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Supplementary Material

Water Assisted Organocatalysis: An Enantioselective Green Protocol for Henry Reaction

Prashant B. Thorat, Santosh V. Goswami, Wamanrao N. Jadhav and Sudhakar R. Bhusare*
Department of Chemistry, Dnyanopasak College, Parbhani-431 401, MS, India
E-mail: bhusare71@yahoo.com

General details

All solvents were used as commercial anhydrous grade without further purification. The column chromatography was carried out over silica gel (100–120 mesh). Optical rotations were measured on a Polax-2L digital polarimeter. Melting points were determined in open capillary tube and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 300 MHz spectrometer in $CDCl_3$ solvent. Mass spectra were taken on Polaris-Q Thermoscintific GC-MS. Entiomeric purity is determined on PerkinElmer Series 200 HPLC Systems.

General procedure for synthesis of Henry reaction

Aromatic aldehydes (2 mmole) was added in solution of nitromethane (4 mmole) in distilled water (20 mL) and 0.12 mmole of organocatalyst (*S*)-*N*-(4-fluorophenyl)-1-tosylpyrrolidine-2-carboxamide. The reaction mixture was stirred for appropriate time at room temperature. Progress of reaction was monitored with thin layer chromatography. After completion of reaction as indicated by TLC, 25mL cool distilled water was added to it. This reaction mixture was then extracted with dichloromethane (15mL x 3). Solvent was removed under *vacuo,* to obtain crude product. The crude mixture was purified with silica gel column chromatography. Spectral data of all compounds is compared to those reported in literature[1, 2] and, it is well in agreement with structure.

(*S*)-2-Nitro-1-(4-nitrophenyl) ethanol (10a)

The product is characterized by comparing the Spectral data, HPLC data and melting point data with those reported in the literature [1]. White solid, M. P. 83-85 °C, $[\alpha]_D^{20}$ **:** +26.0 (c 1.10, CH_2Cl_2)[3a], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.63-7.78 (m, 2H), 7.29-7.46 (m, 2H), 4.60 (m, 1H,), 4.22 (m, 1H), 3.79 (m, 1H), 3.21 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 157.33, 156.71, 124.52, 121.52, 119.00, 75.68; **GC-MS:** *m*/*z* 212.21 (M+); **Elemental Analysis for $C_8H_8N_2O_5$**: Calculated C, 45.29; H, 3.80; N, 13.20; O, 37.71; Found C, 45.31; H, 3.78; N, 13.22; O, 37.70.

HPLC: 92 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 1:4, Flow rate 1.0 mL/min, ƛ = 205 nm; t_R (minor) = 11.4 min, t_R (major) = 13.8 min].

(*S*)-1-(4-Flourophenyl)-2-nitroethanol (10b)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [2]. Yellow oil, $[\alpha]_D^{20}$ **:** +28.6 (c 2.1, $CHCl_3$)[3c], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.03-8.10 (m, 2H), 7.67-7.72 (m, 2H), 4.66 (m, 1H,), 4.31 (m, 1H), 3.82 (m, 1H), 3.24 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 162.91, 153.65, 122.56, 121.78, 110.98, 76.11; **GC-MS:** *m*/*z* 185.22 (M+); **Elemental Analysis for $C_8H_8N_2O_5$**: **Elemental Analysis for $C_8H_8FNO_3$:**Calculated C, 51.90; H, 4.36; F, 10.26; N, 7.56; O, 25.92; Found C, 51.87; H, 4.38; F, 10.27; N, 7.58; O, 25.90.

HPLC: 94 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 210 nm; t_R (minor) = 11.1 min, t_R (major) = 19.1 min].

(*S*)-2-Nitro-1-(3-nitrophenyl) ethanol (10c)

The product is characterized by comparing the Spectral data, HPLC data and melting point data with those reported in the literature [2]. White solid, M. P. 83-85 °C, $[\alpha]_D^{20}$ **:** +28.0 (c 0.8, CH_2Cl_2)[3a], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.23-7.37 (m, 3H), 7.11-7.19 (m, 1H), 4.54 (m, 1H,), 4.27 (m, 1H), 3.77 (m, 1H), 3.22 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 158.17, 150.76, 125.39, 124.23, 122.85, 108.37, 74.86; **GC-MS:** *m*/*z* 212.14 (M+); **Elemental Analysis for$C_8H_8N_2O_5$**: C, 45.29; H, 3.80; N, 13.20; O, 37.71; Found C, 45.27; H, 3.79; N, 13.19; O, 37.69.

HPLC: 91 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 210 nm; t_R (minor) = 21.5 min, t_R (major) = 22.7 min].

(*S*)-1-(4-Chlorophenyl)-2-nitroethanol (10d)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [2]. Yellow oil, $[\alpha]_D^{20}$ **:** +42.0 (c 1.10, CH_2Cl_2)[3a], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.42−7.32 (m, 4H), 4.64 (m, 1H), 4.44 (m, 2H), 3.90 (m, 1H), 3,31 (br s,

1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 143.21, 134.86, 133.27, 130.19, 94.91, 73.38; **GC-MS:** *m/z* 201.04 (M+); **Elemental Analysis for $C_8H_8ClNO_3$:** Calculated C, 47.66; H, 4.00; Cl, 17.59; N, 6.95; O, 23.81; Found C, 47.67; H, 4.02; Cl, 17.58; N, 6.94; O, 23.83.

HPLC: 89 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 210 nm; t_R (minor) = 6.3 min, t_R (major) = 18.3 min].

(*S*)-1-(2-Chlorophenyl)-2-nitroethanol (10e)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [1]. Yellow oil, $[\alpha]_D^{20}$ **:** +23.8 (c 1.10, CH_2Cl_2)[3a], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 6.78-6.83 (m, 1H), 6.26-6.37 (m, 3H), 4.77 (m, 1H), 4.26 (m, 1H), 3.71 (m, 1H), 3.19 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 140.21, 131.74, 123.48, 122.43, 111.07, 71.26; **GC-MS:** *m/z* 212.46 (M+); **Elemental Analysis for $C_8H_8ClNO_3$:** Calculated C, 47.66; H, 4.00; Cl, 17.59; N, 6.95; O, 23.81; Found C, 47.63; H, 3.98; Cl, 17.61; N, 6.99; O, 23.79.

HPLC: 88 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2.5:97.5, Flow rate 1.0 mL/min, ƛ = 205 nm; t_R (minor) = 13.5 min, t_R (major) = 17.2 min].

(*S*)-1-(2-Bromophenyl)-2-nitroethanol (10f)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [1]. Yellow oil, $[\alpha]_D^{20}$ **:** -27.3 (c 1.10, CH_2Cl_2)[3b], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.68-7.81 (m, 1H), 6.87-7.06 (m, 3H), 5.19 (bs, 1H, OH), 4.71 (m, 1H), 4.32 (m, 1H), 3.90 (m, 1H); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 142.73, 131.96, 130.33, 128.00, 123.89, 66.46; **GC-MS:** *m/z* 246 (M+); **Elemental Analysis for $C_8H_8BrNO_3$:** C, 39.05; H, 3.28; Br, 32.47; N, 5.69; O, 19.51; Found C, 39.03; H, 3.31; Br, 32.44; N, 5.71; O, 19.53.

HPLC: 87 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 5:95, Flow rate 1.0 mL/min, ƛ = 205 nm; t_R (minor) = 12.4 min, t_R (major) = 13.5 min].

(*S*)-4-(1-Hydroxy-2-nitroethyl) phenol (10g)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [2]. Yellow oil, $[\alpha]_D^{20}$**:** +25.8 (c 1.10, CH_2Cl_2), **^{1}H NMR (300 MHz, $CDCl_3$):** δ 9.81 (bs, 1H, OH), 7.73-7.89 (m, 2H), 7.29-7.48 (m, 2H), 5.27 (bs, 1H, OH), 4.51 (m, 1H), 4.70 (m, 1H), 4.09 (t, 1H); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 159.27, 145.16, 138.46, 132.00, 119.79, 73.41. **GC-MS:** *m/z* 183 (M+); **Elemental Analysis for $C_8H_9NO_4$:** C, 52.46; H, 4.95; N, 7.65; O, 34.94; Found C, 52.43; H, 4.98; N, 7.63; O, 34.91;

HPLC: 89 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 205 nm; t_R (minor) = 29.8 min, t_R (major) = 40.8 min].

(*S*)-1-(2-Methoxyphenyl)-2-nitroethanol (10h)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [1]. Yellow oil, $[\alpha]_D^{20}$**:** +36.6 (c 1.8, $CHCl_3$)[3c], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.43 (m, 1H), 7.29-7.36 (m, 1H), 6.90-7.04 (m, 2H), 4.85 (m, 1H), 4.67 (m, 1H), 4.52 (m, 1H), 3.88 (s, 3H), 3.29 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ158.71, 140.89, 131.20, 120.11, 114.34, 108.73, 93.45, 78.06, 67.55, 54.77; **GC-MS:** *m*/*z* 197.11 (M+); **Elemental Analysis for $C_9H_{11}NO_4$:** C, 54.82; H, 5.62; N, 7.10; O, 32.46; Found C, 54.80; H, 5.64; N, 7.13; O, 32.45.

HPLC: 94 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 205 nm; t_R (minor) = 11.2 min, t_R (major) = 13.2 min].

(*S*)-1-(4-Methoxyphenyl)-2-nitroethanol (10i)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [2]. Yellow oil, $[\alpha]_D^{20}$**:** +19.0 (c 2.1, $CHCl_3$)[3c], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.12-7.21 (m, 2H), 7.25-7.33 (m, 2H), 4.76 (m, 1H), 4.53 (m, 1H), 3.79 (s, 3H), 3.23 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** 156.93, 129.82, 125.44, 125.38, 112.73, 89.37, 70.47, 54.57; **GC-MS:** *m*/*z* 197.07 (M+); **Elemental Analysis for $C_9H_{11}NO_4$:** C, 54.82; H, 5.62; N, 7.10; O, 32.46; Found C, 54.79; H, 5.65; N, 7.08; O, 32.48.

HPLC: 88 % *ee*. [Determined by chiral HPLC using chiralcel OB-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 205 nm; t_R (minor) = 25.0 min, t_R (major) = 25.6 min].

(*S*)-1-Phenyl-2-nitroethanol (10j)

The product is characterized by comparing the Spectral data and HPLC data with those reported in the literature [2]. Colorless oil, $[\alpha]_D$ **:** +23.7 (c 1.10, CH_2Cl_2)[3a], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 6.67-6.79 (m, 4H), 4.69 (m, 1H), 4.62 (m, 1H), 3.74 (s, 3H), 3.17 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** 139.81, 128.23, 128.11, 84.82, 69.77; **GC-MS:** *m*/*z* 167.05 (M+); **Elemental Analysis for $C_8H_9NO_3$:** C, 57.48; H, 5.43; N, 8.38; O, 28.71; Found C, 57.49; H, 5.45; N, 8.41; O, 28.69.

HPLC: 90 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 1:9, Flow rate 1.0 mL/min, ƛ = 205 nm; t_R (minor) = 13.7 min, t_R (major) = 16.9 min].

***(S)*-1-(4-Bromophenyl)-2-nitroethanol (10k)**

The product is characterized by the Spectral data and HPLC data with those reported in the literature [6].Colorless oil, $[\alpha]_D$ **:** +68.4 (c 1.40, $CHCl_3$)[4], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.42-7.47 (m, 2H), 7.18–7.22 (m, 2H), 4.81 (m, 1H), 4.66 (m, 1H), 4.52 (m, 1H), 3.74 (s, 3H), 3.17 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** 138.11, 131.82, 127.12, 123.11,

81.24, 71.20; **GC-MS:** *m/z* 246.07 (M+); **Elemental Analysis for $C_8H_8BrNO_3$:** C, 39.05; H, 3.28; Br, 32.47; N, 5.69; O, 19.51; Found C, 39.03; H, 3.30; Br, 32.49; N, 5.71; O, 19.53.

HPLC: 89 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 15:85, Flow rate 0.8 mL/min, ƛ = 215 nm; t_R (minor) = 13.8 min, t_R (major) = 17.4 min].

***(S)*-2-(1-hydroxy-2-nitroethyl) phenol (10l)**

The product is characterized by analogy with the Spectral data and HPLC data with those reported in the literature. Yellow oil, $[\alpha]_D^{20}$**:** +25.7 (c 1.10, CH_2Cl_2), **^{1}H NMR (300 MHz, $CDCl_3$):** δ 10.18 (bs, 1H, OH), 7.14-7.21 (m, 2H), 6.89-6.94 (m, 2H), 4.74 (m, 1H), 4.66 (m, 1H), 4.34 (m, 1H) 3.21 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 154.23, 131.45, 128.39, 125.31, 117.87, 71.25. **GC-MS:** *m/z* 183.03 (M+); **Elemental Analysis for $C_8H_9NO_4$:** C, 52.46; H, 4.95; N, 7.65; O, 34.94; Found C, 52.43; H, 4.98; N, 7.63; O, 34.91;

HPLC: 92 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 205 nm; t_R (minor) = 32.6 min, t_R (major) = 41.4 min].

(*S*)-1-Nitro-3-phenylpropan-2-ol (10m)

The product is characterized by the Spectral data and HPLC data with those reported in the literature [5].Colorless oil, $[\alpha]_D^{20}$**:** -21.9 (c 1.9, CH_2Cl_2)[5], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.15 (m, 5H), 4.67 (m, 1H), 4.55 (m, 1H), 4.41 (m, 1H), 2.89 (m, 1H), 2.81 (m, 1H), 2.60 (bs, 1H, OH). **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 135.89, 1228.74, 128.04, 126.81, 80.59, 70.34, 42.65; **GC-MS:** *m/z* 181.20 (M+); **Elemental Analysis for $C_9H_{11}NO_3$:** C, 59.66; H, 6.12; N, 7.73; O, 26.49; Found C, 59.64; H, 6.14; N, 7.69; O, 26.52;

HPLC: 76 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 10:90, Flow rate 0.5 mL/min, ƛ = 215 nm; t_R (minor) = 30.8 min, t_R (major) = 36.9 min].

(*S*)- 1-Nitro-4-phenyl-but-3-en-2-ol (10n)

The product is characterized by the Spectral data and HPLC data with those reported in the literature [2]. Colorless oil, $[\alpha]_D^{20}$**:** +22.6 (c 1.8, CH_2Cl_2)[2], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.17-7.39 (m, 5H), 6.74 (m, 1H), 6.34 (m, 1H), 4.89 (m, 1H), 4.69 (m, 1H), 4.54 (m, 1H), 3.01 (bs, 1H, OH); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 136.32, 132.44, 130.11, 128.56, 127.69, 125.97, 80.34, 71.19 **GC-MS:** *m/z* 193.20 (M+); **Elemental Analysis for $C_{10}H_{11}NO_3$:** C, 62.17; H, 5.74; N, 7.25; O, 24.84; Found C, 62.20; H, 5.77; N, 7.23; O, 24.82;

HPLC: 81 % *ee*. [Determined by chiral HPLC using chiralcel OD-H, IPA/Hexane 2:8, Flow rate 0.8 mL/min, ƛ = 215 nm; t_R (minor) = 12.5 min, t_R (major) = 16.8 min].

(*S*)-2-Nitro-1-cyclohexylethanol (10o)

The product is characterized by the Spectral data and HPLC data with those reported in the literature [6]. Colorless oil, $[\alpha]_D^{20}$**:** +16.5 (c 0.6, CH_2Cl_2)[6], **^{1}H NMR (300 MHz, $CDCl_3$):** δ

4.49 (m, 2H), 4.38 (m, 1H), 4.14 (m, 1H), 2.78 (bs, 1H, OH), 1.81-1.97 (m, 5H), 1.62-1.71 (m, 1H), 1.33-1.52 (m, 5H), **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 80.34, 70.76, 42.17, 30.24, 28.75, 26.22, 25.87; **GC-MS:** *m/z* 173.19 (M+); **Elemental Analysis for $C_8H_{15}NO_3$:** C, 55.47; H, 8.73; N, 8.09; O, 27.71; Found C, 55.49; H, 8.75; N, 8.11; O, 27.73;

HPLC: 70 % *ee*. [Determined by chiral HPLC using chiralcel AD-H, IPA/Hexane 3:97 v/v, Flow rate 0.8 mL/min, ƛ = 215 nm; t_R (minor) = 12.0 min, t_R (major) = 14.2 min].

(*S*)-3-Methyl-1-nitrobutan-2-ol (10p)

The product is characterized by the Spectral data and HPLC data with those reported in the literature [6].Colorless oil, $[\alpha]_D^{20}$**:** +20.1 (c 1.0, CH_2Cl_2)[6], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 4.57 (m, 2H), 4.38 (m, 1H), 4.15 (m, 1H), 3.01 (bs, 1H, OH), 1.78 (m, 1H), 0.96-1.05 (m, 6H); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 79.83, 74.26, 32.19, 19.11, 18.37; **GC-MS:** *m/z* 133.15 (M+); **Elemental Analysis for $C_5H_{11}NO_3$:** C, 45.10; H, 8.33; N, 10.52; O, 36.05; Found C, 45.07; H, 8.31; N, 10.50; O, 36.03.

HPLC: 65 % *ee*. [Determined by chiral HPLC using Chiralcel OD-H, IPA/Hexane 3:97 v/v, Flow rate 0.6 mL/min, ƛ = 215 nm; t_R (minor) = 27.8 min, t_R (major) = 30.1 min].

(S)-4-Methyl-1-nitropentan-2-ol (10q)

The product is characterized by the Spectral data and HPLC data with those reported in the literature [6 and 7].Colorless oil, $[\alpha]_D^{20}$**:** -2.3 (c 0.5, CH_2Cl_2)[7], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 4.41 (m, 2H), 4.29 (m, 1H), 2.90 (bs, 1H, OH), 1.62 (m, 1H), 0.91-1.00 (m, 6H); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 82.14, 68.72, 43.16, 25.00, 22.94, 20.76; **GC-MS:** *m/z* 147.19 (M+); **Elemental Analysis for $C_6H_{13}NO_3$:** C, 48.97; H, 8.90; N, 9.52; O, 32.61; Found C, 49.00; H, 8.87; N, 9.55; O, 32.59.

HPLC: 62 % *ee*. [Determined by chiral HPLC using Chiralcel OJ-H, IPA/Hexane 15:85 v/v, Flow rate 0.8 mL/min, ƛ = 215 nm; t_R (minor) = 11.5 min, t_R (major) = 14.00 min].

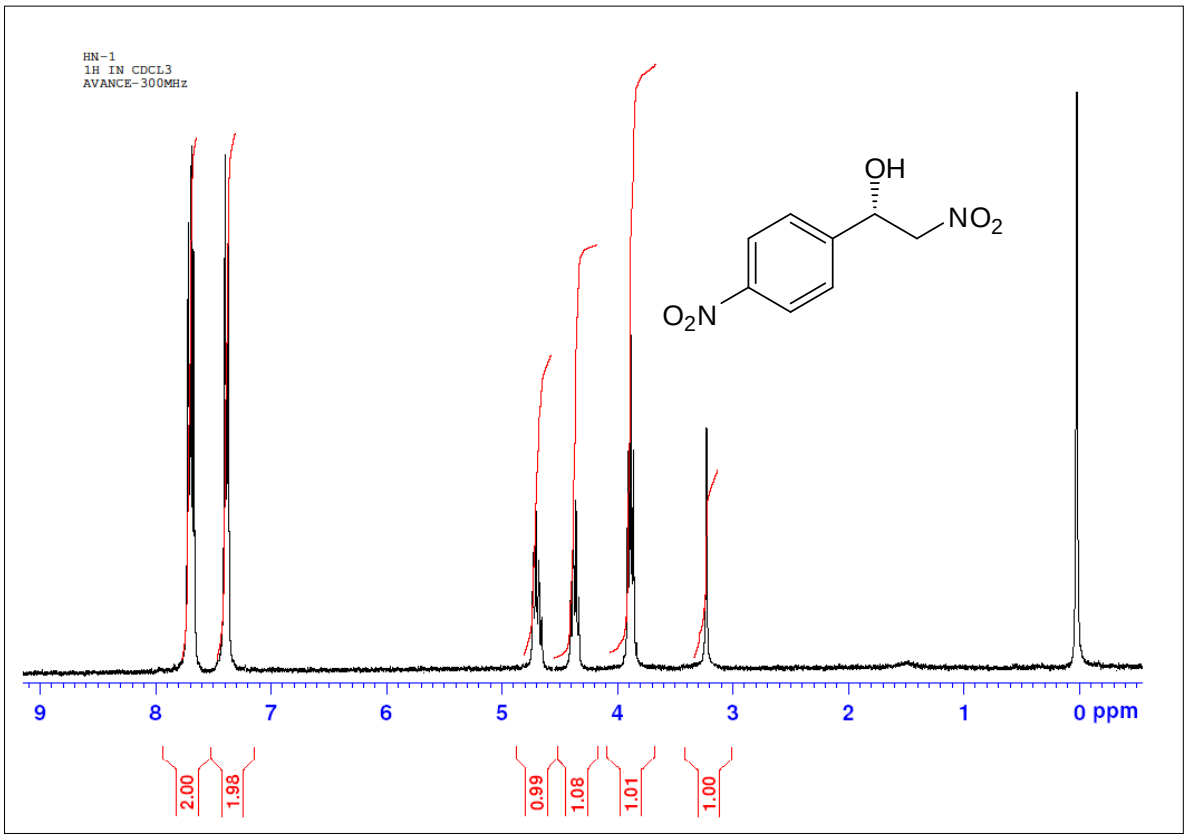
(*S*)-1-Nitrooctan-2-ol (10r)

The product is characterized by the Spectral data and HPLC data with those reported in the literature [3c].]. Colorless oil, $[\alpha]_D^{20}$**:** +6.2 (c 1.5, $CHCl_3$)[3c], **^{1}H NMR (300 MHz, $CDCl_3$):** δ 4.48 (m, 2H), 4.34 (m, 1H), 2.84 (bs, 1H, OH), 1.51 (m, 2H), 1.18-1.30 (m, 8H), 0.91 (t, *J* = 7.2 Hz, 3H); **^{13}C-NMR (300 MHz, $CDCl_3$):** δ 80.69, 69.16, 35.03, 30.89, 29.63, 24.56, 21.49, 15.43; **GC-MS:** *m/z* 175.24 (M+); **Elemental Analysis for $C_8H_{17}NO_3$:** C, 54.84; H, 9.78; N, 7.99; O, 27.39; Found C, 54.82; H, 9.81; N, 8.02; O, 27.42.

HPLC: 64 % *ee*. [Determined by chiral HPLC using Chiralcel OJ-H, IPA/Hexane 1:10 v/v, Flow rate 1.0 mL/min, ƛ = 222 nm; t_R (minor) = 7.8 min, t_R (major) = 11.5 min].

