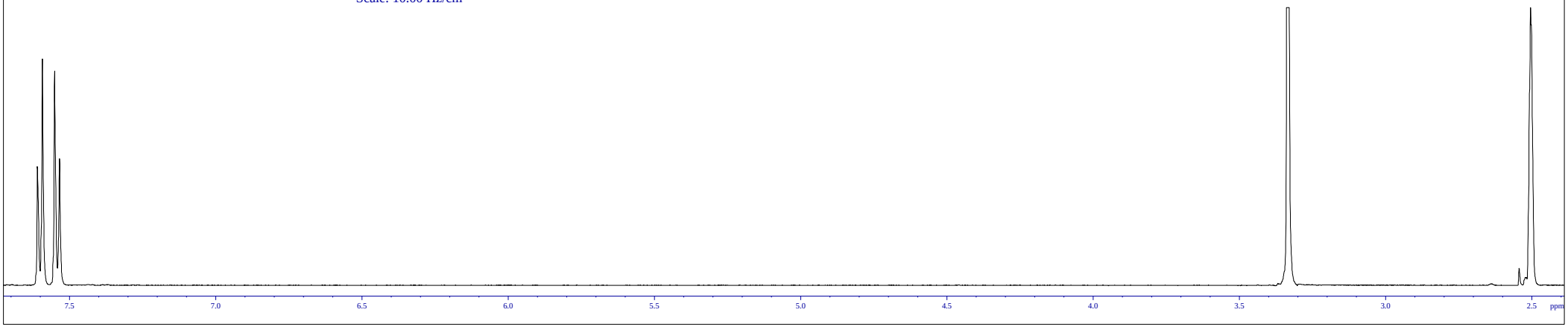

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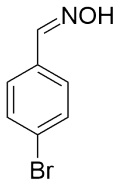

***E*-1b**

Peaks List

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2	16150.2	4069.014	8.1359	7.92
3	17012.3	3805.919	7.6099	4.49
4	17039.9	3797.492	7.5930	8.54
5	17108.1	3776.668	7.5514	8.08
6	17135.9	3768.208	7.5345	4.77
7	24016.1	1668.512	3.3362	85.76
8	25314.0	1272.436	2.5442	0.63
9	25353.8	1260.309	2.5200	0.29
10	25378.0	1252.919	2.5052	10.96
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The Best Applied NMR!

NMR/29210027

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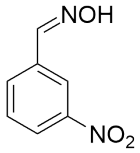

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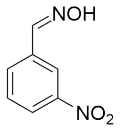

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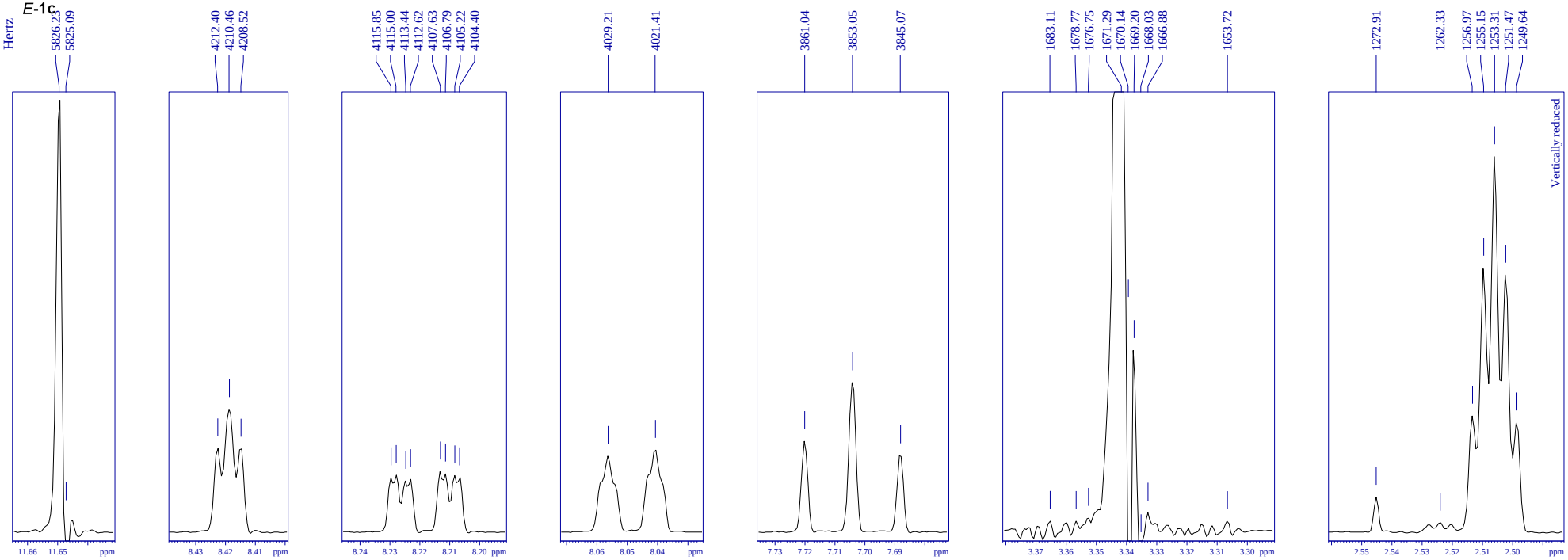

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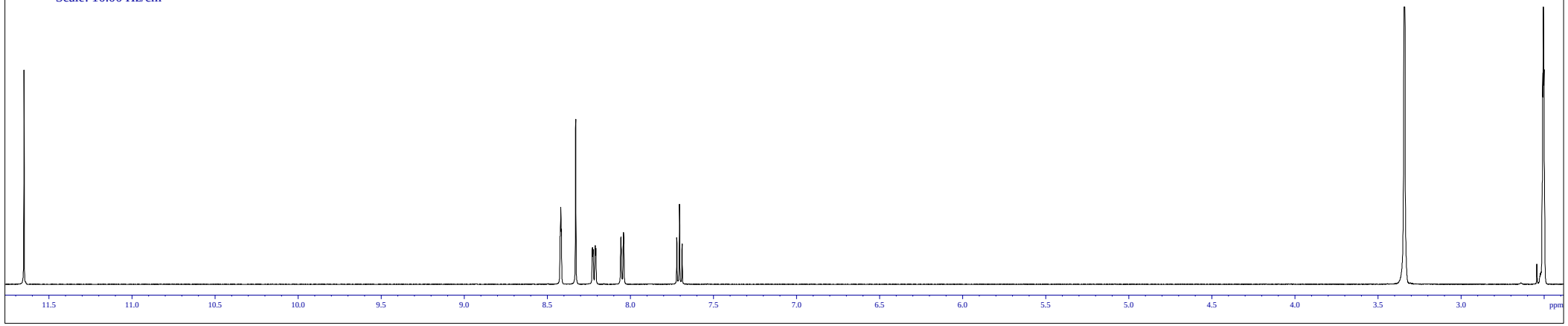
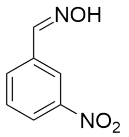


NMR/29210027



***E*-1c**

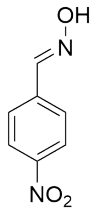
Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	10393.6	5826.235	11.6494	8.34
2	10397.3	5825.094	11.6472	−1.38
3	15681.8	4212.397	8.4226	1.56
4	15688.2	4210.457	8.4187	2.29
5	15694.5	4208.516	8.4148	1.59
6	15835.0	4165.647	8.3291	5.89
7	15998.2	4115.852	8.2296	1.02
8	16001.0	4115.003	8.2279	1.06
9	16006.1	4113.443	8.2247	0.95
10	16008.8	4112.617	8.2231	0.99
11	16025.1	4107.626	8.2131	1.13
12	16027.9	4106.786	8.2114	1.09
13	16033.0	4105.223	8.2083	1.05
14	16035.7	4104.397	8.2067	1.03
15	16282.1	4029.207	8.0563	1.41
16	16307.7	4021.407	8.0407	1.54
17	16833.2	3861.037	7.7201	1.70
18	16859.3	3853.054	7.7041	2.82
19	16885.5	3845.074	7.6881	1.47
20	23969.8	1683.106	3.3653	0.21
21	23984.0	1678.774	3.3567	0.21
22	23990.6	1676.748	3.3526	0.27
23	24008.5	1671.291	3.3417	106.34
24	24012.3	1670.136	3.3394	−13.79
25	24015.4	1669.197	3.3375	3.71
26	24019.2	1668.032	3.3352	−0.56
27	24023.0	1666.881	3.3329	0.36
28	24066.1	1653.723	3.3066	0.20
29	25313.9	1272.907	2.5452	0.87
30	25348.6	1262.325	2.5240	0.24
31	25366.1	1256.975	2.5133	2.88
32	25372.1	1255.147	2.5096	6.53
33	25378.2	1253.312	2.5060	9.29
34	25384.2	1251.473	2.5023	6.37
35	25390.2	1249.637	2.4986	2.71
36	29485.0	0.002	0.0000	3.98

The Best Applied NMR!

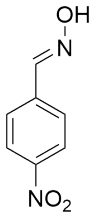
NMR/27290144

Found protons = 6 impurity* = 0.5 %

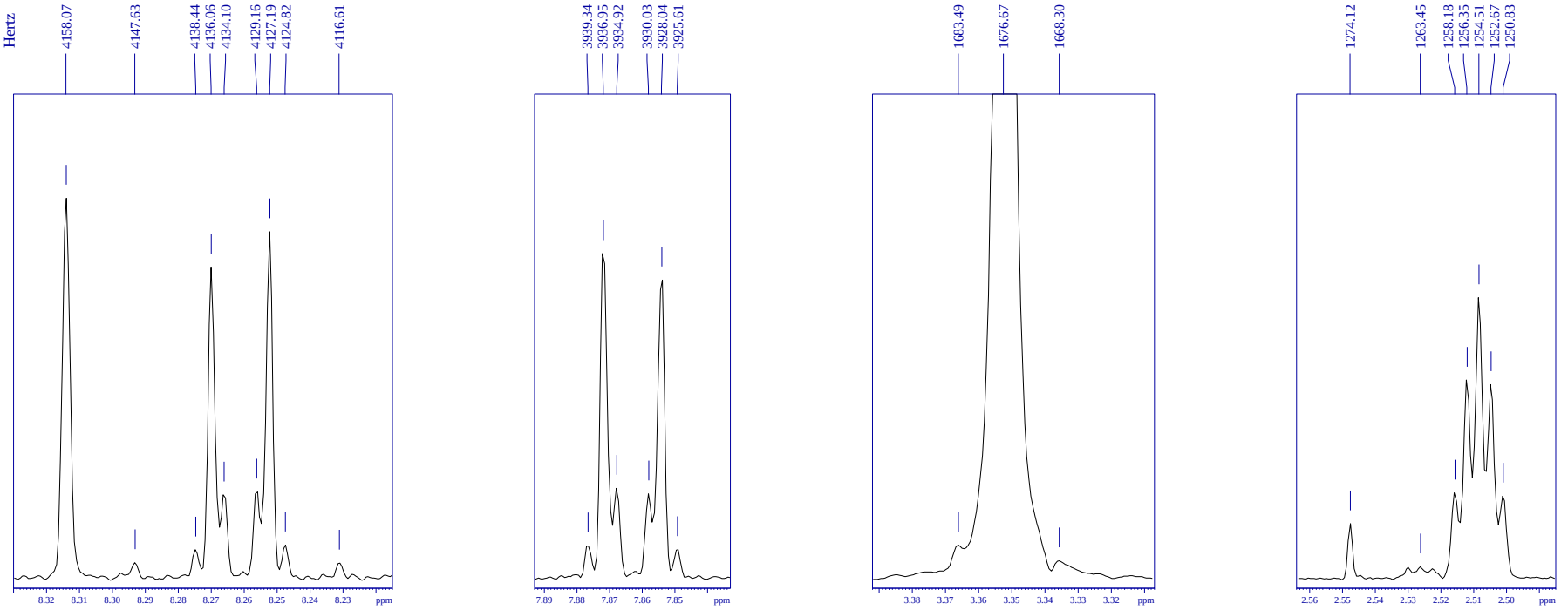


***E*-1d**

NMR/27290144



***E*-1d**



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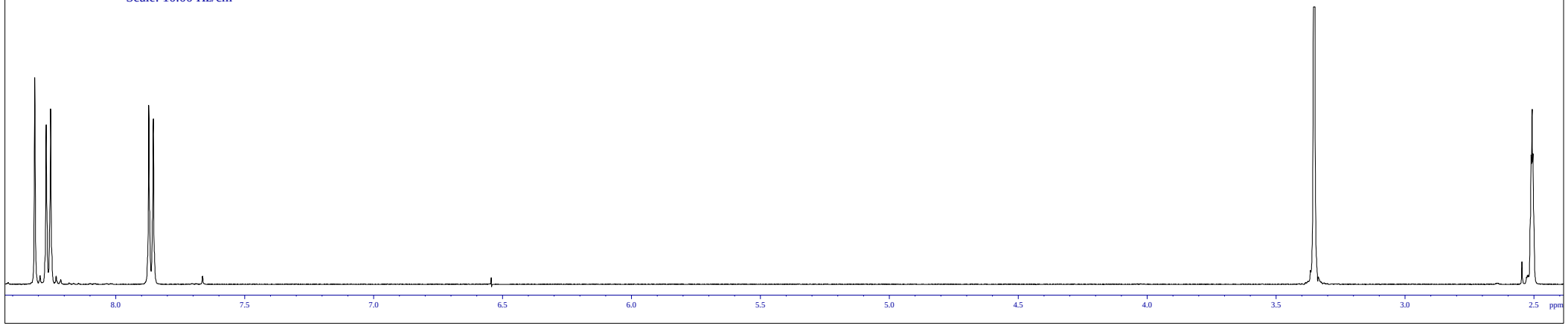
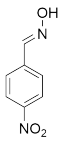




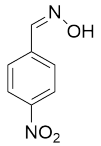
E-**1d**

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	9432.2	6120.838	12.2385	0.23
2	10059.9	5929.300	11.8555	9.25
3	15863.8	4158.072	8.3140	6.55
4	15898.0	4147.631	8.2931	0.28
5	15928.2	4138.439	8.2747	0.49
6	15936.0	4136.058	8.2700	5.35
7	15942.4	4134.104	8.2661	1.47
8	15958.6	4129.158	8.2562	1.53
9	15965.0	4127.188	8.2522	5.95
10	15972.8	4124.820	8.2475	0.58
11	15999.7	4116.615	8.2311	0.27
12	16580.6	3939.335	7.8766	0.58
13	16588.4	3936.948	7.8719	5.74
14	16595.1	3934.917	7.8678	1.55
15	16611.1	3930.033	7.8580	1.46
16	16617.6	3928.042	7.8540	5.27
17	16625.6	3925.614	7.8492	0.52
18	16930.3	3832.624	7.6633	0.27
19	18765.5	3272.540	6.5434	0.43
20	23955.8	1688.614	3.3764	0.22
21	23958.3	1687.844	3.3748	−0.23
22	23964.8	1685.843	3.3708	−0.22
23	23968.4	1684.763	3.3687	0.30
24	23970.7	1684.051	3.3672	−0.32
25	23973.7	1683.125	3.3654	0.67
26	23981.4	1680.776	3.3607	0.47
27	23984.4	1679.877	3.3589	−0.70
28	23988.8	1678.540	3.3562	0.86
29	23994.9	1676.668	3.3525	71.48
30	24001.6	1674.610	3.3483	−0.51
31	24004.1	1673.853	3.3468	0.55
32	24013.4	1671.033	3.3412	0.55
33	24016.4	1670.101	3.3393	−0.31
34	24023.6	1667.899	3.3349	0.41
35	24028.1	1666.541	3.3322	0.36
36	24031.0	1665.642	3.3304	0.33
37	24036.8	1663.871	3.3269	0.21
38	24040.8	1662.666	3.3245	−0.50
39	24043.4	1661.874	3.3229	0.34
40	25314.0	1274.123	2.5476	0.94
41	25348.9	1263.446	2.5262	0.20
42	25366.2	1258.182	2.5157	1.48
43	25372.2	1256.348	2.5120	3.43
44	25378.2	1254.510	2.5084	4.86
45	25384.2	1252.673	2.5047	3.36
46	25390.3	1250.832	2.5010	1.43
47	29489.0	0.001	0.0000	1.75

