

SUPPLEMENTARY DATA

Waste-to-useful: Biowaste-derived heterogeneous catalyst for a green and sustainable Henry reaction

Kalyani Rajkumari, Diparjun Das, Gunindra Pathak and

Samuel Lalthazuala Rokhum*

Department of Chemistry, National Institute of Technology Silchar, Silchar-10,

Assam, India

* Corresponding author. Tel.: +91 3842 242915; fax: +91 3842-224797; email
address: rokhum@che.nits.ac.in (L. Rokhum)

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Table S1: Metallic and non-metallic concentration in recovered MAPA after 10th recyclability test as given by XRF analysis.

Sl No	Name of the component in the MAPA sample	% Mass fraction in fresh MAPA	% Mass fraction in recovered MAPA after 10 th recycles.
1.	K ₂ O	65.110	64.76
2.	SiO ₂	10.864	2.38
3.	CaO	7.787	4.42
4.	P ₂ O ₅	6.067	1.80
5.	SO ₃	2.857	0.79
6.	MgO	2.427	0.69
7.	Fe ₂ O ₃	1.152	1.29
8.	Al ₂ O ₃	0.737	0.19
9.	MnO	0.227	0.40
10.	CuO	0.192	0.092

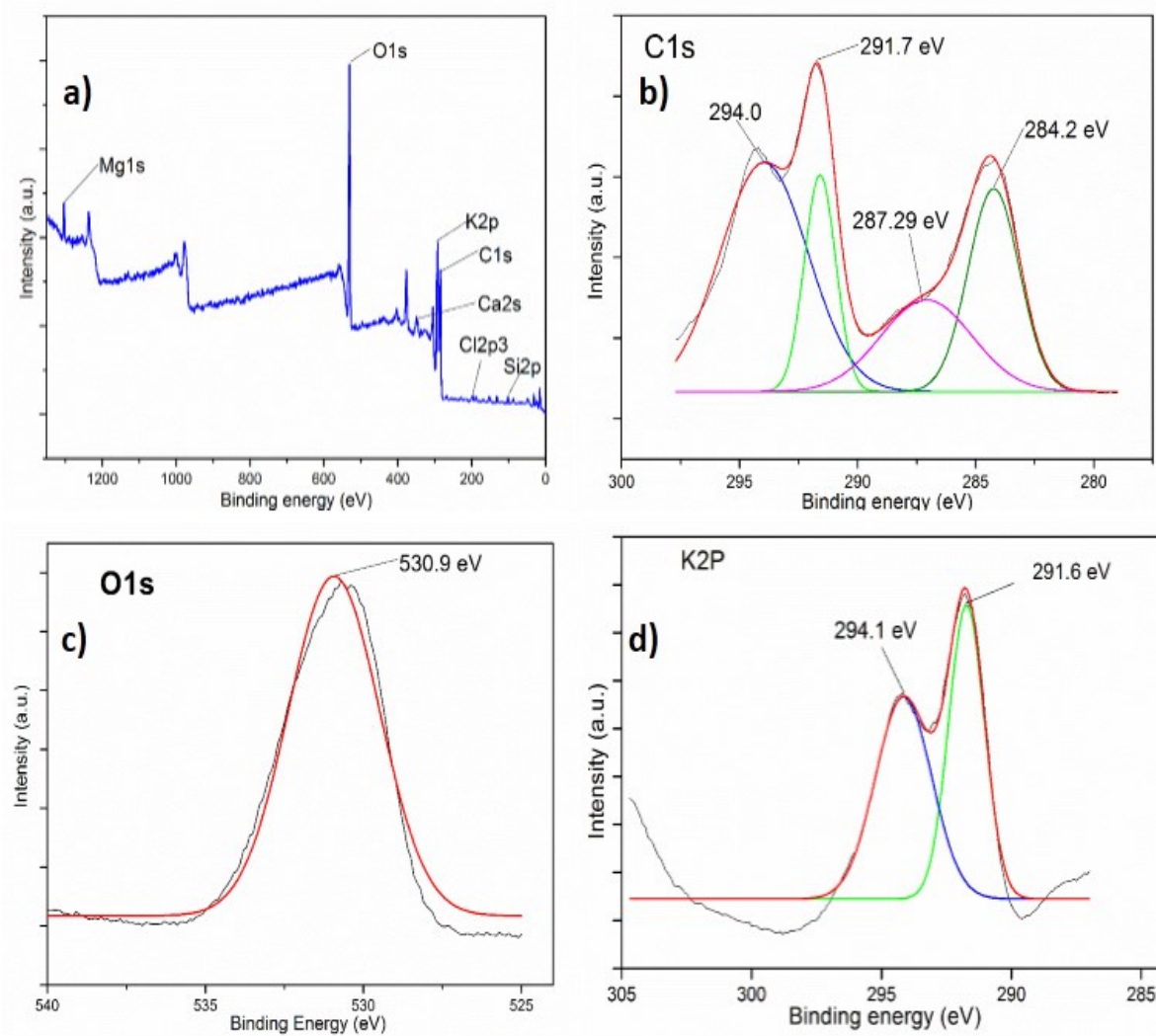


Fig: S1 a) XPS survey spectrum, b) C1s, c) O1s, d) K2p spectra of recovered MAPA.

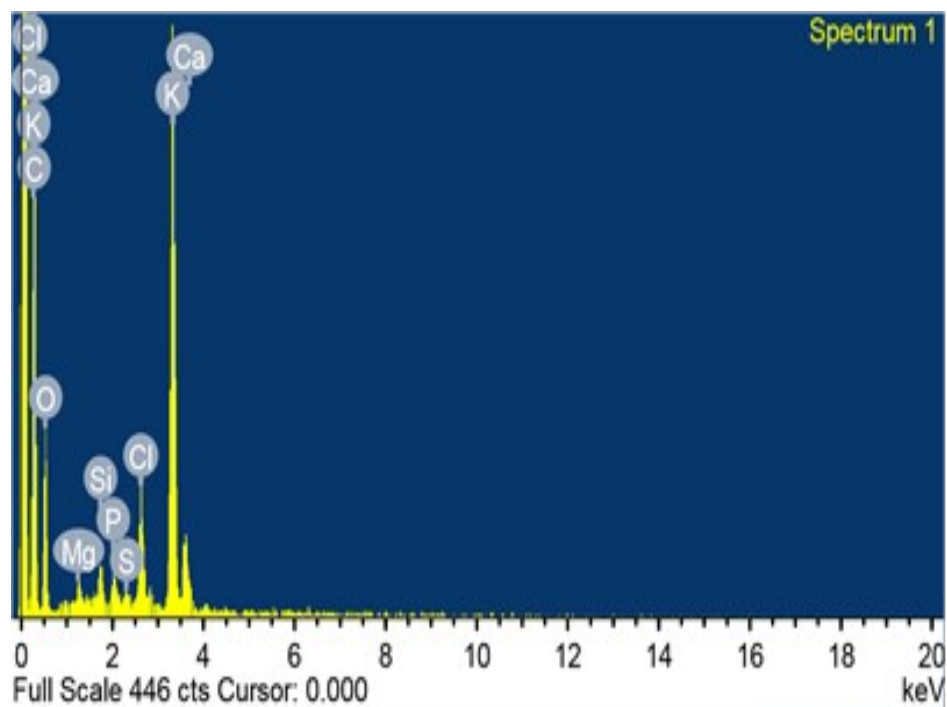


Fig. S2: EDS analysis of the recovered catalyst (after 10th cycle).

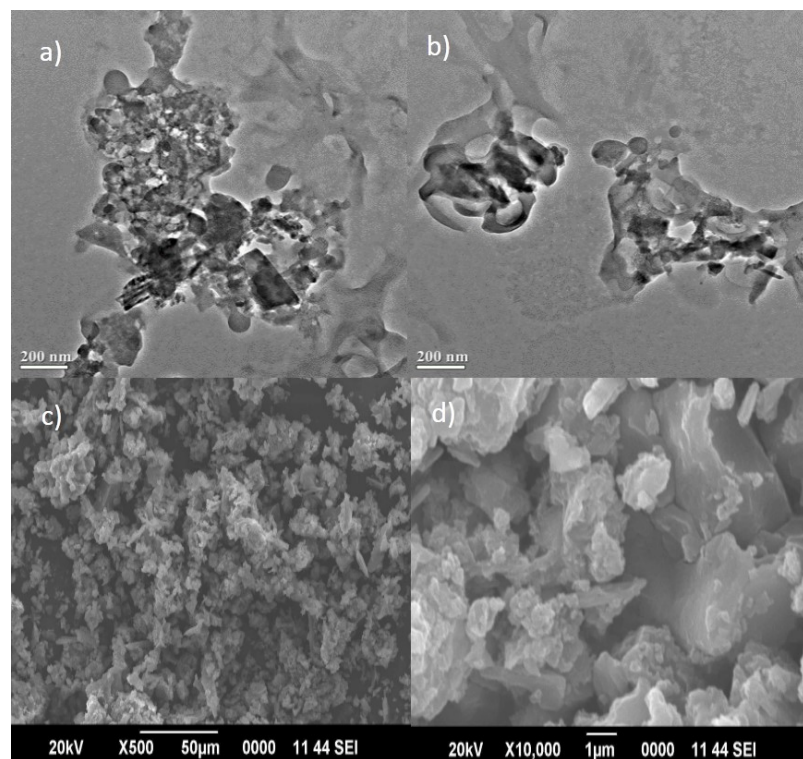


Fig S3: a-b) TEM and b-c) SEM images of the recycled catalyst.

Calculation of Atom Economy and E-factor:

$$\text{Atom economy} = \frac{\text{Mass of atoms in desired product}}{\text{Mass of atoms in reactant}}$$

$$= \frac{0.212g}{(0.151 + 0.061)g} \times 100\%$$
$$= 100\%$$

$$\text{E-factor} = \frac{\text{Total waste (g)}}{\text{Product (g)}}$$

Mass in the process = Aldehyde + Nitroalkane + Catalyst

$$= (0.151 + 0.061 + 0.020) \text{ g}$$

$$= 0.232 \text{ g}$$

$$\text{Product} = 0.208 \text{ g}$$

$$\text{Total waste} = (0.232 - 0.208) \text{ g}$$

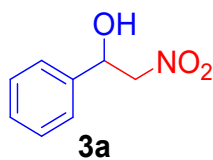
$$= 0.024 \text{ g}$$

$$\text{E-factor} = \frac{0.024 \text{ g}}{0.208 \text{ g}}$$

$$= 0.115$$

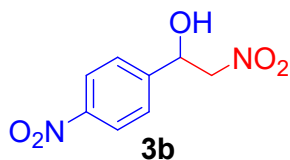
Spectral data:

2-Nitro-1-phenylethanol (Table 4, entry 3a)



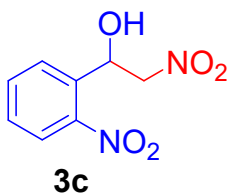
Colorless oil, ^1H NMR (400 MHz, CDCl_3): δ 2.68 (s, 1H), δ 4.61-4.32 (m, 2H), δ 5.41-5.28 (m, 1H), δ 7.47-7.20 (m, 5H). ^{13}C NMR (100 MHz, CDCl_3): δ 73.08, 77.71, 113.65, 117.63, 127.14, 135.08; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3429, 3018, 2408, 1553, 1433, 1221, 1035, 963, 777, 677.

2-nitro-1-(4-nitrophenyl)ethan-1-ol (Table 4, entry 3b)



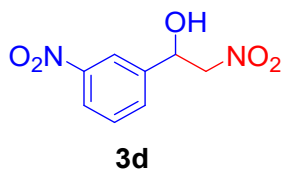
Brown solid, ^1H NMR (CDCl_3 , 400 MHz): δ 3.62 (1H, s), δ 4.61 (2H, d, $J=40$ Hz), δ 5.62 (1H, m), δ 7.61 (2H, d, $J=8$ Hz), δ 8.21 (2H, d, $J=7.6$ Hz); ^{13}C NMR (CDCl_3 , 125 MHz): δ 69.98, 80.67, 124.13, 127.01, 145.31, 147.95; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3320, 3075, 2965, 2885, 1608, 1532, 1508, 1430, 1358, 1320, 1112, 1058, 765, 654.

2-Nitro-1-(2-nitrophenyl)ethan-1-ol (Table 4, entry 3c)



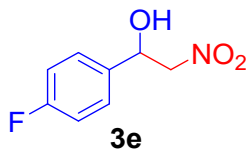
Oily liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 4.58-4.52 (m, 1H), δ 4.87 (1H, d, $J=13.6$ Hz), δ 6.05 (1H, d, $J=9.2$ Hz), δ 7.56 (1H, t, $J=8$ Hz), δ 7.97 (1H, d, $J=7.6$), δ 8.07 (1H, d, $J=8$ Hz), δ 8.13 (1H, d, $J=7.6$ Hz), ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 134.37, 134.16, 133.81, 131.31, 129.64, 128.77, 124.95, 66.79; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3305, 3025, 2939, 2889, 2787, 1553, 1432, 1379, 1323, 1281, 1178, 1121, 845.

2-nitro-1-(3-nitrophenyl)ethanol (3d)



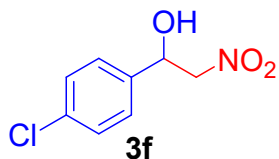
Yellow solid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.25 (1H, s), δ 4.49–4.71 (2H, m), δ 5.61–5.64 (1H, m), δ 7.61 (1H, t, $J=8$ Hz), δ 7.79 (1H, d, $J=8$ Hz), δ 8.19 (1H, d, $J=8$ Hz), δ 8.31 (1H, s); ^{13}C NMR (CDCl_3 , 125 MHz): δ 69.84, 80.71, 121.14, 123.77, 130.14, 132.15, 140.35, 148.45; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3304, 3075, 2956, 2870, 1612, 1545, 1511, 1437, 1368, 1329, 1095, 1058, 775, 668.

1-(4-Fluorophenyl)-2-nitroethan-1-ol (3e)



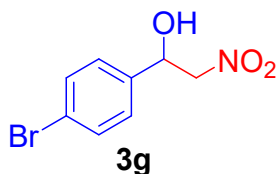
Light yellow liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 2.92 (1H, s), δ 4.59–4.50 (1H, m), δ 4.59–4.50 (1H, m), δ 4.78 (1H, t, $J=6.8$ Hz), δ 5.47–5.44 (m, 1H), δ 7.12 (2H, d, $J=8.4$ Hz), 7.39–7.37 (1H, dd, $J=8$ Hz), δ 7.41–7.39 (1H, dd, $J=8$ Hz); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 161.66, 133.86, 127.74, 116.14, 115.93, 70.32; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3425, 3012, 2909, 2100, 1704, 1526, 1132, 879, 745.