1H NMR

1H NMR compound 10a



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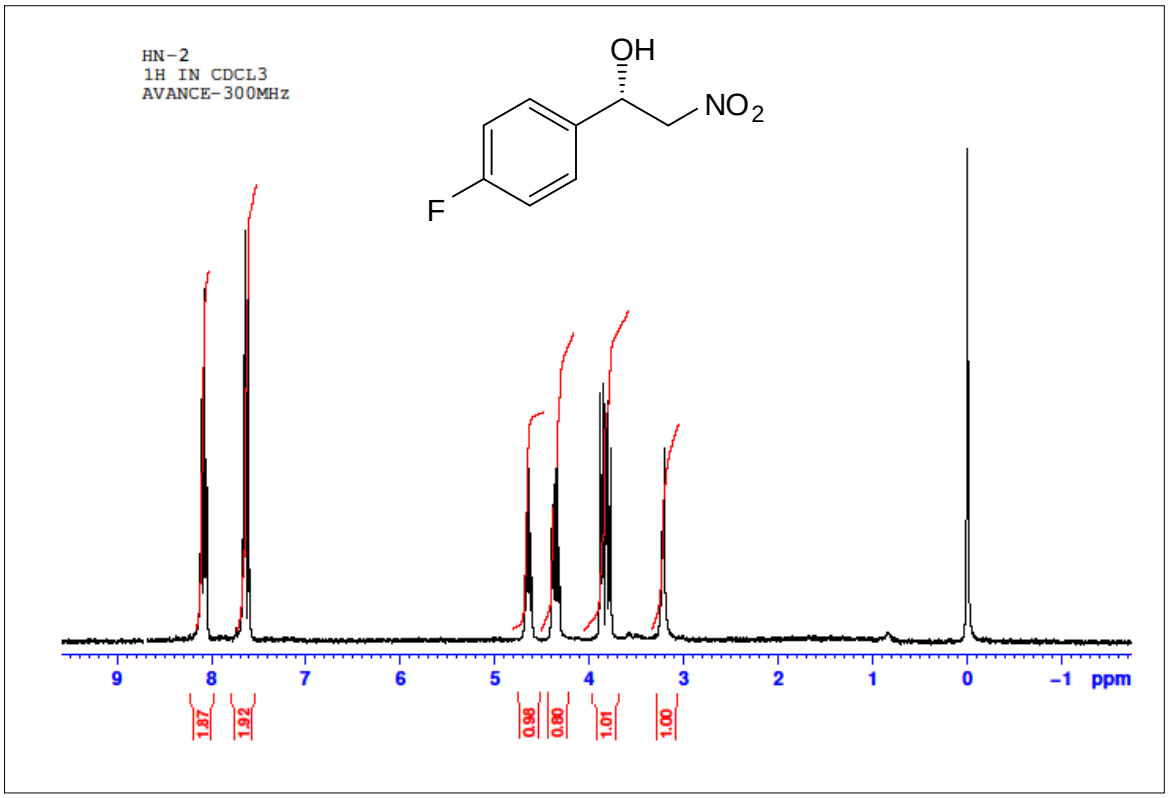

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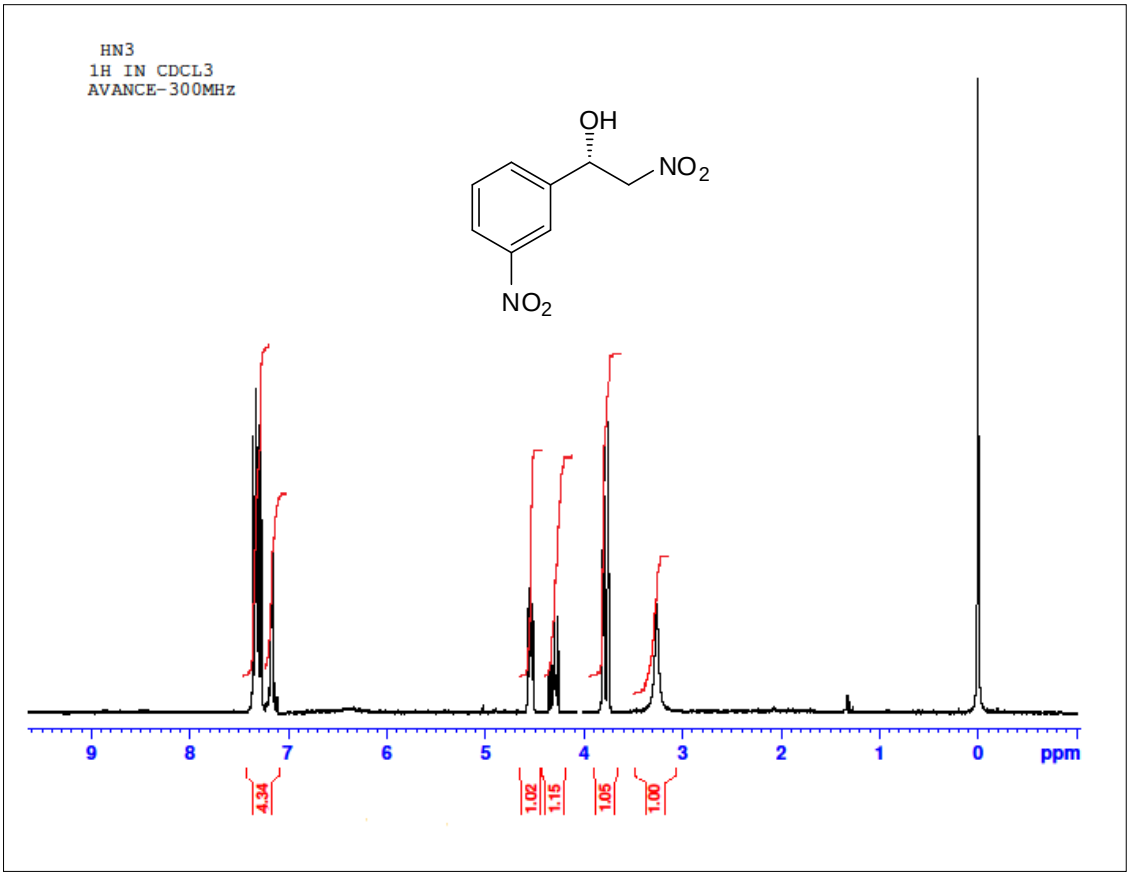

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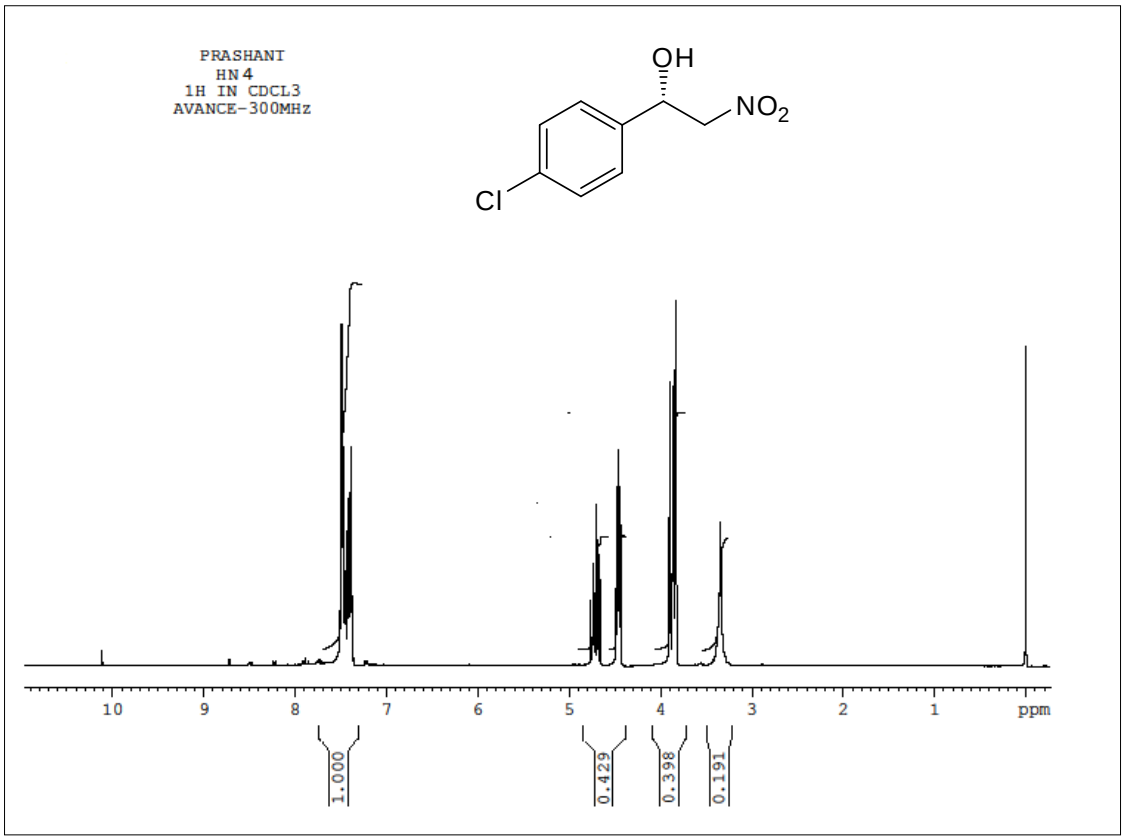

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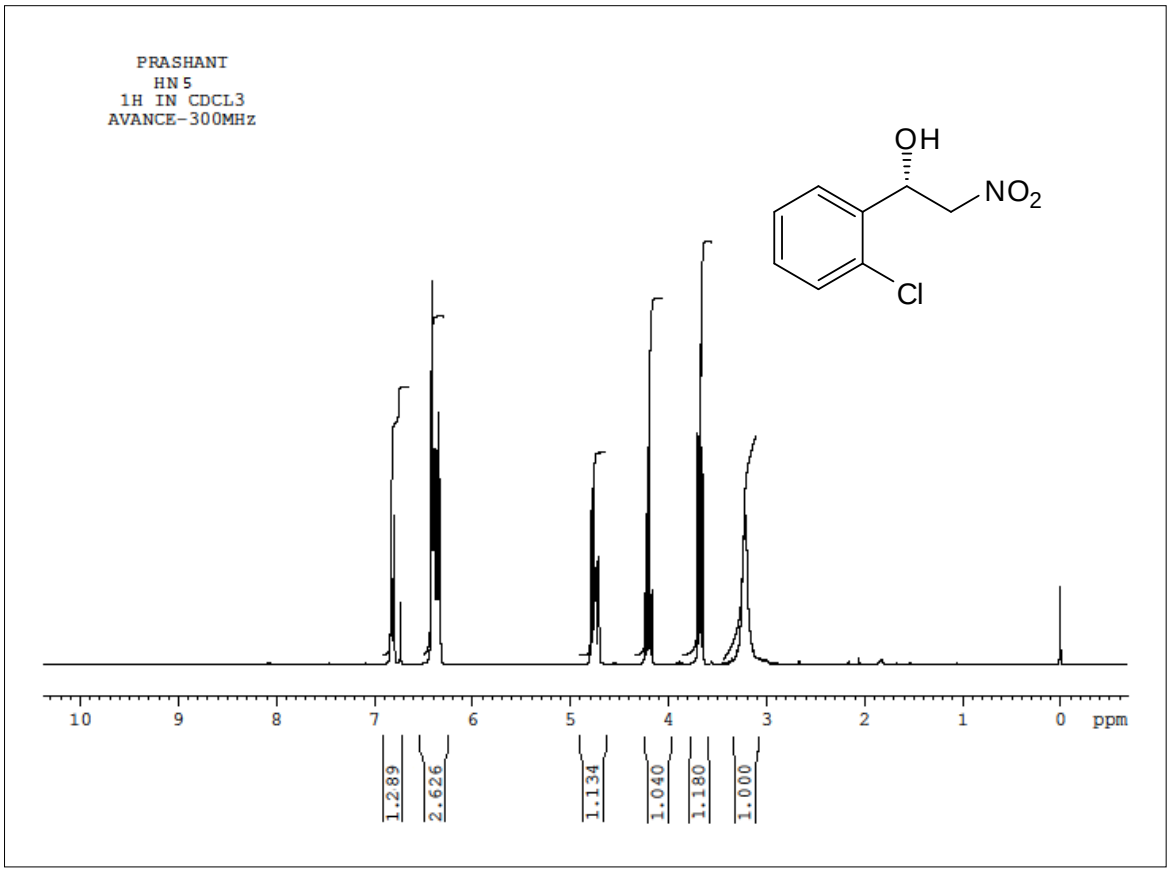

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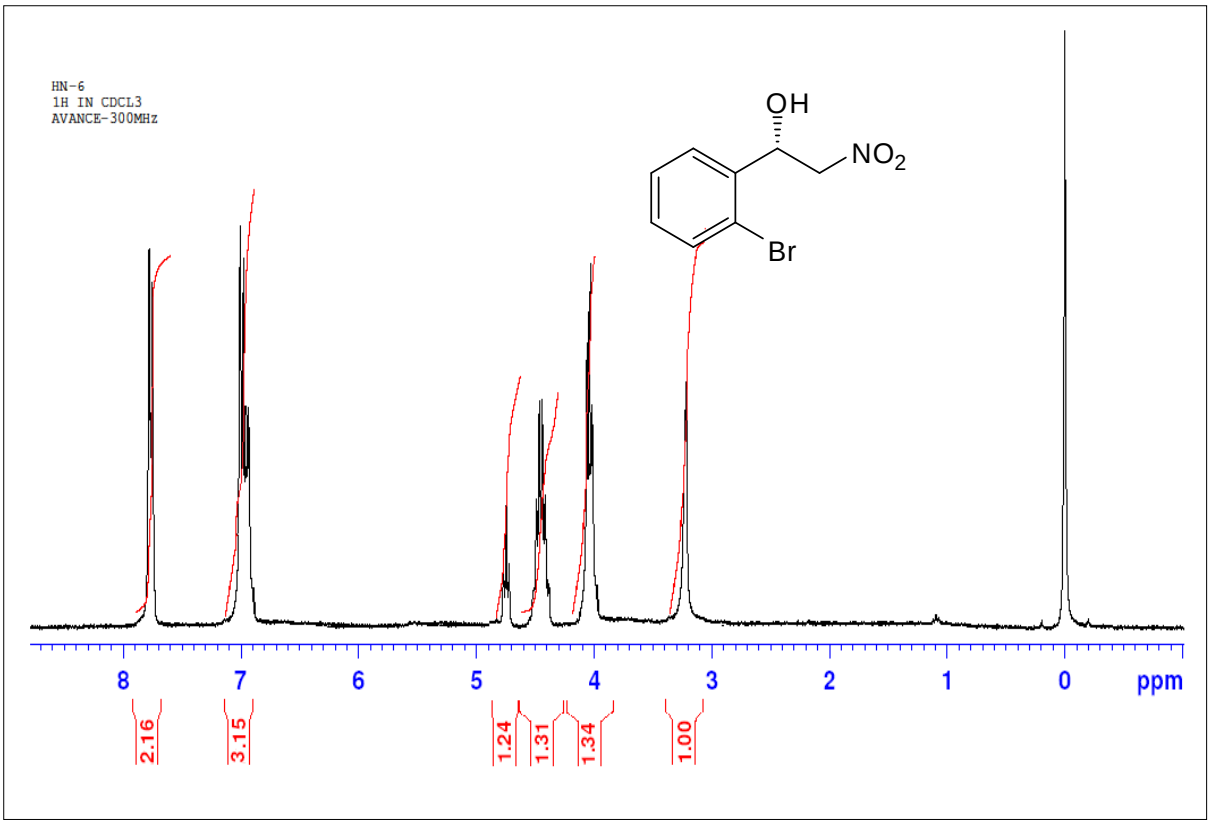

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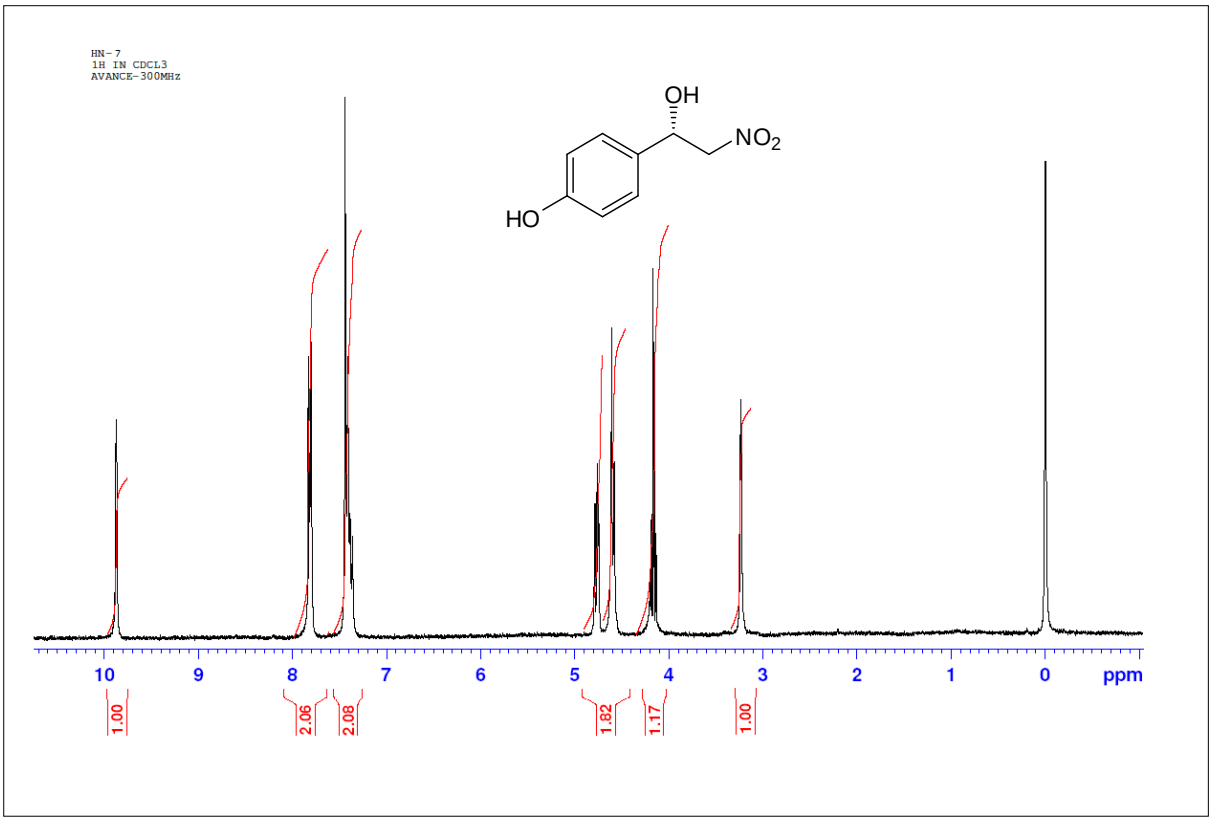
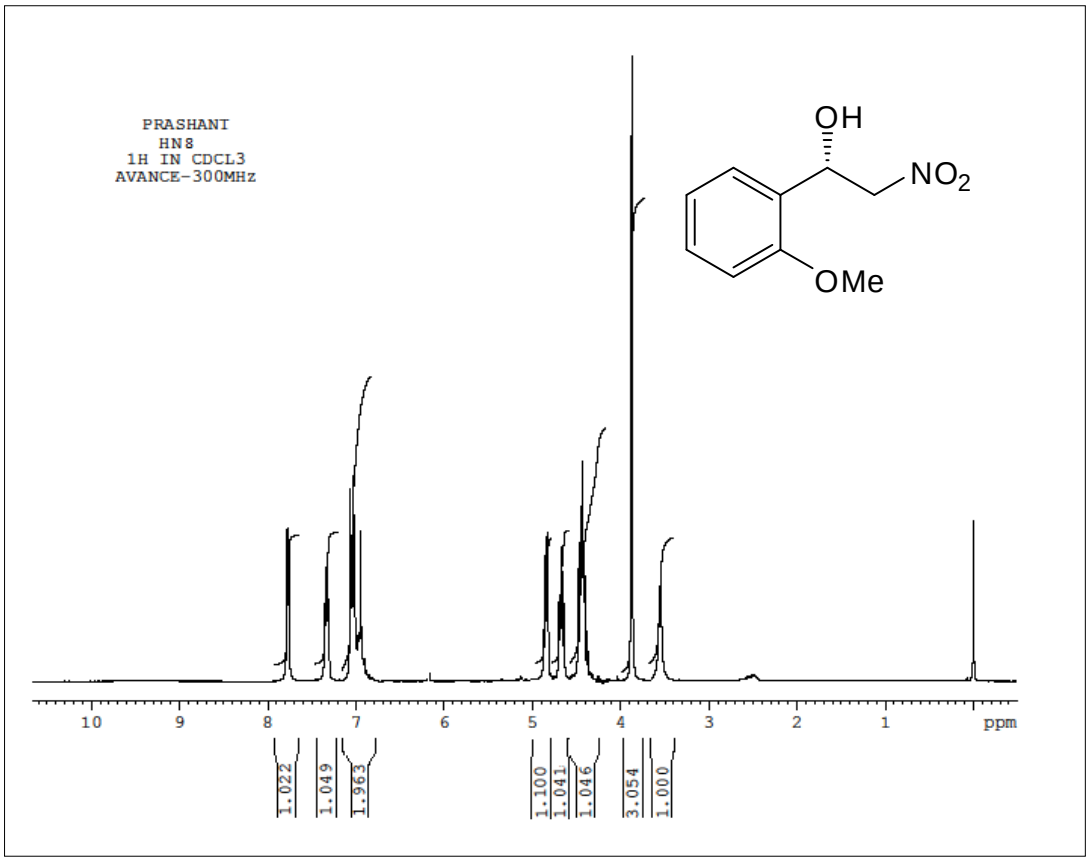
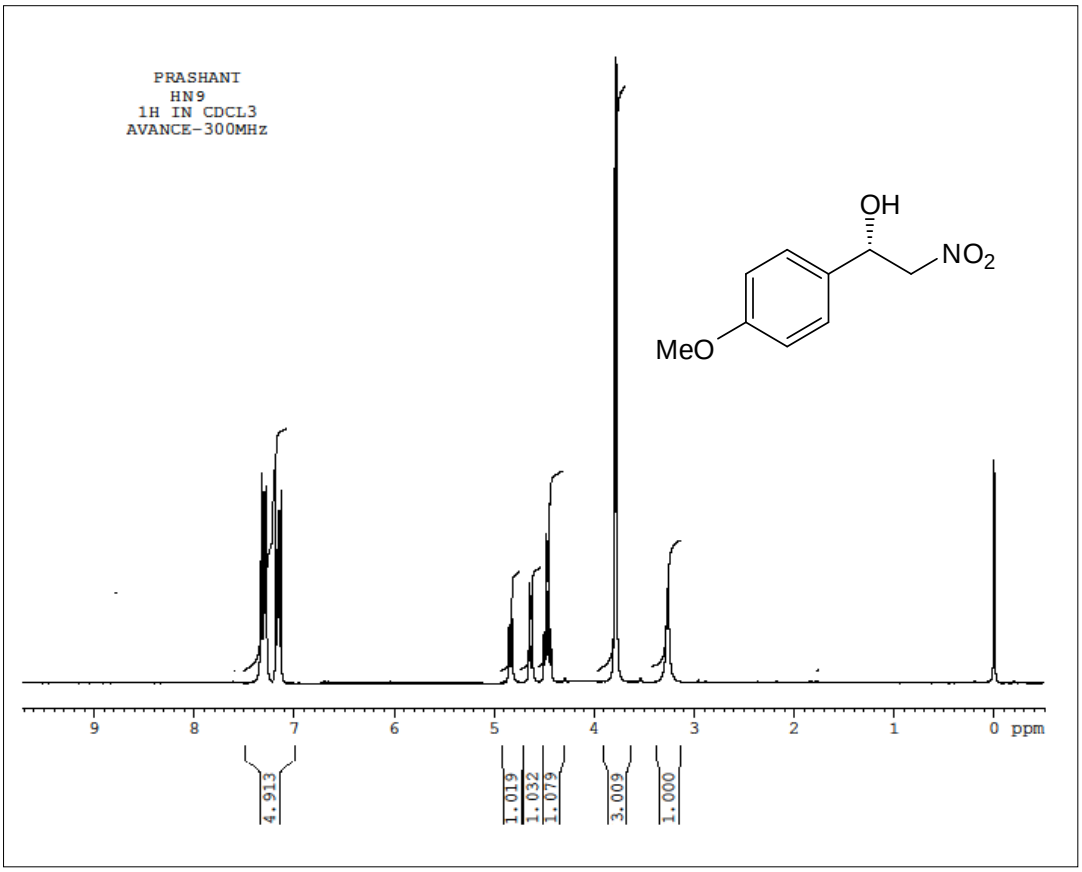