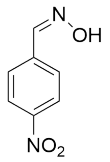
NMR/27290144

NMR/27290143

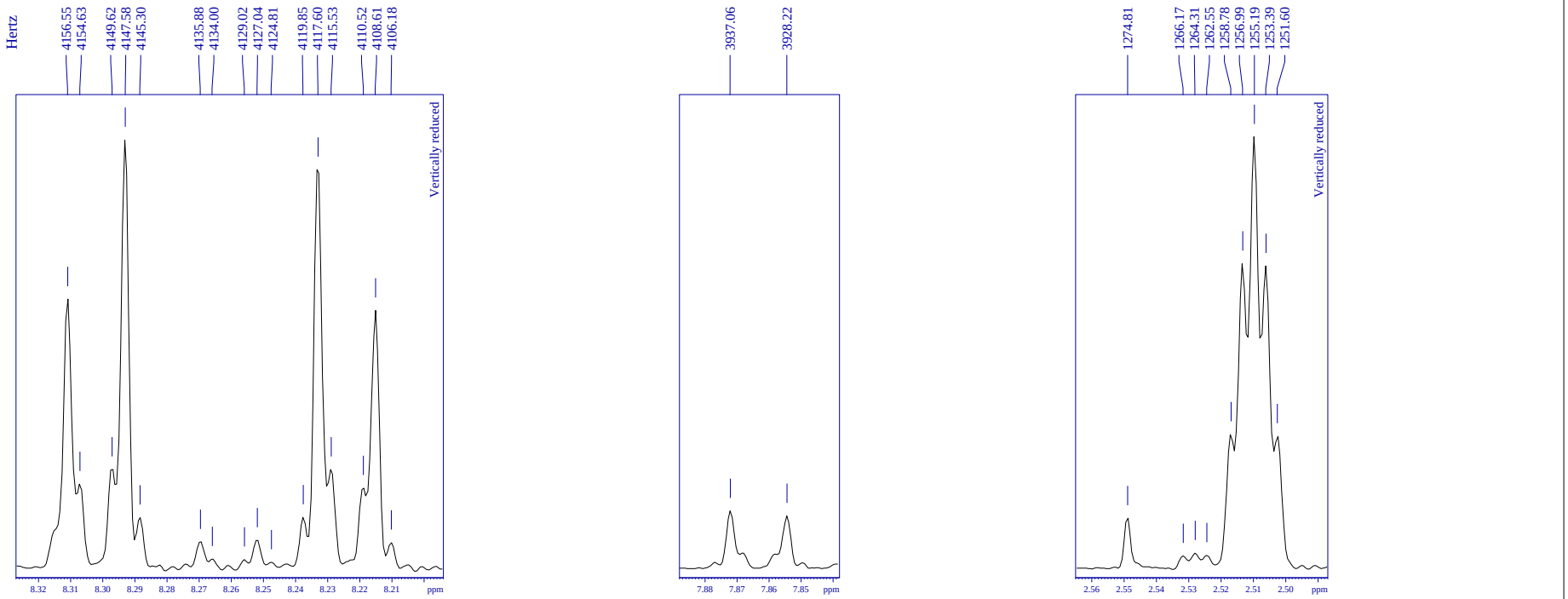


Z-**1d**

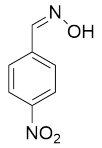
NMR/27290143



***Z*-1d**



NMR/27290143

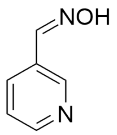


***Z*-1d**

Peaks List

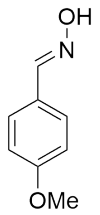
#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	15871.8	4156.549	8.3109	9.57
2	15878.1	4154.633	8.3071	2.99
3	15894.5	4149.622	8.2971	3.56
4	15901.2	4147.577	8.2930	15.28
5	15908.7	4145.300	8.2884	1.82
6	15939.6	4135.878	8.2696	0.95
7	15945.7	4134.000	8.2659	0.33
8	15962.0	4129.024	8.2559	0.31
9	15968.5	4127.042	8.2519	1.02
10	15975.8	4124.814	8.2475	0.21
11	15992.1	4119.849	8.2376	1.81
12	15999.5	4117.595	8.2330	14.52
13	16006.2	4115.526	8.2289	3.52
14	16022.6	4110.521	8.2189	2.86
15	16028.9	4108.609	8.2151	9.14
16	16036.9	4106.179	8.2102	0.91
17	16591.0	3937.059	7.8721	0.93
18	16620.0	3928.217	7.8544	0.85
19	16932.8	3832.756	7.6635	16.00
20	18767.2	3272.960	6.5442	−0.50
21	23984.4	1680.793	3.3607	5.04
22	25314.7	1274.806	2.5489	1.59
23	25343.0	1266.173	2.5317	0.38
24	25349.1	1264.312	2.5280	0.47
25	25354.9	1262.552	2.5244	0.41
26	25367.2	1258.782	2.5169	4.21
27	25373.1	1256.995	2.5133	9.53
28	25379.0	1255.191	2.5097	13.48
29	25384.9	1253.388	2.5061	9.46
30	25390.8	1251.601	2.5026	4.15
31	29492.0	0.000	0.0000	2.76

/BROD SCR598



***E*-1e**

/BROD SCR408

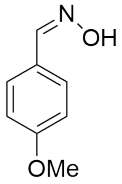


***E*-1f**

The Best Applied NMR!

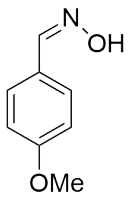
NMR/27290150

Found protons = 9 impurity* < 0.1 %

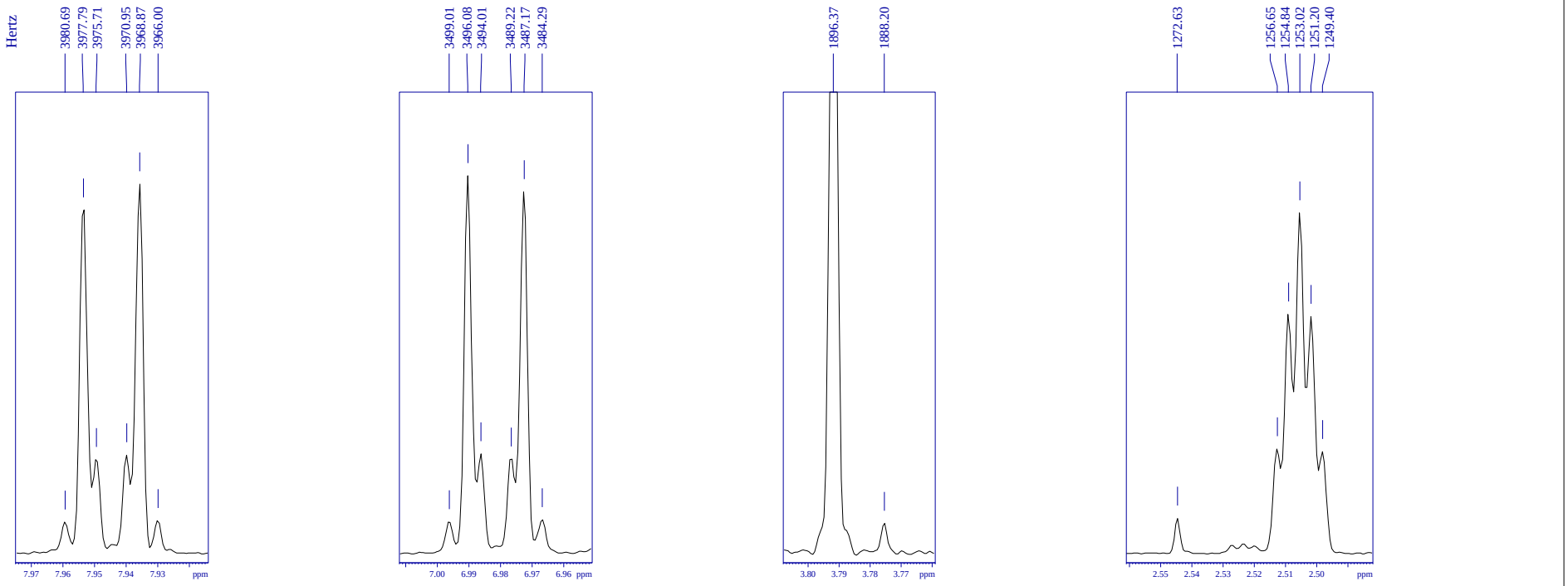


***Z*-1f**

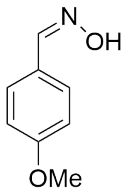
NMR/27290150



***Z*-1f**



NMR/27290150

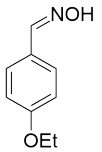


***Z*-1f**

Peaks List

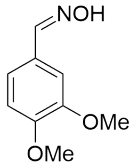
#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	10858.4	5686.517	11.3701	0.68
2	16448.1	3980.688	7.9593	0.51
3	16457.6	3977.792	7.9535	5.66
4	16464.4	3975.710	7.9494	1.54
5	16480.0	3970.951	7.9398	1.59
6	16486.8	3968.872	7.9357	5.99
7	16496.2	3966.003	7.9299	0.53
8	17509.9	3656.649	7.3114	7.86
9	18026.4	3499.014	6.9962	0.52
10	18036.0	3496.082	6.9903	6.09
11	18042.8	3494.009	6.9862	1.61
12	18058.5	3489.222	6.9766	1.55
13	18065.2	3487.172	6.9725	5.87
14	18074.7	3484.289	6.9668	0.55
15	23278.0	1896.371	3.7918	27.32
16	23304.7	1888.204	3.7754	0.49
17	23996.8	1677.006	3.3531	21.30
18	25321.9	1272.628	2.5446	0.57
19	25374.2	1256.650	2.5126	1.69
20	25380.1	1254.839	2.5090	3.86
21	25386.1	1253.020	2.5054	5.49
22	25392.1	1251.201	2.5018	3.82
23	25398.0	1249.397	2.4981	1.64
24	29492.0	0.000	0.0000	9.62

/BROD SCR719



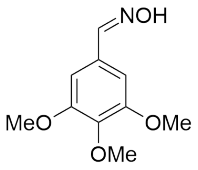
E-**1g**

/BROD SCR356



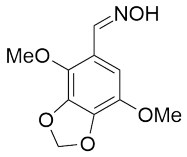
***E*-1h**

/BROD SCR680



E-**1i**

/BROD SCR597

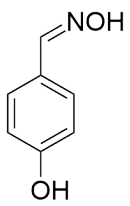


E-**1j**

The Best Applied NMR!

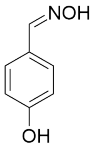
NMR/29210025

Found protons = 29 impurity* = 2.3 %

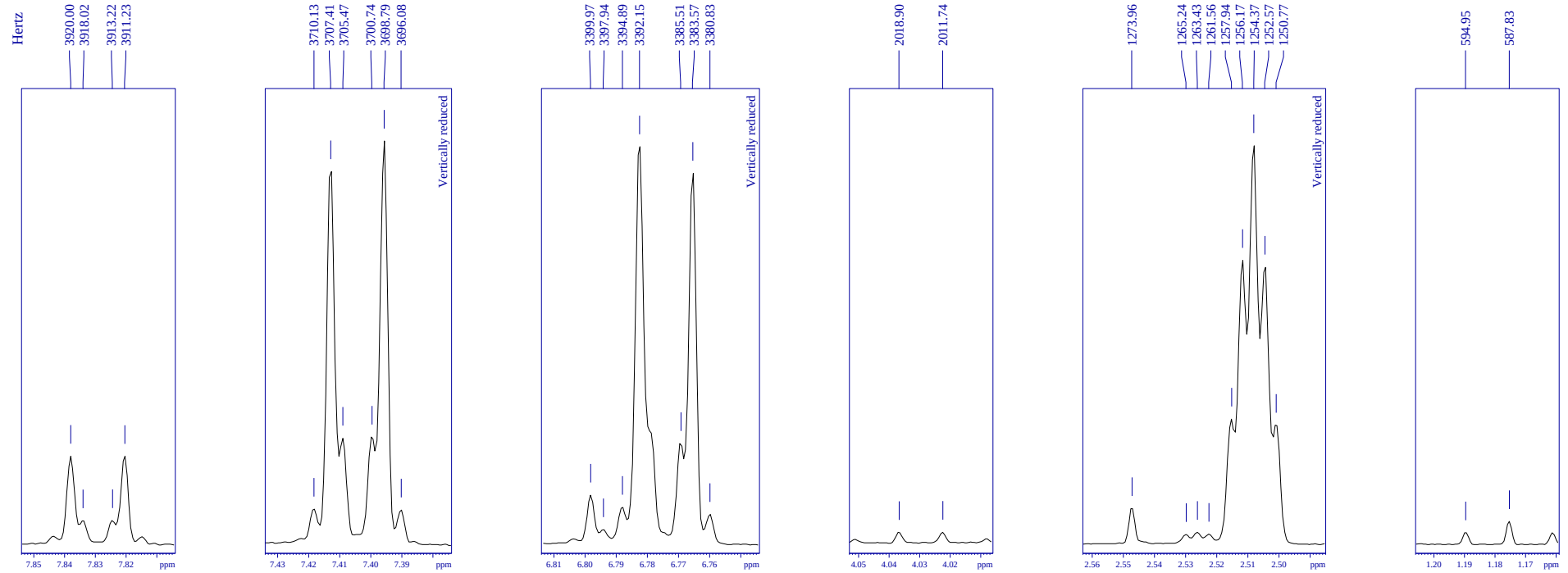


E-**1k**

NMR/29210025



E-**1k**



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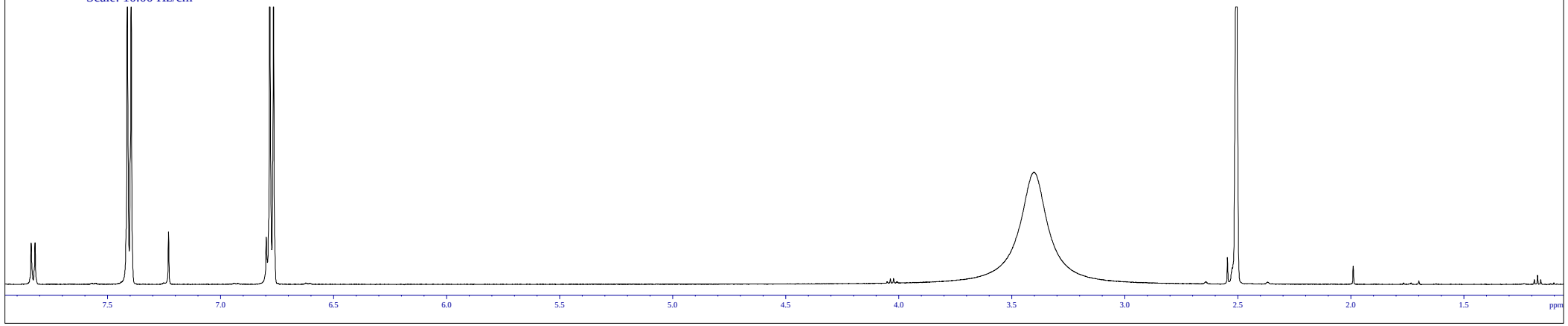
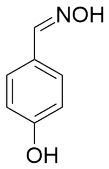