1-(4-Chlorophenyl)-2-nitroethan-1-ol (3f)



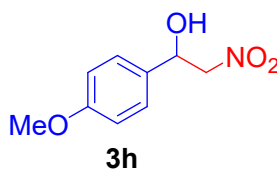
Colorless liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 2.57 (1H, s), δ 4.56 (1H, d, $J=3.6\text{ Hz}$), δ 4.80 (1H, t, $J=7.2\text{ Hz}$), δ 5.44-5.41 (1H, m), δ 7.18 (2H, d, $J=8.4\text{ Hz}$), δ 7.35 (1H, d, $J=8.4\text{ Hz}$); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 70.29, 127.37, 129.18, 128.80, 132.67, 138.37; IR (KBr, $\nu_{\text{max}}/\text{cm}^{-1}$): 3408, 3035, 2979, 2989, 2756, 1536, 1428, 1389, 1326, 1275, 1185, 1115, 840, 756.

1-(4-Bromophenyl)-2-nitroethan-1-ol (3g)



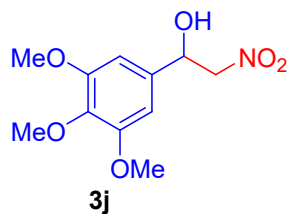
Pale yellow oil, ^1H NMR (CDCl_3 , 400 MHz): δ 2.03 (1H, s), δ 4.50-4.57 (1H, m), δ 4.79 (1H, t, $J=7.2\text{ Hz}$), δ 5.44-5.41 (1H, m), δ 7.29 (2H, d, $J=8.4\text{ Hz}$), δ 7.54 (1H, d, $J=8.4\text{ Hz}$); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 70.33, 122.89, 127.68, 129.12, 132.14, 138.05; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3415, 3025, 2939, 2889, 2787, 1550, 1440, 1381, 1331, 1280, 1184, 1120, 840.

1-(4-methoxyphenyl)-2-nitroethan-1-ol (3h)



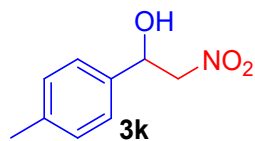
Yellow liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 2.92 (1H, s), δ 3.80 (3H, s), δ 4.46 (1H, d, $J=12.4\text{ Hz}$); δ 4.58 (1H, t, $J=10\text{ Hz}$), δ 5.382 (1H, d, $J=8\text{ Hz}$), δ 6.90 (2H, d, $J=7.6\text{ Hz}$), δ 7.30 (2H, d, $J=7.2\text{ Hz}$); ^{13}C NMR (CDCl_3 , 125 MHz): δ 55.35, 70.65, 80.26, 114.35, 127.3, 128.55, 130.55, 159.96; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3378, 3083, 2943, 2896, 2780, 1612, 1536, 1425, 1182, 1050, 790, 663.

2-nitro-1-(3,4,5-trimethoxyphenyl)ethan-1-ol (3j)



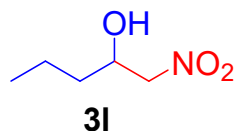
Brown solid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.25 (1H, s), δ 3.82 (3H, s), δ 3.86 (6H, s), δ 4.482-4.631 (2H, m), δ 5.38-5.41 (1H, m), δ 6.60 (2H, s); ^{13}C NMR (CDCl_3 , 125 MHz): δ 56.13, 60.85, 81.33, 102.69, 133.97, 137.93, 153.58; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3308, 3025, 2960, 2856, 2775, 1608, 1556, 1423, 1110, 1043, 771.

2-Nitro-1-(p-tolyl)ethan-1-ol (3k)



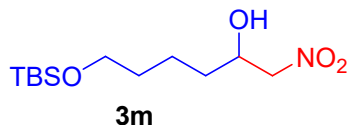
Light yellow oil, ^1H NMR (CDCl_3 , 400 MHz): δ 1.52 (1H, s), 2.34 (3H, s), δ 4.55-4.61 (1H, m), δ 4.71-4.74 (1H, m), δ 5.38-5.41 (1H, m), δ 7.26-7.27 (1H, dd, $J=7.6\text{Hz}$); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 21.16, 70.90, 125.89, 129.67, 129.93, 138.89, 139.04; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3429, 3018, 2408, 1553, 1433, 1221, 1035, 963, 777, 677.

1-Nitropentan-2-ol (3l)



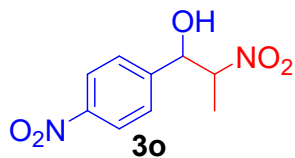
Yellow liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 0.96 (1H, t, $J=6.4$ Hz), δ 1.40-1.53 (1H, s), 3.19 (1H, s), 3.91 (1H, s), 4.48-4.57 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 15.95, 18.89, 35.14, 65.19, 86.47; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3361, 2846, 1614, 1520, 1206, 1171, 853, 736.

6-((tert-butyldimethylsilyl)oxy)-1-nitrohexan-2-ol (3m)



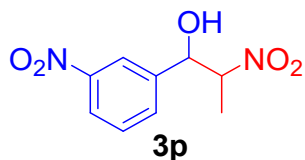
Colorless oil; ^1H -NMR (400 MHz, CDCl_3 , TMS): δ 0.26 (6H,s), δ 0.83 (9H, s), δ 1.49–1.39 (6H, m), δ 3.64–3.57 (1H, m), δ 3.89 (2H, t, $J \frac{1}{4} 7.2$ Hz), δ 4.14–4.11 (1H, m), δ 4.51–4.41 (1H, m), δ 5.25 (1H, s); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 80.60, 68.58, 62.83, 36.01, 33.35, 32.13, 25.95, 21.66, 5.31; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 1753, 1628, 1528, 1201, 1119, 865, 769, 678.

2-Nitro-1-(4-nitrophenyl)propan-1-ol (3o)



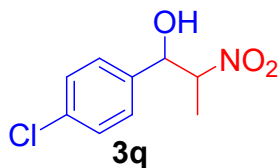
Reddish liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.36-1.38 (1H, dd, $J=6.8$ Hz), δ 1.46-1.48 (2H, dd, $J=6.8$ Hz), δ 3.26 (1H, s), δ 4.71-4.82 (1H, m), δ 5.21 (1H, d, $J=8.4$ Hz), δ 7.62 (2H, d, $J=4.8$ Hz), δ 8.21-8.22 (1H, dd, $J=4$ Hz), δ 8.23-8.24 (1H, dd, $J=4.4$ Hz); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 16.16, 75.03, 87.88, 124.36, 128.01, 147.71, 148.11; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3435, 3330, 3025, 2889, 2789, 1547, 1440, 1320, 1284, 1223, 1185.

2-Nitro-1-(3-nitrophenyl)propan-1-ol (3p)



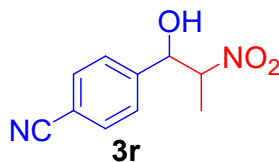
Reddish liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.37-1.39 (1.5H, dd, $J=6$ Hz), δ 1.48-1.50 (1.5H, dd, $J=6$ Hz), δ 4.77-4.88 (1H, m), δ 5.22 (1H, d, $J=8.4$ Hz), δ 7.58-7.64 (1H, dd, $J=8.4$ Hz), δ 7.78 (1H, d, $J=7.6$ Hz), δ 8.50 (1H, d, $J=7.6$ Hz) 8.69 (1H, s); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 16.11, 74.97, 88.0, 121.95, 123.84, 133.21, 135.00, 140.83, 148.38; IR (KBr, pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3445, 3310, 3055, 2819, 2779, 1536, 1441, 1327, 1282, 1242, 1158.

1-(4-Chlorophenyl)-2-nitropropan-1-ol (3q)



Colorless oil, ^1H NMR (CDCl_3 , 400 MHz): δ 1.47 (3H, d, $J=6.8$ Hz), δ 4.69-4.75 (1H, m), δ 5.01 (1H, d, $J=8.8$ Hz), δ 7.52 (2H, d, $J=7.6$ Hz), δ 7.81 (2H, d, $J=7.6$ Hz); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 16.33, 31.77, 88.25, 127.40, 128.32, 131.47, 136.87; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3401, 3025, 2949, 2889, 2786, 1546, 1438, 1381, 1323, 1281, 1179, 1121, 845, 786.

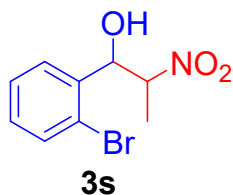
4-(1-Hydroxy-2-nitropropyl)benzonitrile (3r)



Light green liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.33-1.35 (1.5 H, d, $J=6.8$ Hz), δ 1.45-1.47 (1.5 H, dd, $J=6.8$ Hz), δ 4.66-4.77 (1H, m), δ 5.12 (1H, d, $J=8.8$ Hz), δ 7.86 (2H, d, $J=8$ Hz), δ 8.01

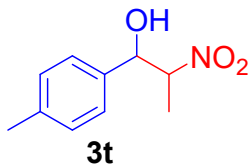
(2H, d, J=8 Hz); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 15.95, 73.13, 87.93, 112.07, 118.32, 126.97, 132.57, 143.87; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3555, 3059, 2914, 2055, 1976, 1528, 1448, 1280, 845.

1-(2-Bromophenyl)-2-nitropropan-1-ol (3s)



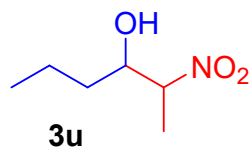
Yellow liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.36-1.37 (1.5 H, dd, J=4 Hz), δ 1.38-1.40 (1.5 H, dd, J=6.8 Hz), δ 4.81-4.87 (1H, m), δ 5.55 (1H, d, J= 6.8 Hz), δ 5.75 (1H, s), δ 7.2 (1H, t, J= 5.2 Hz), δ 7.45 (1H, d, J=6.8 Hz), δ 7.55 (1H, t, J=7.2 Hz), δ 7.59 (1H, d, J=7.6 Hz); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 16.01, 73.91, 88.33, 121.53, 129.94, 130.32, 132.32, 137.98; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3351, 2957, 2863, 2756, 1527, 1379, 883.

2-Nitro-1-(p-tolyl)propan-1-ol (3t)



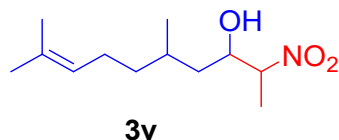
Colorless liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.37-1.39 (1.5 H, dd, J=6 Hz), δ 1.48-1.50 (1.5 H, dd, J=6 Hz), δ 4.77-4.85 (1H, m), δ 5.22 (1H, d, J= 8.4 Hz), δ 5.56 (1H, s), δ 7.58-7.64 (1H, dd, J= 8.4 Hz), δ 7.78 (1H, d, J=7.6 Hz), δ 8.69 (1H, s); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 16.11, 74.97, 88.0, 121.53, 129.95, 123.84, 133.21, 135.00, 140.38, 148.83; IR (KBr pellet, pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): ν 3445, 3310, 3055, 2819, 2779, 1536, 1441, 1327, 1282, 1242, 1158.

2-nitrohexan-3-ol (3u)



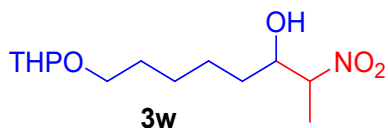
Light yellow liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 0.95- 0.98 (3H, m), δ 1.38-1.46 (4H, m), δ 2.047 (3H, d, $J=4.4$), δ 2.69 (1H, s), δ 3.90-3.94 (1H, m), δ 4.18-4.20 (1H, m); ^{13}C NMR (CDCl_3 , 125 MHz): δ 13.74, 16.12, 18.35, 34.91, 71.8, 86.41; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3306, 2946, 2830, 1608, 1536, 1206, 1148, 1035, 838, 755.

5,9-Dimethyl-2-nitrodec-8-en-3-ol (3v)



Colorless liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 0.93 (3H, d, $J=6.8$ Hz), δ 0.96 (3H, dd, $J=6.4$ Hz), δ 1.54 (6H, t, $J=6.4$ Hz), δ 1.06-1.49 (8H, m), δ 1.60 (6H, s), δ 1.68 (6H, s), δ 1.55-1.73 (2H, m), δ 1.95-2.02 (4H, m), δ 2.35-2.39 (1H, m), δ 2.40-2.46 (1H, m), δ 3.94-4.03 (1H, m), δ 4.25-4.34 (1H, m), δ 4.45-4.55 (2H, m), δ 5.06-5.10 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 10.1, 10.2, 17.6, 18.6, 18.7, 20.0, 20.3, 25.14, 25.19, 25.3, 25.7, 28.4, 25.7, 28.6, 28.8, 29.1, 35.7, 36.1, 37.6, 37.8, 40.1, 40.4, 69.8, 70.1, 70.8, 71.1, 86.8, 87.9, 88.4, 124.3, 131.5, 131.6; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3540, 3025, 2925, 1620, 1553, 1454, 1381, 1215.

2-nitro-7-((tetrahydro-2H-pyran-2-yl)oxy)heptan-3-ol (3w)



Light yellow liquid, ^1H NMR (CDCl_3 , 400 MHz): δ 1.39-1.85 (13H, m) , δ 2.51 (1H, s), δ 3.37-3.43 (2H, m), δ 3.48-3.53 (1H, m), δ 3.63-3.78 (2H, m), δ 3.85-3.95 (1H, m), δ 4.48-4.56 (1H, m); ^{13}C -NMR (100 MHz, CDCl_3 , TMS): δ 10.1, 10.2, 17.6, 18.6, 18.7, 20.0, 20.3, 25.14, 25.19, 25.3, 25.7, 28.4, 25.7, 28.6, 28.8, 29.1, 35.7, 36.1, 37.6, 37.8, 40.1, 40.4, 69.8, 70.1, 70.8, 71.1, 86.8, 87.9, 88.4, 124.3, 131.5, 131.6; IR (KBr pellet, $\nu_{\text{max}}/\text{cm}^{-1}$): 3310, 3016, 2940, 1656, 1530, 1403, 1350, 1180, 875, 761.