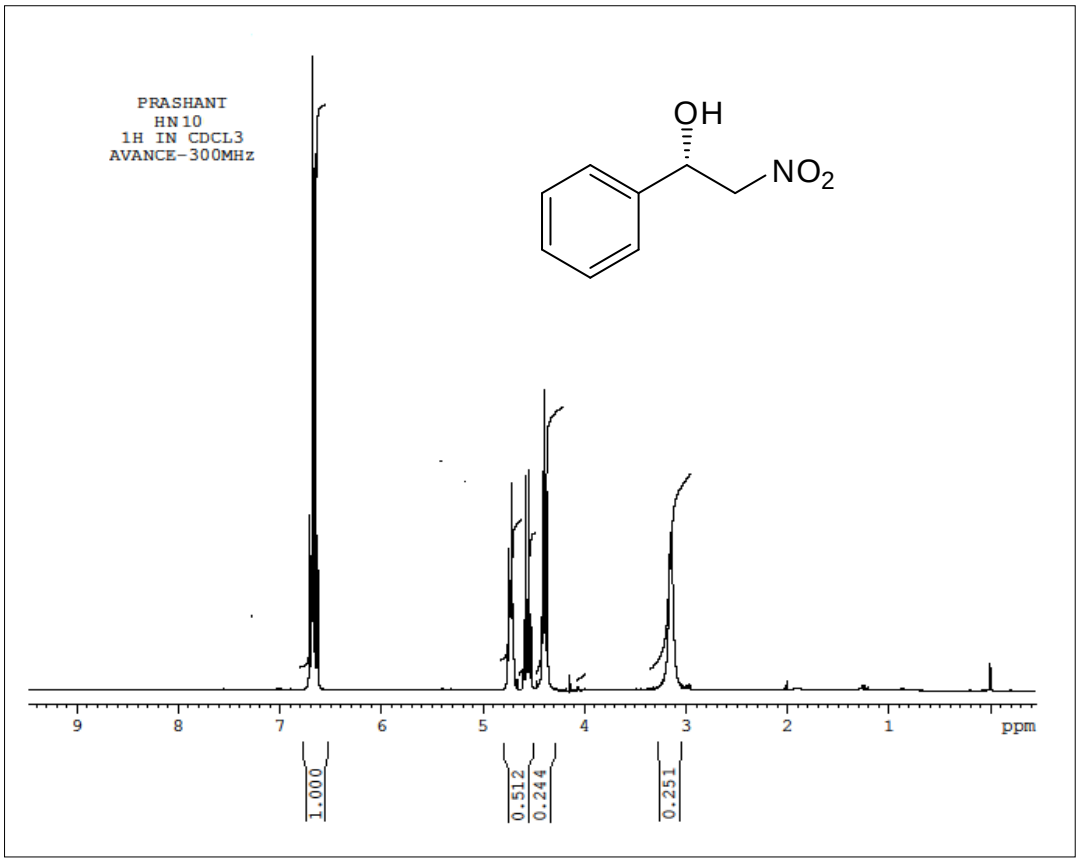
^{1}H NMR compound 10h



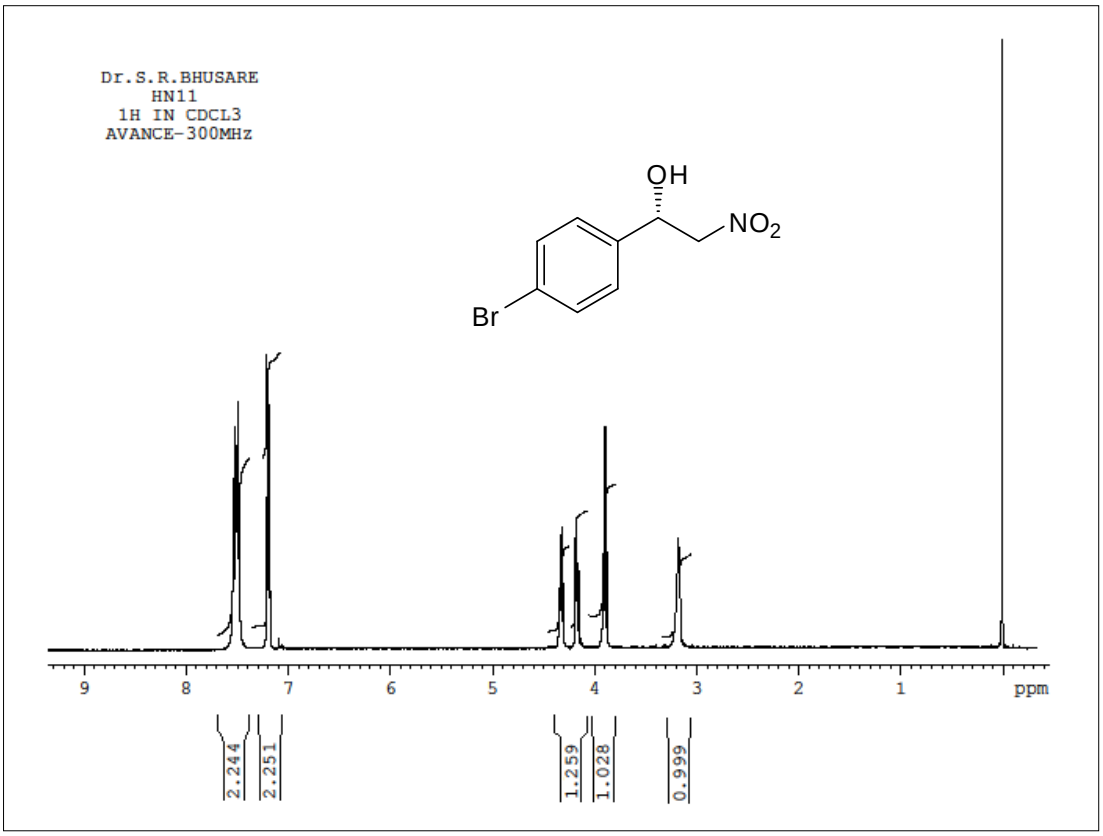
^{1}H NMR compound 10i



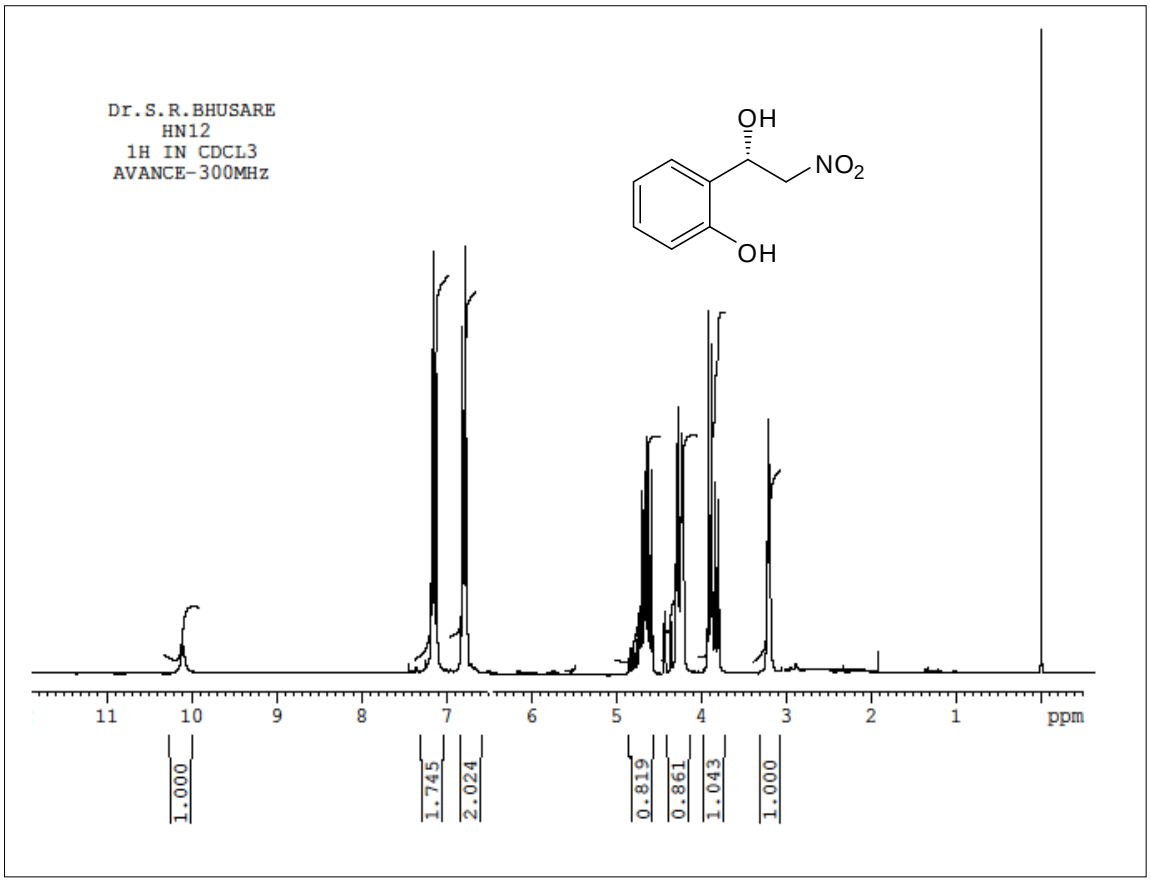
^{1}H NMR compound 10j



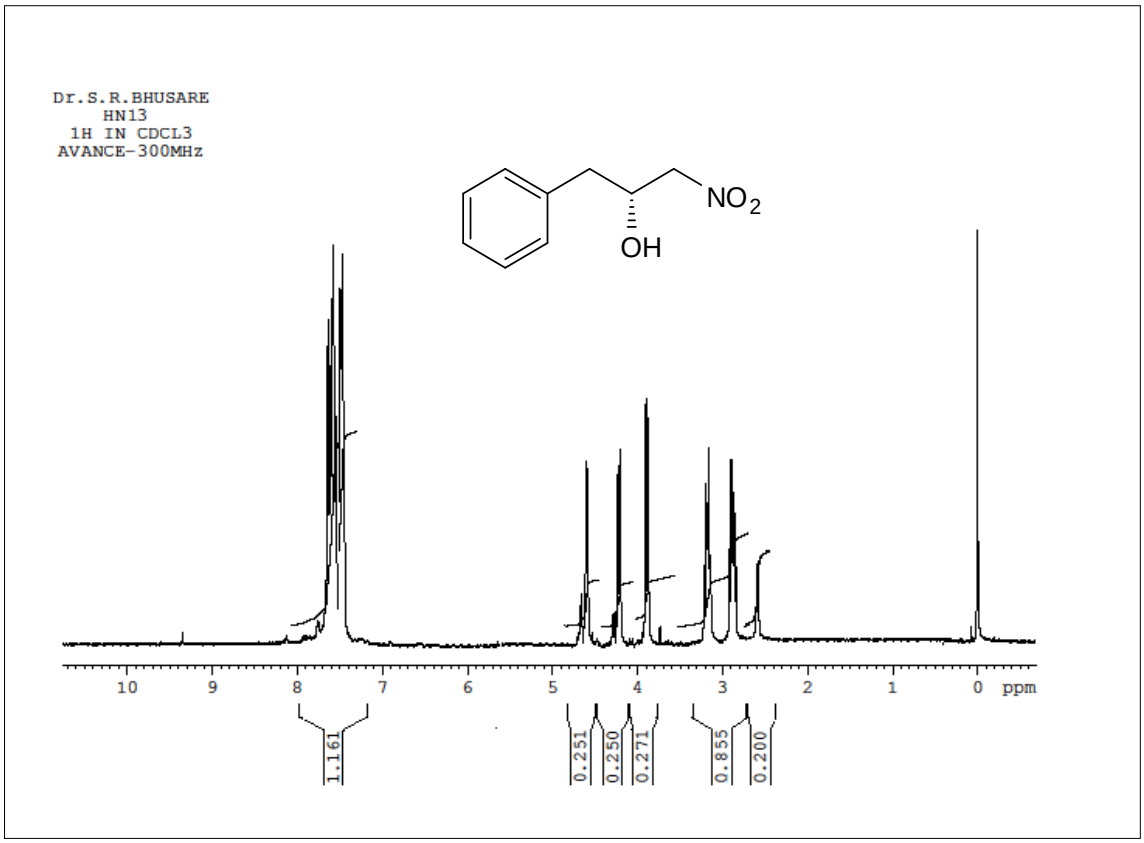
^{1}H NMR compound 10k



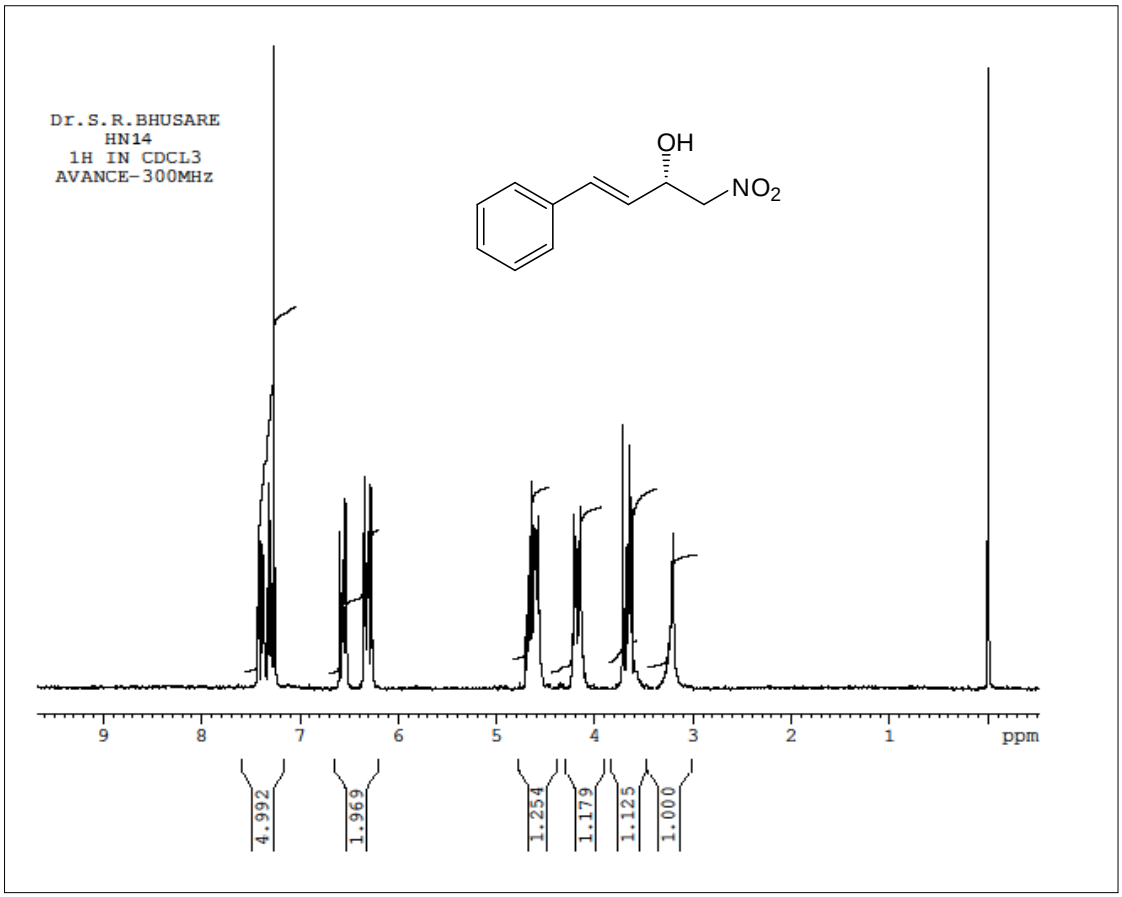
^{1}H NMR compound 10l



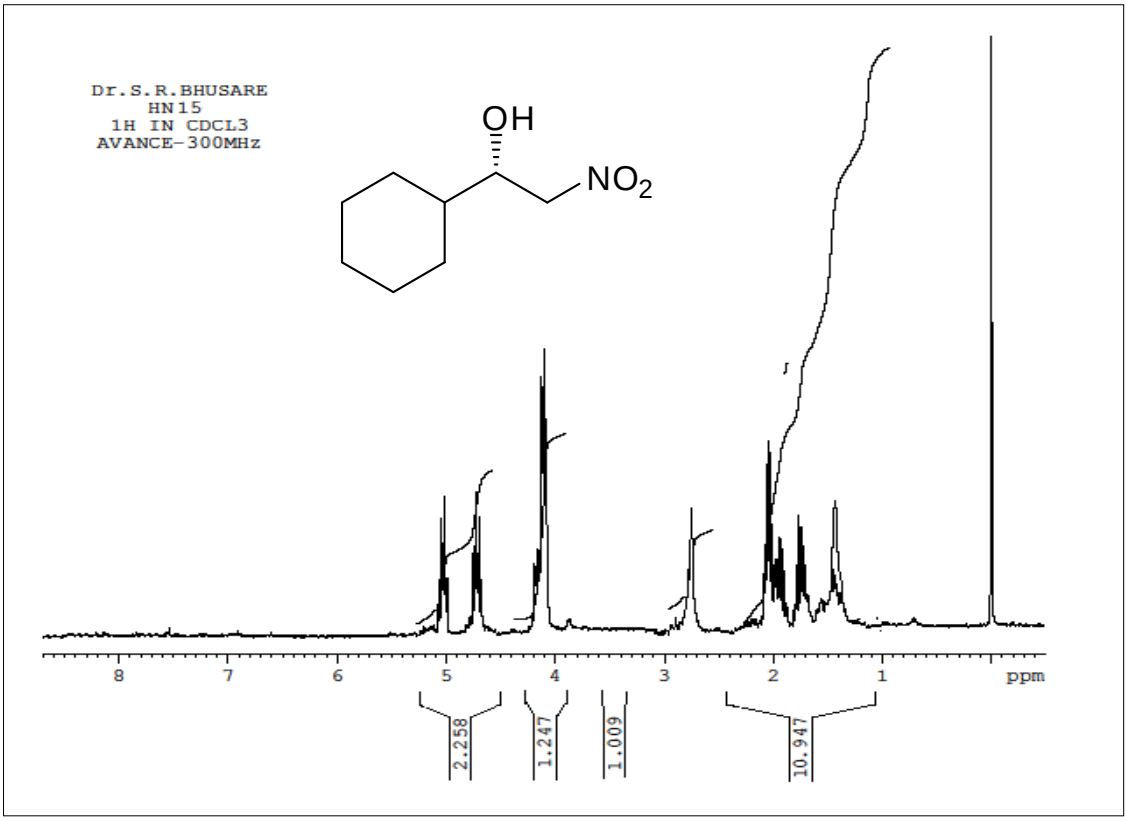
^{1}H NMR compound 10m



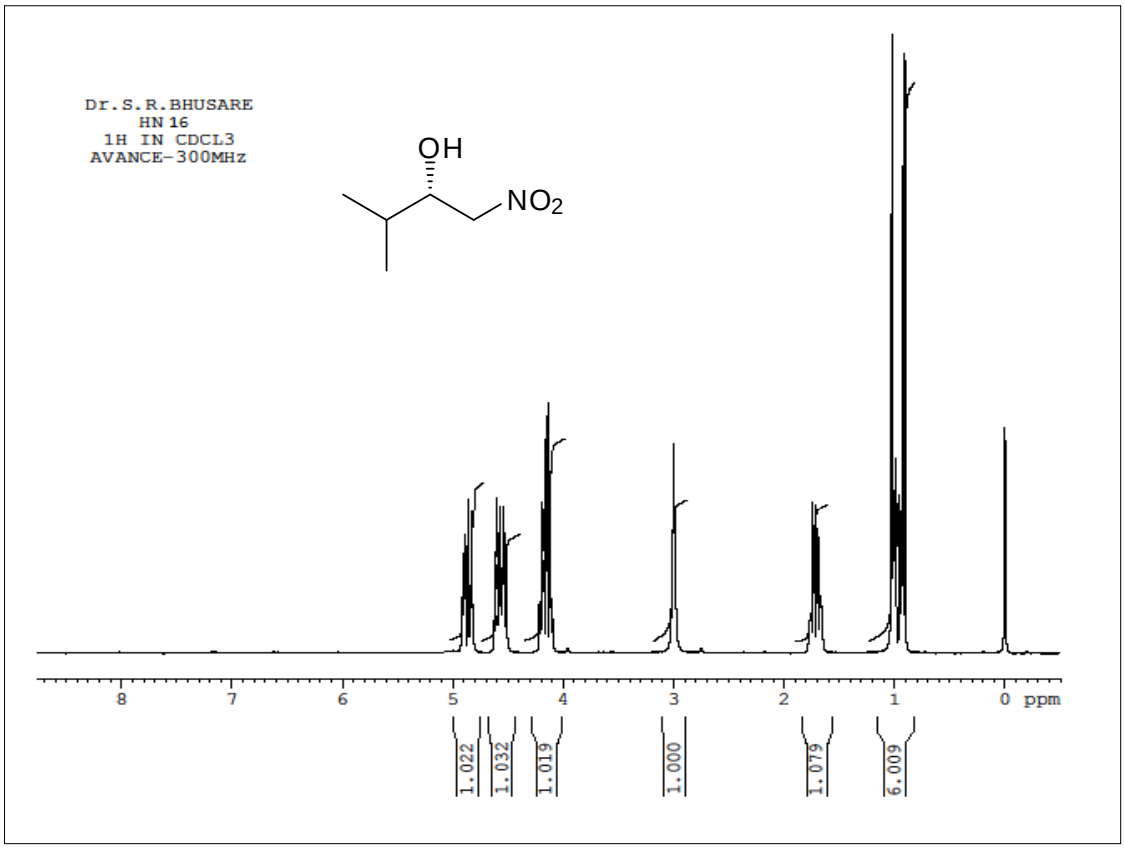
^{1}H NMR compound 10n



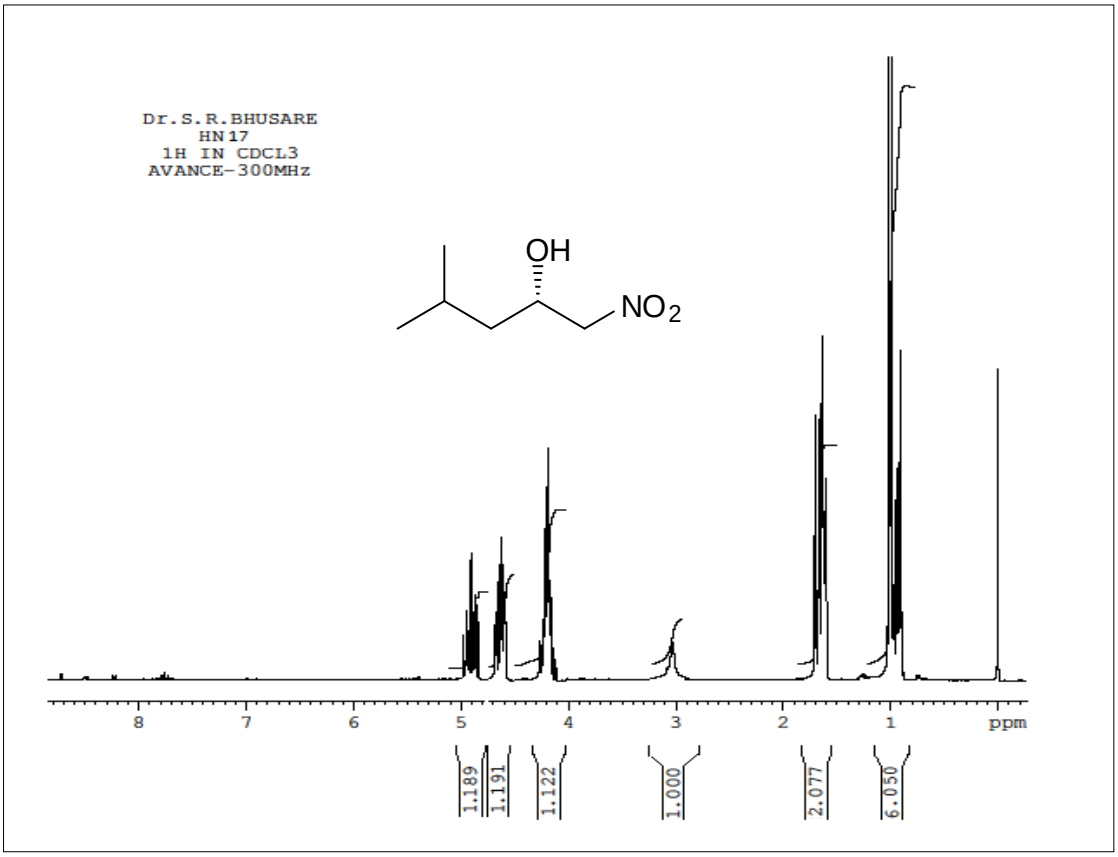
^{1}H NMR compound 10o



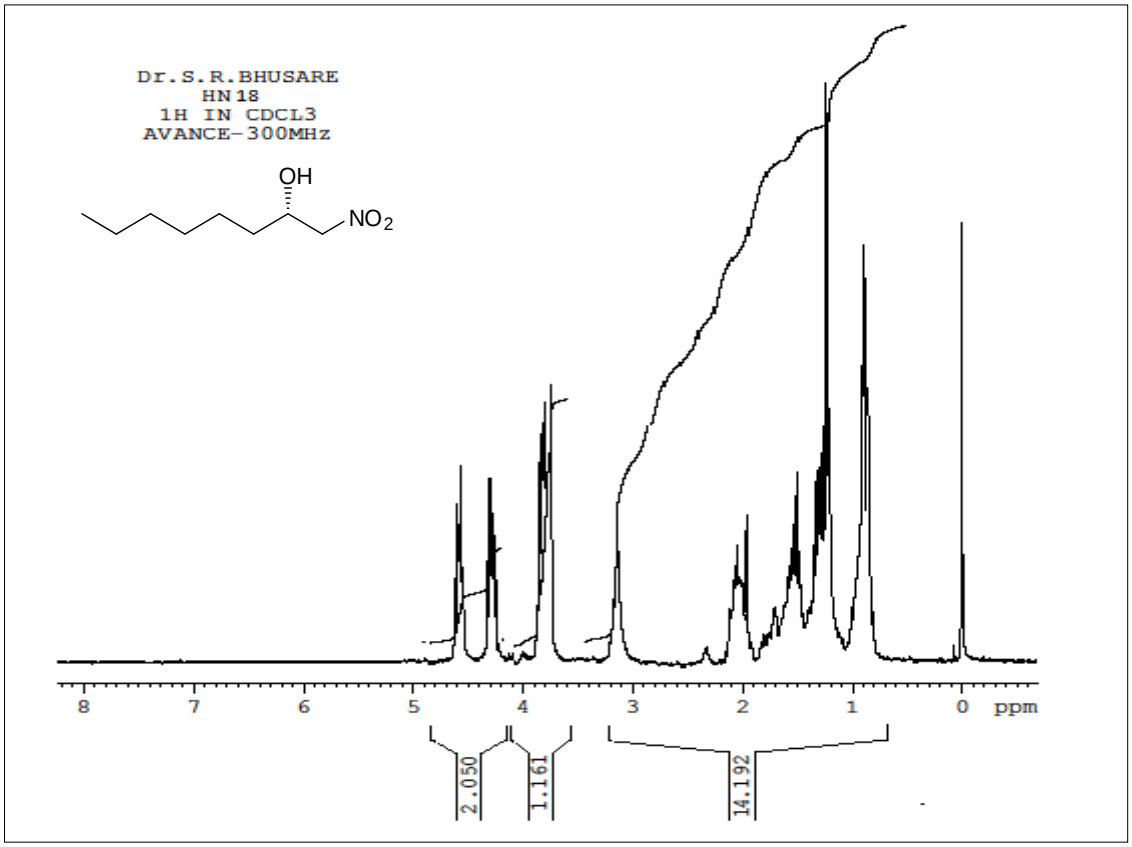
^{1}H NMR compound 10p


Dr.S.R.BHUSARE
HN 16
1H IN CDCL3
AVANCE-300MHz
OH
NO2
8
7
6
5
4
3
2
1
0 ppm
1.022
1.032
1.019
1.000
1.079
6.009

^{1}H NMR compound 10q

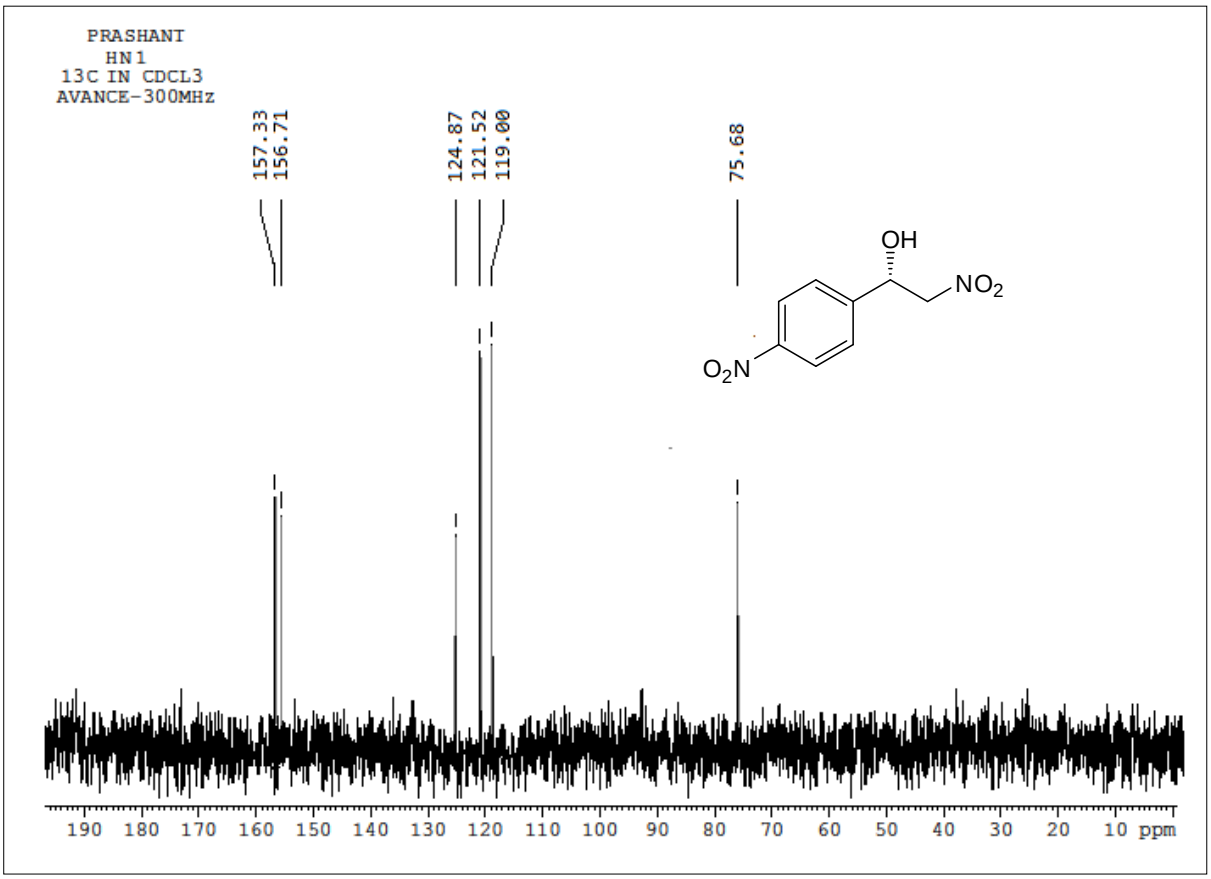