NMR/29210025

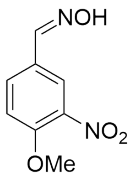


E-**1k**

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	16373.6	4002.494	8.0029	16.00
2	16643.9	3919.999	7.8380	1.53
3	16650.4	3918.022	7.8340	0.41
4	16666.1	3913.225	7.8244	0.41
5	16672.7	3911.227	7.8204	1.54
6	17331.7	3710.130	7.4183	1.13
7	17340.6	3707.409	7.4129	12.08
8	17346.9	3705.470	7.4090	3.37
9	17362.4	3700.745	7.3996	3.45
10	17368.8	3698.790	7.3957	12.85
11	17377.7	3696.077	7.3902	1.10
12	17640.0	3616.016	7.2302	2.02
13	18348.0	3399.971	6.7982	1.65
14	18354.6	3397.940	6.7941	0.50
15	18364.6	3394.885	6.7880	1.26
16	18373.6	3392.154	6.7825	13.60
17	18395.4	3385.505	6.7692	3.44
18	18401.7	3383.572	6.7654	12.61
19	18410.7	3380.833	6.7599	1.01
20	22873.5	2018.899	4.0367	0.21
21	22896.9	2011.742	4.0224	0.21
22	23913.9	1701.393	3.4019	2.74
23	25314.5	1273.956	2.5472	1.13
24	25343.0	1265.245	2.5298	0.30
25	25349.0	1263.433	2.5262	0.36
26	25355.1	1261.561	2.5225	0.30
27	25367.0	1257.944	2.5152	3.79
28	25372.8	1256.174	2.5117	8.63
29	25378.7	1254.373	2.5081	12.20
30	25384.6	1252.568	2.5045	8.53
31	25390.5	1250.773	2.5009	3.64
32	26226.5	995.649	1.9908	0.78
33	27539.5	594.946	1.1896	0.21
34	27562.8	587.827	1.1753	0.40
35	29489.0	0.001	0.0000	8.19

/BROD SCR561



E-**1l**

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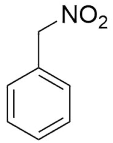
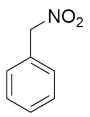
3.141

NMR/29310035

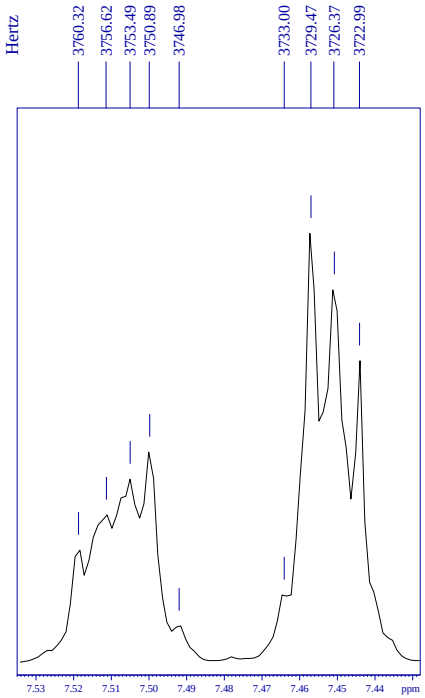


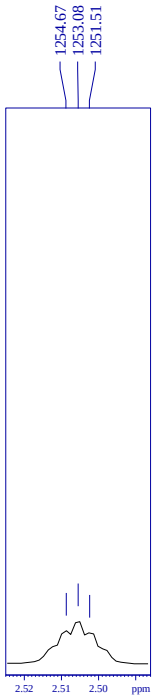
2a

NMR/29310035

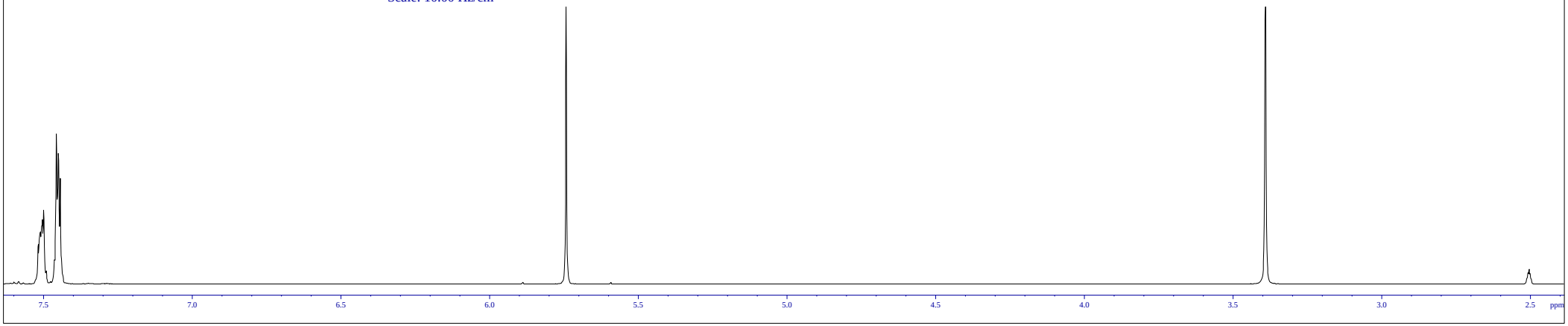


2a

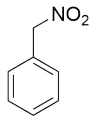




Scale: 10.00 Hz/cm



NMR/29310035

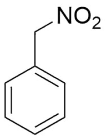


2a

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	8581.7	3760.320	7.5187	1.52
2	8587.8	3756.622	7.5113	1.97
3	8592.9	3753.491	7.5050	2.44
4	8597.2	3750.887	7.4998	2.81
5	8603.6	3746.978	7.4920	0.52
6	8626.5	3733.004	7.4641	0.95
7	8632.3	3729.466	7.4570	5.79
8	8637.3	3726.374	7.4508	5.02
9	8642.9	3722.993	7.4441	4.03
10	10037.0	2872.057	5.7426	12.75
11	11963.0	1696.516	3.3921	16.00
12	12687.0	1254.673	2.5087	0.44
13	12689.6	1253.078	2.5055	0.58
14	12692.1	1251.512	2.5024	0.41
15	14742.6	0.001	0.0000	0.31

NMR/29310035

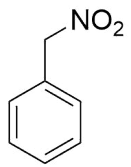


2a

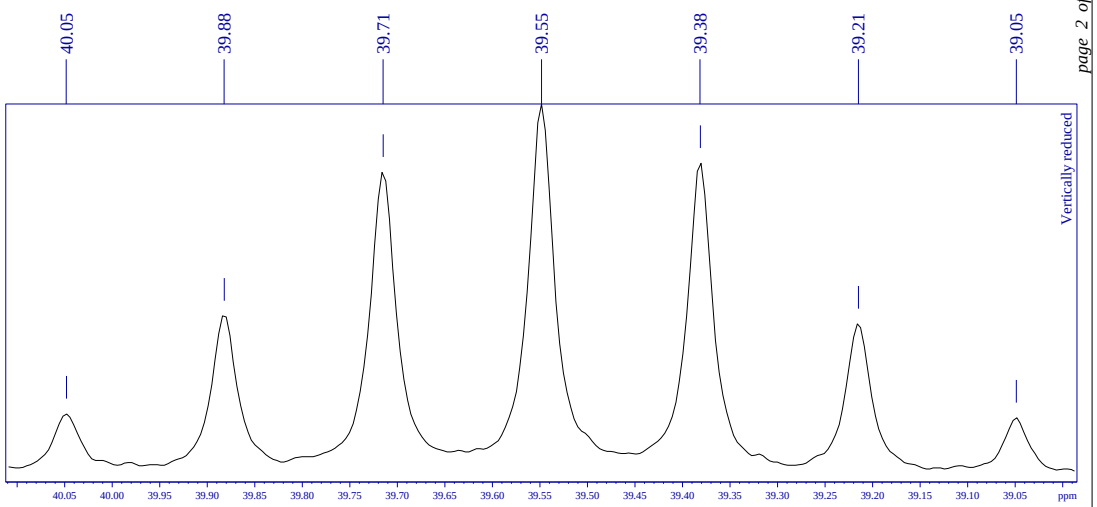
130.61
130.45
129.54
128.81
79.23
40.05
39.88
39.71
39.55
39.38
39.21
39.05

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

NMR/29310035



2a



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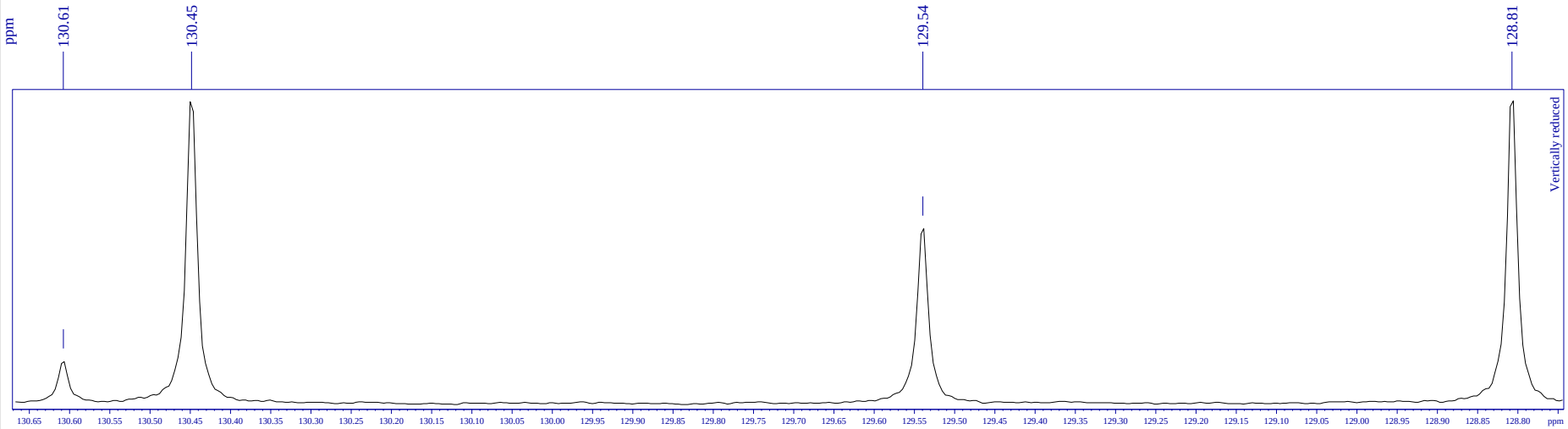
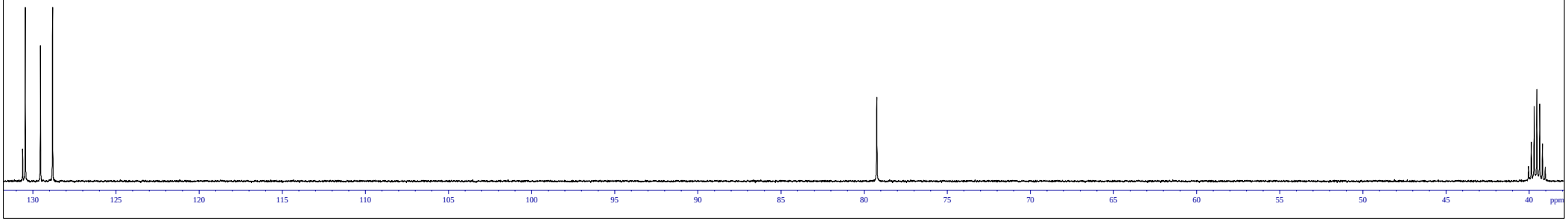
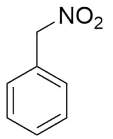




NMR/29310035



2a

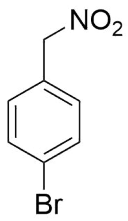
Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	26056.6	16424.943	130.6077	1.92
2	26098.4	16404.889	130.4482	13.88
3	26336.6	16290.604	129.5395	8.02
4	26528.6	16198.491	128.8070	14.00
5	39521.5	9964.001	79.2316	4.92
6	49790.9	5036.368	40.0481	0.87
7	49834.4	5015.482	39.8821	2.29
8	49878.3	4994.460	39.7149	4.32
9	49921.9	4973.510	39.5483	5.29
10	49965.7	4952.497	39.3812	4.46
11	50009.3	4931.584	39.2149	2.16
12	50052.8	4910.694	39.0488	0.81

The Best Applied NMR!