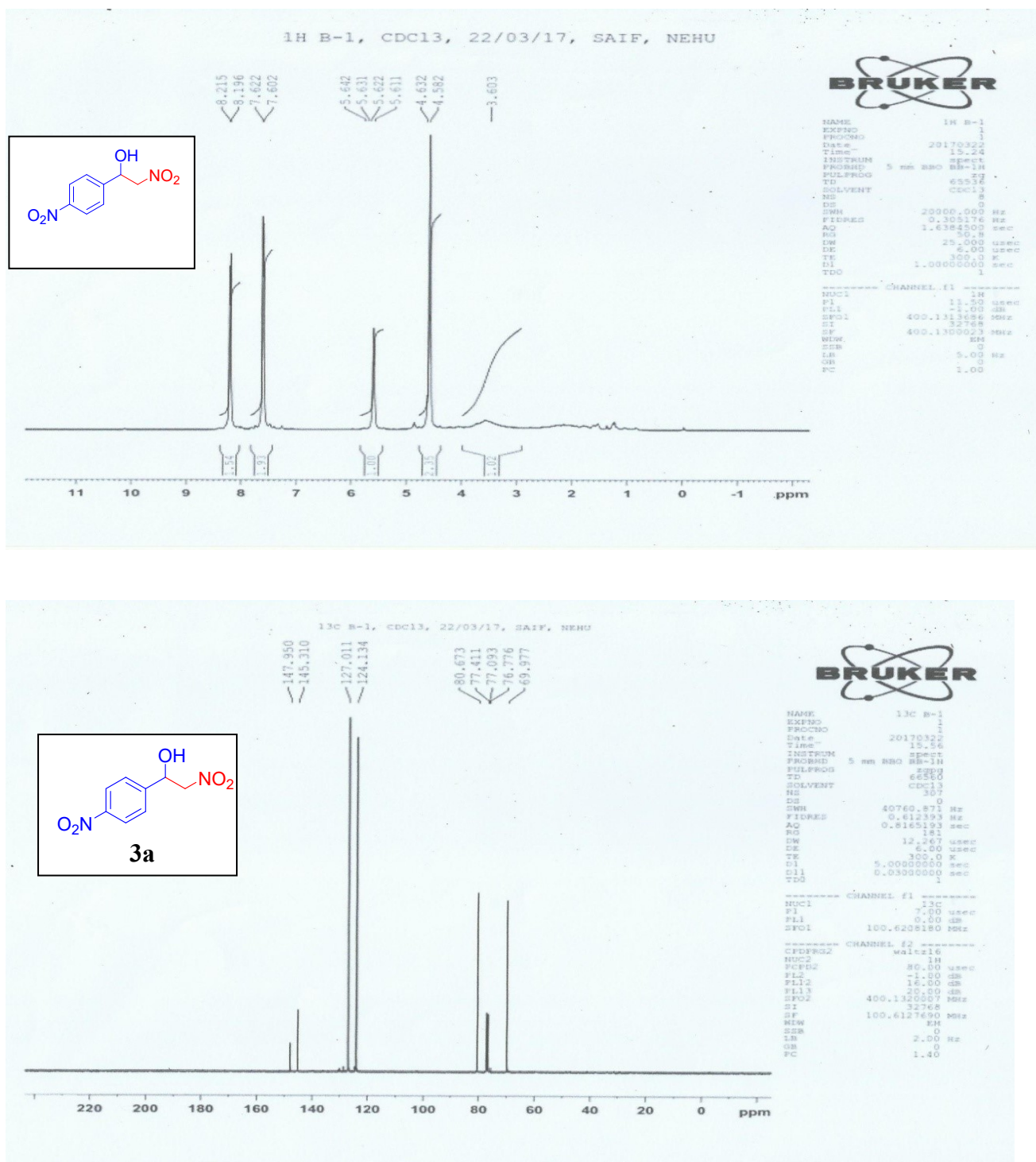
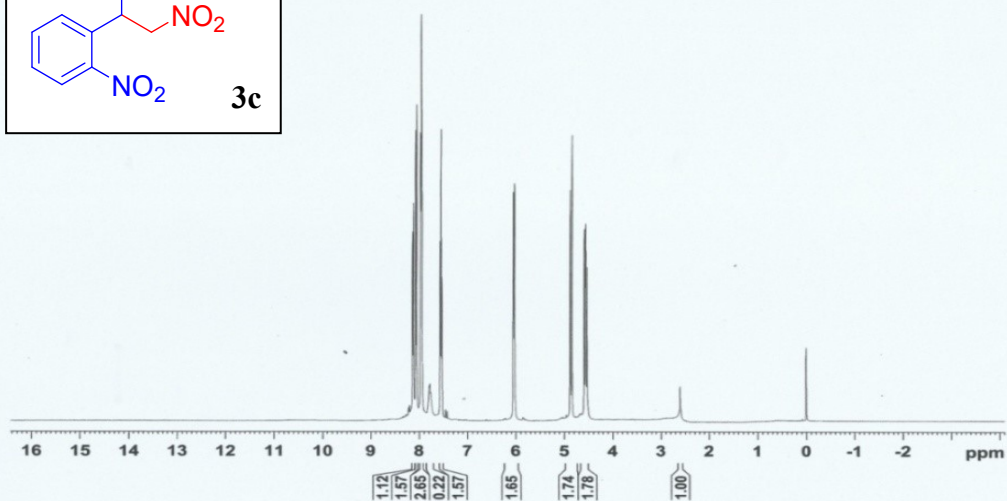
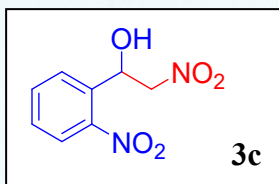


Fig: S4 : ¹H NMR and ¹³C NMR Spectra of 2-nitro-1-(4-nitrophenyl)ethanol (Table 3, Entry 3a)

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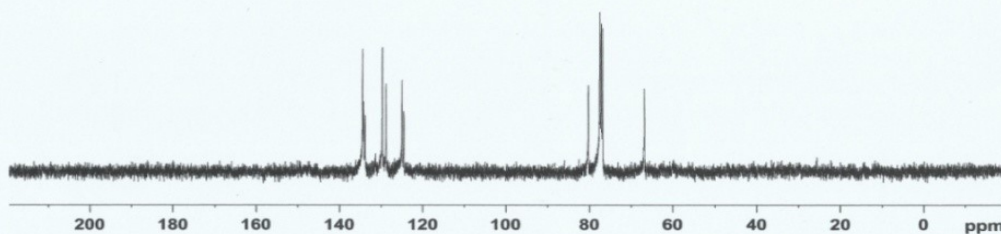
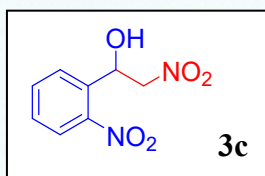
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PROCNO 1

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SOLVENT CDCl3
NS 512
DS 4
SWH 8223.485 Hz
FIDRES 0.125483 Hz
AQ 3.3646387 sec
RG 43.11
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.0000000 sec
TD0

===== CHANNEL f1 =====
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P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2604718 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TI

Signature SIF VIT VELLORE
H41



Current Data Parameters
NAME EXT40616
EXPNO 47
PROCNO 1

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TD 65536
SOLVENT CDCl3
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DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO1 100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW3 0.3509700 W
PLW13 0.28428999 W
SFO2 400.2536010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TI

Fig S5: ^1H NMR and ^{13}C NMR Spectra of 2-Nitro-1-(2-nitrophenyl)ethan-1-ol (Table 3, Entry 3c)

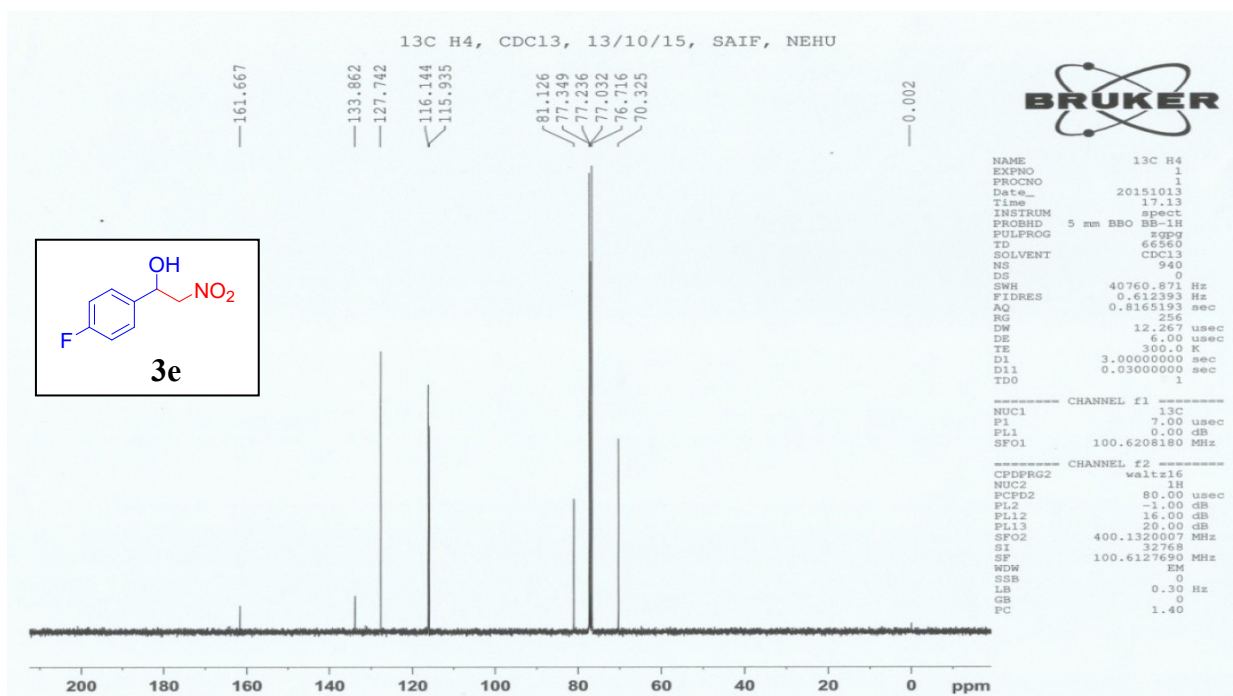
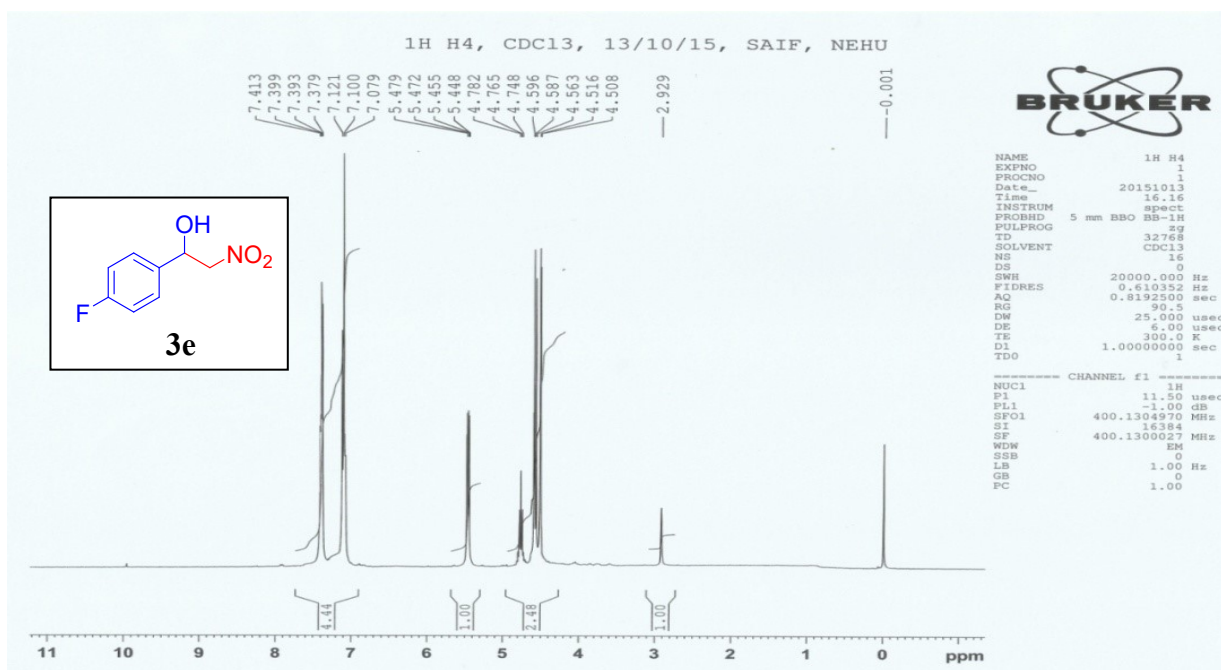


Fig S7: ^1H NMR and ^{13}C NMR Spectra of 1-(4-Fluorophenyl)-2-nitroethan-1-ol (Table 3, Entry 3e)

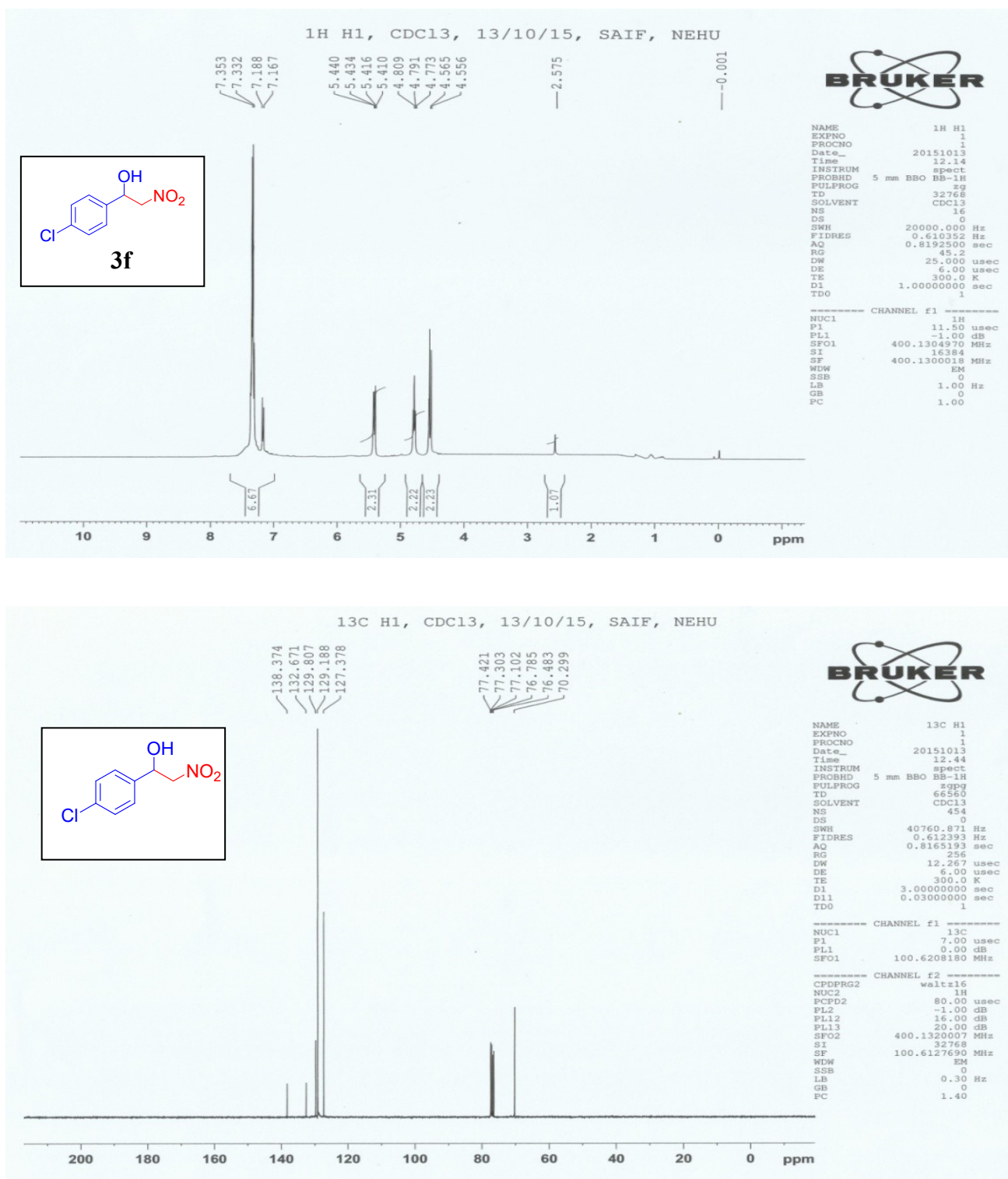


Fig S8:- ^1H NMR and ^{13}C NMR Spectra of 1-(4-Chlorophenyl)-2-nitroethan-1-ol (Table 3, Entry 3f)