^{1}H NMR compound 10r

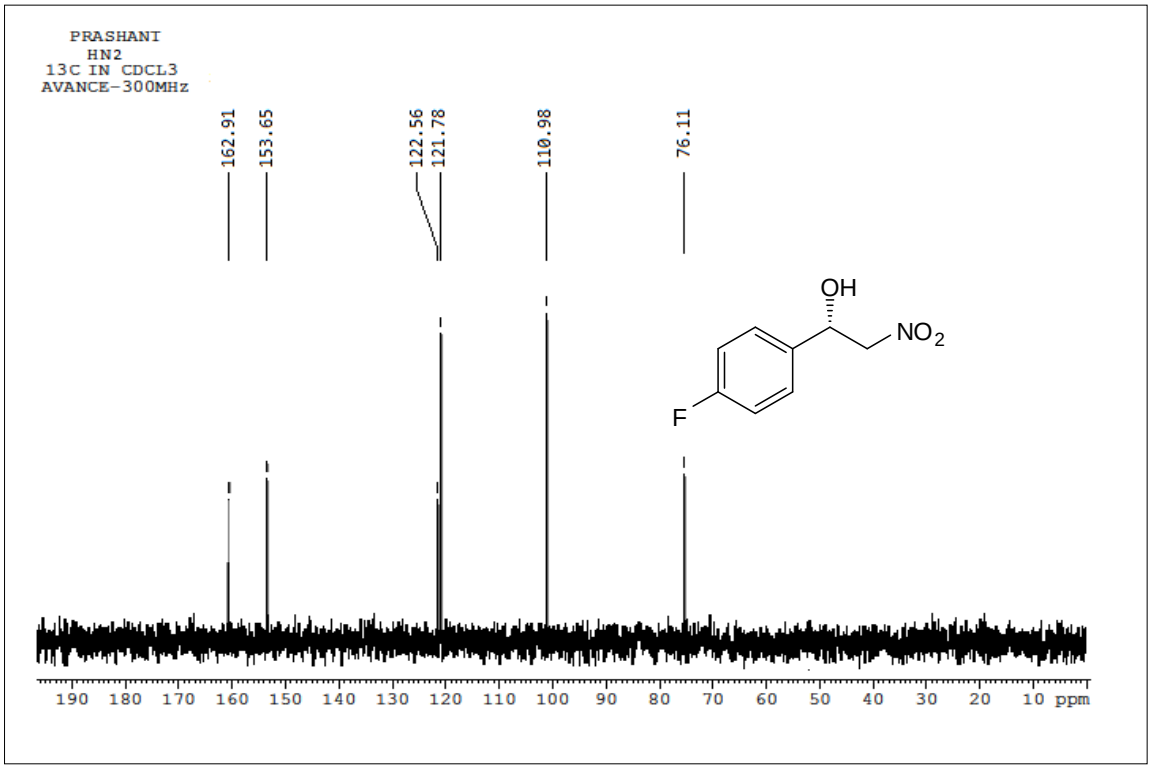


^{13}C NMR

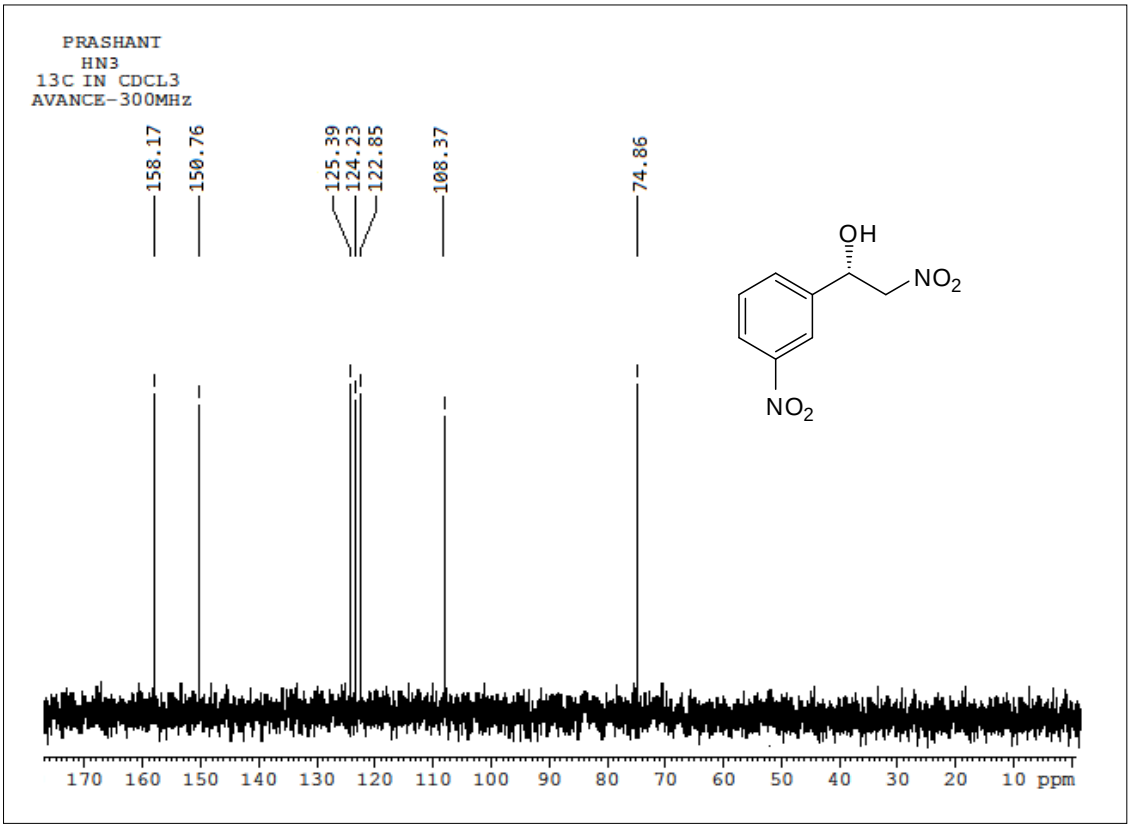
^{13}C NMR for compound 10a



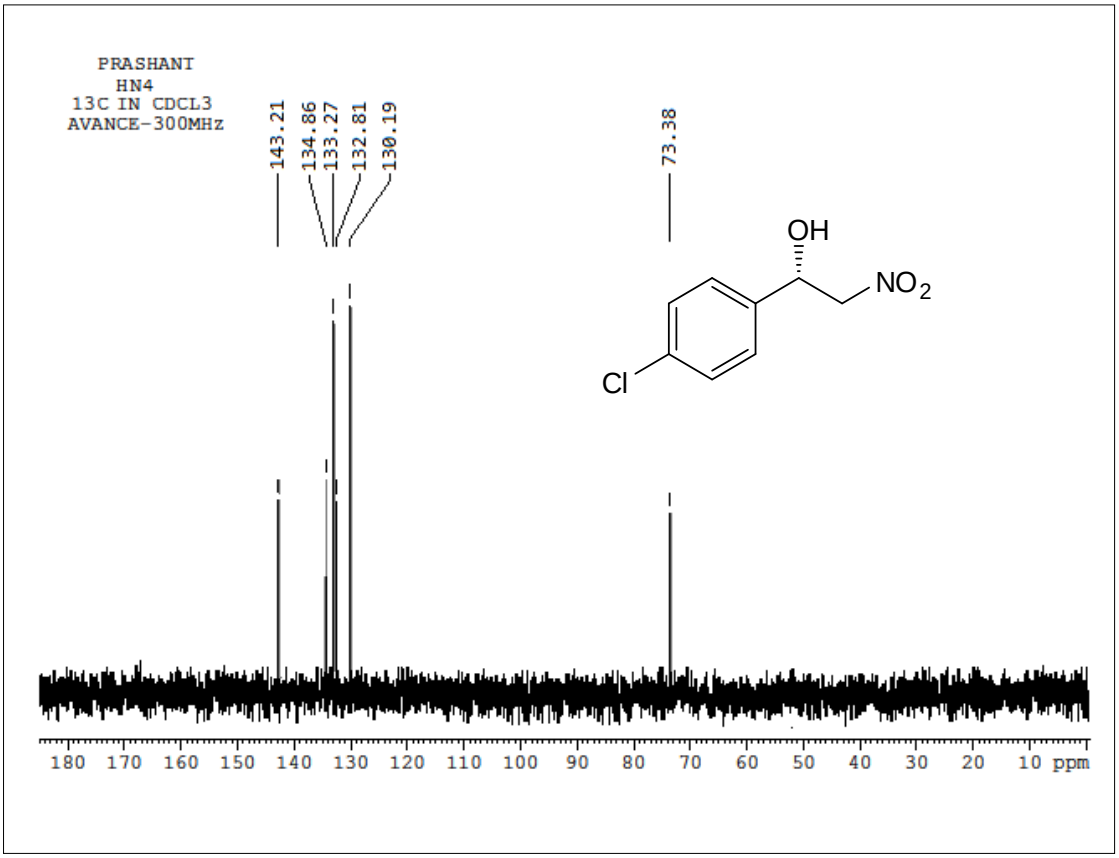
^{13}C NMR for compound 10b



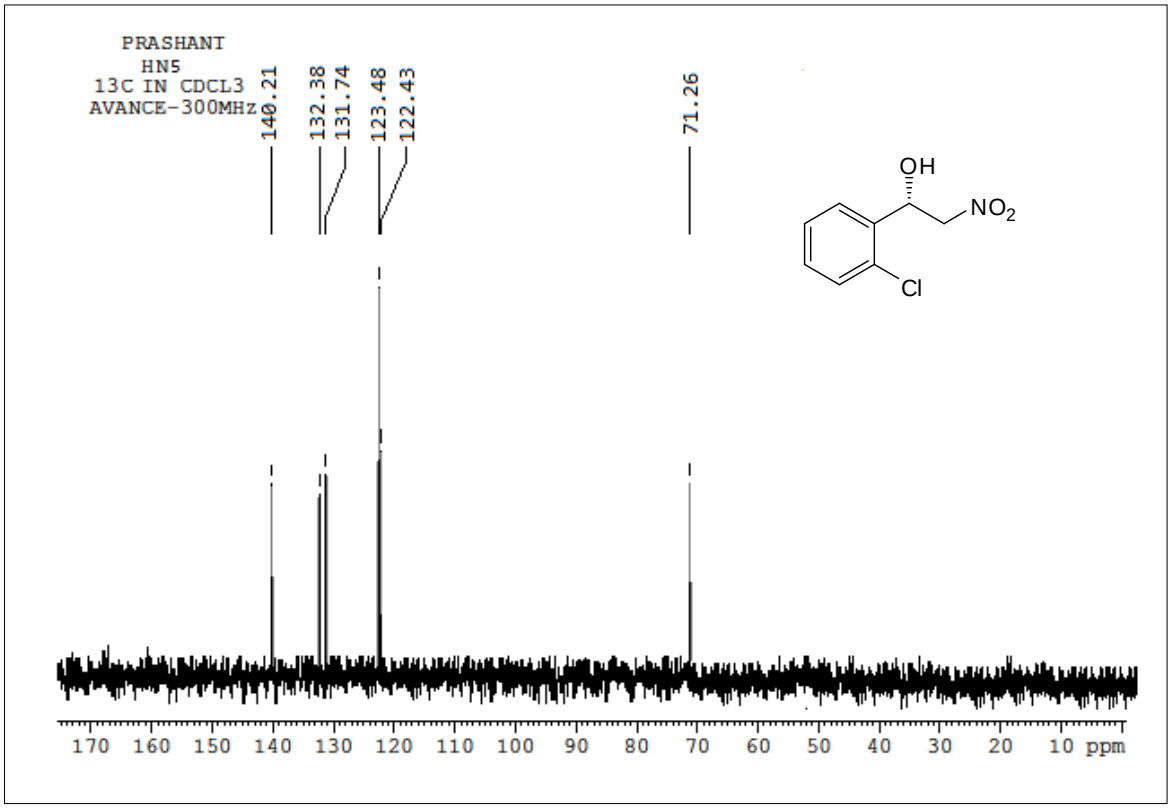
^{13}C NMR for compound 10c



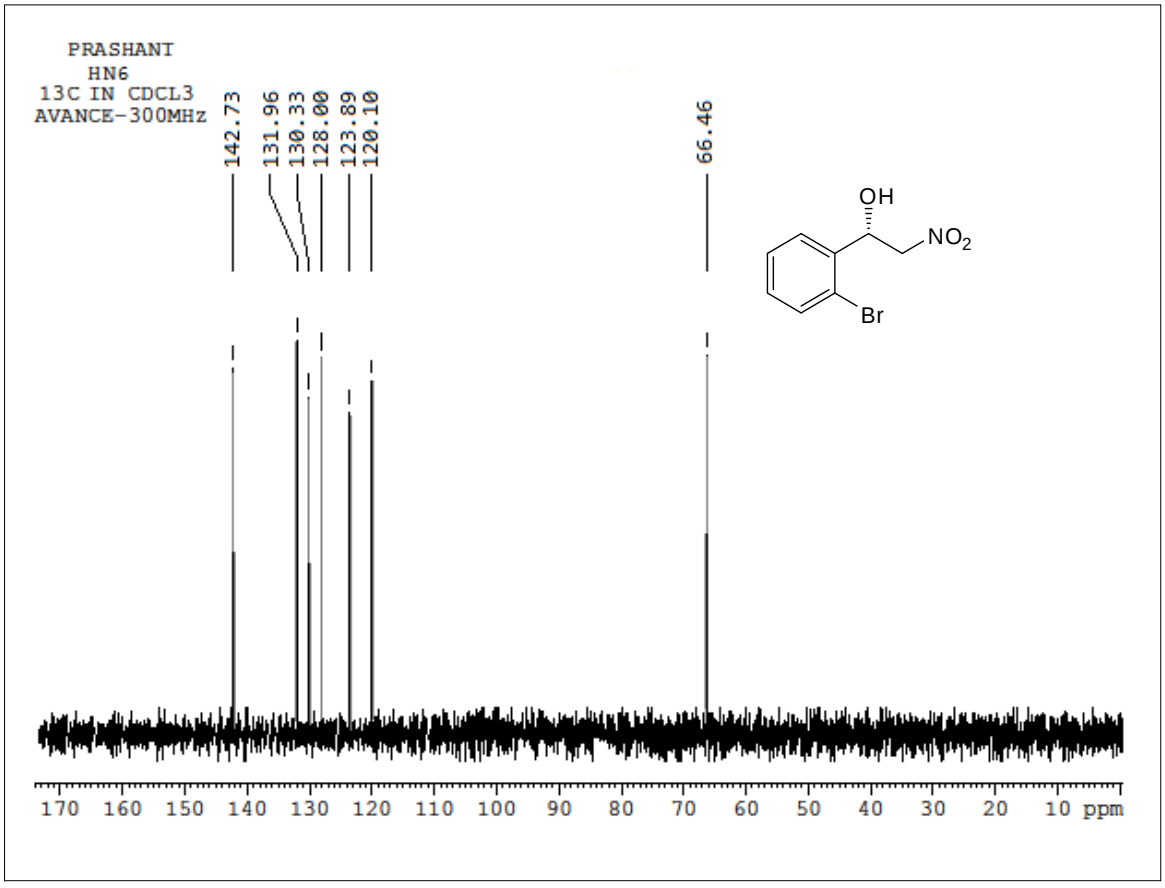
^{13}C NMR for compound 10d



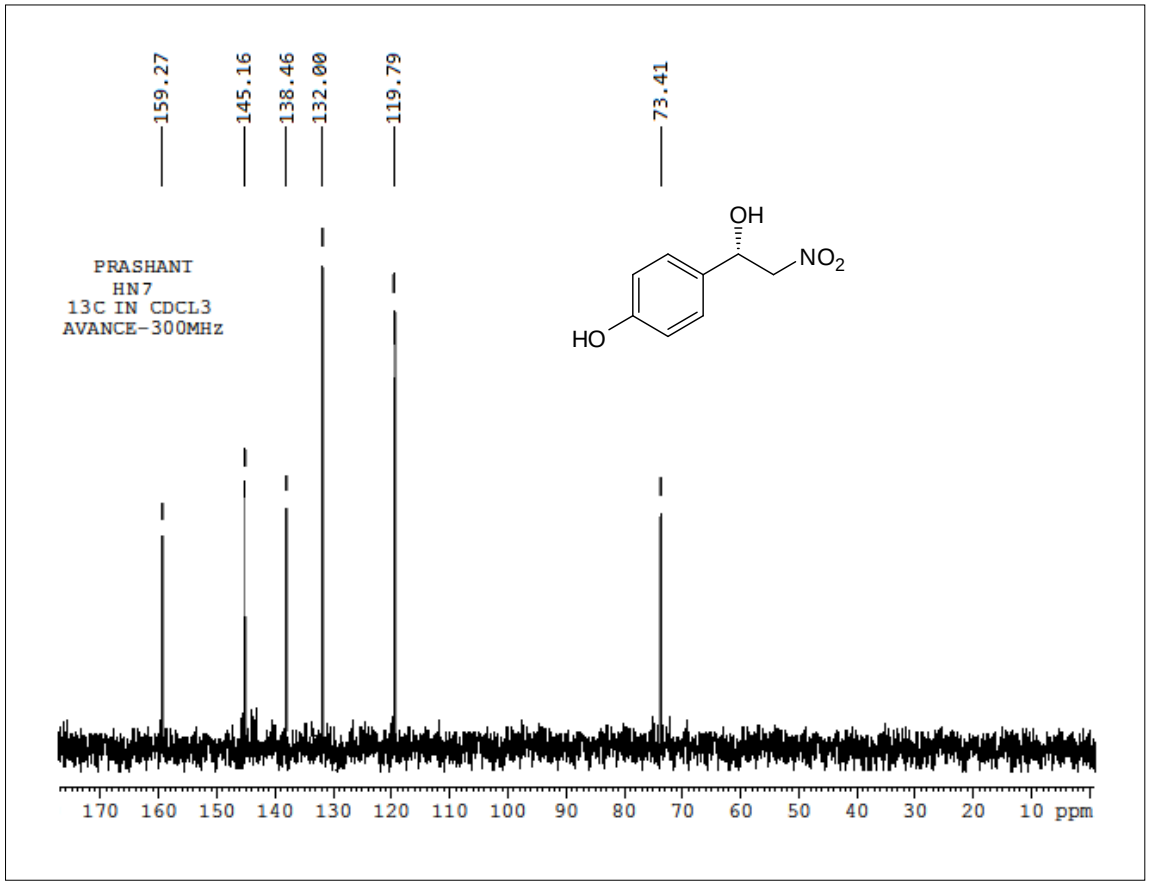
^{13}C NMR for compound 10e



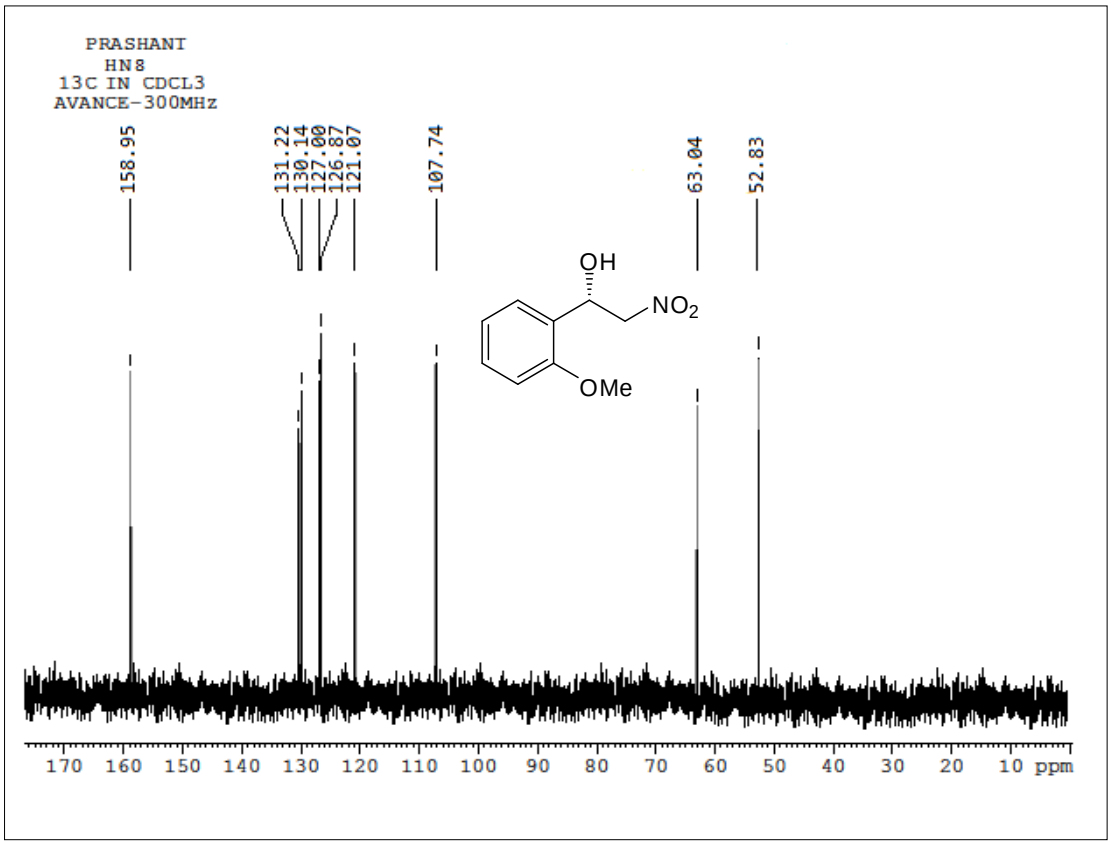
^{13}C NMR for compound 10f



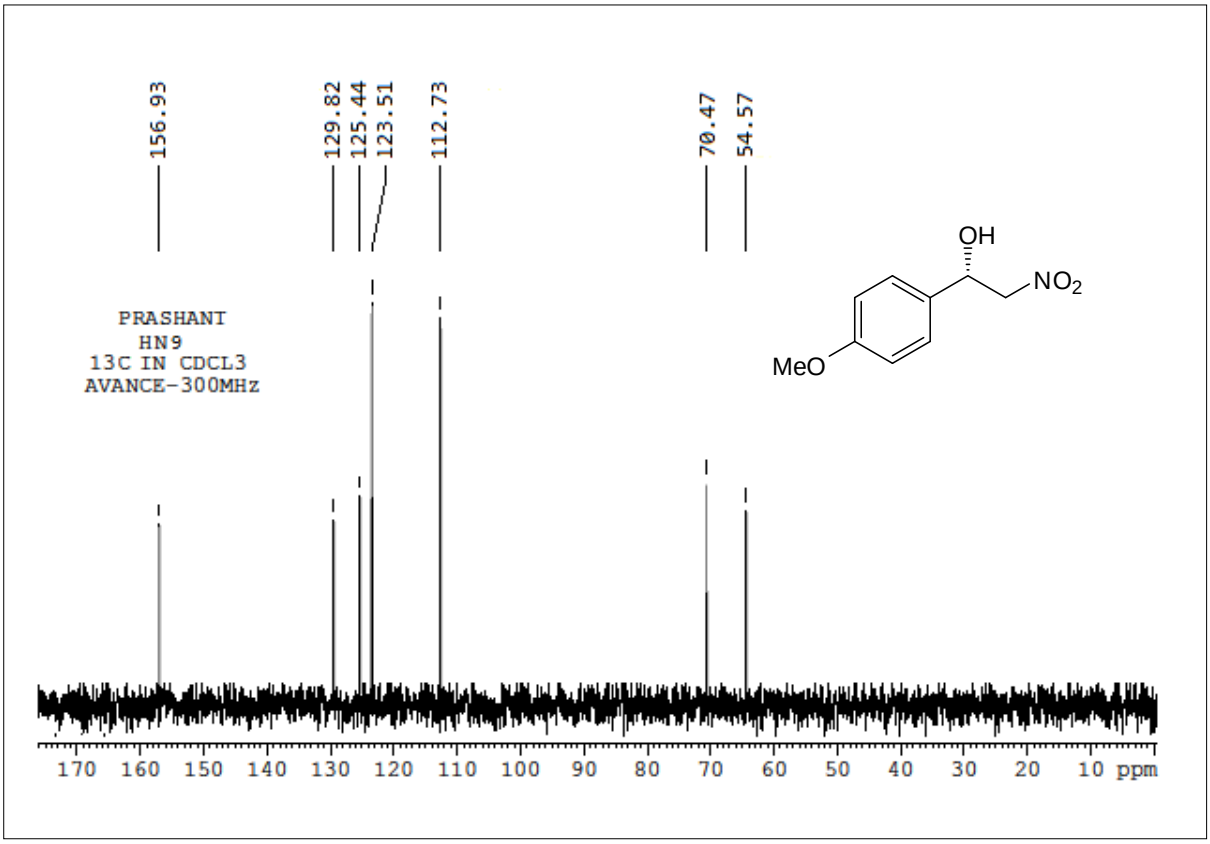
^{13}C NMR for compound 10g



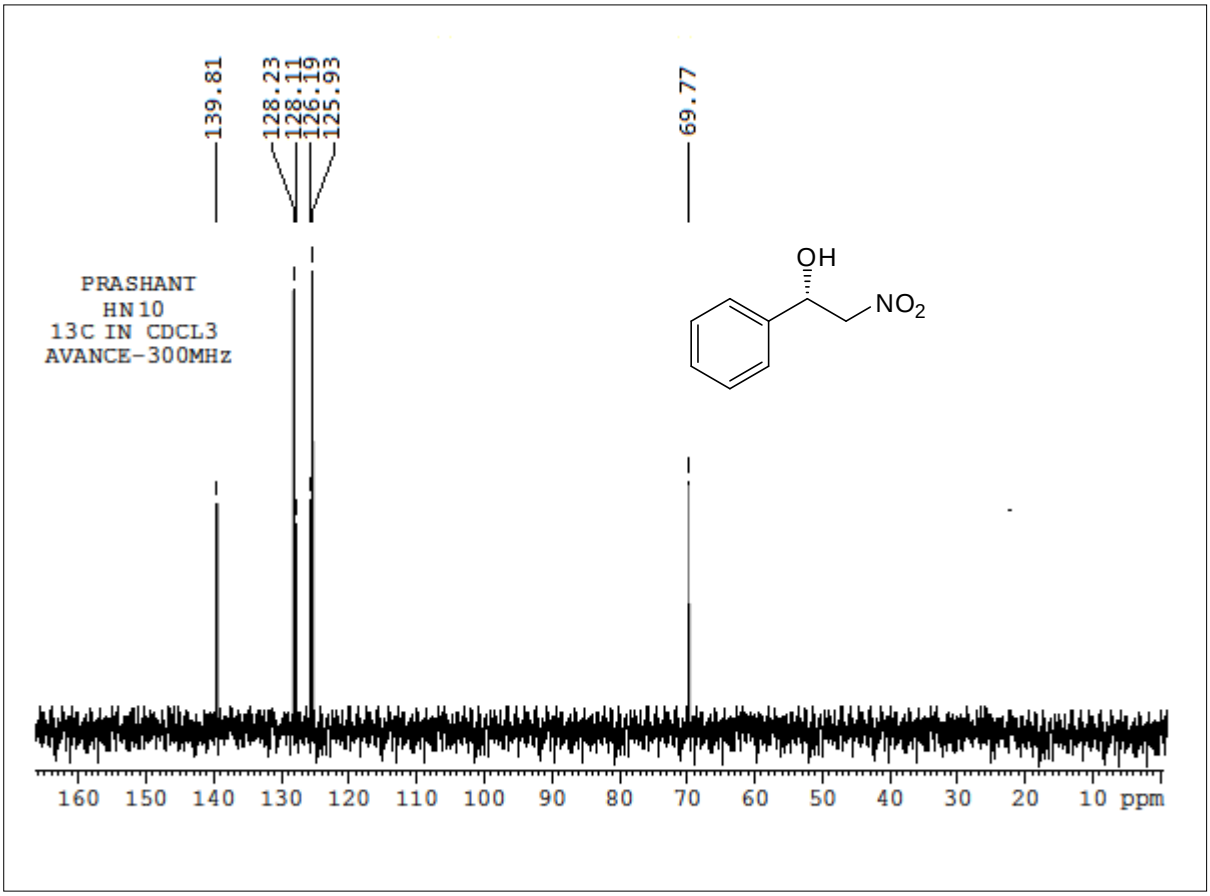
^{13}C NMR for compound 10h



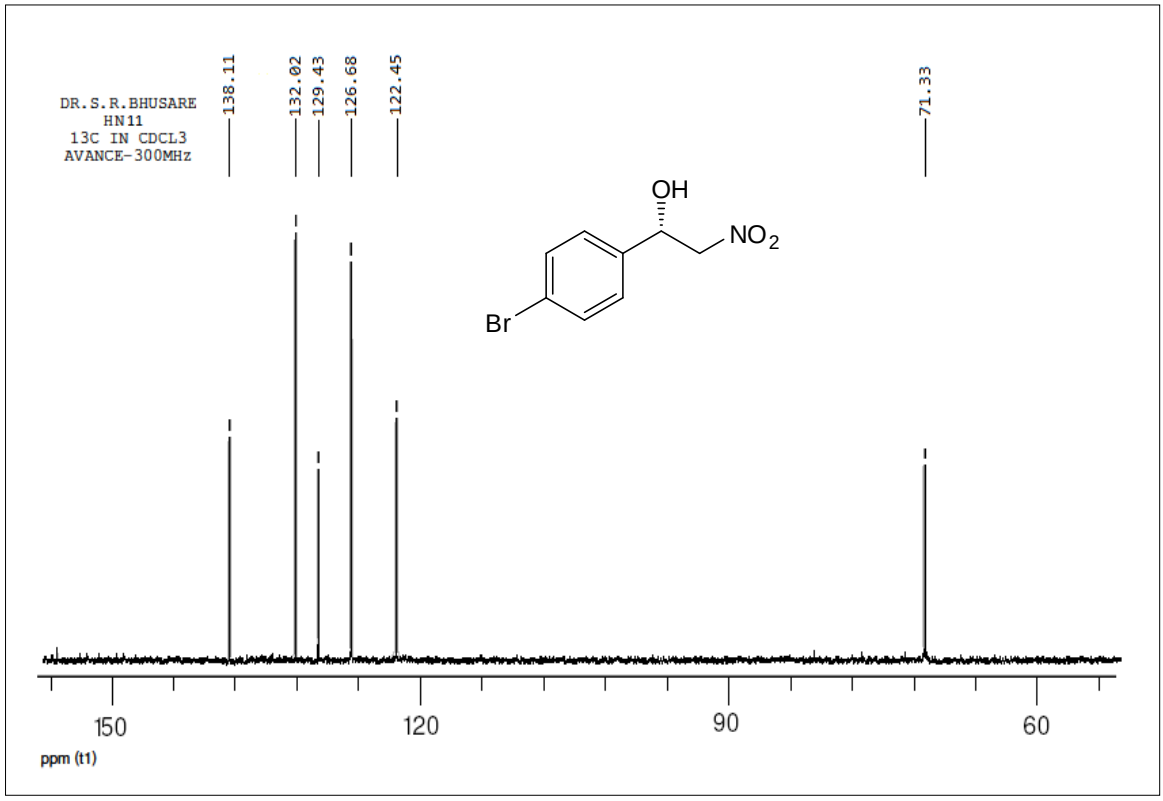
^{13}C NMR for compound 10i



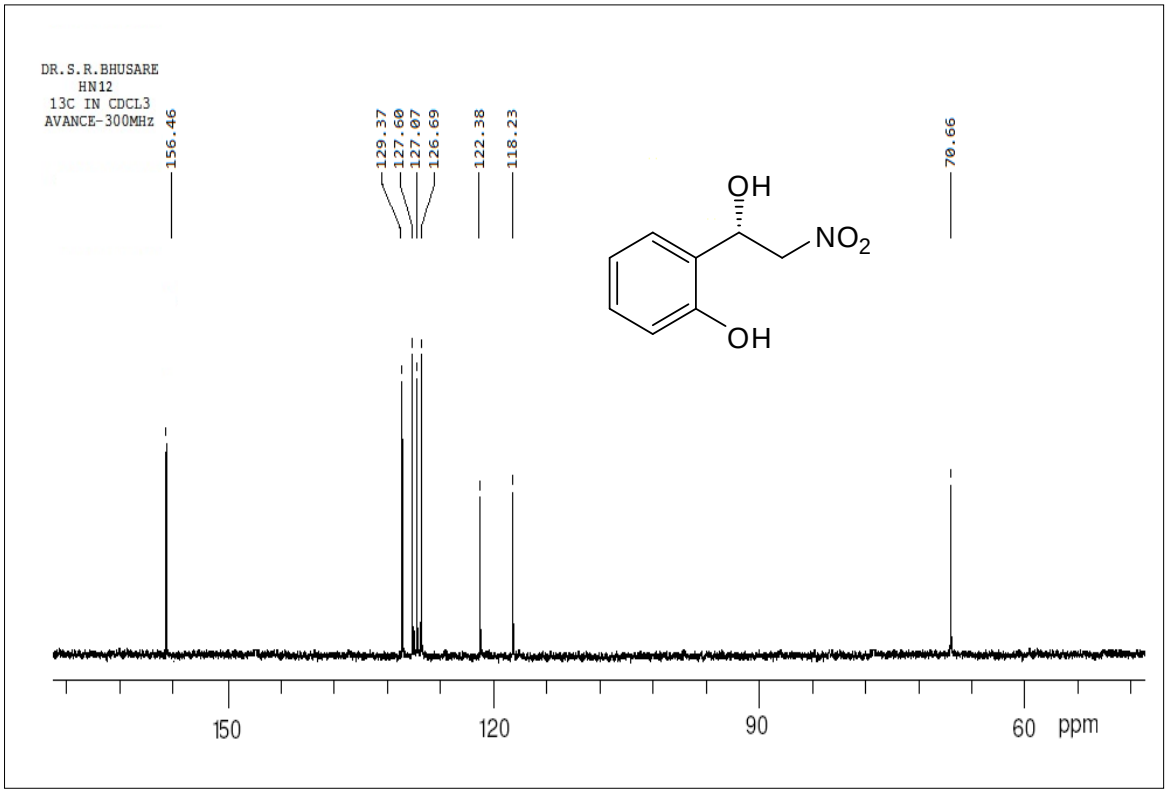