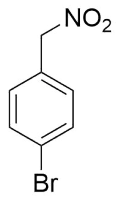
NMR/29330084

Found protons = 3 impurity* = 1.4 %

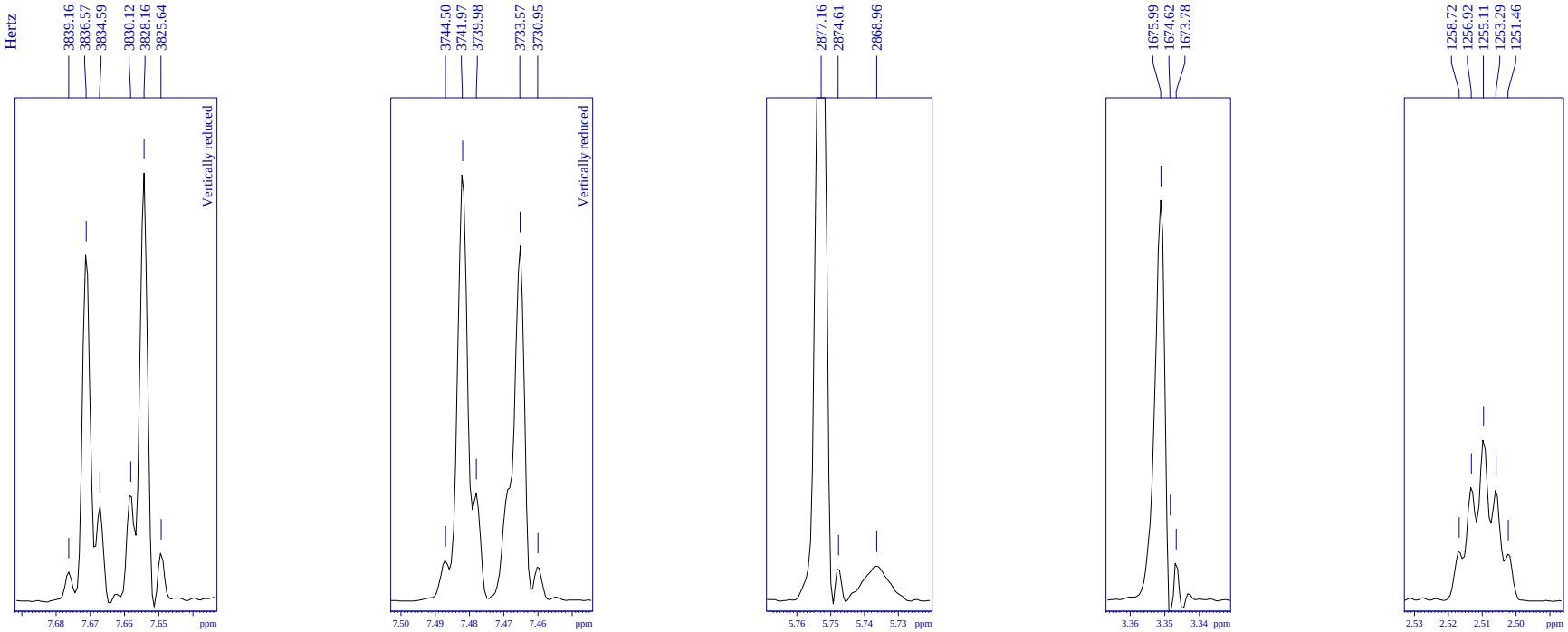


2b

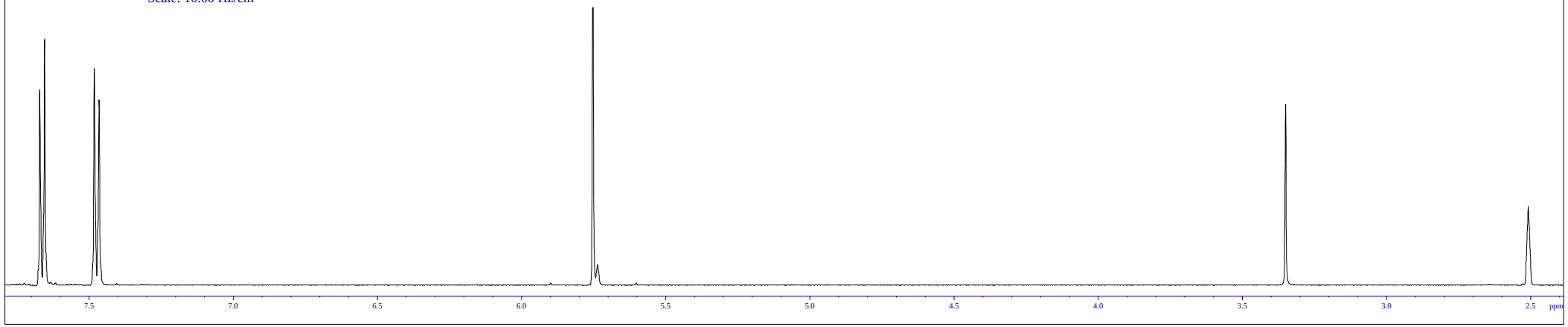
NMR/29330084



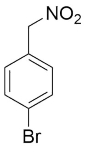
2b



Scale: 10.00 Hz/cm



NMR/29330084

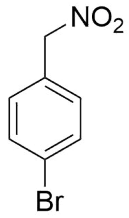


2b

Peaks List

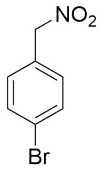
#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	16910.8	3839.158	7.6763	0.66
2	16919.3	3836.573	7.6712	7.97
3	16925.8	3834.586	7.6672	2.17
4	16940.5	3830.118	7.6582	2.48
5	16946.9	3828.163	7.6543	9.73
6	16955.2	3825.636	7.6493	1.09
7	17221.0	3744.496	7.4870	0.75
8	17229.3	3741.972	7.4820	7.88
9	17235.8	3739.982	7.4780	1.98
10	17256.8	3733.570	7.4652	6.52
11	17265.4	3730.949	7.4600	0.63
12	20063.1	2877.157	5.7528	16.00
13	20071.5	2874.612	5.7477	0.55
14	20090.0	2868.964	5.7364	0.57
15	23999.1	1675.991	3.3511	6.53
16	24003.6	1674.616	3.3484	−0.75
17	24006.4	1673.781	3.3467	0.66
18	25366.4	1258.725	2.5168	0.82
19	25372.3	1256.924	2.5132	1.87
20	25378.3	1255.111	2.5096	2.64
21	25384.2	1253.285	2.5059	1.81
22	25390.2	1251.462	2.5023	0.77
23	29491.0	0.000	0.0000	3.13

NMR/29330084

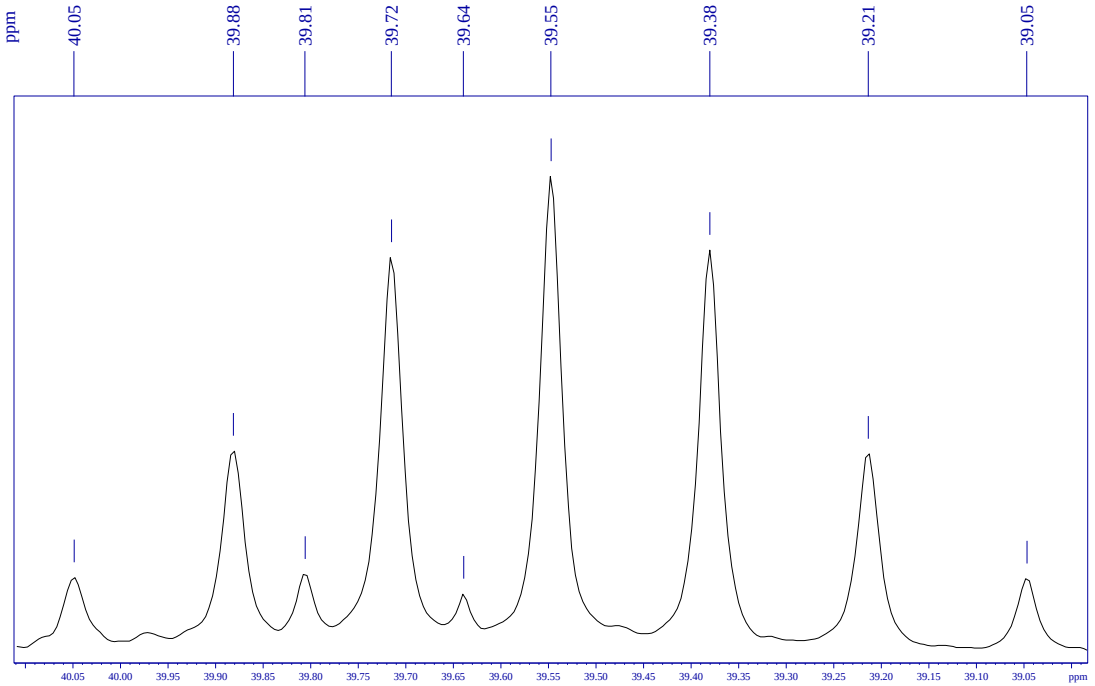


2b

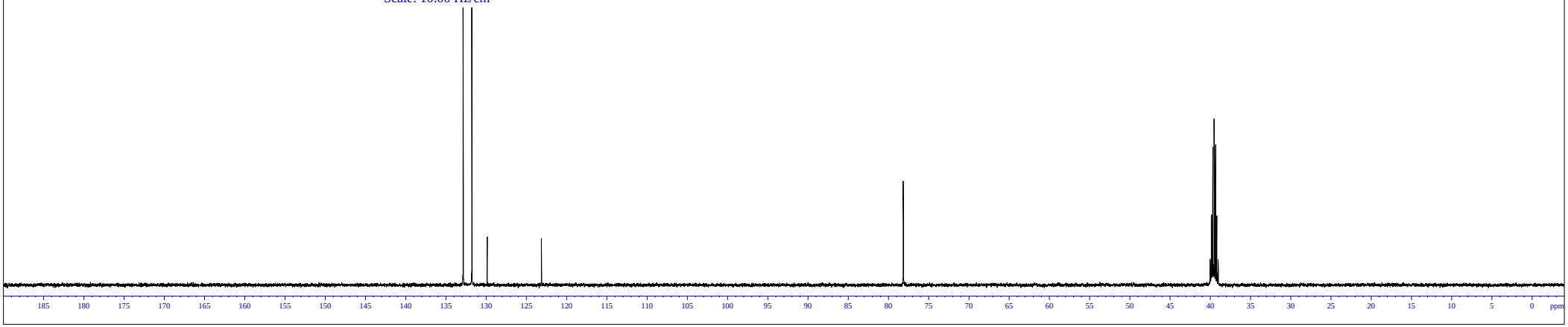
NMR/29330084



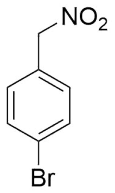
2b



Scale: 10.00 Hz/cm



NMR/29330084



2b

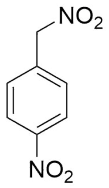
Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	25470.6	16706.119	132.8436	11.42
2	25753.8	16570.250	131.7632	14.00
3	26256.8	16328.912	129.8441	1.73
4	28019.3	15483.191	123.1191	1.69
5	39808.0	9826.554	78.1387	3.70
6	49790.8	5036.438	40.0487	0.93
7	49834.7	5015.383	39.8813	2.52
8	49854.4	5005.897	39.8058	0.98
9	49878.2	4994.473	39.7150	4.92
10	49898.1	4984.925	39.6391	0.72
11	49922.2	4973.372	39.5472	5.93
12	49965.9	4952.382	39.3803	5.00
13	50009.6	4931.425	39.2137	2.49
14	50053.4	4910.442	39.0468	0.92

The Best Applied NMR!

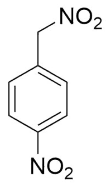
NMR/27290142

Found protons = 3 impurity* = 0.3 %

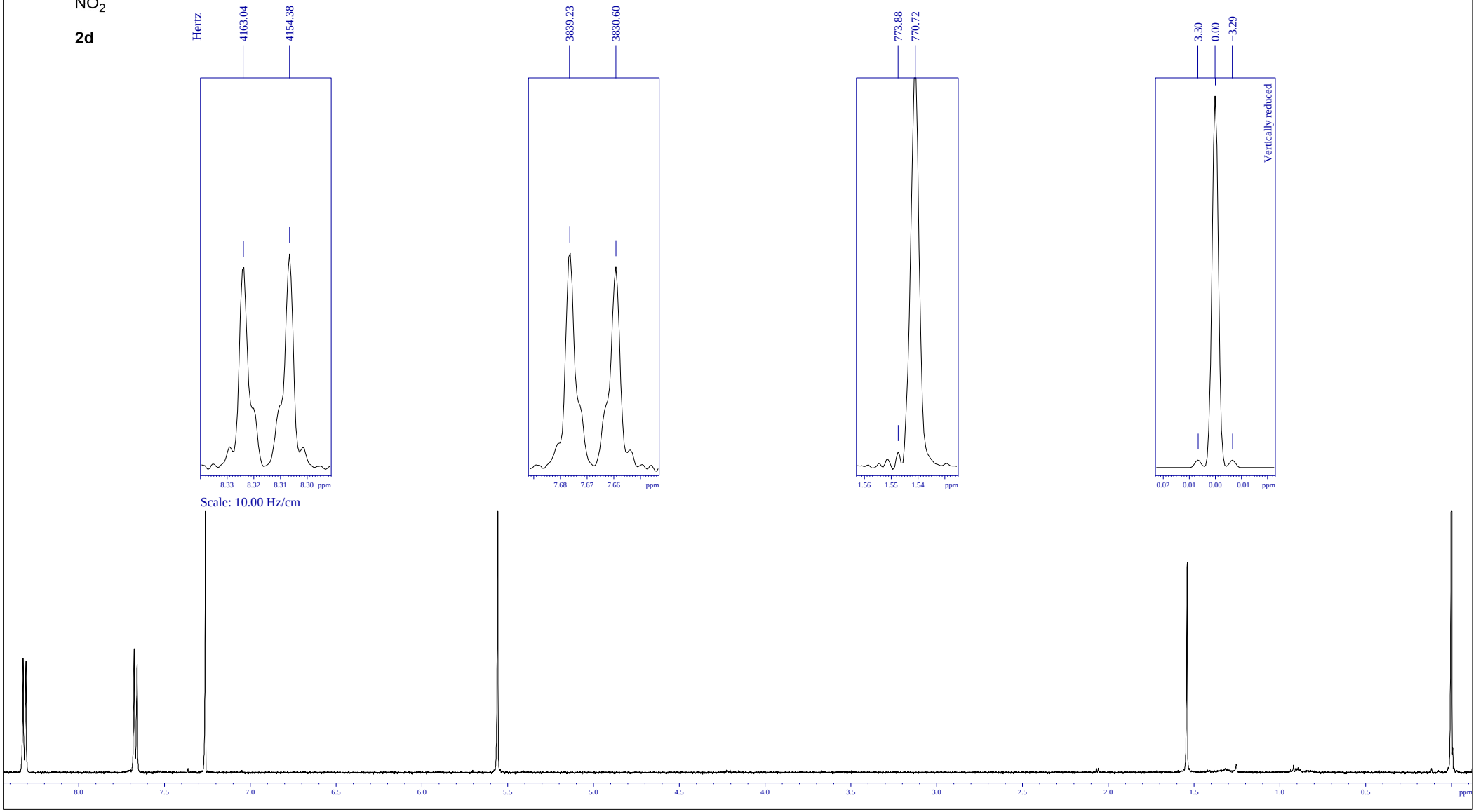


2d

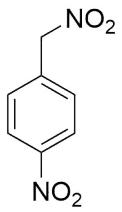
NMR/27290142



2d



NMR/27290142



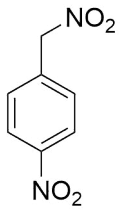
2d

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	15838.6	4163.038	8.3239	3.83
2	15866.9	4154.379	8.3066	4.03
3	16899.6	3839.233	7.6765	4.09
4	16927.9	3830.598	7.6592	3.78
5	17580.6	3631.414	7.2609	11.34
6	20372.4	2779.430	5.5574	11.04
7	26944.2	773.881	1.5474	0.30
8	26954.5	770.716	1.5410	7.65
9	27423.8	627.516	1.2547	0.23
10	27970.8	460.577	0.9209	0.29
11	29469.2	3.296	0.0066	0.65
12	29480.0	0.002	0.0000	32.46
13	29490.8	−3.293	−0.0066	0.65

The Best Applied NMR!