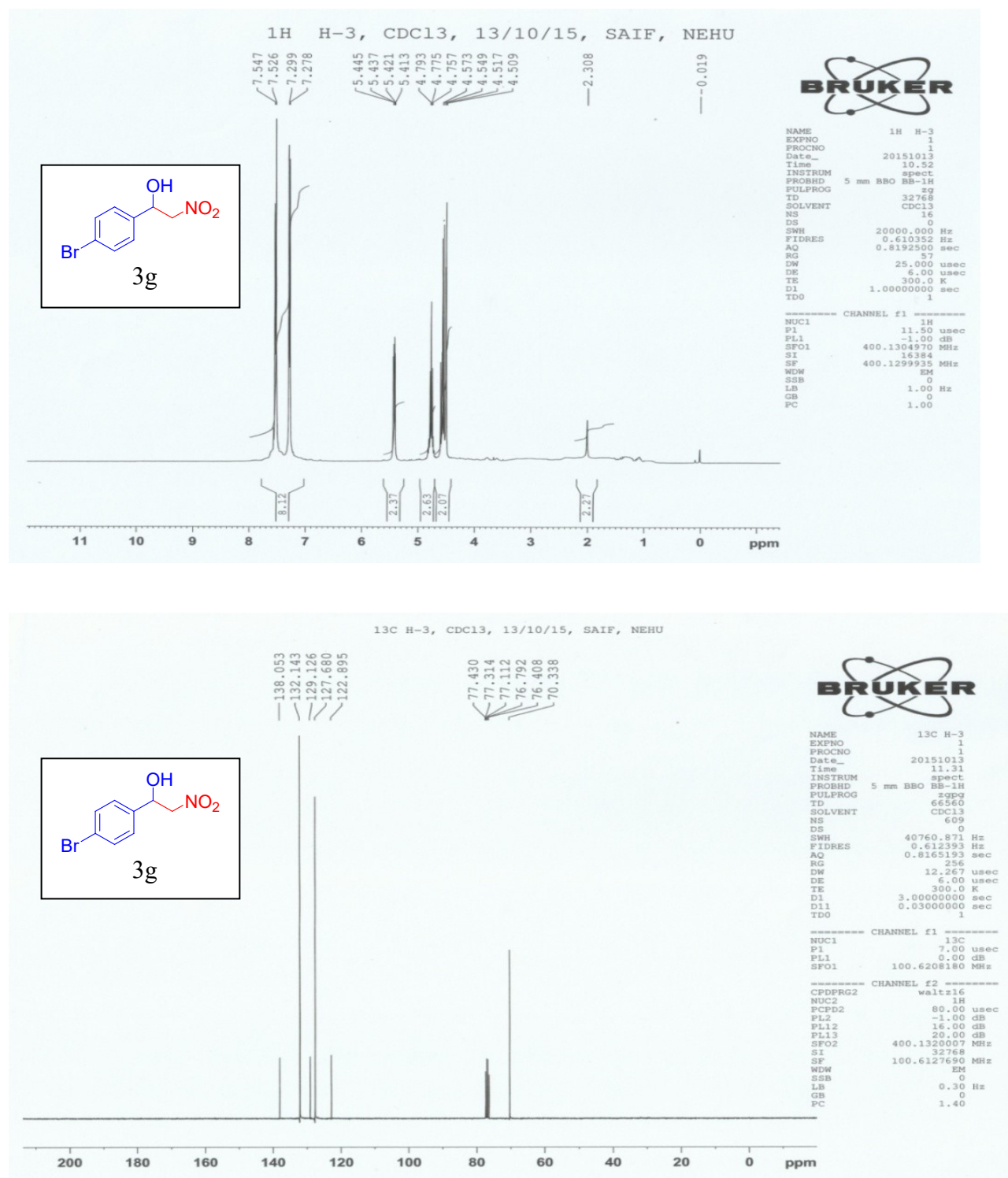


Fig S9: ^1H NMR and ^{13}C NMR Spectra of 1-(4-Bromophenyl)-2-nitroethan-1-ol (Table 3, Entry 3g)

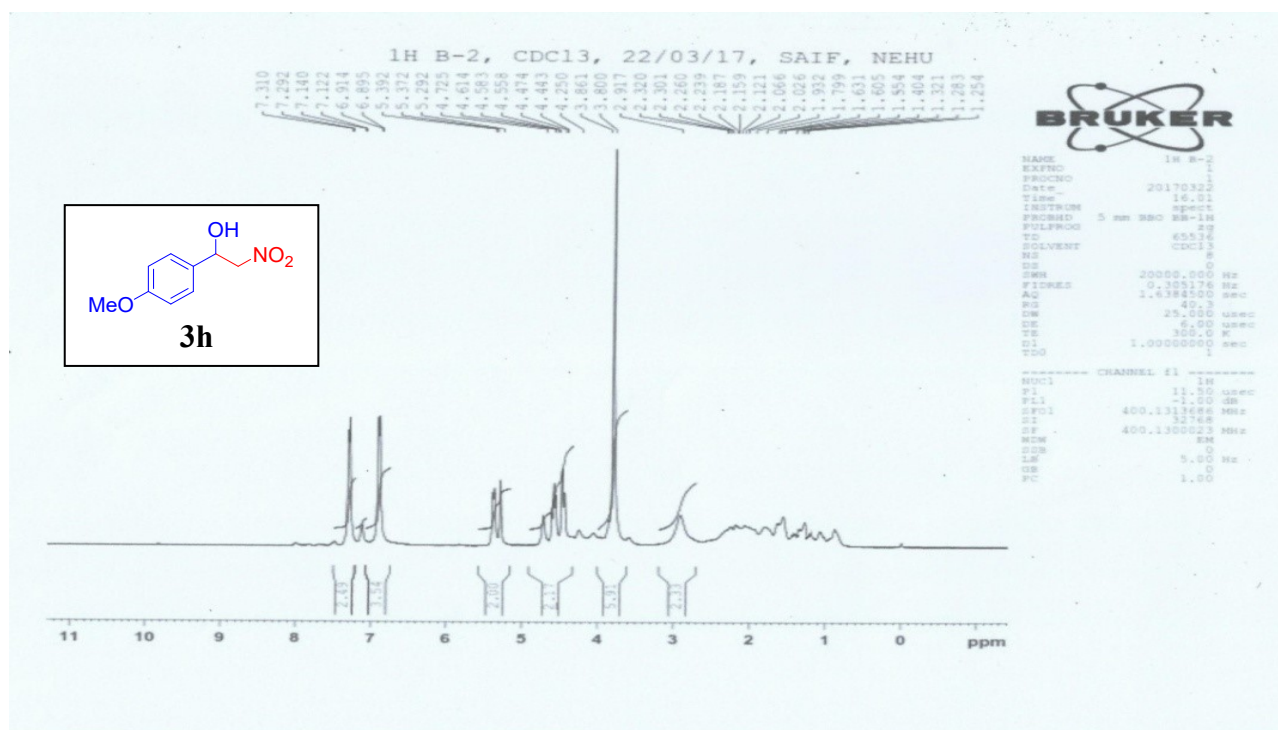
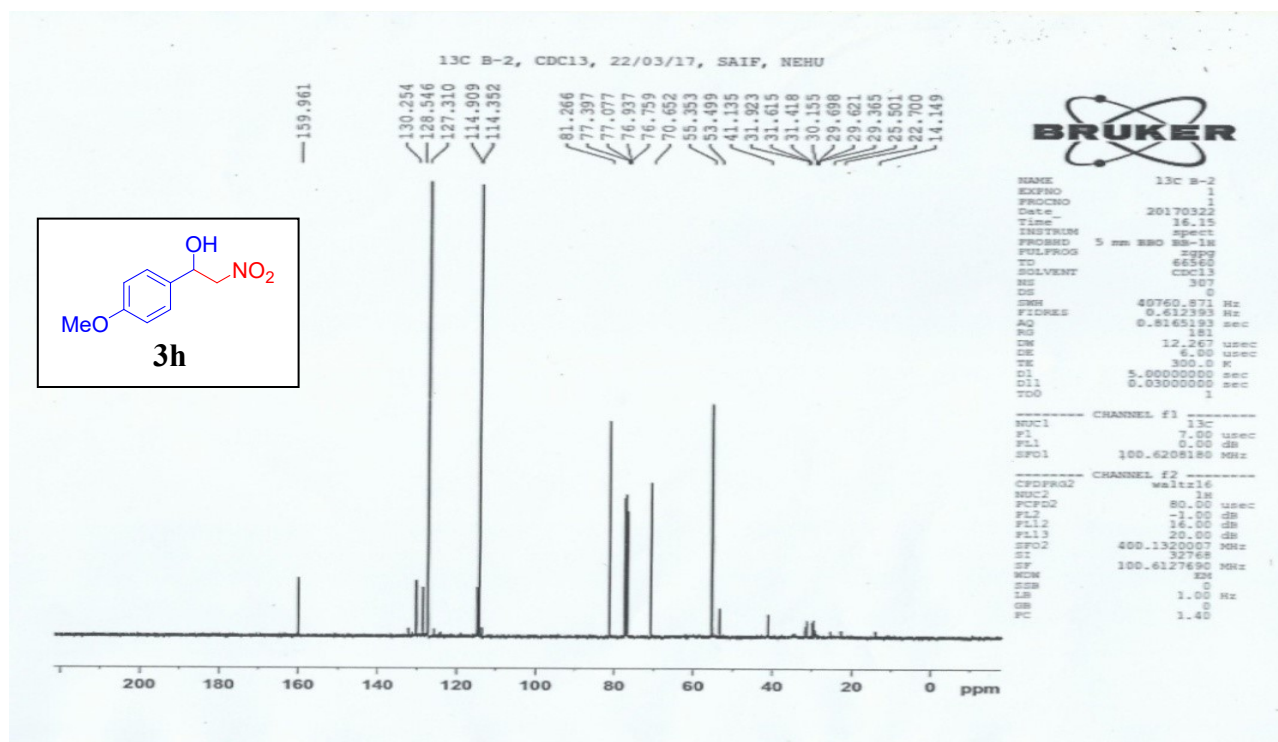


Fig S10: ^1H NMR and ^{13}C NMR Spectra of 1-(4-methoxyphenyl)-2-nitroethan-1-ol (Table 3, Entry 3h)

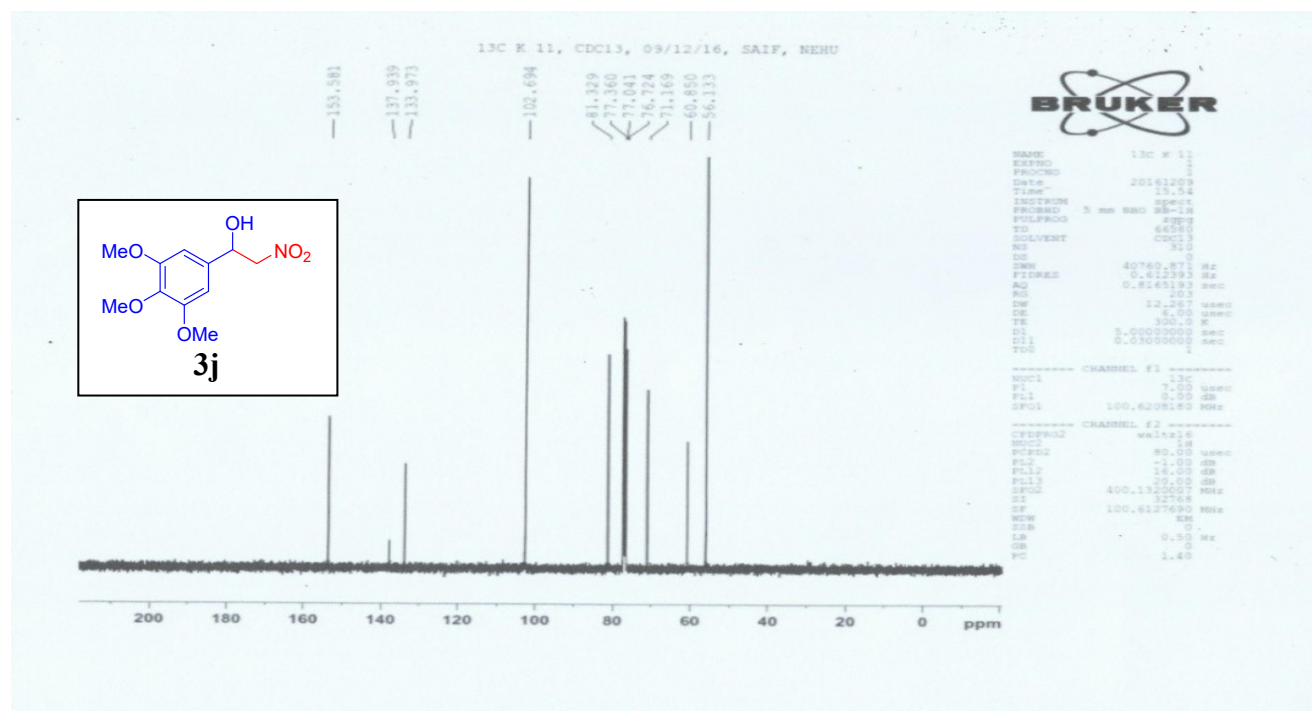
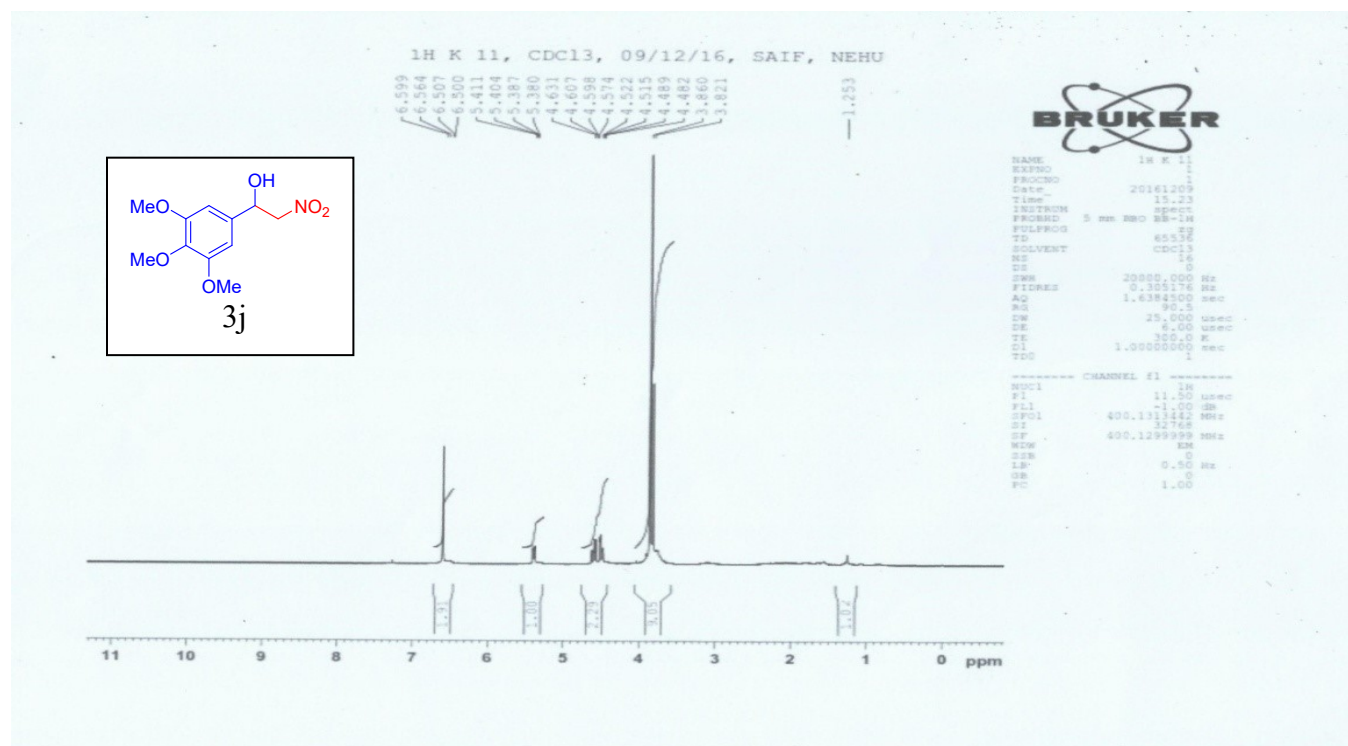