^{13}C NMR for compound 10j



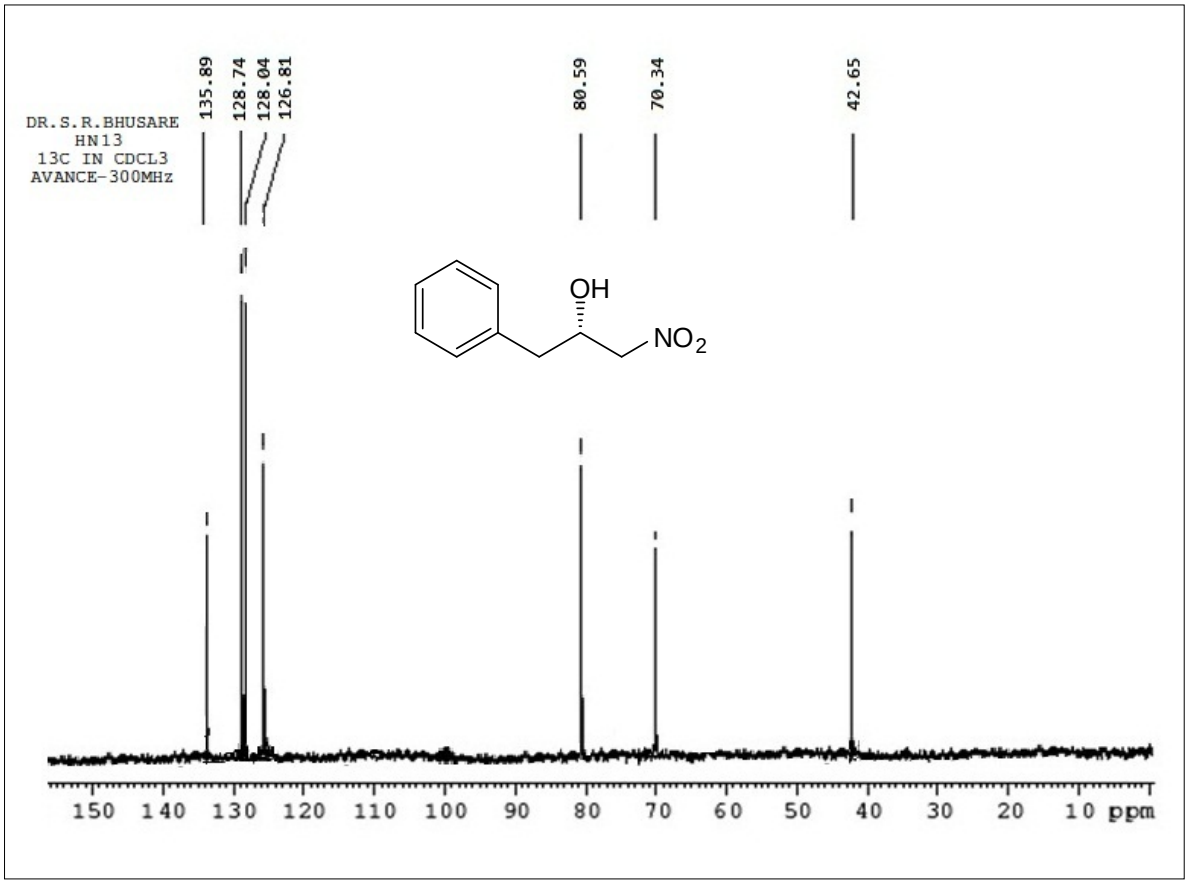
^{13}C NMR for compound 10k



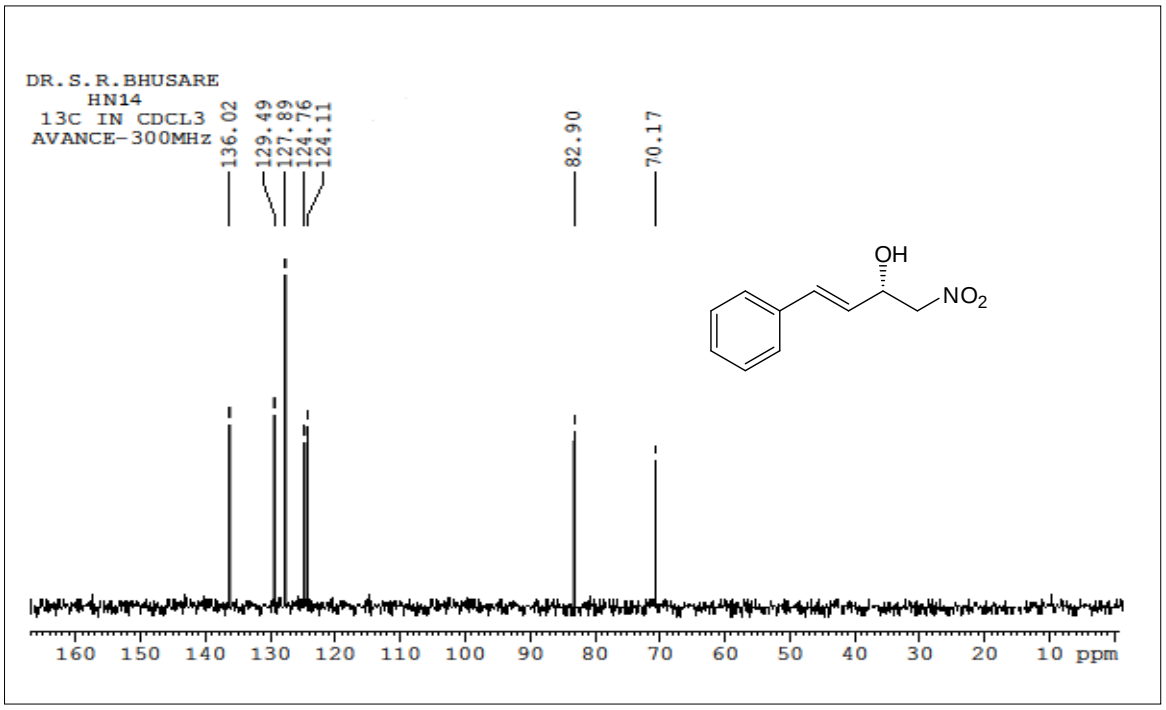
^{13}C NMR for compound 10l



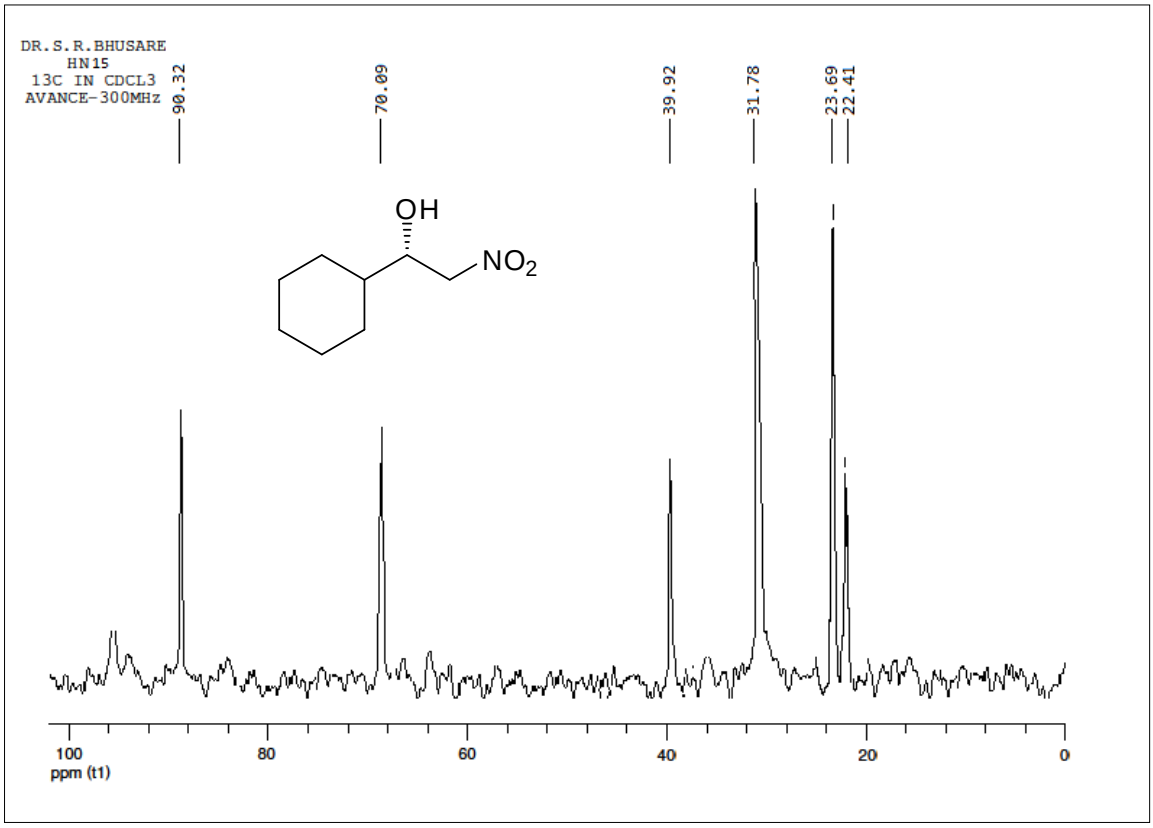
^{13}C NMR for compound 10m



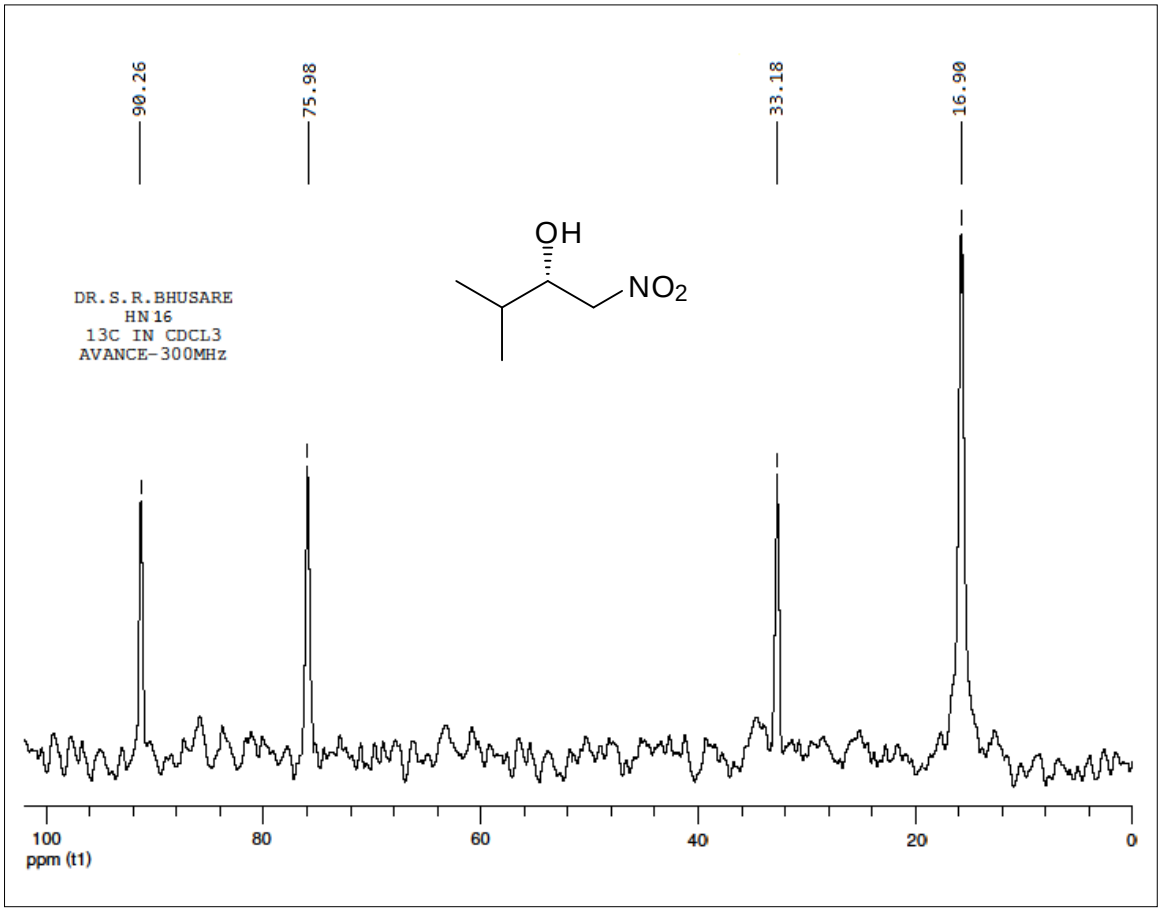
^{13}C NMR for compound 10n



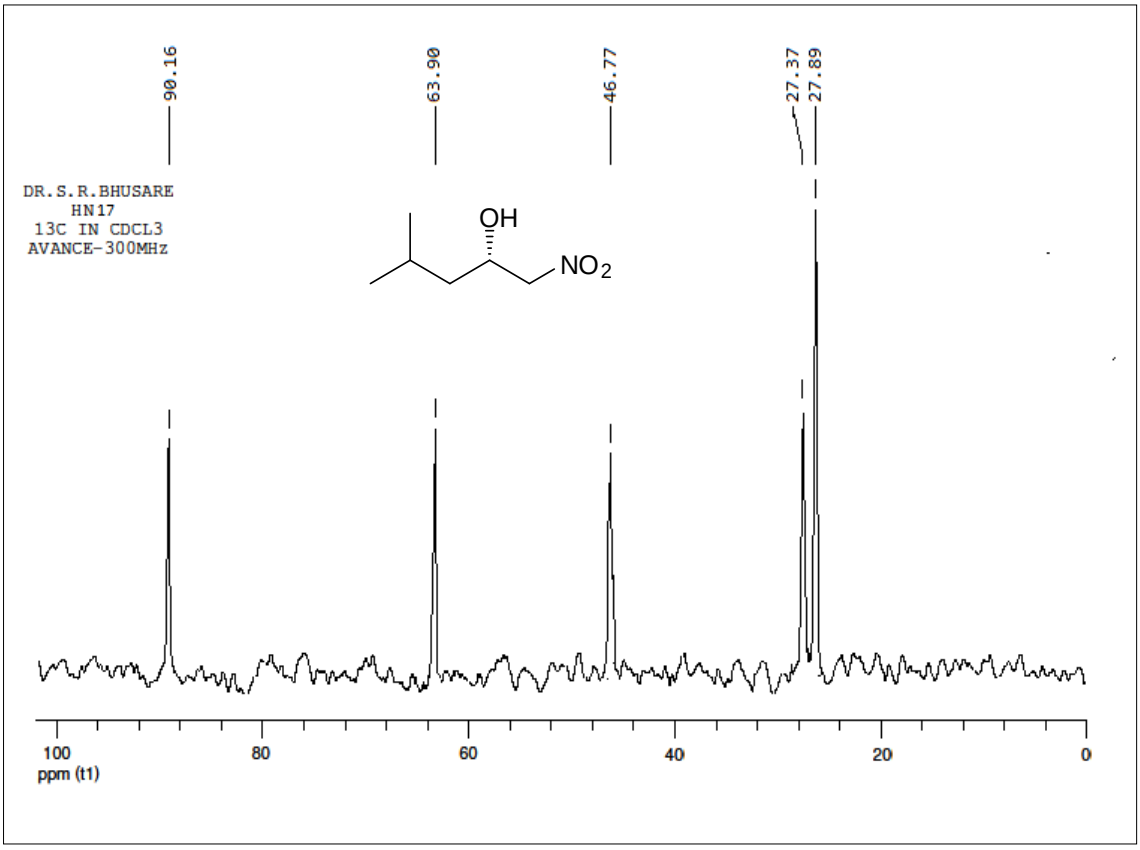
^{13}C NMR for compound 10o



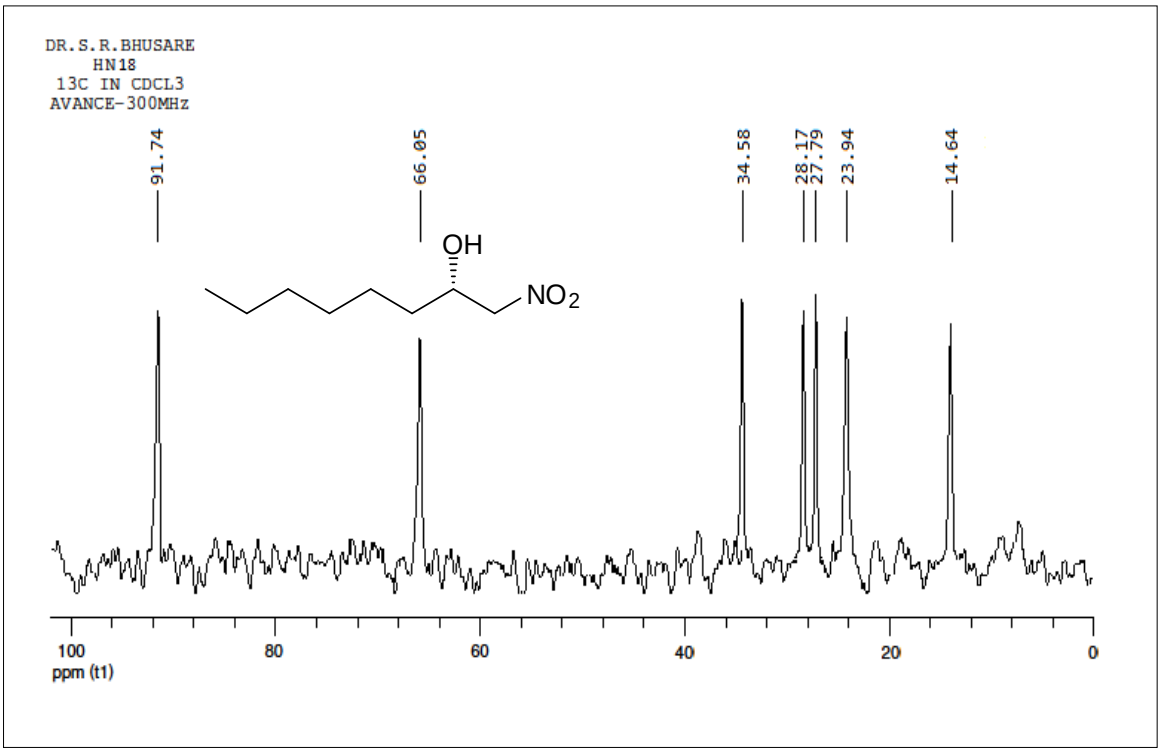
^{13}C NMR for compound 10p



^{13}C NMR for compound 10q

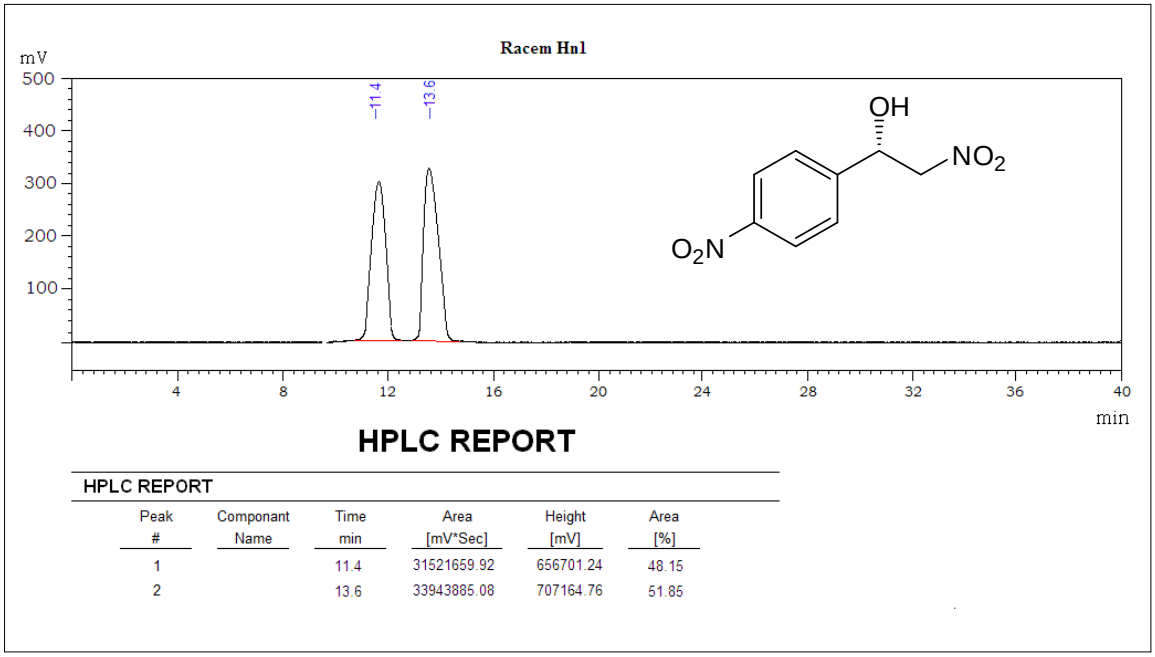


^{13}C NMR for compound 10r



HPLC chromatograms for compounds (10a-r)

HPLC Chromatograms of racemic compound **10a**

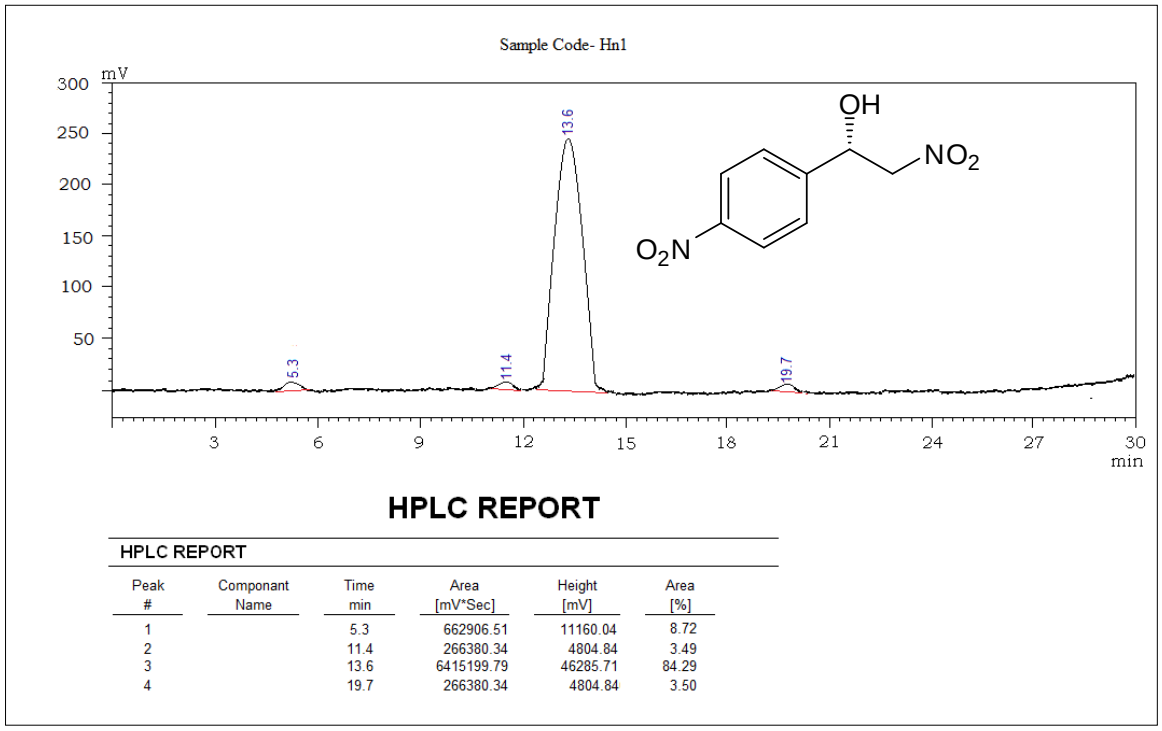


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		11.4	31521659.92	656701.24	48.15