NMR/27290142

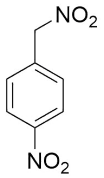


2d

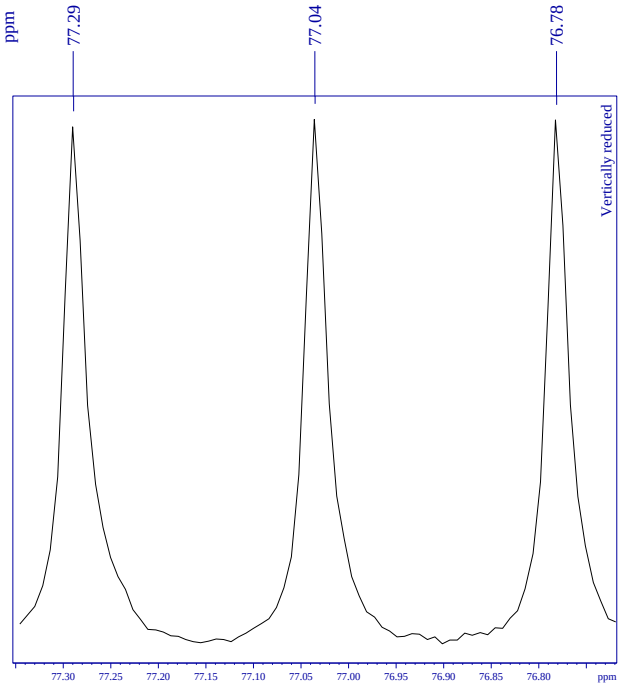
148.93
135.73
131.14
124.29
78.73
77.29
77.04
76.78
-0.00

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

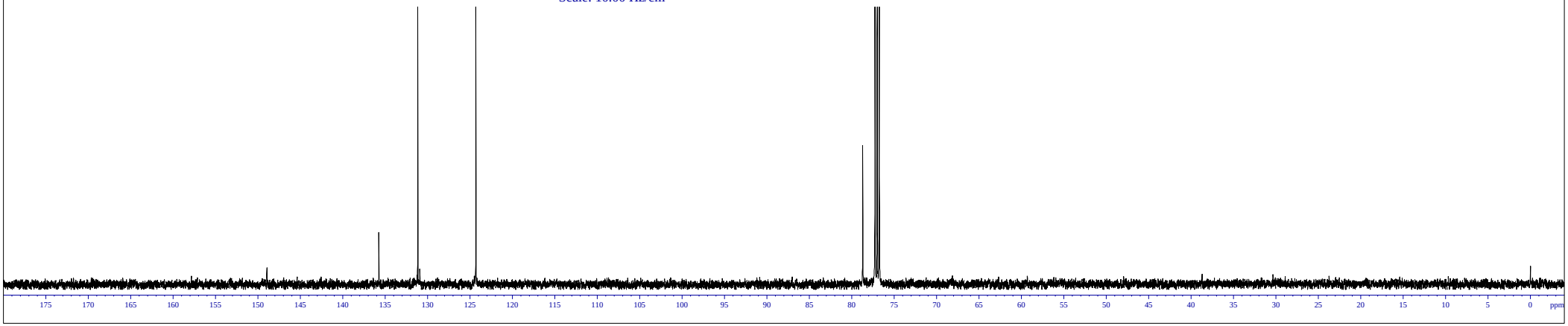
NMR/27290142



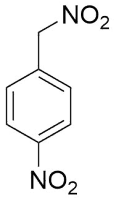
2d



Scale: 10.00 Hz/cm



NMR/27290142



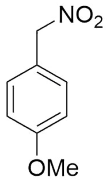
2d

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	11483.0	18728.502	148.9252	0.62
2	13147.2	17068.787	135.7275	1.95
3	13725.8	16491.670	131.1384	14.00
4	14589.7	15630.175	124.2879	13.84
5	20334.2	9901.091	78.7314	5.23
6	20516.1	9719.704	77.2891	13.60
7	20548.1	9687.776	77.0352	13.80
8	20580.1	9655.831	76.7812	13.80
9	30262.1	−0.006	−0.0001	0.68

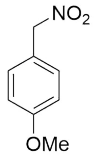
NMR/29310046

Found protons = 41 impurity* = 3.2 %

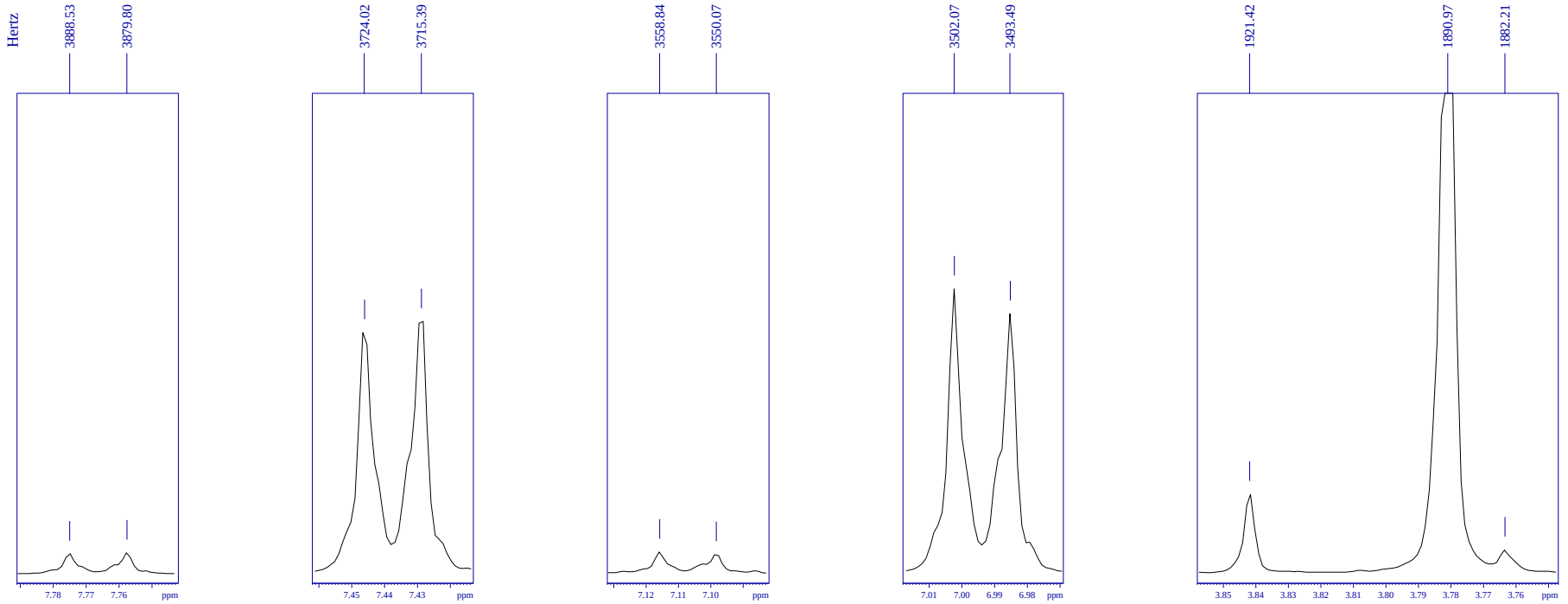


2f

NMR/29310046



2f



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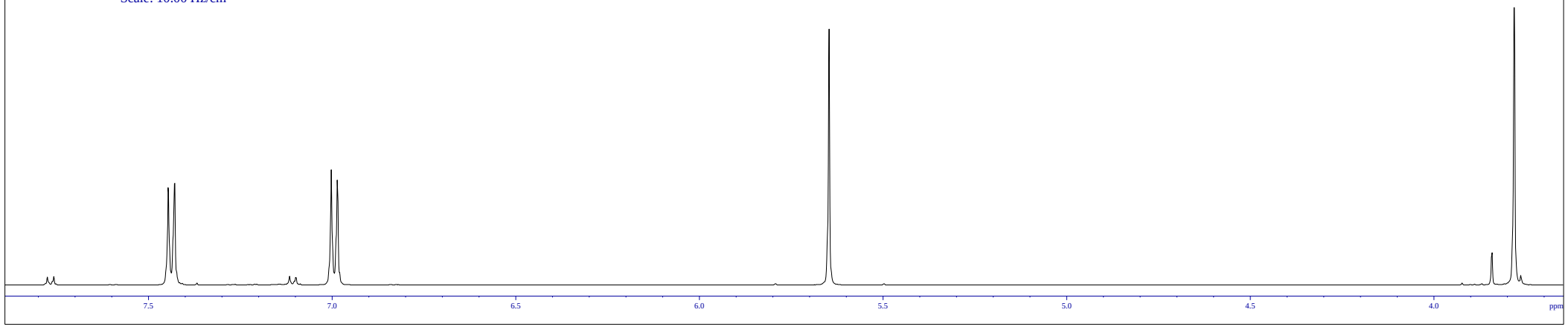
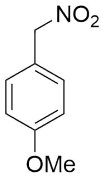


NMR/29310046

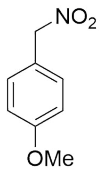


2f

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	8373.8	3888.534	7.7750	0.29
2	8388.1	3879.805	7.7576	0.31
3	8643.4	3724.017	7.4461	3.68
4	8657.5	3715.390	7.4288	3.90
5	8914.0	3558.837	7.1158	0.32
6	8928.4	3550.073	7.0983	0.29
7	9007.0	3502.066	7.0023	4.21
8	9021.1	3493.493	6.9852	3.85
9	10117.8	2824.113	5.6468	9.46
10	11596.7	1921.425	3.8419	1.20
11	11646.6	1890.974	3.7810	16.00
12	11661.0	1882.210	3.7634	0.35
13	11970.7	1693.158	3.3854	10.59
14	12689.4	1254.549	2.5084	0.45
15	12927.7	1109.092	2.2176	0.81
16	14744.8	0.001	0.0000	0.23

NMR/29310046

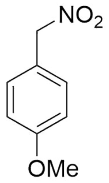


2f

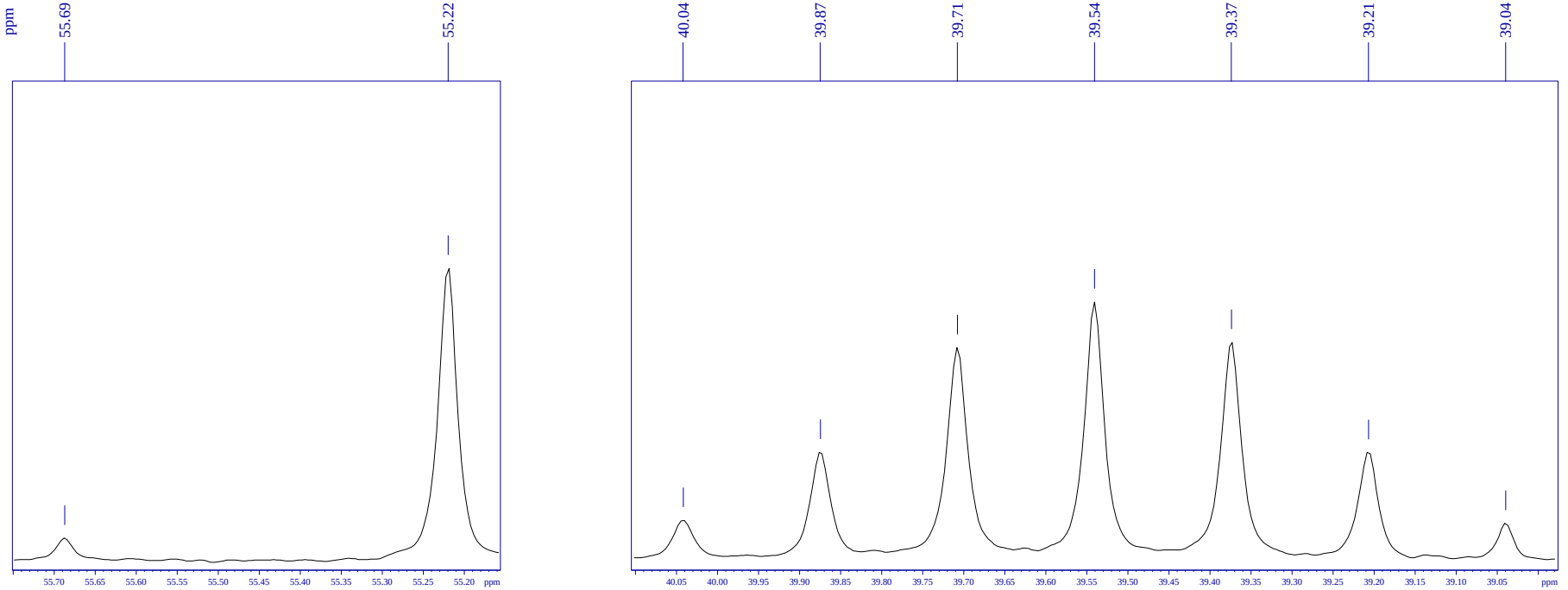
160.16
134.20
132.01
122.72
115.15
114.13
78.74
55.69
55.22
40.04
39.87
39.71
39.54
39.37
39.21
39.04

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

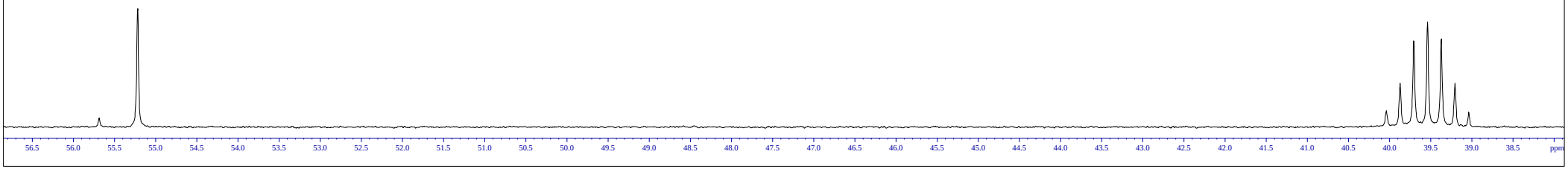
NMR/29310046



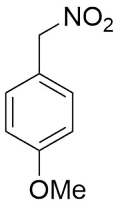
2f



Scale: 10.00 Hz/cm



NMR/29310046



2f

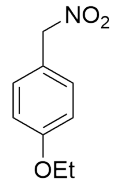
Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	18312.2	20141.002	160.1570	1.59
2	25115.2	16876.658	134.1996	0.92
3	25688.6	16601.555	132.0121	13.57
4	28122.9	15433.468	122.7237	2.11
5	30107.0	14481.431	115.1533	0.92
6	30375.7	14352.489	114.1280	14.00
7	39649.2	9902.743	78.7445	4.79
8	45692.2	7003.104	55.6872	0.32
9	45814.7	6944.308	55.2197	4.26
10	49792.6	5035.561	40.0417	0.59
11	49836.4	5014.545	39.8746	1.58
12	49880.1	4993.559	39.7077	3.08
13	49923.9	4972.550	39.5407	3.74
14	49967.7	4951.565	39.3738	3.18
15	50011.4	4930.569	39.2068	1.58
16	50055.2	4909.551	39.0397	0.54

The Best Applied NMR!