Fig S11: ¹H NMR and ¹³C NMR Spectra of 1-(3, 4-Dimethoxyphenyl)-2-nitroethanol (Table 3, Entry 3j)

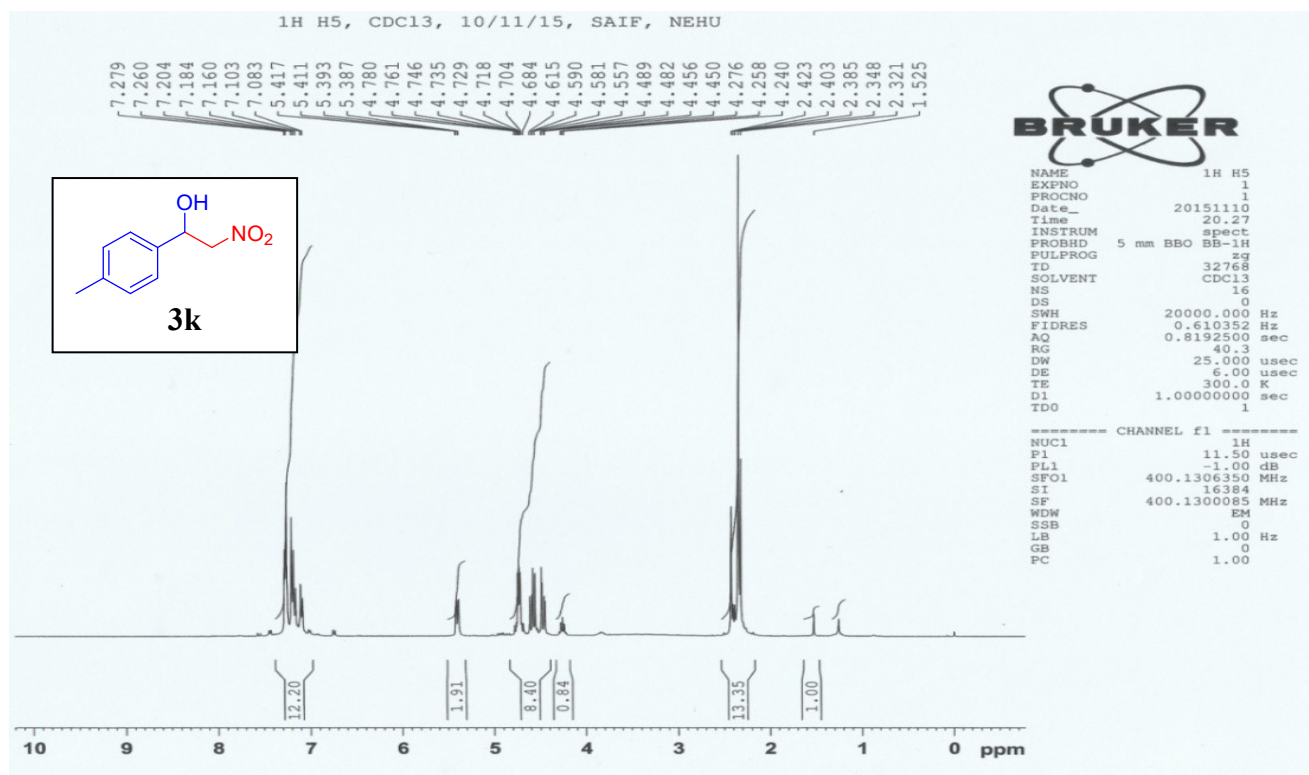
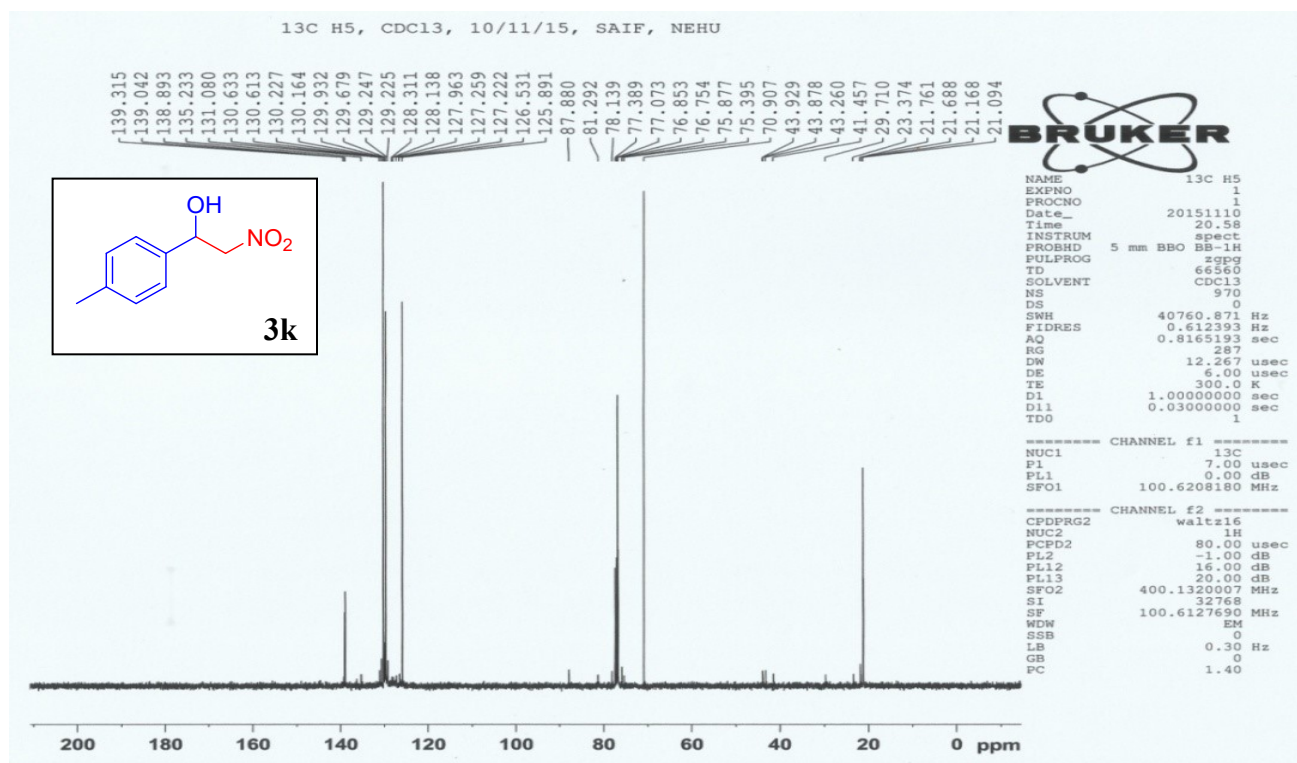
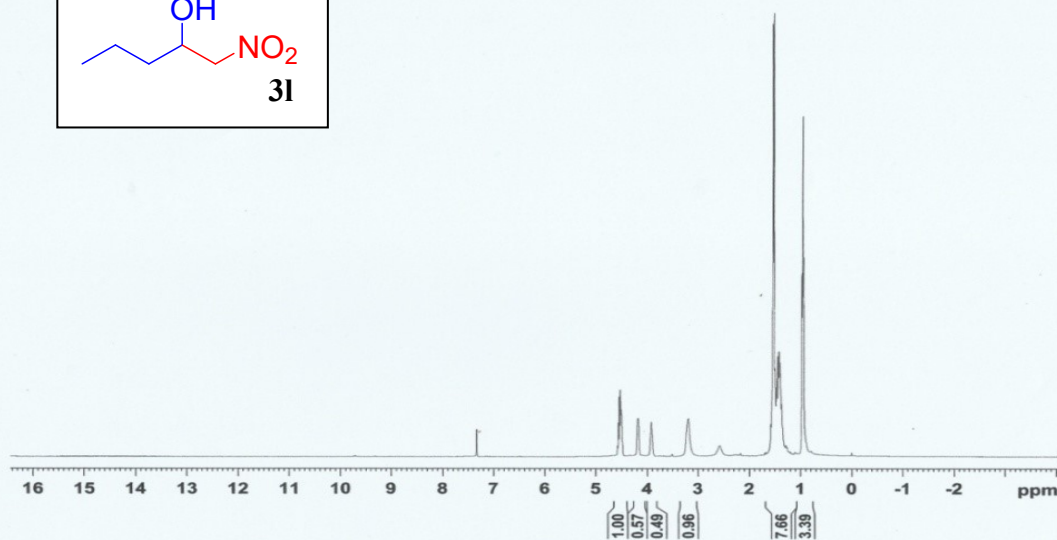
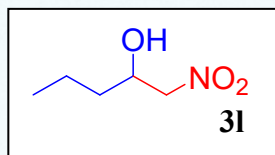


Fig S12: ¹H NMR and ¹³C NMR Spectra of 2-Nitro-1-(p-tolyl)ethan-1-ol (Table 3, Entry 3k)

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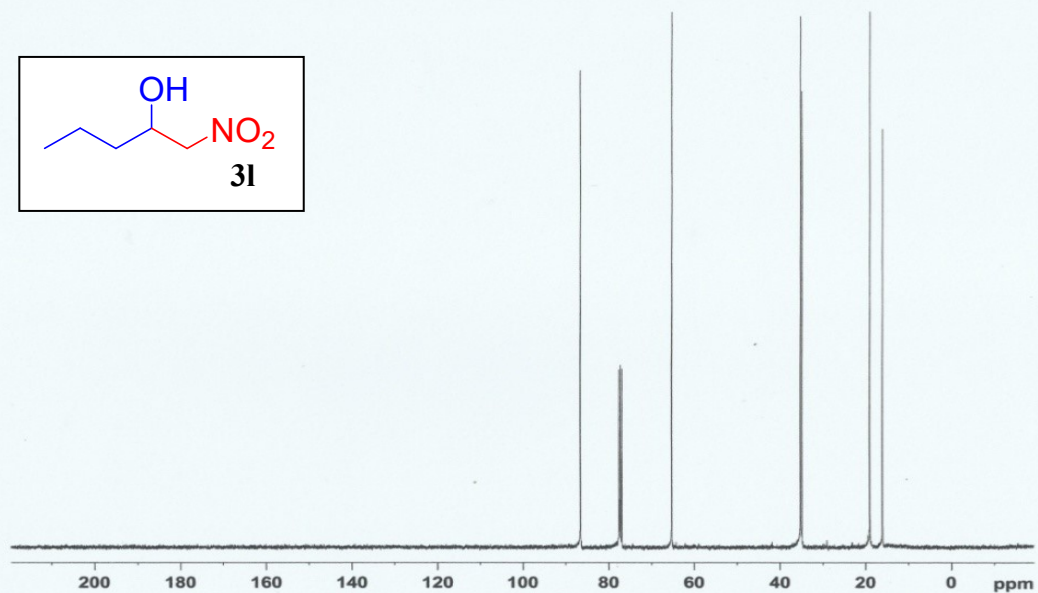
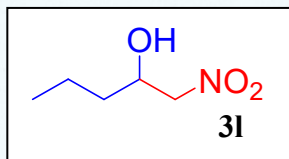
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PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.861287 sec
RG 16.75
DM 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.0000000 sec
TDS 4

===== CHANNEL f1 =====
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P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 45336
SF 400.2579813 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TI

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H43



Current Data Parameters
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EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
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Time 15.12
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 199.6
DM 20.000 usec
DE 6.50 usec
TE 301.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDS 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO1 100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2536610 MHz

F2 - Processing parameters
SI 32768
SF 100.6449940 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TI

Fig S13: ^1H NMR and ^{13}C NMR Spectra of 1-Nitropentan-2-ol (Table 3, Entry 3l)