2		13.6	33943885.08	707164.76	51.85

HPLC Chromatograms of compound **10a** [ref1]

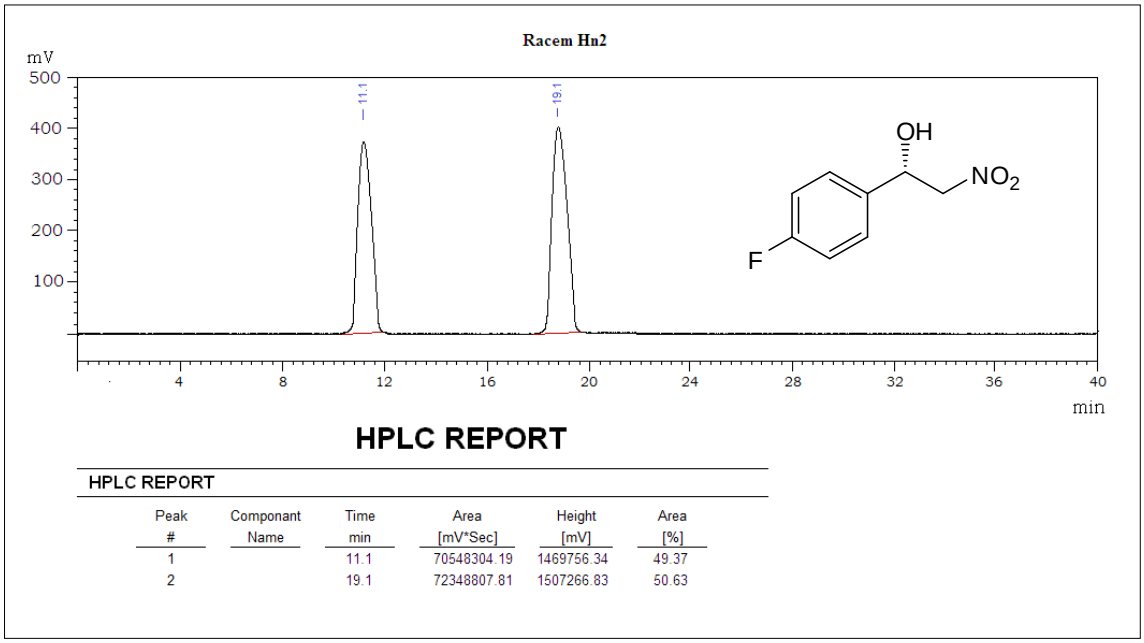


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		5.3	662906.51	11160.04	8.72
2		11.4	266380.34	4804.84	3.49
3		13.6	6415199.79	46285.71	84.29
4		19.7	266380.34	4804.84	3.50

HPLC Chromatograms of Racemic compound **10b**

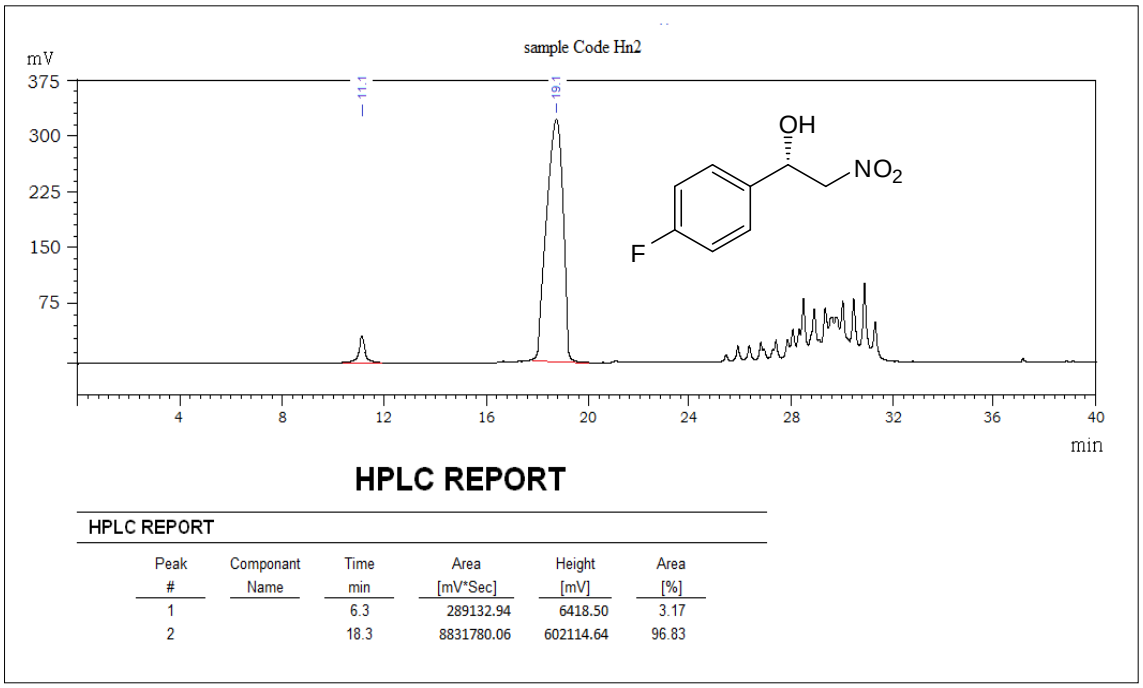


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		11.1	70548304.19	1469756.34	49.37
2		19.1	72348807.81	1507266.83	50.63

HPLC Chromatograms of compound **10b** [ref2]

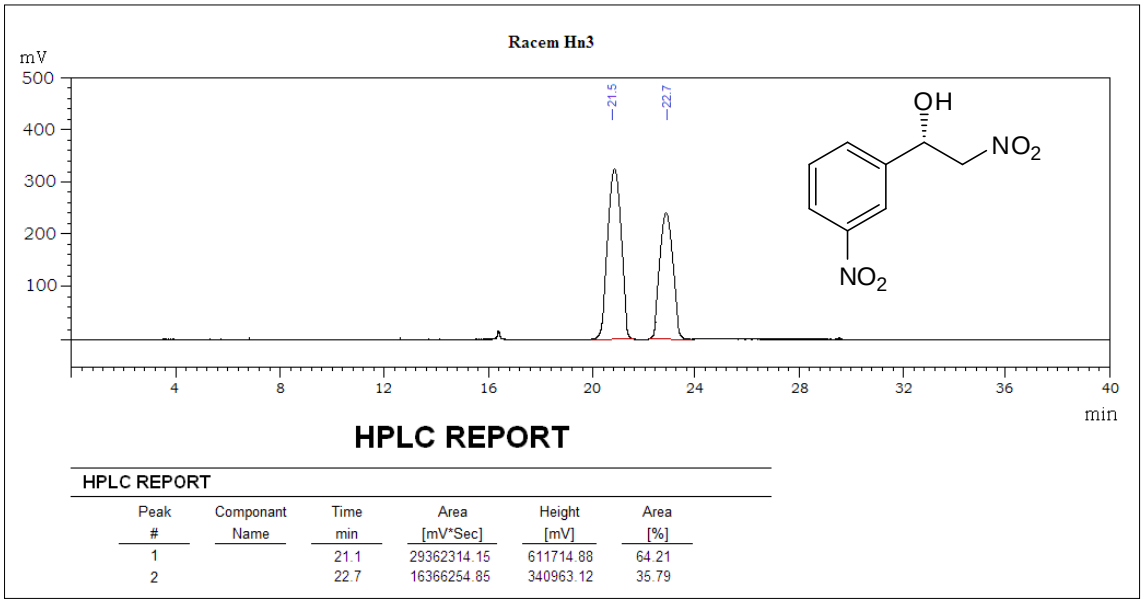


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		6.3	289132.94	6418.50	3.17
2		18.3	8831780.06	602114.64	96.83