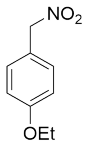
NMR/29330042

Found protons = 11 impurity* = 0.4 %

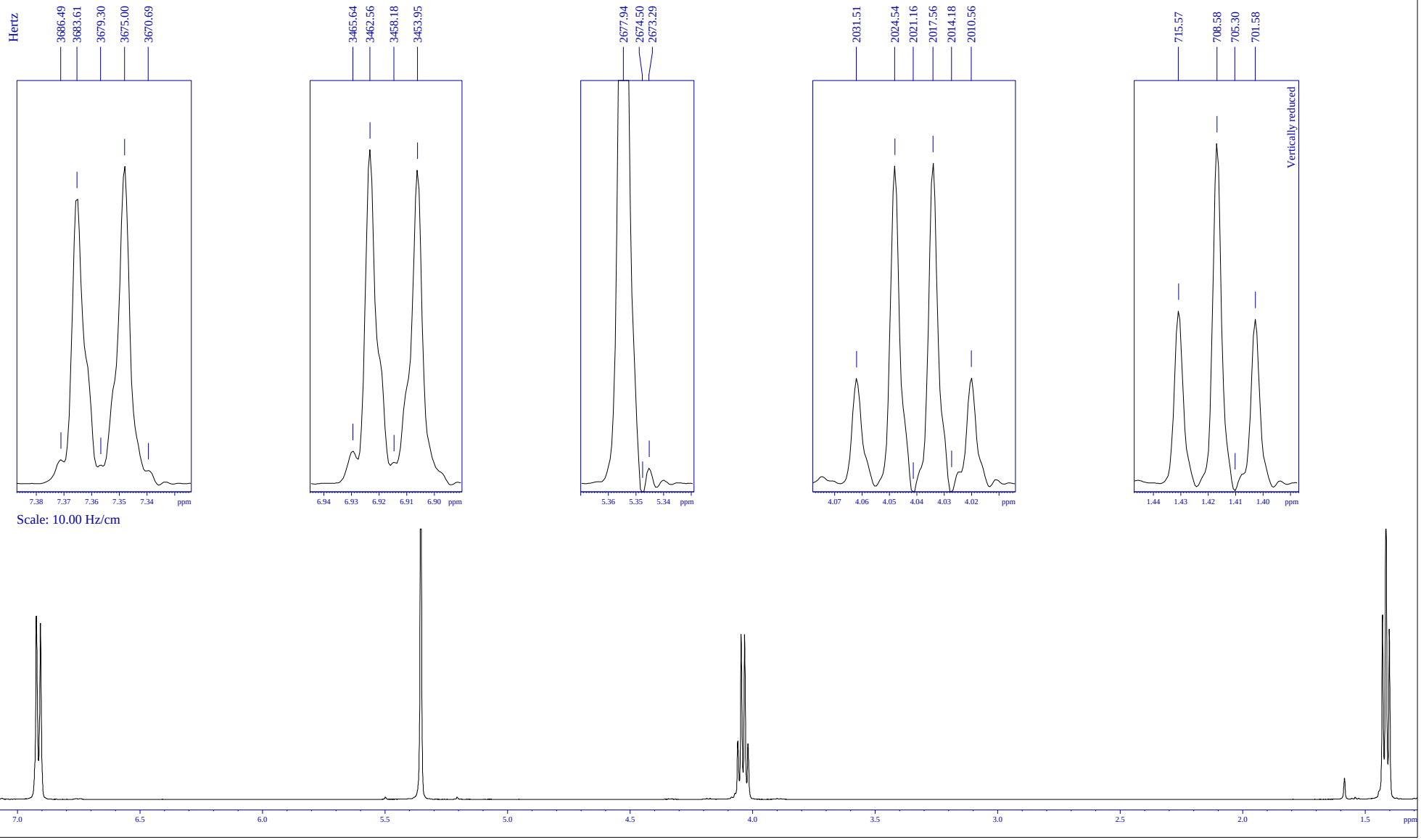


2g

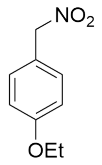
NMR/29330042



2g



NMR/29330042



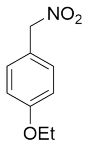
2g

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	17389.1	3686.492	7.3711	0.49
2	17398.6	3683.607	7.3653	5.90
3	17412.7	3679.300	7.3567	0.38
4	17426.7	3675.004	7.3481	6.53
5	17440.9	3670.690	7.3395	0.27
6	17580.5	3628.077	7.2543	1.07
7	18112.8	3465.641	6.9295	0.67
8	18122.9	3462.559	6.9233	6.85
9	18137.2	3458.177	6.9146	0.44
10	18151.1	3453.950	6.9061	6.43
11	20693.9	2677.940	5.3545	16.00
12	20705.2	2674.496	5.3476	−0.33
13	20709.1	2673.292	5.3452	0.32
14	22812.2	2031.507	4.0620	2.16
15	22835.0	2024.544	4.0480	6.51
16	22846.1	2021.159	4.0413	−0.22
17	22857.9	2017.556	4.0341	6.57
18	22868.9	2014.185	4.0273	−0.22
19	22880.8	2010.564	4.0201	2.18
20	26870.4	793.035	1.5857	0.75
21	27124.2	715.568	1.4308	7.25
22	27147.1	708.576	1.4168	14.25
23	27157.9	705.302	1.4102	−0.28
24	27170.1	701.581	1.4028	6.88
25	29469.0	−0.002	−0.0000	3.74

The Best Applied NMR!

NMR/29330042

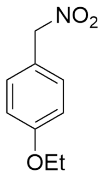


2g

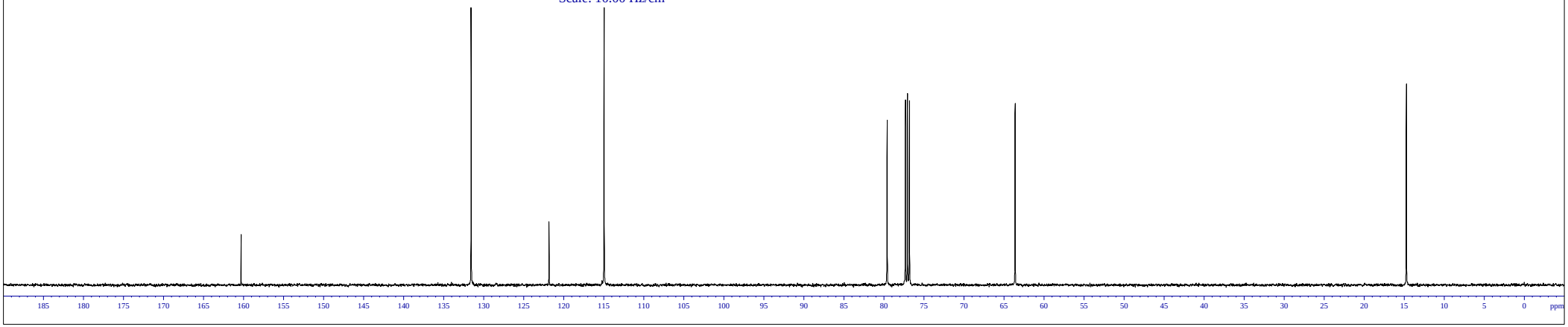
160.29
131.55
121.82
114.94
79.63
77.35
77.10
76.84
63.64
14.76

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

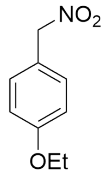
NMR/29330042



2g



NMR/29330042



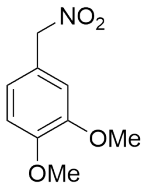
2g

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	10053.9	20157.480	160.2881	1.81
2	13677.1	16544.039	131.5548	14.00
3	14904.9	15319.562	121.8180	2.27
4	15772.2	14454.626	114.9402	13.96
5	20224.3	10014.499	79.6332	5.99
6	20511.9	9727.664	77.3524	6.65
7	20544.0	9695.713	77.0983	6.87
8	20576.0	9663.773	76.8443	6.61
9	22240.7	8003.596	63.6429	6.64
10	28404.1	1856.758	14.7646	7.22

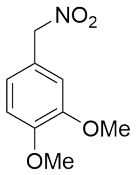
NMR/29310157

Found protons = 6 impurity* = 0.8 %

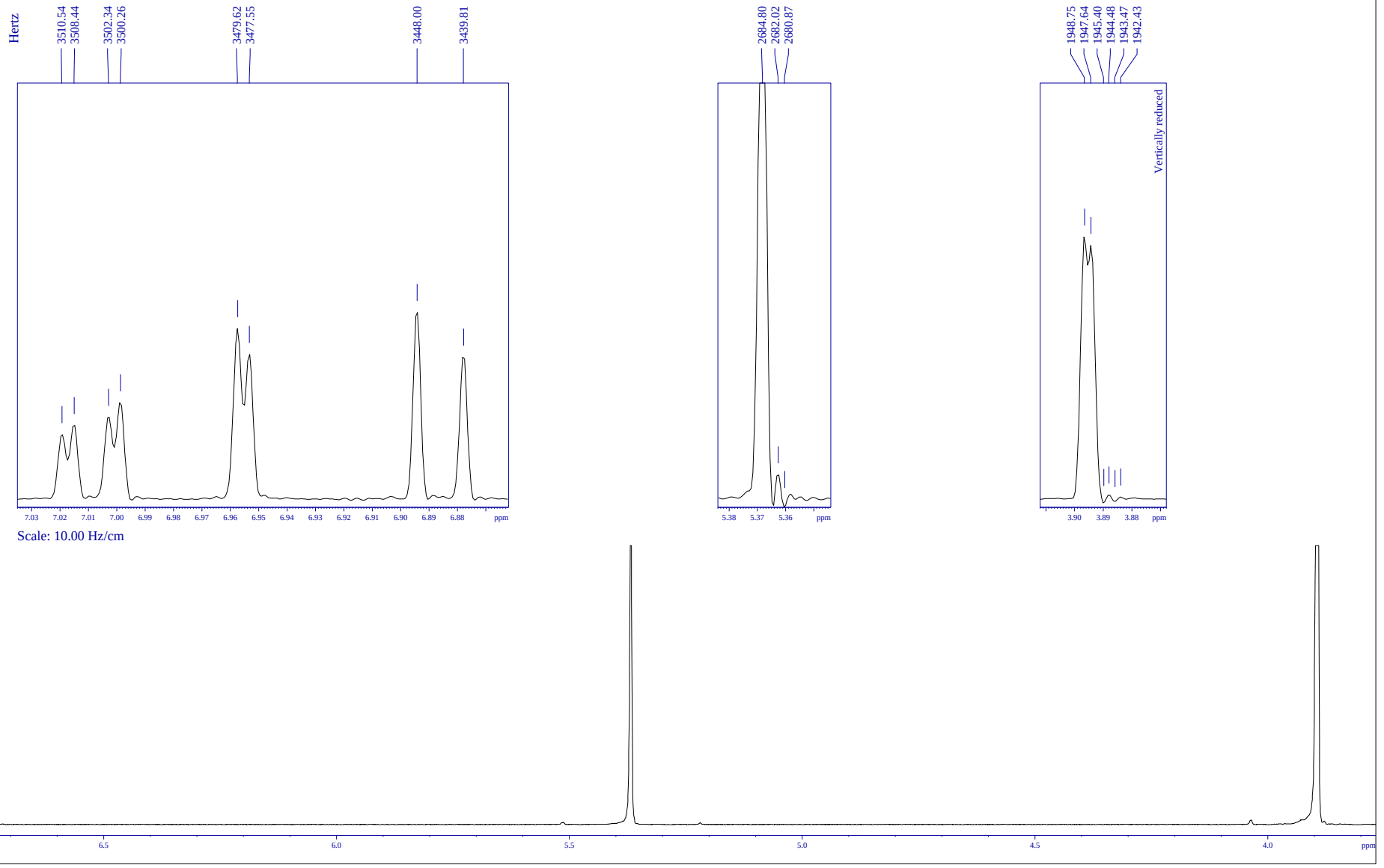


2h

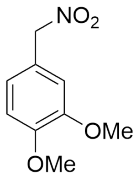
NMR/29310157



2h



NMR/29310157



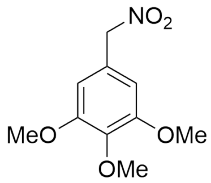
2h

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	17579.5	3637.860	7.2738	0.99
2	17996.7	3510.539	7.0193	1.72
3	18003.6	3508.436	7.0150	1.98
4	18023.5	3502.338	7.0029	2.20
5	18030.3	3500.264	6.9987	2.57
6	18098.0	3479.620	6.9574	4.50
7	18104.7	3477.555	6.9533	3.85
8	18201.6	3448.000	6.8942	5.02
9	18228.4	3439.807	6.8778	3.83
10	20702.4	2684.804	5.3682	17.14
11	20711.6	2682.016	5.3626	0.67
12	20715.3	2680.867	5.3603	−0.22
13	23114.3	1948.748	3.8965	32.00
14	23118.0	1947.637	3.8943	30.64
15	23125.3	1945.398	3.8898	−0.51
16	23128.3	1944.483	3.8880	0.51
17	23131.6	1943.473	3.8859	−0.29
18	23135.0	1942.433	3.8839	0.25
19	26841.1	811.429	1.6224	0.42
20	29500.0	0.000	0.0000	3.20

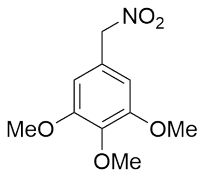
NMR/29317564

Found protons = 7 impurity* = 0.9 %



2i

NMR/29317564



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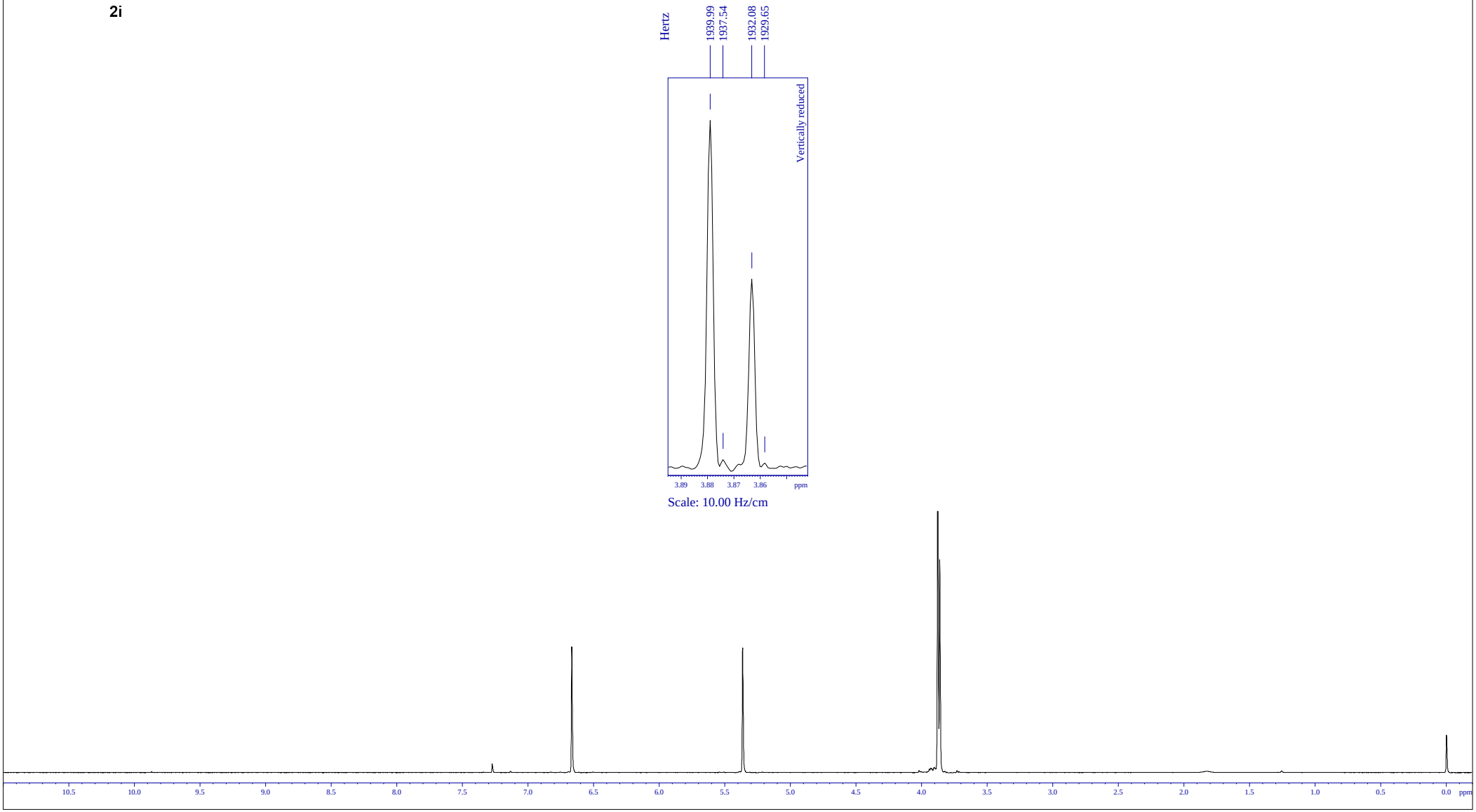
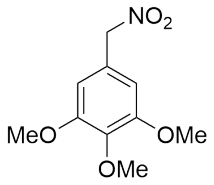