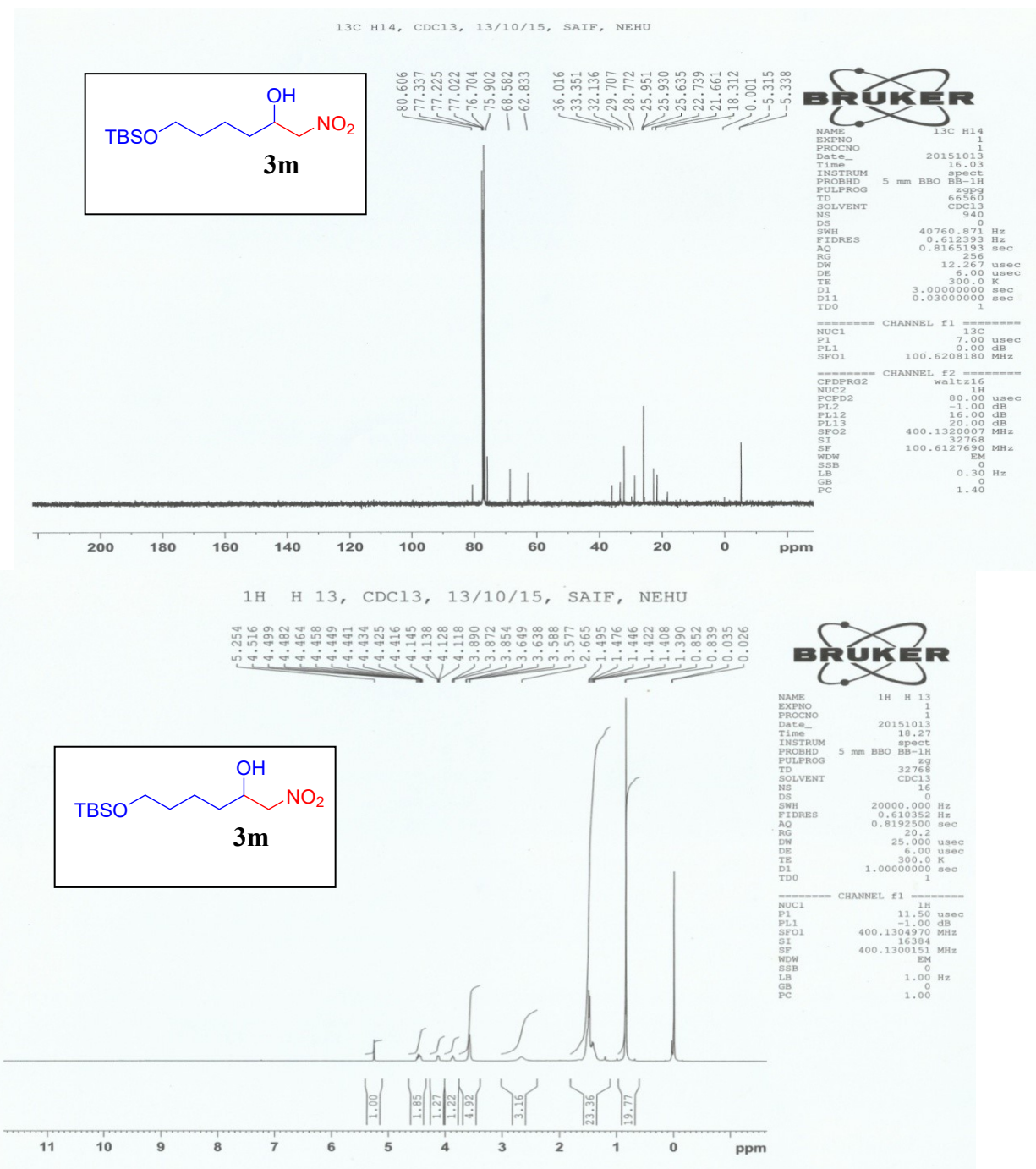


Fig S14: ¹H NMR and ¹³C NMR Spectra of 6-((tert-butyldimethylsilyl)oxy)-1-nitrohexan-2-ol (Table 3, Entry 3m)

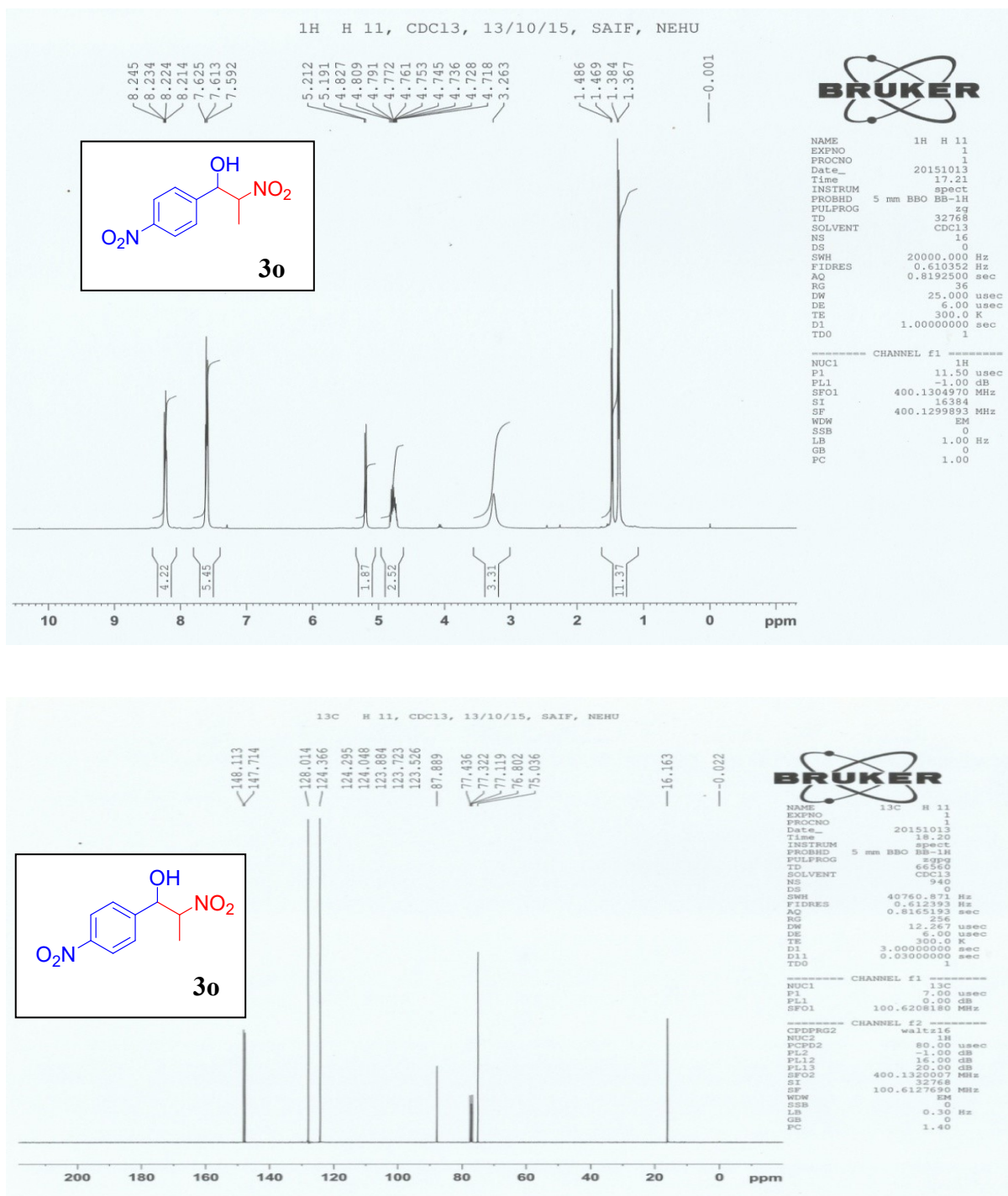
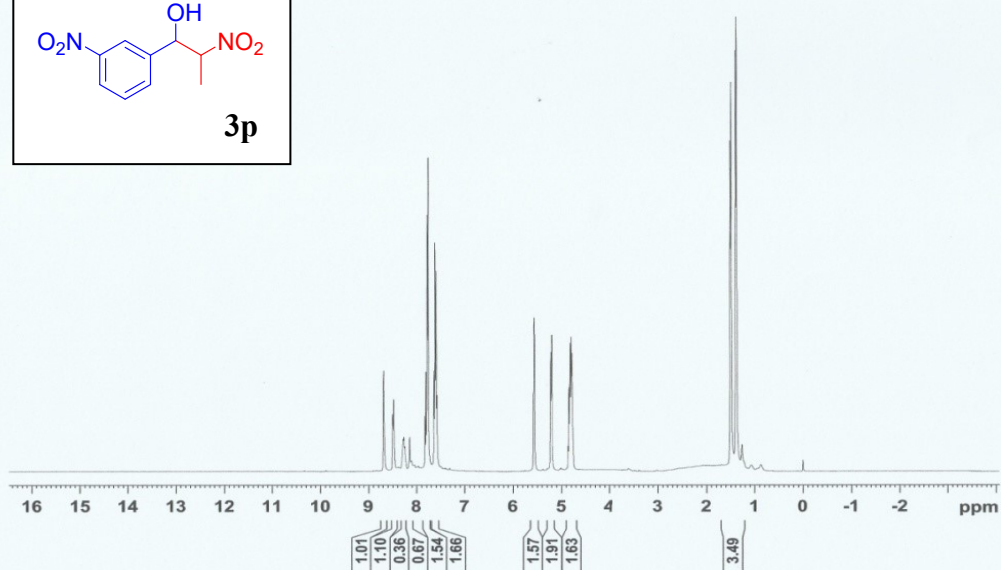
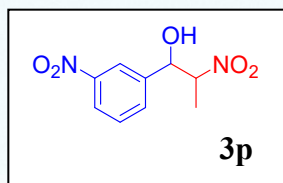


Fig S15 : ^1H NMR and ^{13}C NMR Spectra of 2-Nitro-1-(4-nitrophenyl)propan-1-ol (Table 3, Entry 3o)

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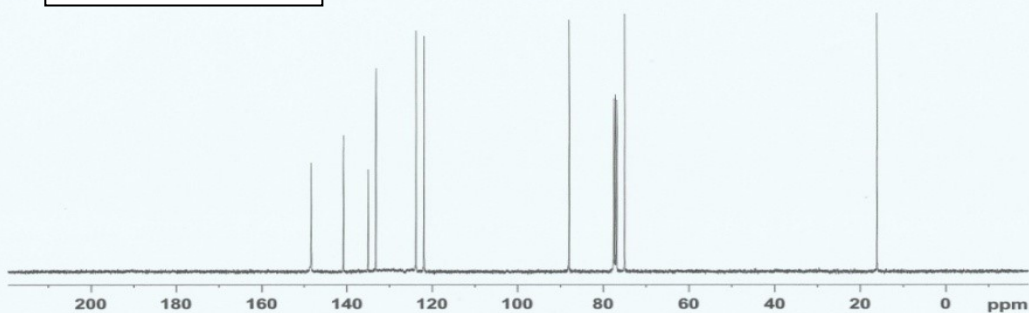
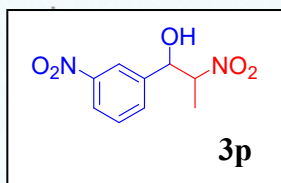
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PROCNO 1

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SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 35.49
DW 60.800 usec
DE 6.50 usec
TE 302.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLN1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2579882 MHz
WDW EM
SSB 0
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GB 0
PC 1.00
TI

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Current Data Parameters
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EXPNO 40
PROCNO 1

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SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLN1 58.0000000 W
SFO1 100.6250182 MHz

===== CHANNEL f2 =====
CFDPFG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLN2 14.0000000 W
PLN12 0.35097000 W
PLN13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TI

Fig S16 : ^1H NMR and ^{13}C NMR Spectra of 2-Nitro-1-(3-nitrophenyl)propan-1-ol (Table 3, Entry 3p)

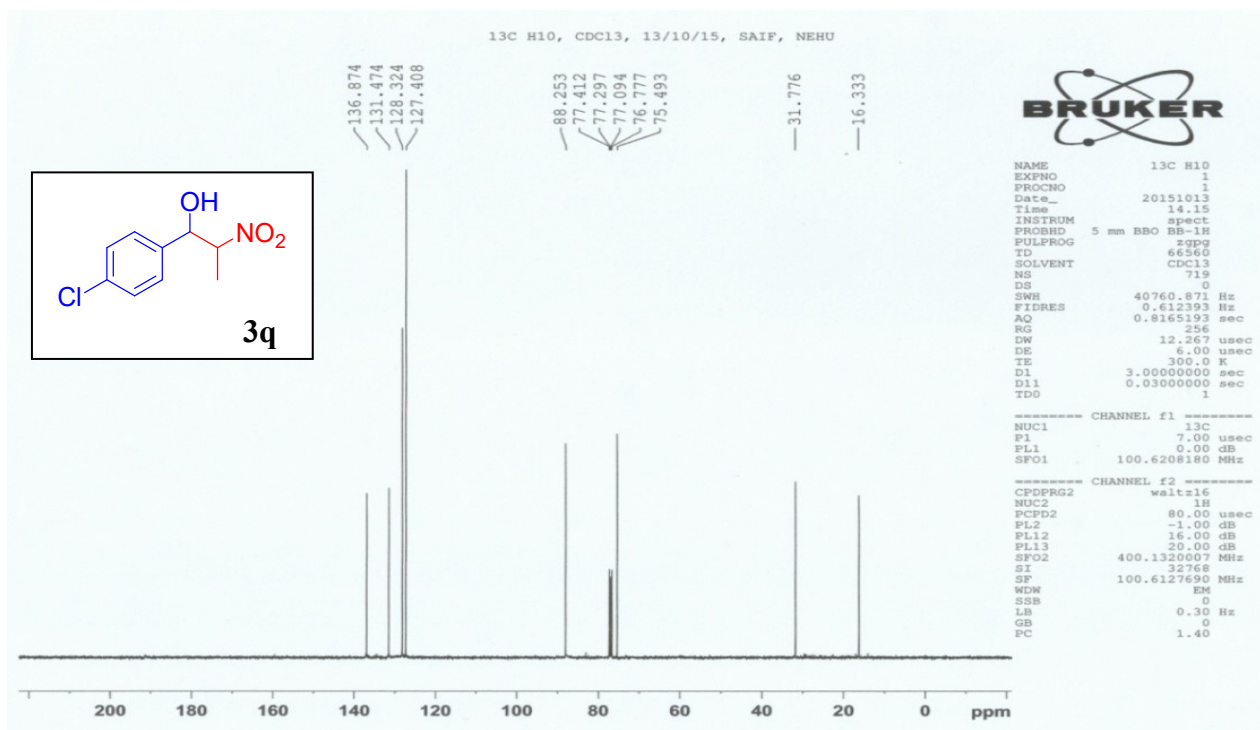
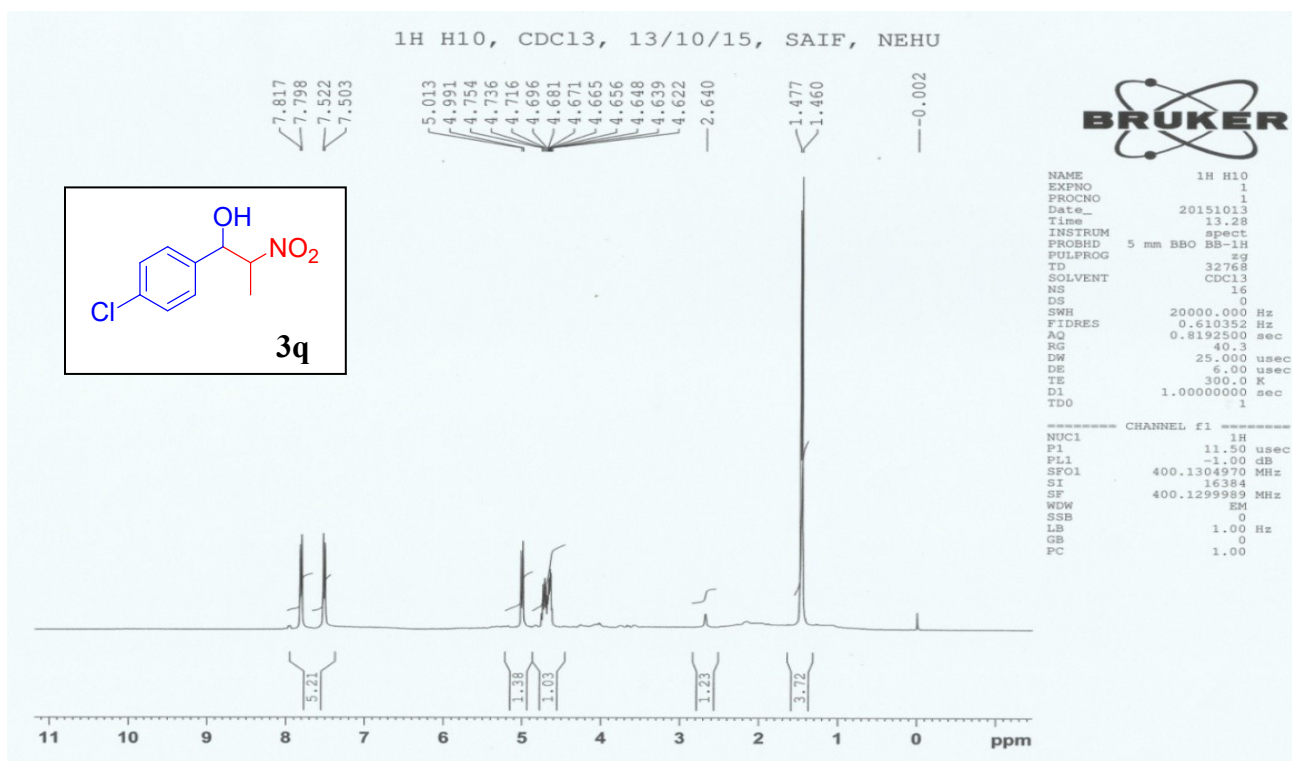