HPLC Chromatograms of Racemic compound **10c**

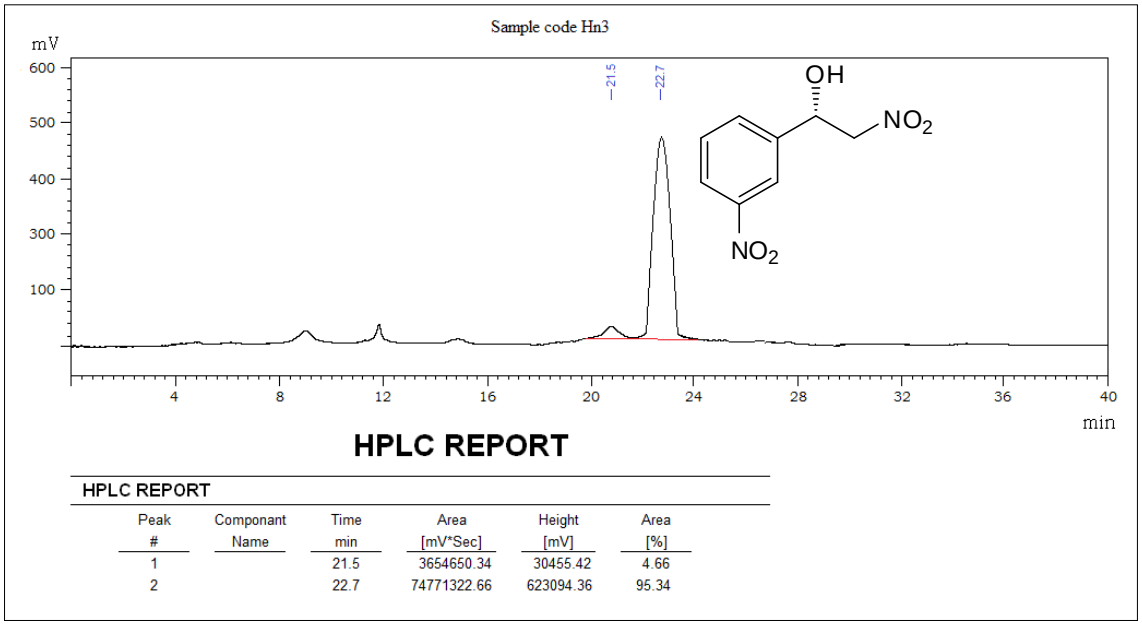


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		21.1	29362314.15	611714.88	64.21
2		22.7	16366254.85	340963.12	35.79

HPLC Chromatograms of compound **10c** [ref2]

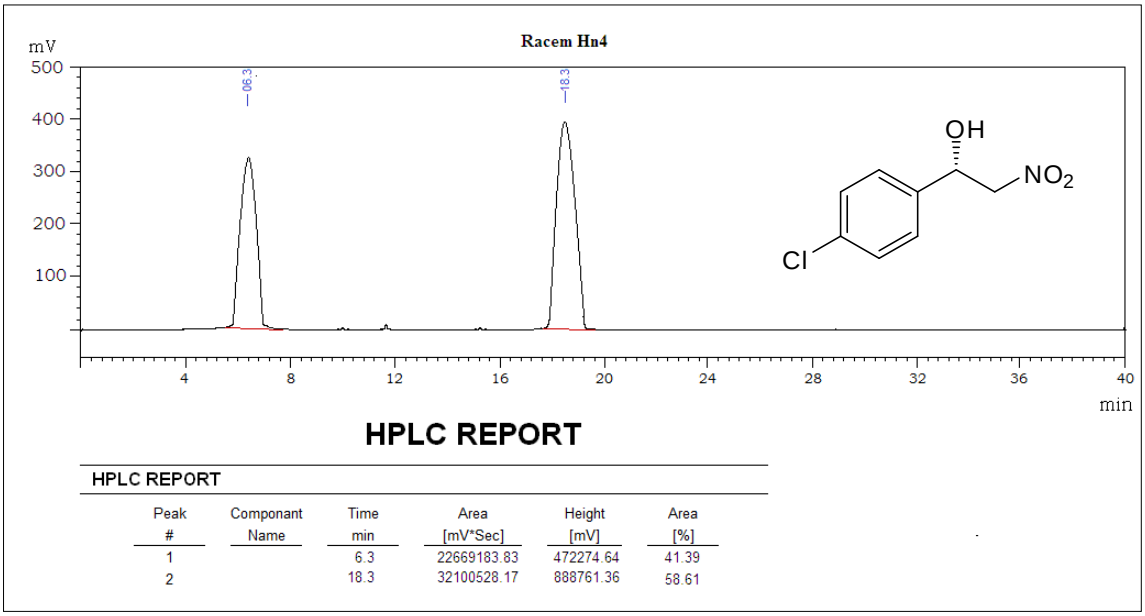


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		21.5	3654650.34	30455.42	4.66
2		22.7	74771322.66	623094.36	95.34

HPLC Chromatograms of Racemic compound **10d**

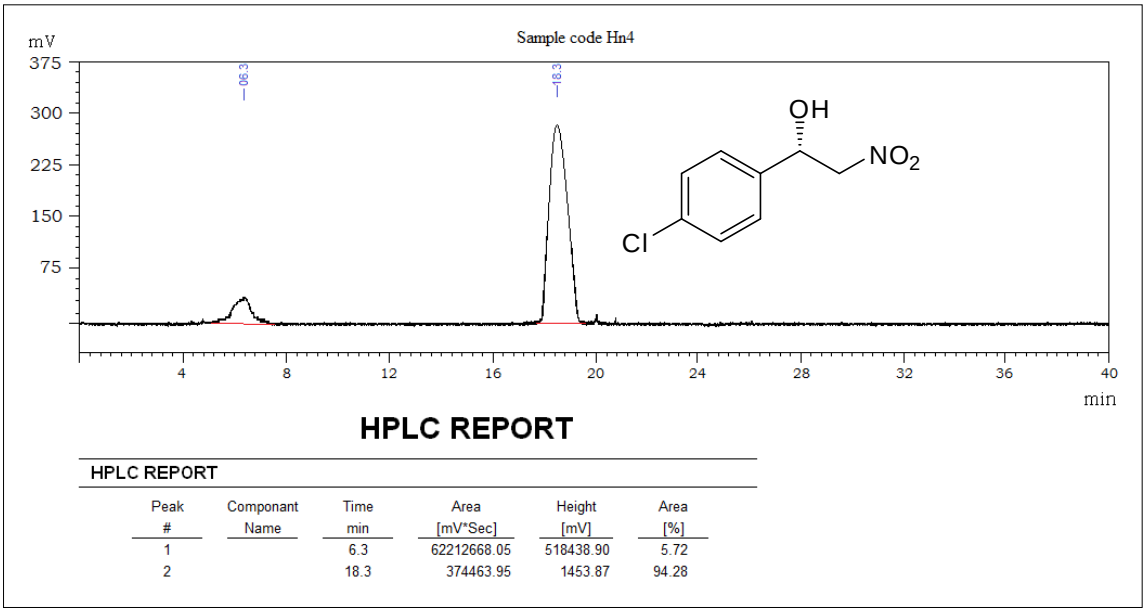


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		6.3	22669183.83	472274.64	41.39
2		18.3	32100528.17	888761.36	58.61

HPLC Chromatograms of compound **10d** [ref2]

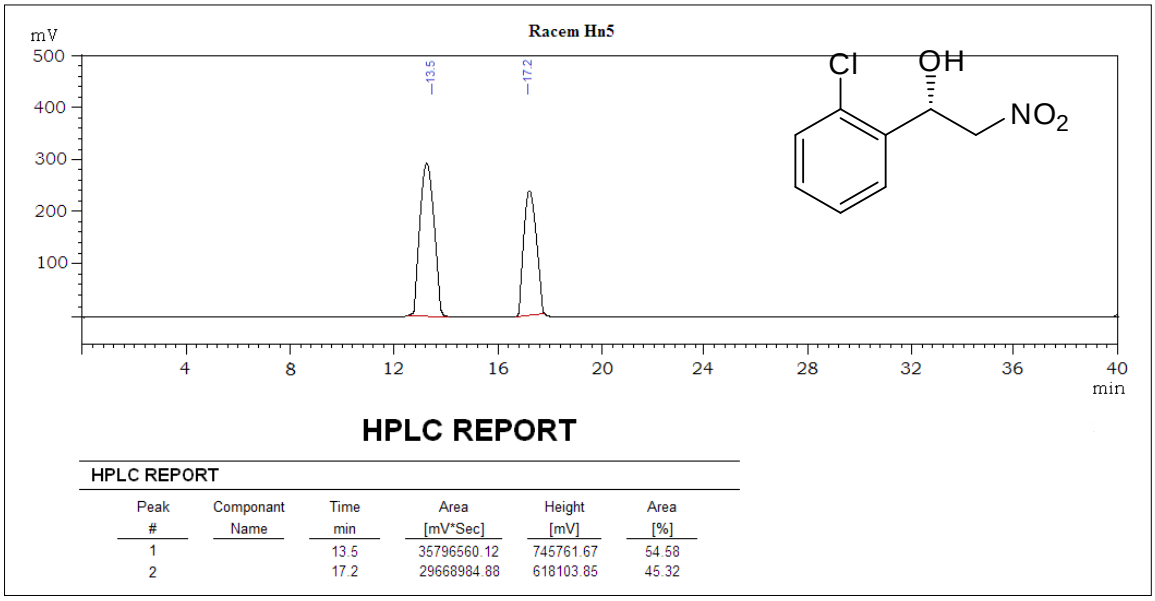


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		6.3	62212668.05	518438.90	5.72
2		18.3	374463.95	1453.87	94.28

HPLC Chromatograms of Racemic compound **10e**

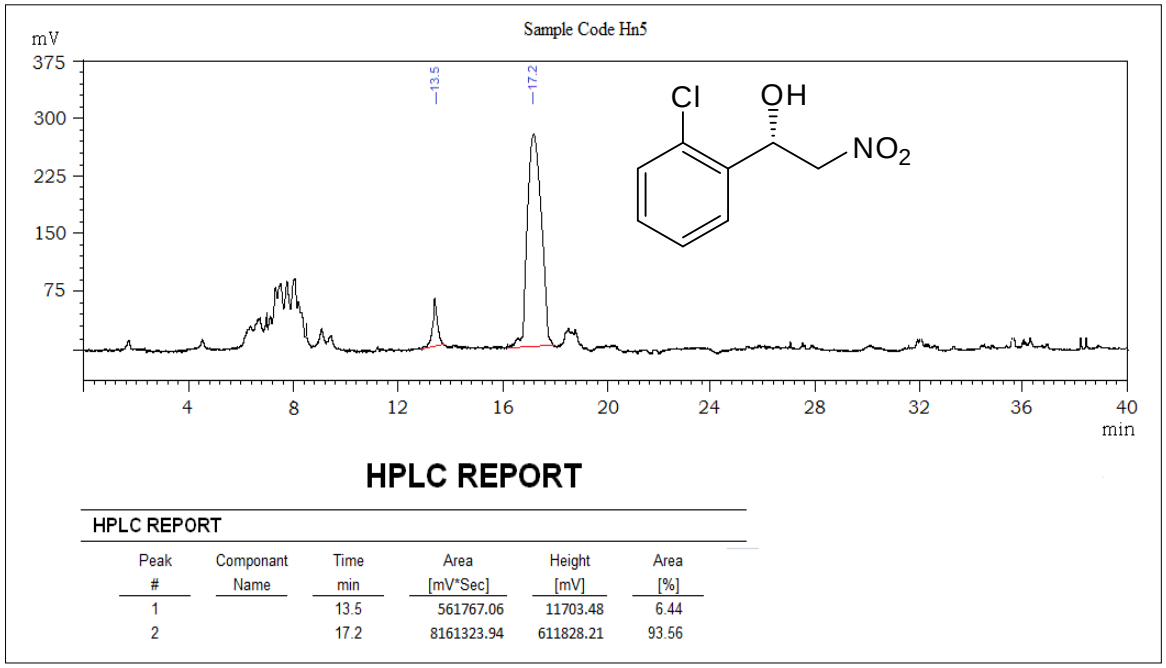


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		13.5	35796560.12	745761.67	54.58
2		17.2	29668984.88	618103.85	45.32

HPLC Chromatograms of compound **10e** [ref1]

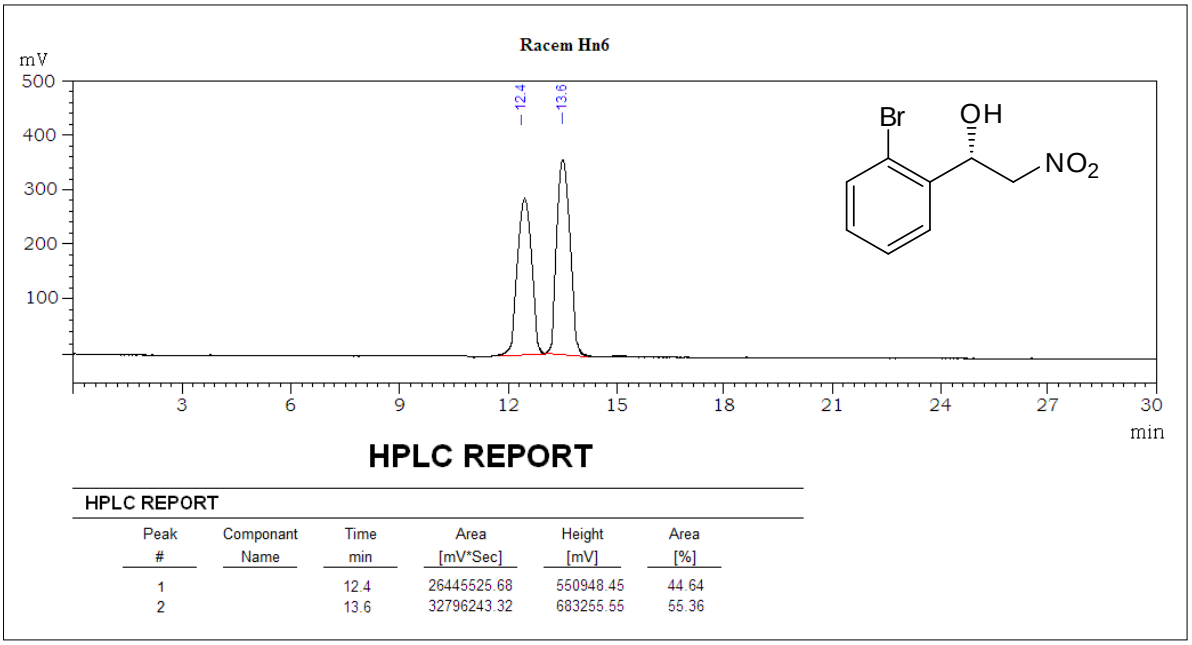


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		13.5	561767.06	11703.48	6.44
2		17.2	8161323.94	611828.21	93.56

HPLC Chromatograms of Racemic compound **10f**

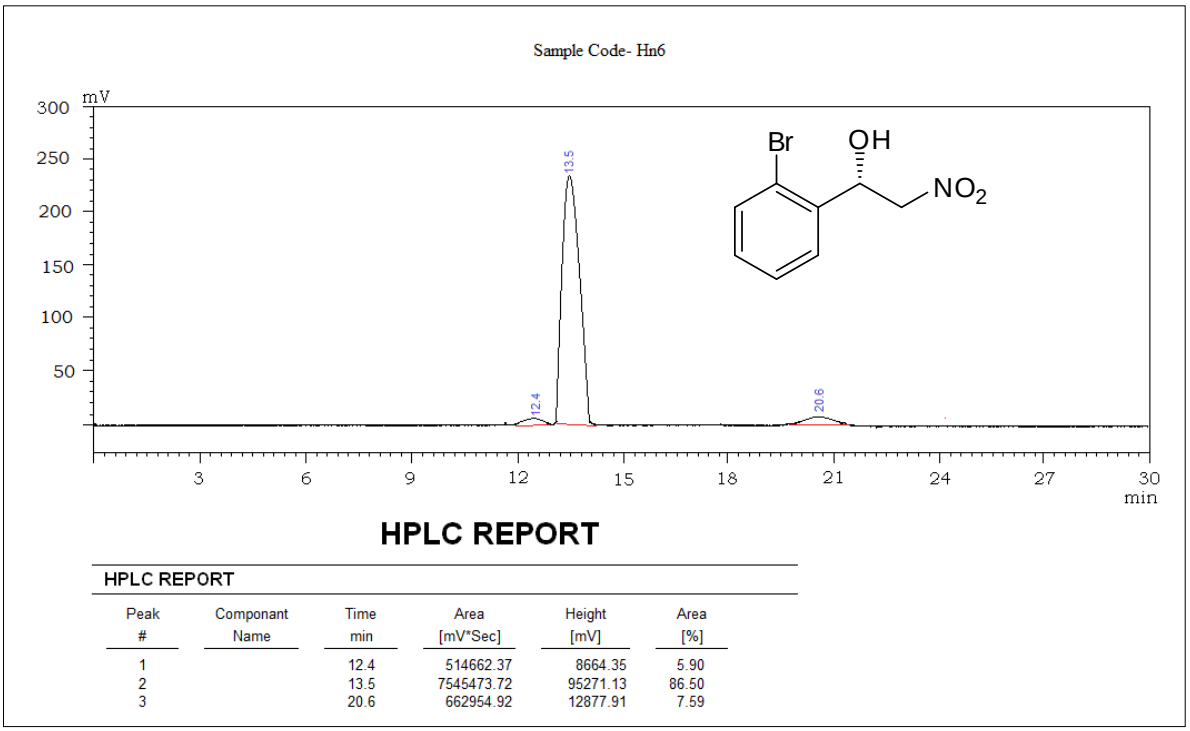


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		12.4	26445525.68	550948.45	44.64
2		13.6	32796243.32	683255.55	55.36

HPLC Chromatograms of compound **10f** [ref1]

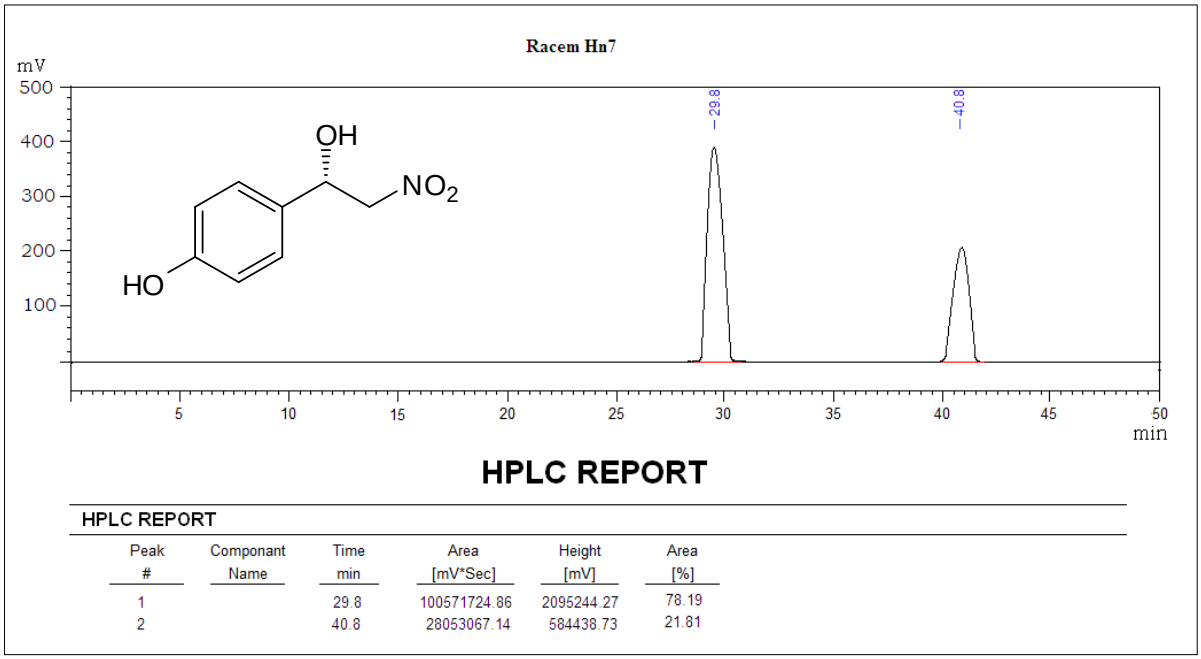


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		12.4	514662.37	8664.35	5.90
2		13.5	7545473.72	95271.13	86.50
3		20.6	662954.92	12877.91	7.59

HPLC Chromatograms of Racemic compound **10g**

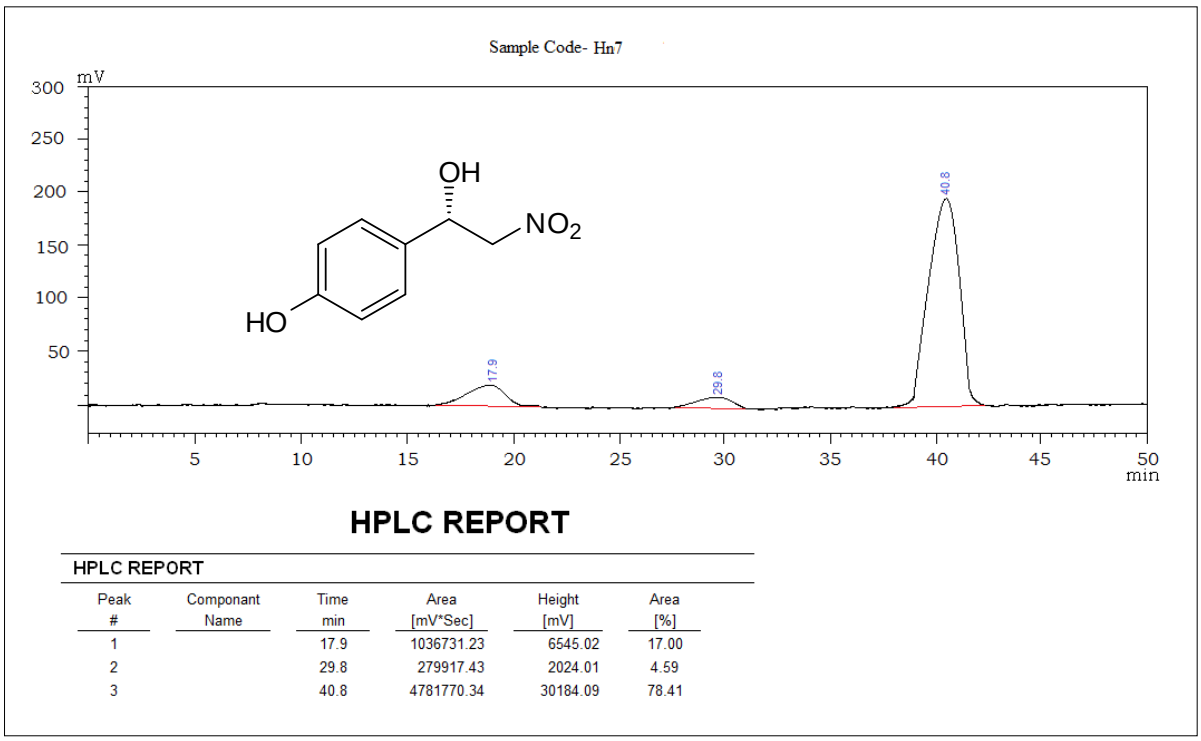


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		29.8	100571724.86	2095244.27	78.19
2		40.8	28053067.14	584438.73	21.81

HPLC Chromatograms of compound **10g** [ref2]