NMR/29317564



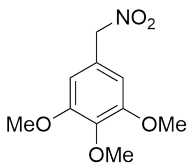
2i

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	17578.6	3638.120	7.2743	0.38
2	18571.9	3334.993	6.6683	4.53
3	20706.6	2683.543	5.3657	4.36
4	23143.0	1939.995	3.8790	16.00
5	23151.1	1937.541	3.8741	0.37
6	23169.0	1932.083	3.8632	8.69
7	23176.9	1929.652	3.8583	0.21
8	29500.0	0.000	0.0000	1.61

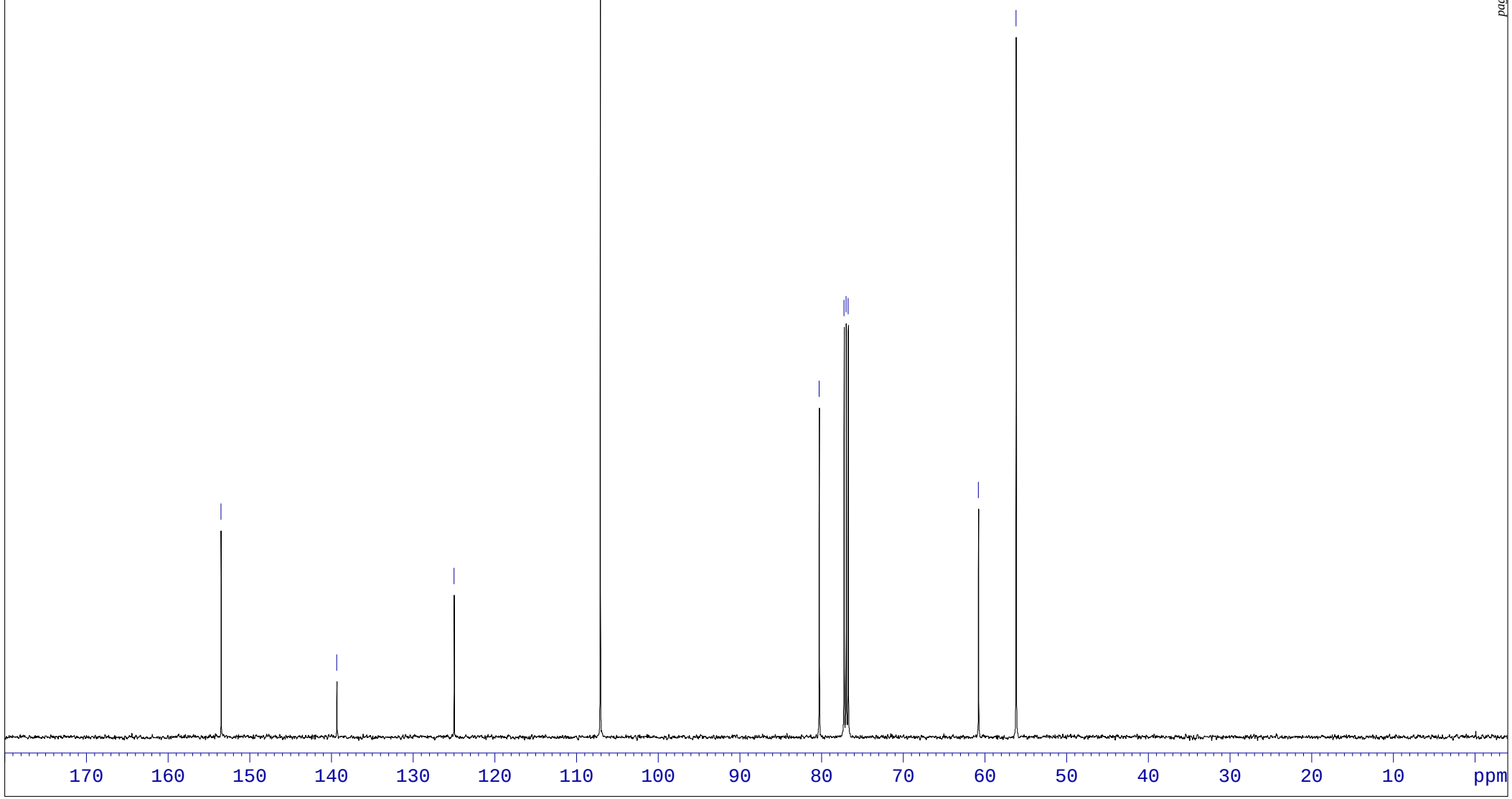
The Best Applied NMR!

NMR/29317564

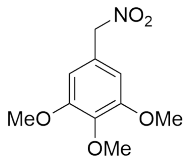


2i

153.53 139.36 125.00 107.11 80.30 77.26 77.00 76.75 60.81 56.20



NMR/29317564



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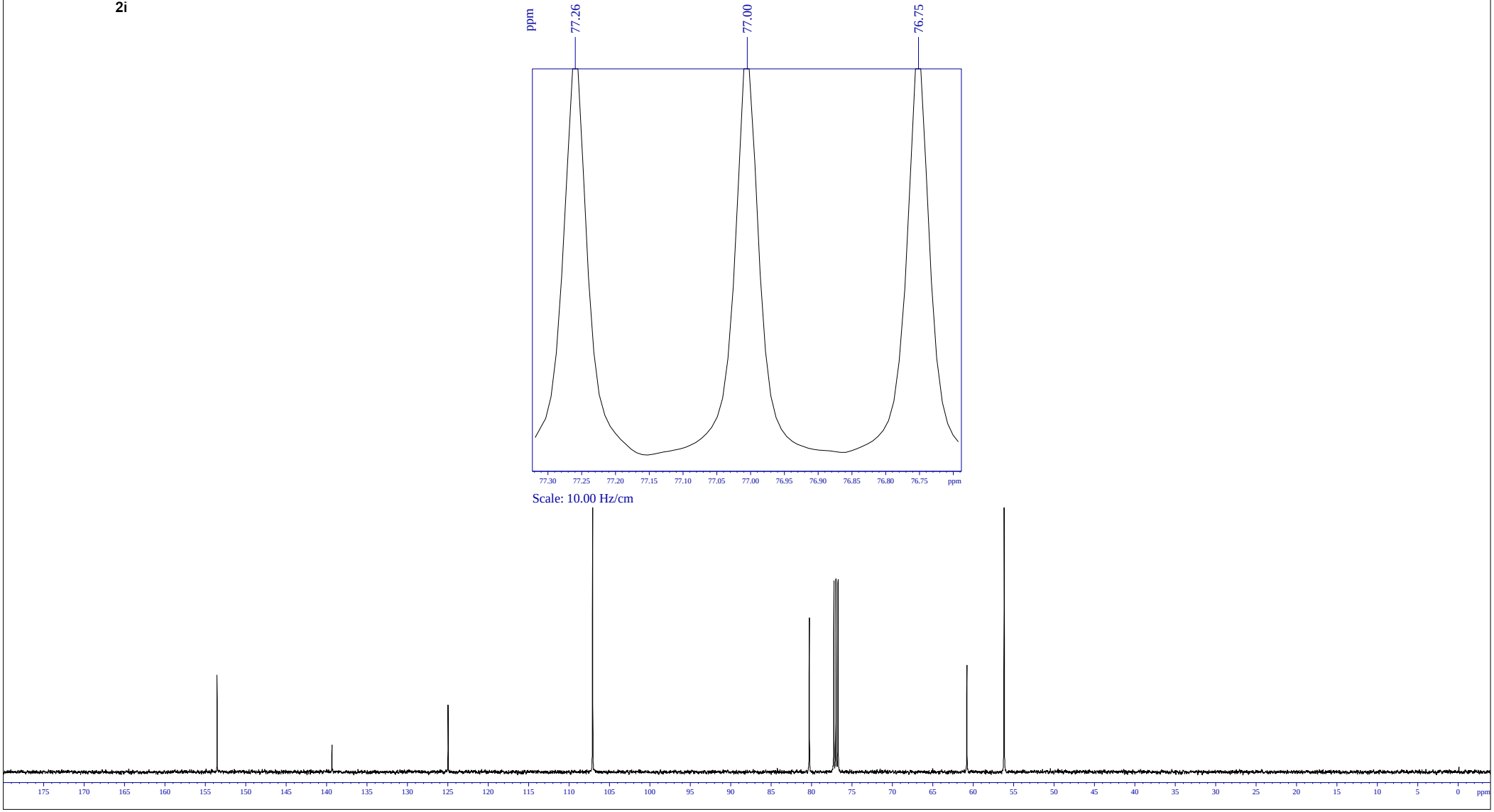
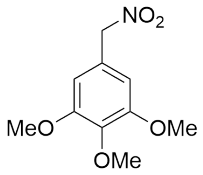


NMR/29317564



2i

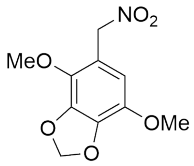
Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	10895.0	19307.602	153.5300	3.63
2	12681.7	17525.709	139.3608	1.03
3	14492.7	15719.601	124.9990	2.57
4	16748.3	13470.071	107.1112	14.00
5	20128.9	10098.553	80.3016	5.77
6	20512.5	9715.990	77.2595	7.40
7	20544.6	9683.966	77.0049	7.41
8	20576.6	9652.087	76.7514	7.41
9	22586.5	7647.526	60.8115	4.12
10	23168.2	7067.374	56.1983	12.32

The Best Applied NMR!

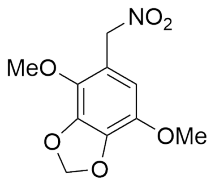
NMR/29210024

Found protons = 36 impurity* = 2.6 %

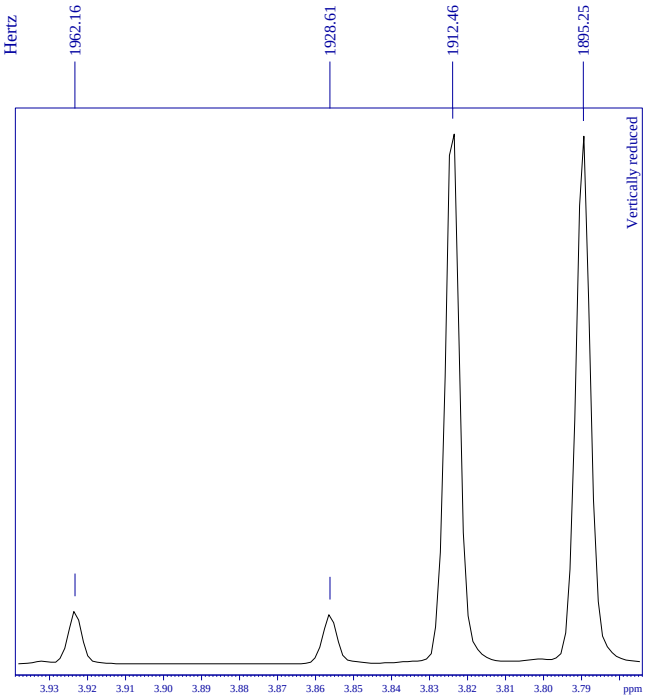


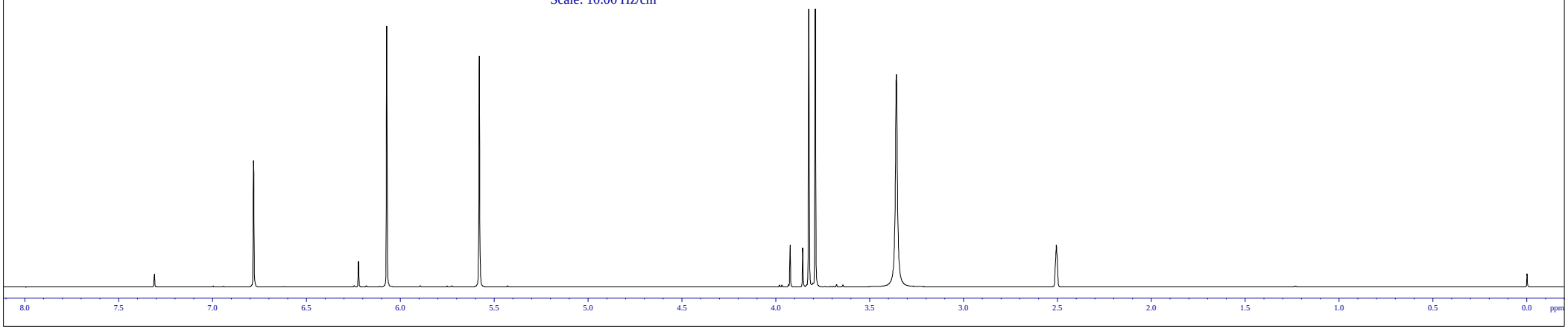
2j

NMR/29210024

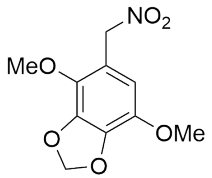


2j





NMR/29210024



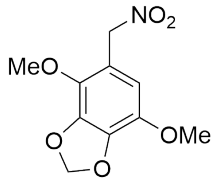
2j

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	8752.1	3655.900	7.3099	0.46
2	9185.2	3391.555	6.7813	4.65
3	9643.1	3112.131	6.2226	0.94
4	9766.4	3036.867	6.0722	9.75
5	10170.3	2790.309	5.5792	8.57
6	11527.2	1962.162	3.9233	1.54
7	11582.1	1928.608	3.8562	1.44
8	11608.6	1912.461	3.8239	16.00
9	11636.8	1895.248	3.7895	15.52
10	11990.9	1679.114	3.3574	7.75
11	12689.2	1252.917	2.5052	1.53
12	14742.0	0.001	0.0000	0.49

The Best Applied NMR!