Fig S17 : ^1H NMR and ^{13}C NMR Spectra of 1-(4-Chlorophenyl)-2-nitropropan-1-ol (Table 3, Entry 3q)

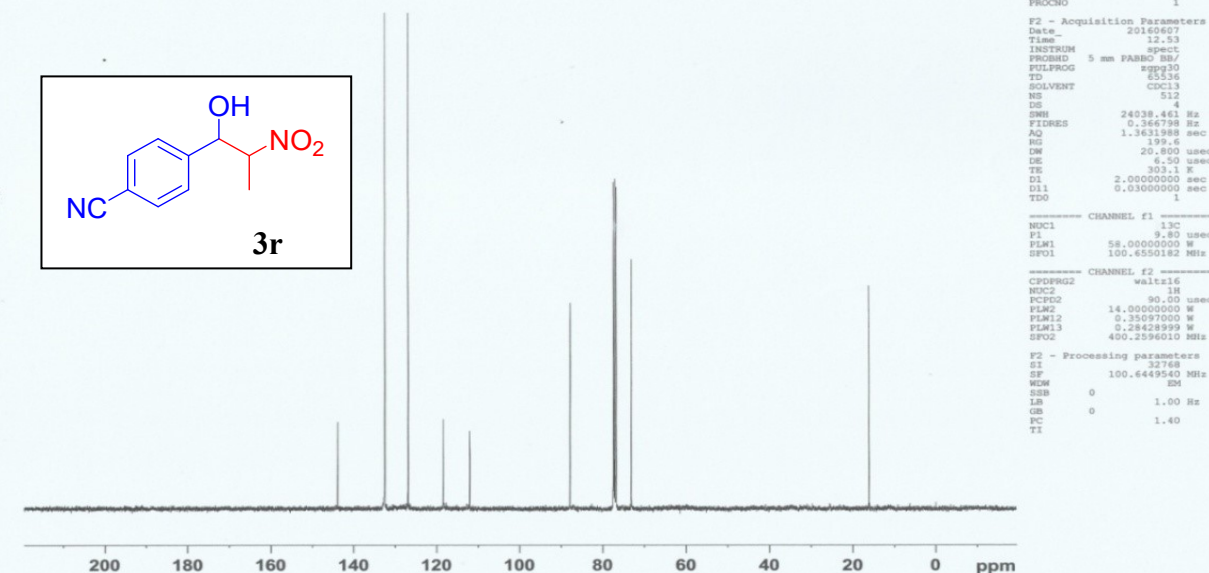
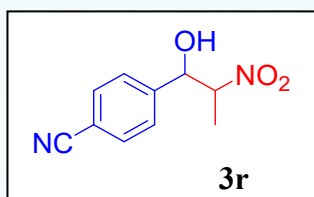
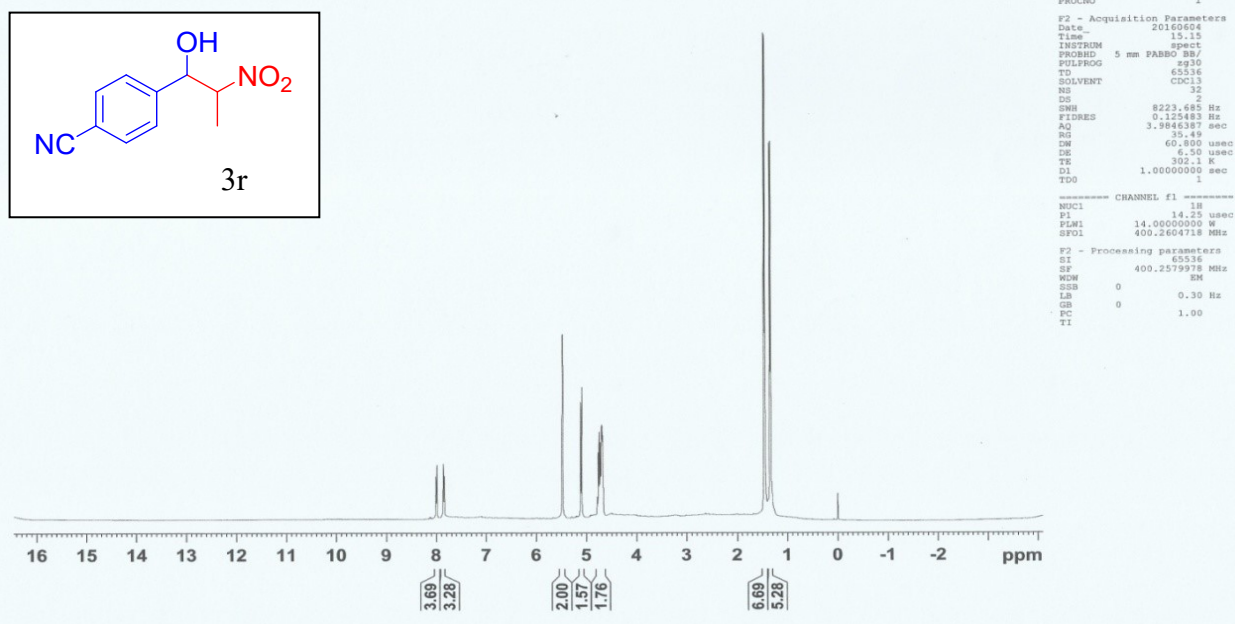
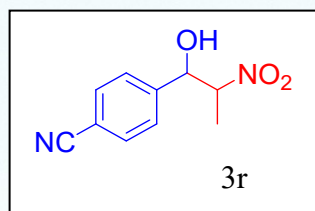
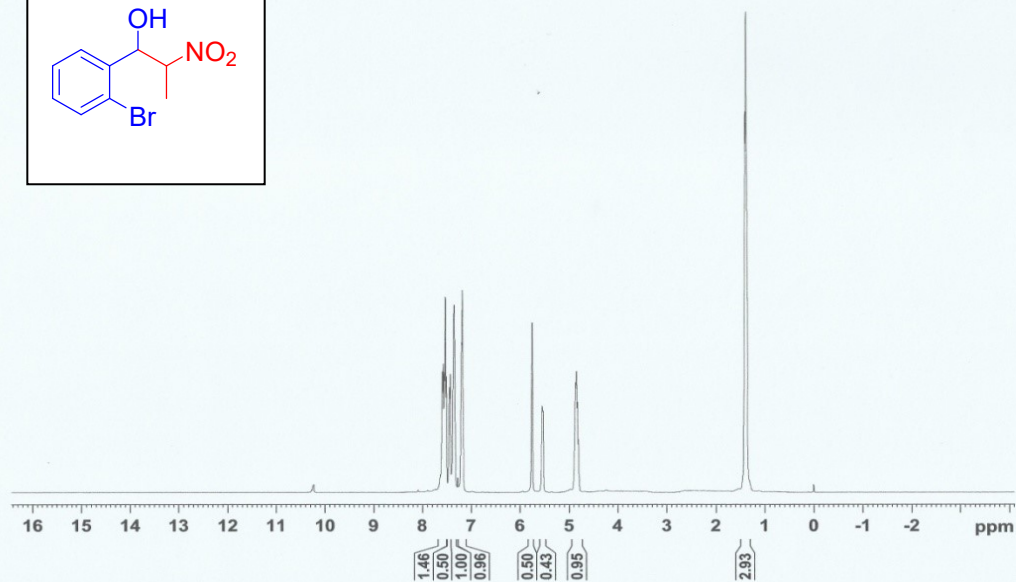
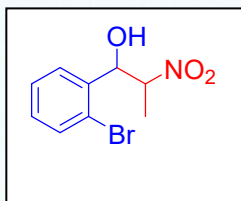


Fig S 18: ^1H NMR and ^{13}C NMR Spectra of 4-(1-Hydroxy-2-nitropropyl)benzonitrile (Table 3, Entry 3r)

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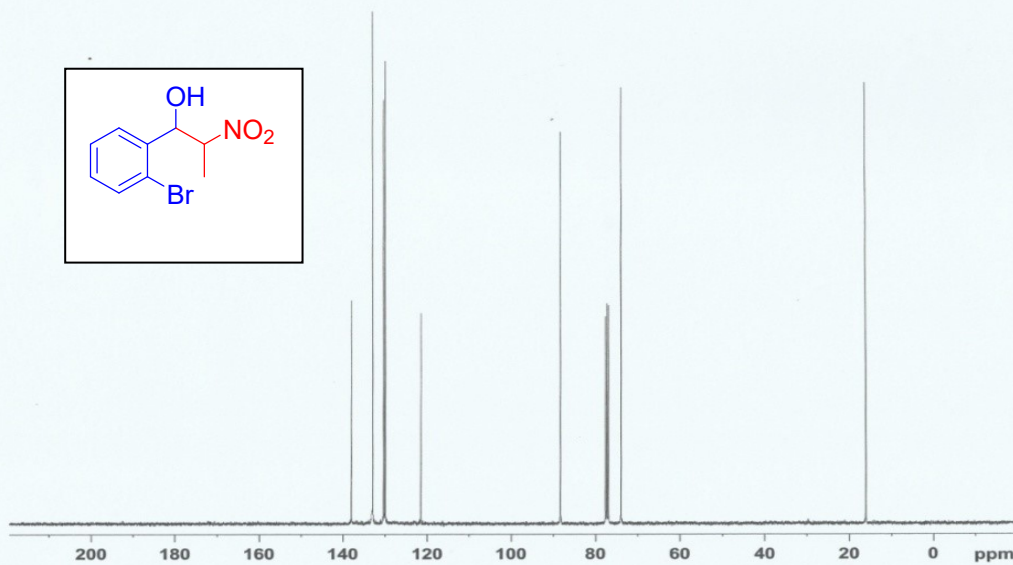
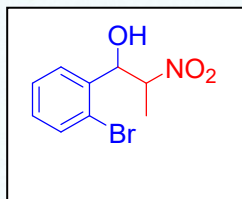
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NS 32
DS 4
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 22.56
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLM1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
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SF 400.2580051 MHz
WDW EM
SSB 0
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GB 0
PC 1.00
TI

Signature SIF VIT VELLORE
H40



Current Data Parameters
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PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 302.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLM1 58.00000000 W
SFO1 100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLM2 14.00000000 W
PLM12 0.35087000 W
PLM13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TI

Fig S19 : ^1H NMR and ^{13}C NMR Spectra of 1-(2-Bromophenyl)-2-nitropropan-1-ol (Table 3, Entry)

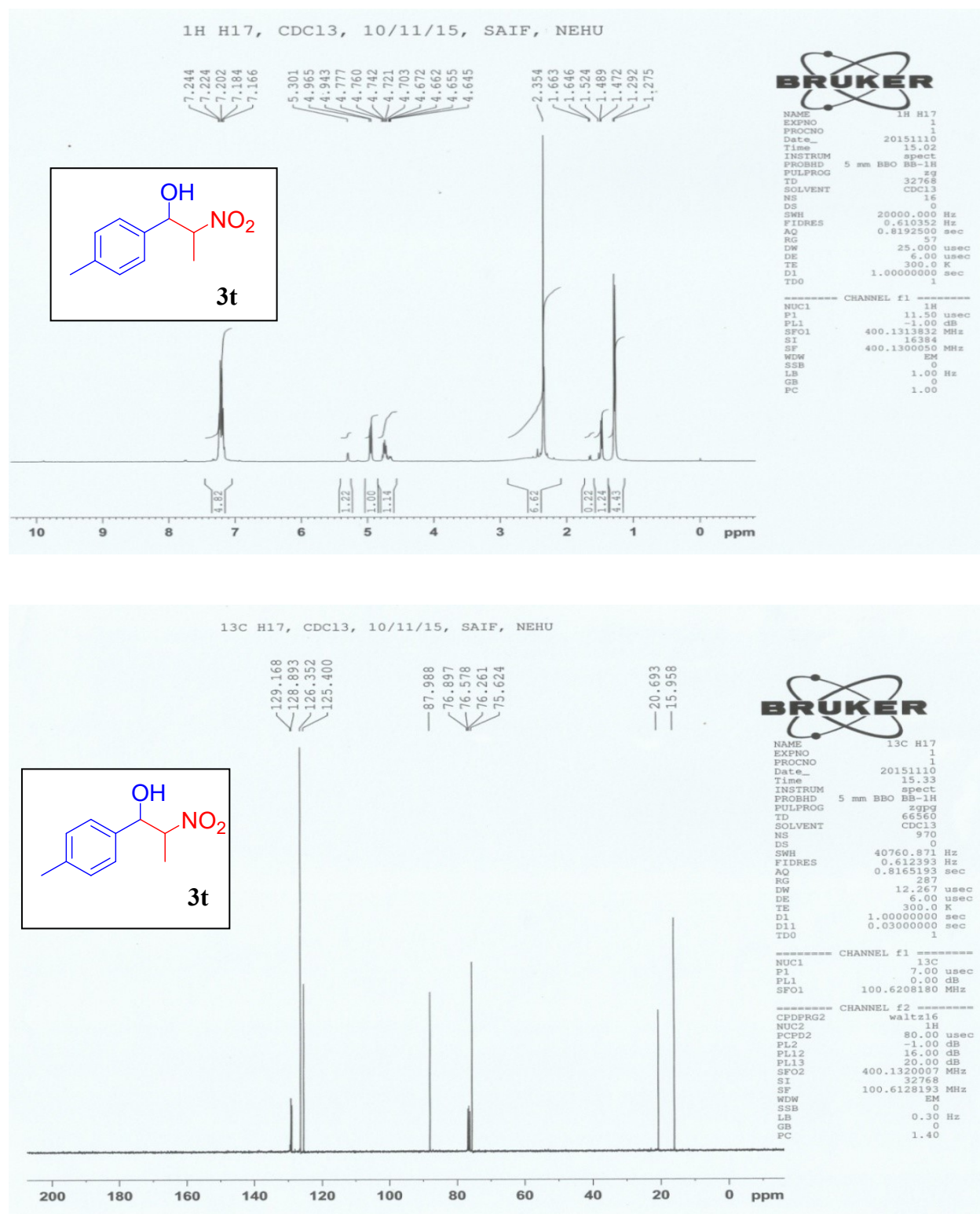


Fig S20 : ¹H NMR and ¹³C NMR Spectra of 2-Nitro-1-(p-tolyl)propan-1-ol (Table 3, Entry 3t)