NMR/29210024

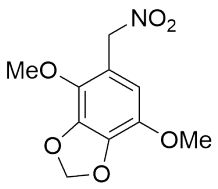


2j

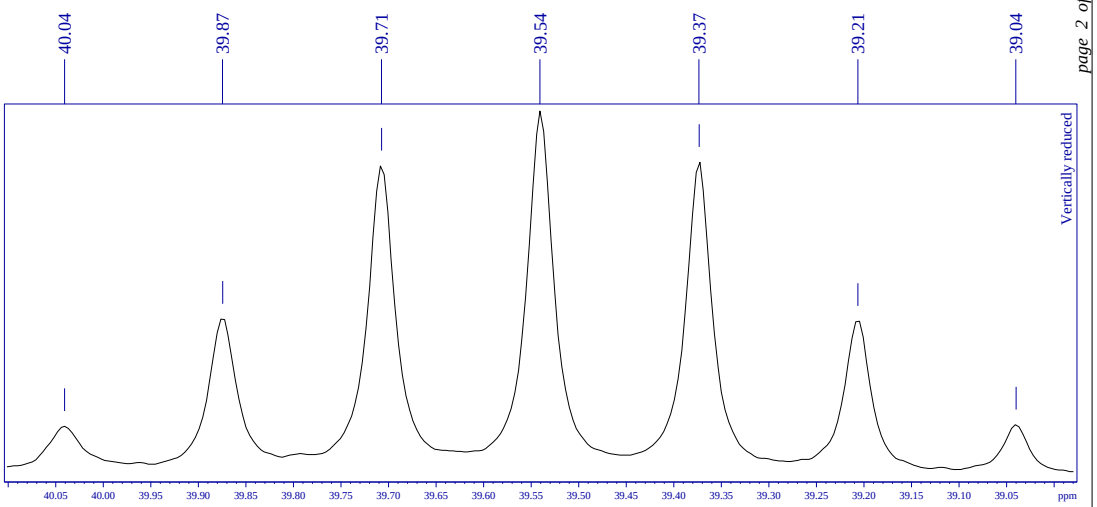
138.47
138.09
137.87
136.95
115.75
111.40
102.16
74.35
59.69
56.68
40.04
39.87
39.71
39.54
39.37
39.21
39.04

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

NMR/29210024



2j



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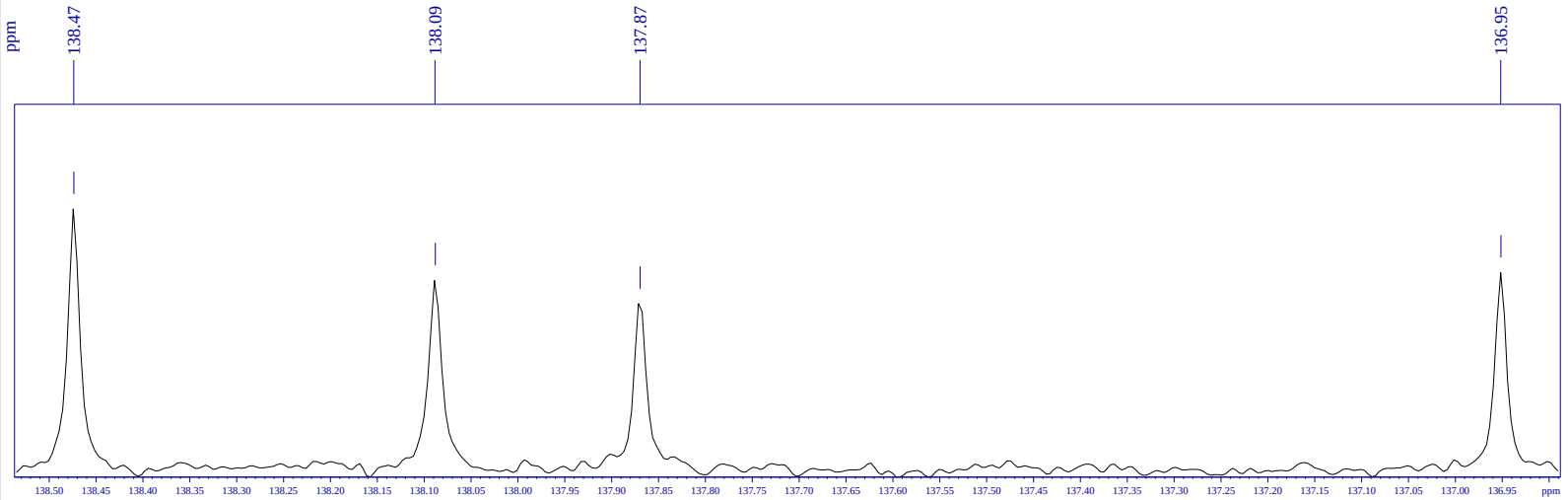
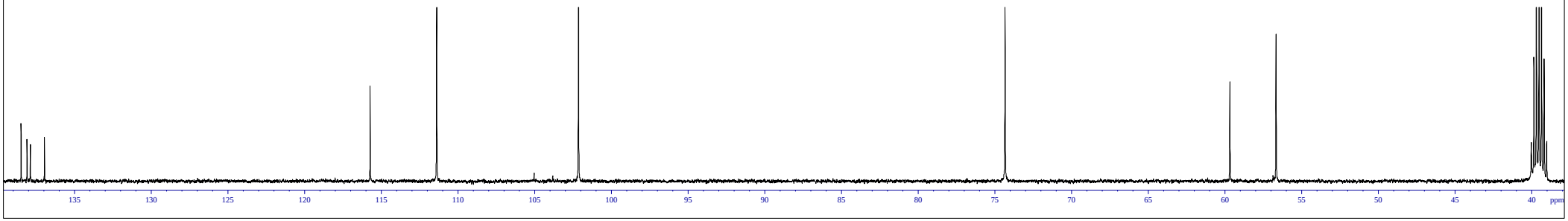
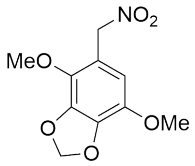




NMR/29210024

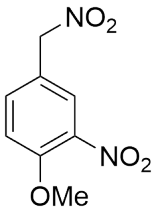


2j

Peaks List

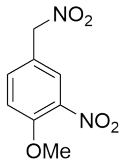
#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	23995.1	17414.150	138.4737	3.40
2	24096.1	17365.664	138.0881	2.47
3	24153.4	17338.186	137.8696	2.22
4	24394.0	17222.715	136.9514	2.57
5	29951.8	14555.871	115.7452	5.61
6	31089.4	14010.032	111.4048	13.42
7	33512.1	12847.537	102.1609	11.70
8	40800.7	9350.206	74.3509	12.08
9	44643.1	7506.496	59.6901	5.84
10	45431.9	7127.965	56.6801	8.64
11	49792.9	5035.428	40.0407	2.26
12	49836.5	5014.519	39.8744	7.35
13	49880.2	4993.507	39.7073	14.49
14	49924.0	4972.498	39.5403	17.00
15	49967.8	4951.507	39.3733	14.66
16	50011.5	4930.507	39.2064	7.26
17	50055.1	4909.589	39.0400	2.33

NMR/29210026

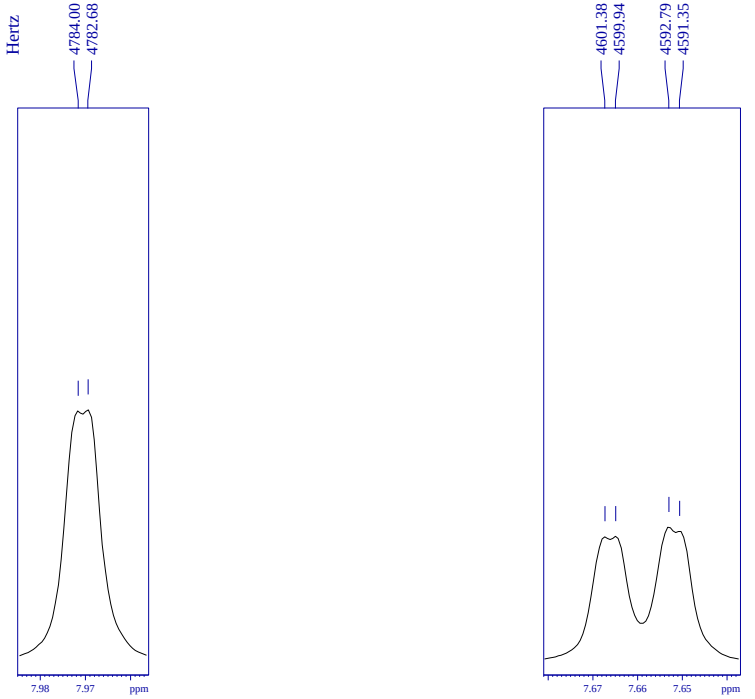


2l

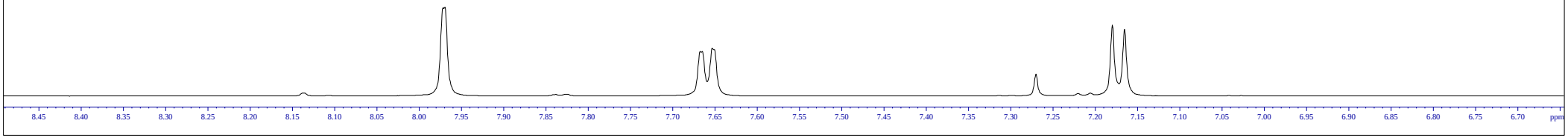
NMR/29210026



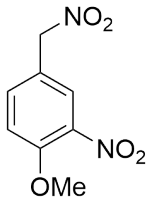
2l



Scale: 10.00 Hz/cm



NMR/29210026



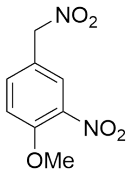
2l

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	16431.2	4783.996	7.9716	3.31
2	16434.8	4782.676	7.9694	3.33
3	16929.0	4601.377	7.6673	1.67
4	16933.0	4599.936	7.6649	1.67
5	16952.4	4592.795	7.6530	1.79
6	16956.3	4591.355	7.6506	1.74
7	17727.0	4308.693	7.1796	2.65
8	17750.5	4300.052	7.1652	2.51
9	20585.5	3260.206	5.4325	10.04
10	22922.5	2402.981	4.0041	16.00
11	29474.1	−0.120	−0.0002	2.33

The Best Applied NMR!

NMR/29210026

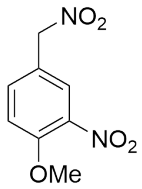


2l

153.65
139.02
135.46
127.15
121.23
113.71
77.67
76.76
76.55
76.34
56.29

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

NMR/29210026



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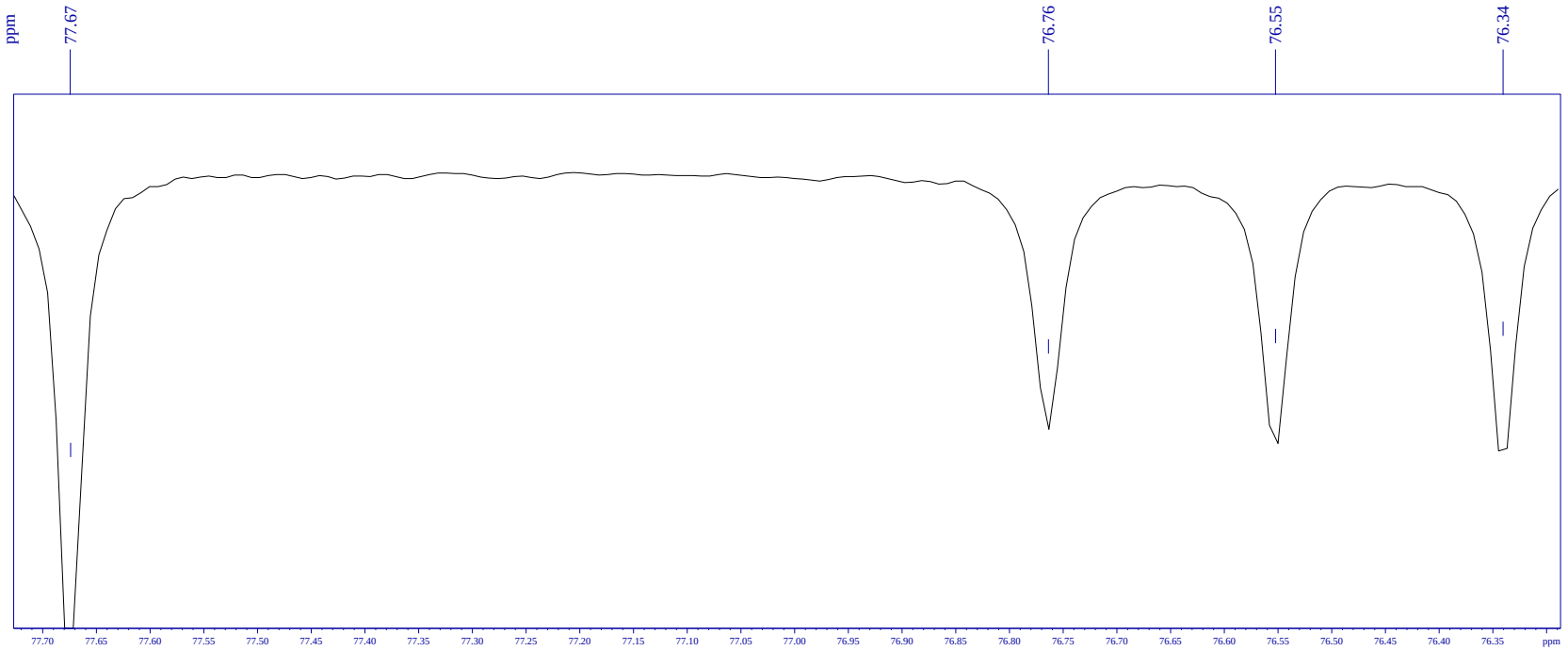
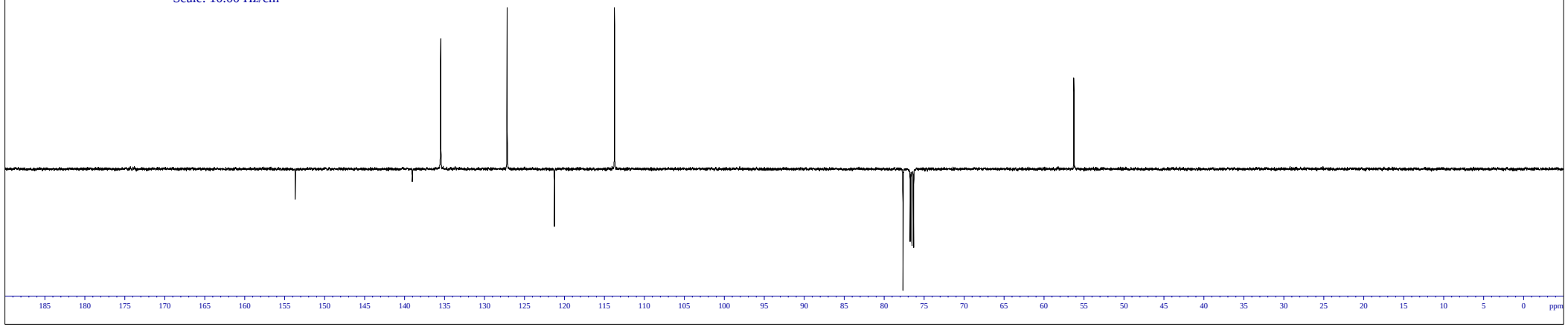
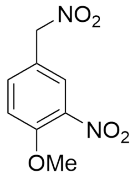


Scale: 10.00 Hz/cm



NMR/29210026



2l

Peaks List

#	Address [points]	Frequency [Hz]	[ppm]	Intensity [cm]
1	11944.6	23186.892	153.6544	−2.07
2	13797.6	20977.900	139.0159	−0.82
3	14248.1	20440.837	135.4569	8.53
4	15299.9	19187.030	127.1482	10.58
5	16049.1	18293.911	121.2297	−3.77
6	17001.0	17159.182	113.7101	14.00
7	21562.7	11721.231	77.6740	−9.74
8	21677.9	11583.864	76.7637	−4.74
9	21704.7	11551.963	76.5523	−5.09
10	21731.5	11520.002	76.3405	−5.34
11	24269.2	8494.746	56.2928	6.07