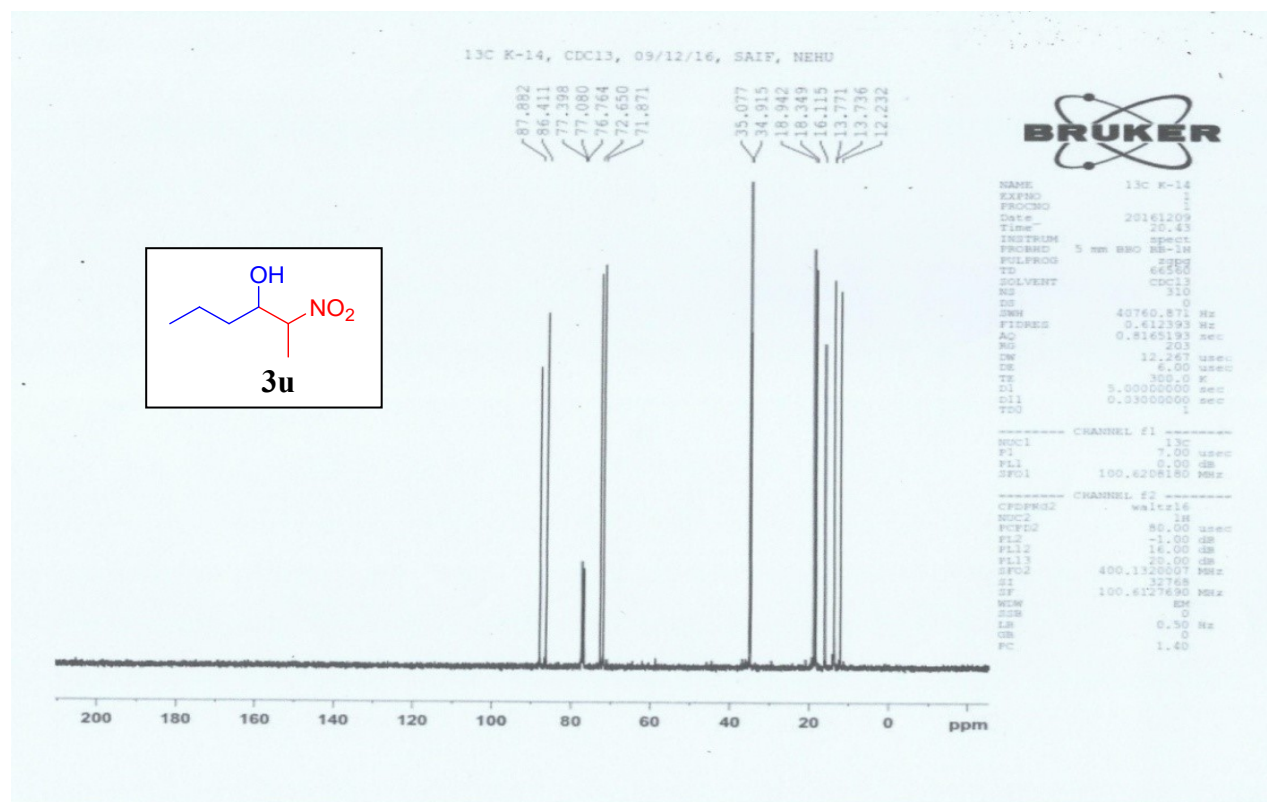
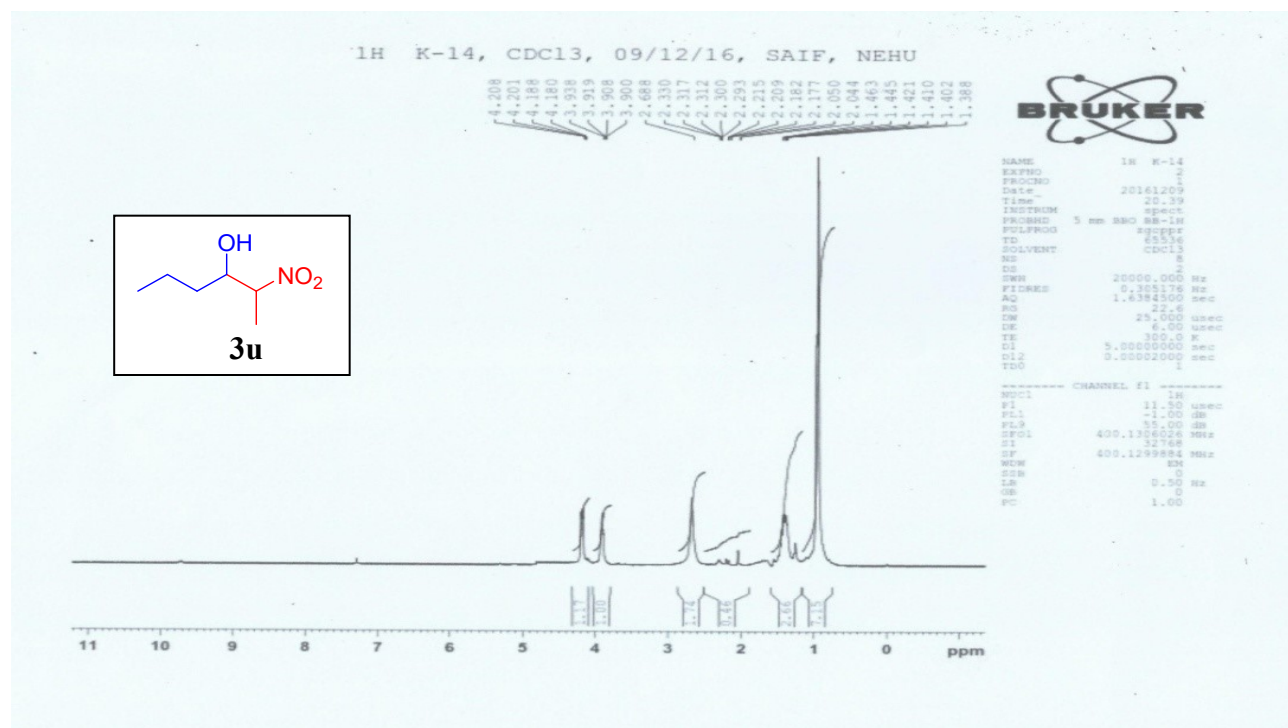


Fig S 21 : ¹H NMR and ¹³C NMR Spectra of 2-nitrohexan-3-ol (Table 3, Entry 3u)

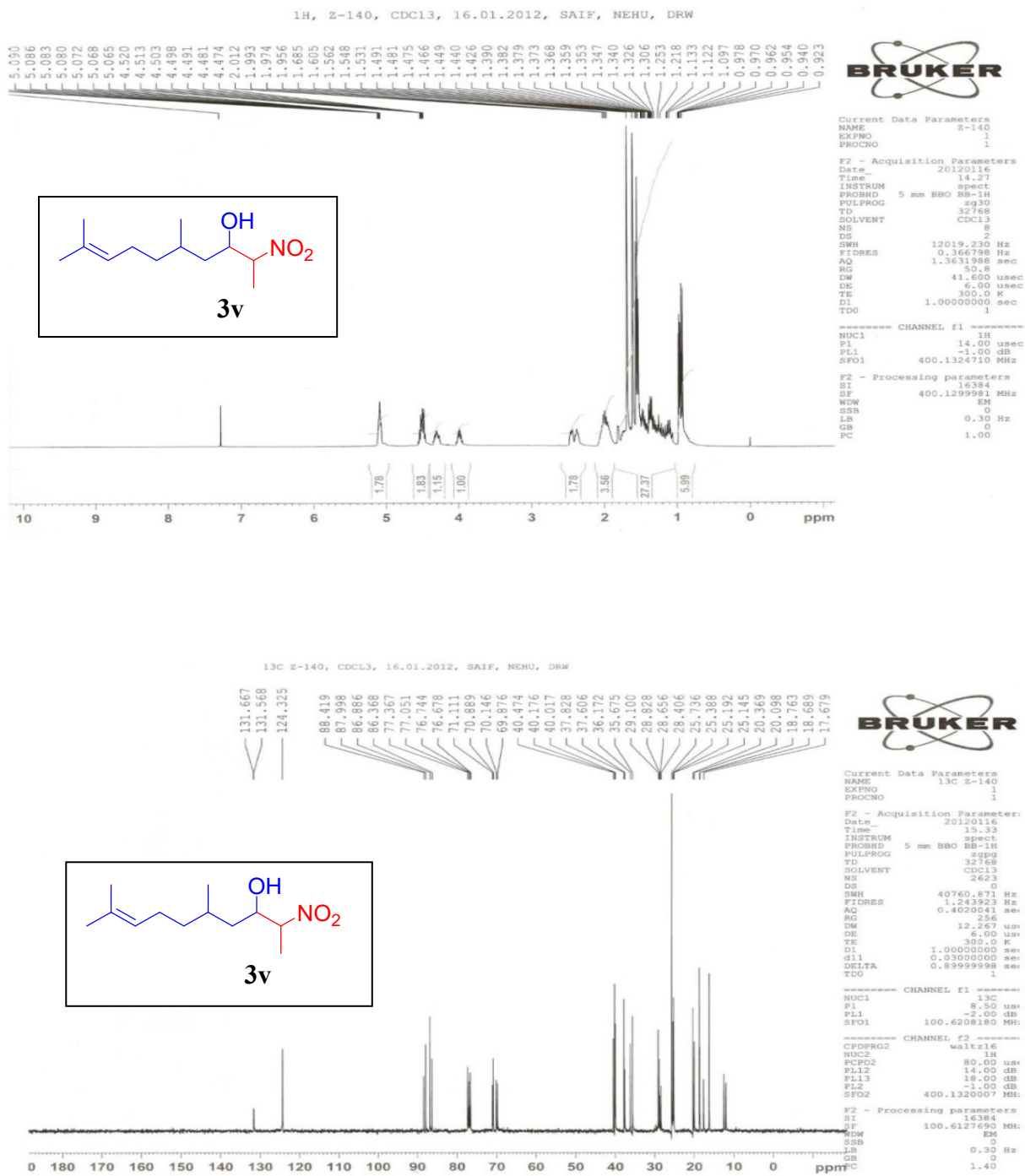


Fig S 22 : ^1H NMR and ^{13}C NMR Spectra of 5,9-Dimethyl-2-nitrodec-8-en-3-ol (Table 3, Entry)

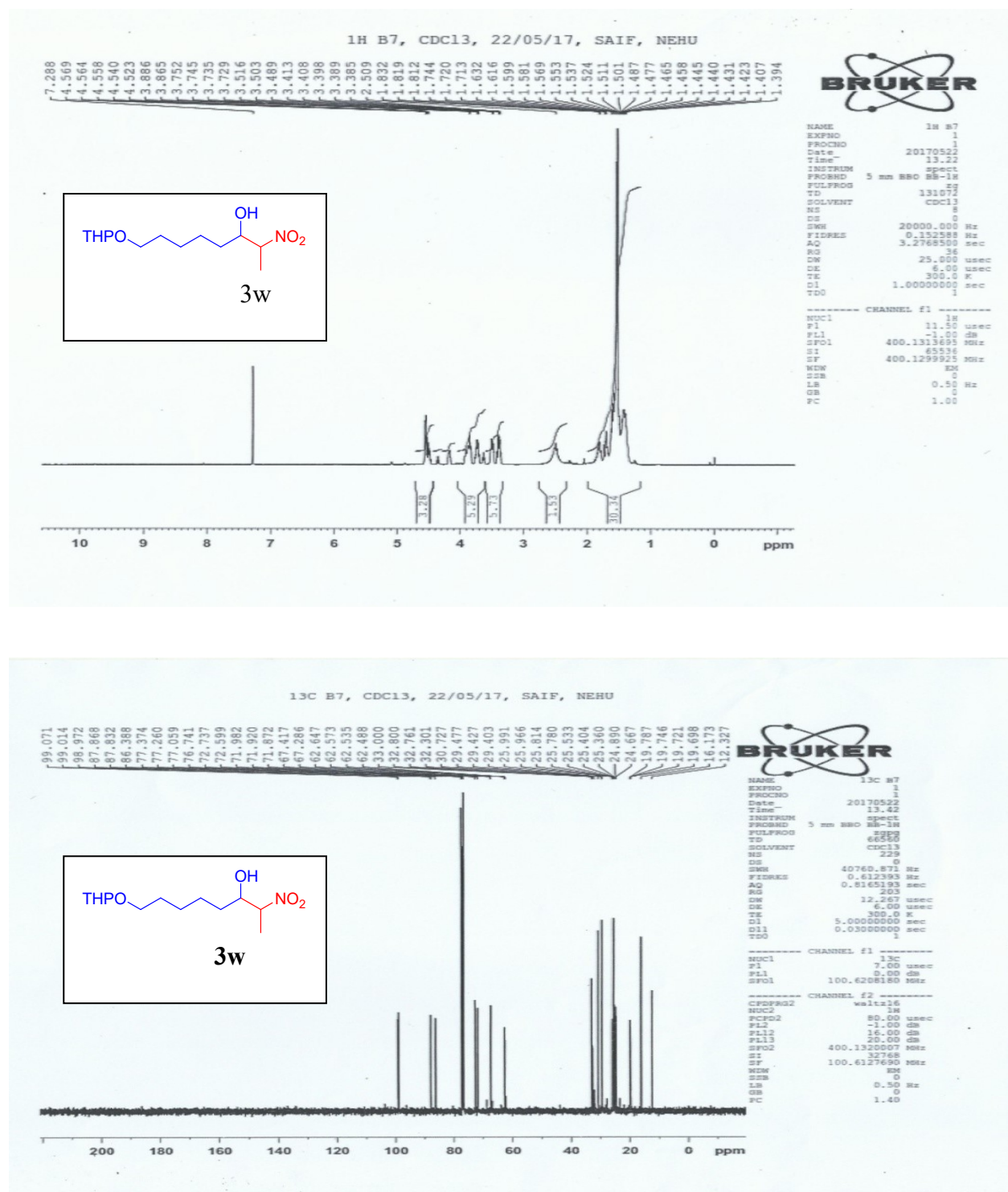


Fig S 23 : ^1H NMR and ^{13}C NMR Spectra of 2-nitro-7-((tetrahydro-2H-pyran-2-yl)oxy)heptan-3-ol (Table 3, Entry 3w)