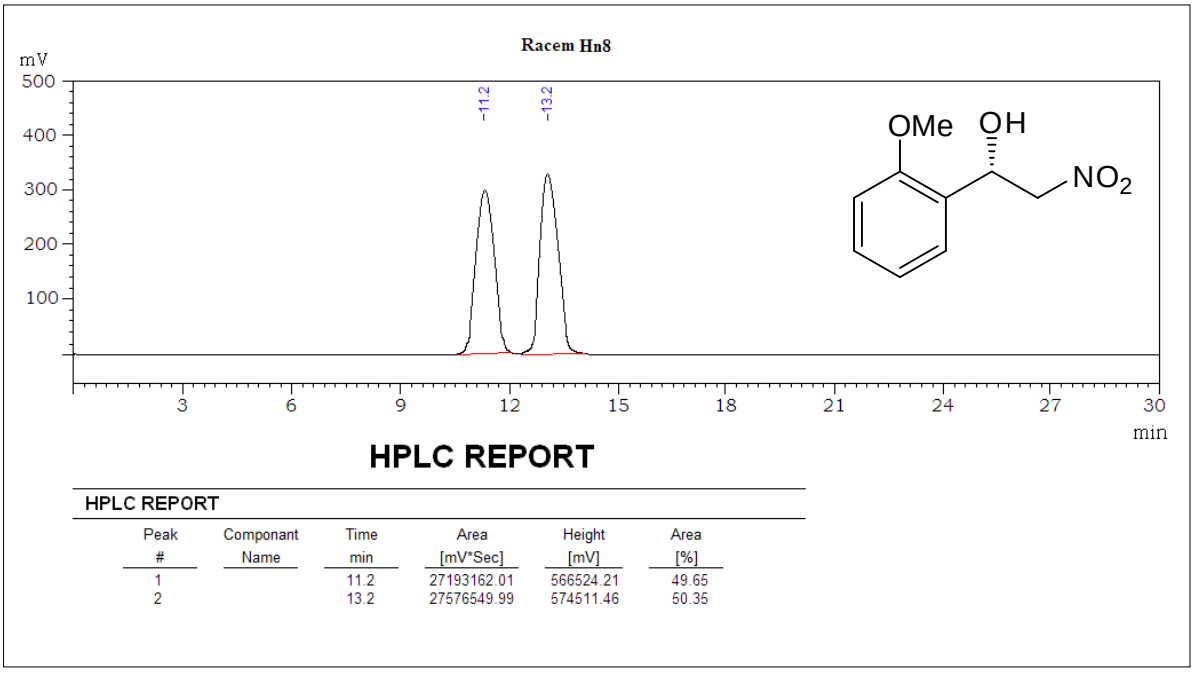


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		17.9	1036731.23	6545.02	17.00
2		29.8	279917.43	2024.01	4.59
3		40.8	4781770.34	30184.09	78.41

HPLC Chromatograms of Racemic compound **10h**

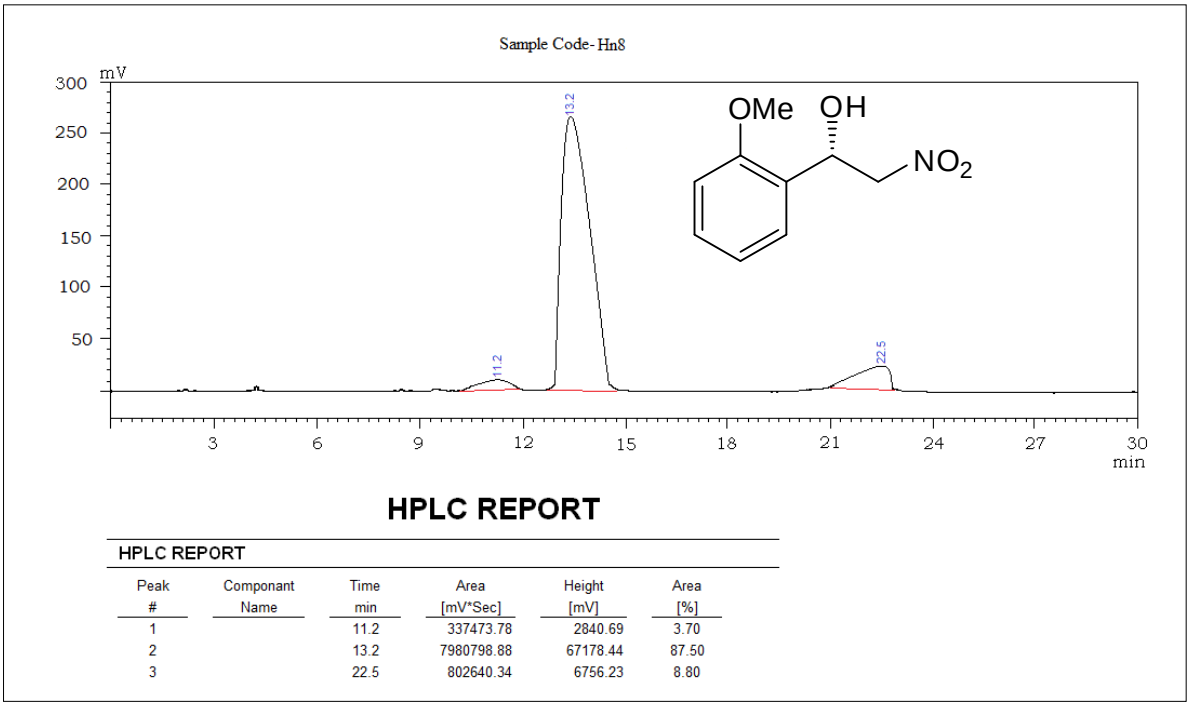


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		11.2	27193162.01	566524.21	49.65
2		13.2	27576549.99	574511.46	50.35

HPLC Chromatograms of compound **10h** [ref1]

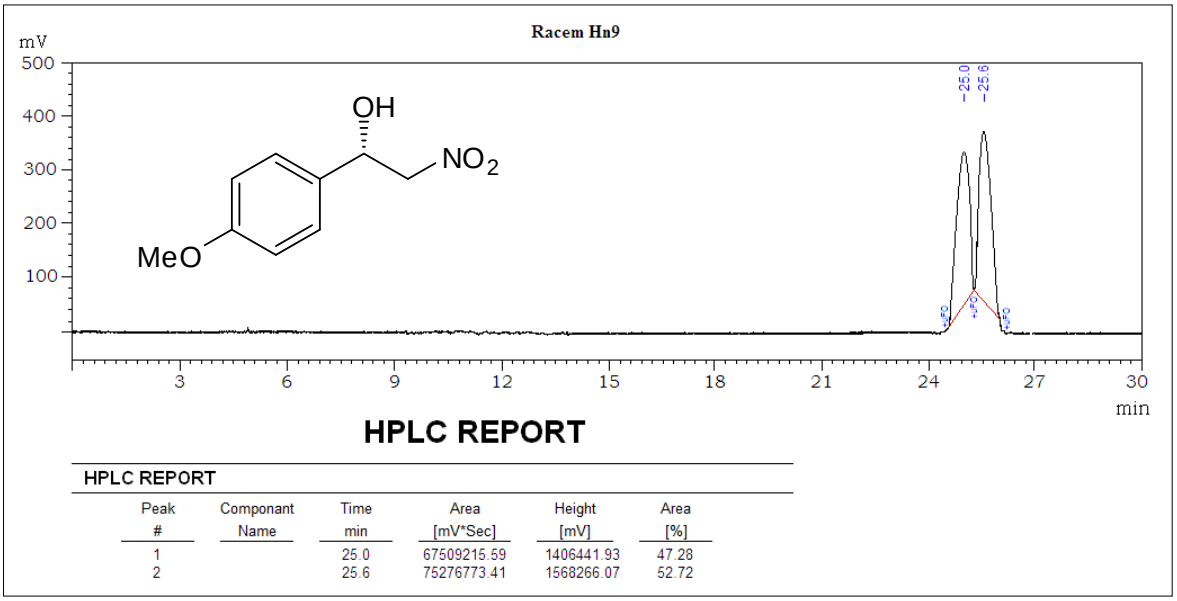


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		11.2	337473.78	2840.69	3.70
2		13.2	7980798.88	67178.44	87.50
3		22.5	802640.34	6756.23	8.80

HPLC Chromatograms of Racemic compound **10i**

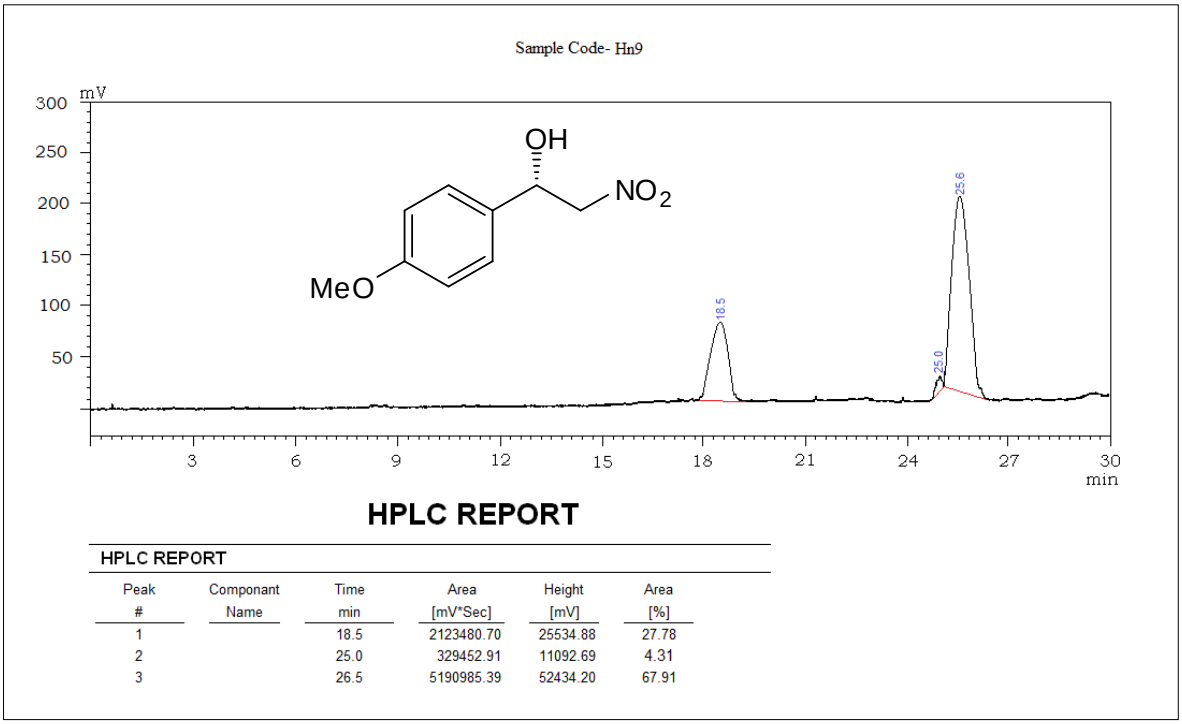


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		25.0	67509215.59	1406441.93	47.28
2		25.6	75276773.41	1568266.07	52.72

HPLC Chromatograms of compound **10i** [ref2]

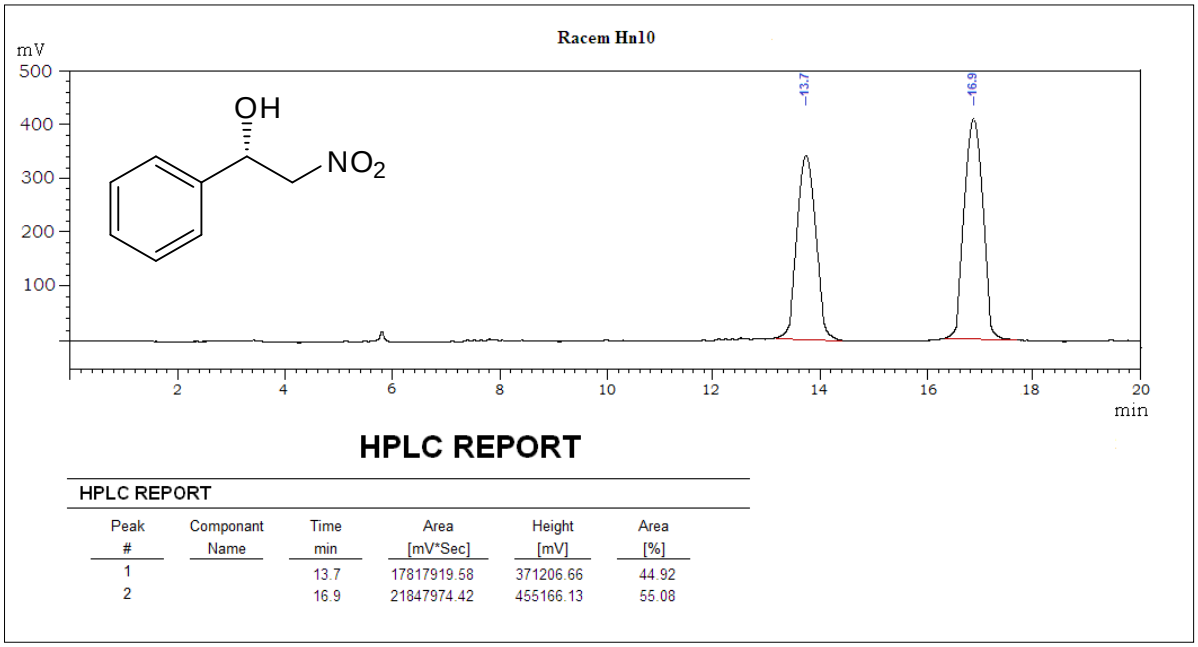


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		18.5	2123480.70	25534.88	27.78
2		25.0	329452.91	11092.69	4.31
3		26.5	5190985.39	52434.20	67.91

HPLC Chromatograms of Racemic compound **10j**

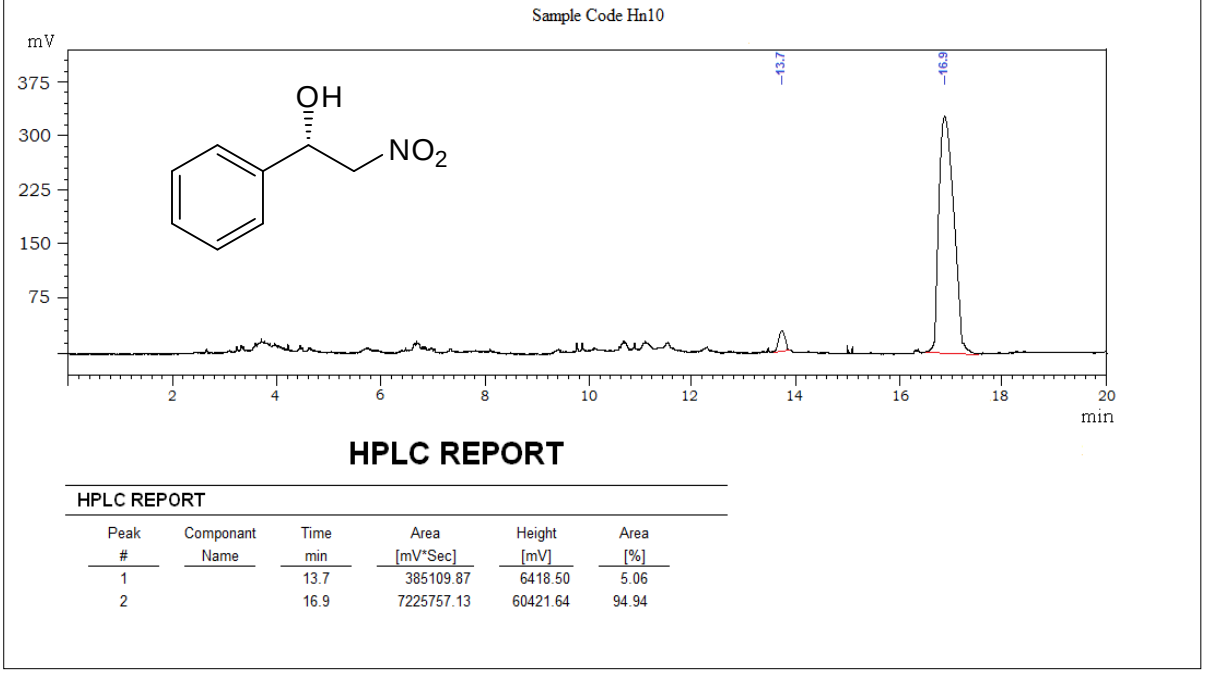


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		13.7	17817919.58	371206.66	44.92
2		16.9	21847974.42	455166.13	55.08

HPLC Chromatograms of compound **10j** [ref2]

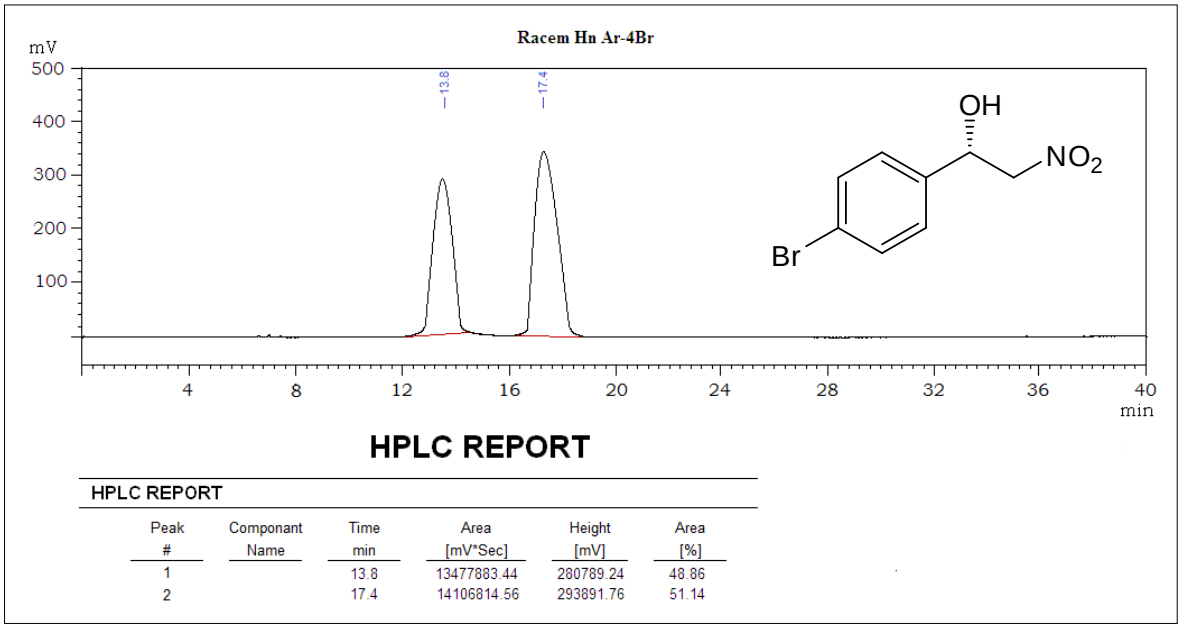


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		13.7	385109.87	6418.50	5.06
2		16.9	7225757.13	60421.64	94.94

HPLC Chromatograms of Rcemic compound **10k**

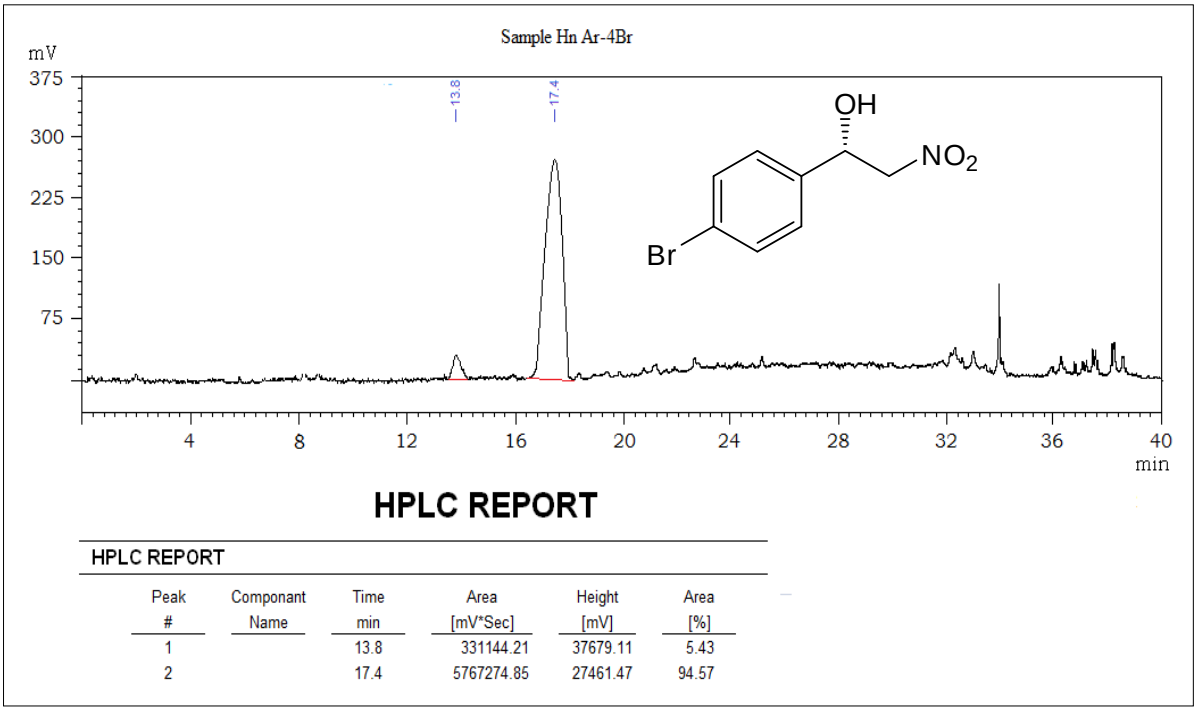


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		13.8	13477883.44	280789.24	48.86
2		17.4	14106814.56	293891.76	51.14

HPLC Chromatograms of compound **10k** [ref6]

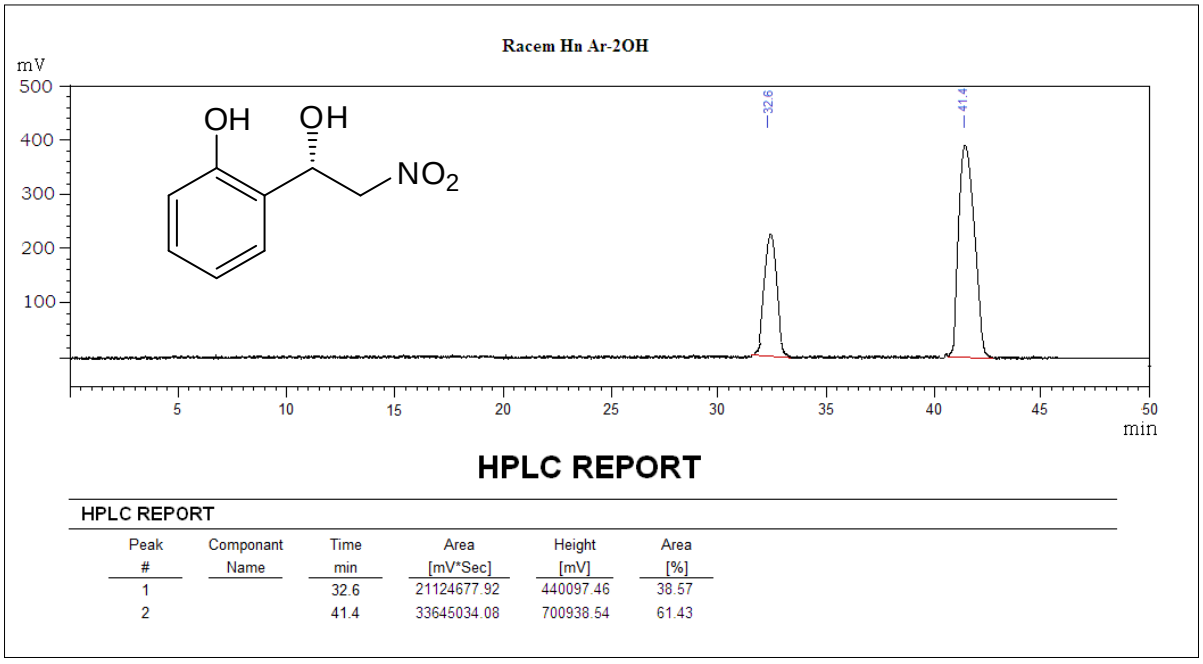


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		13.8	331144.21	37679.11	5.43
2		17.4	5767274.85	27461.47	94.57

HPLC Chromatograms of Racemic compound **10l**

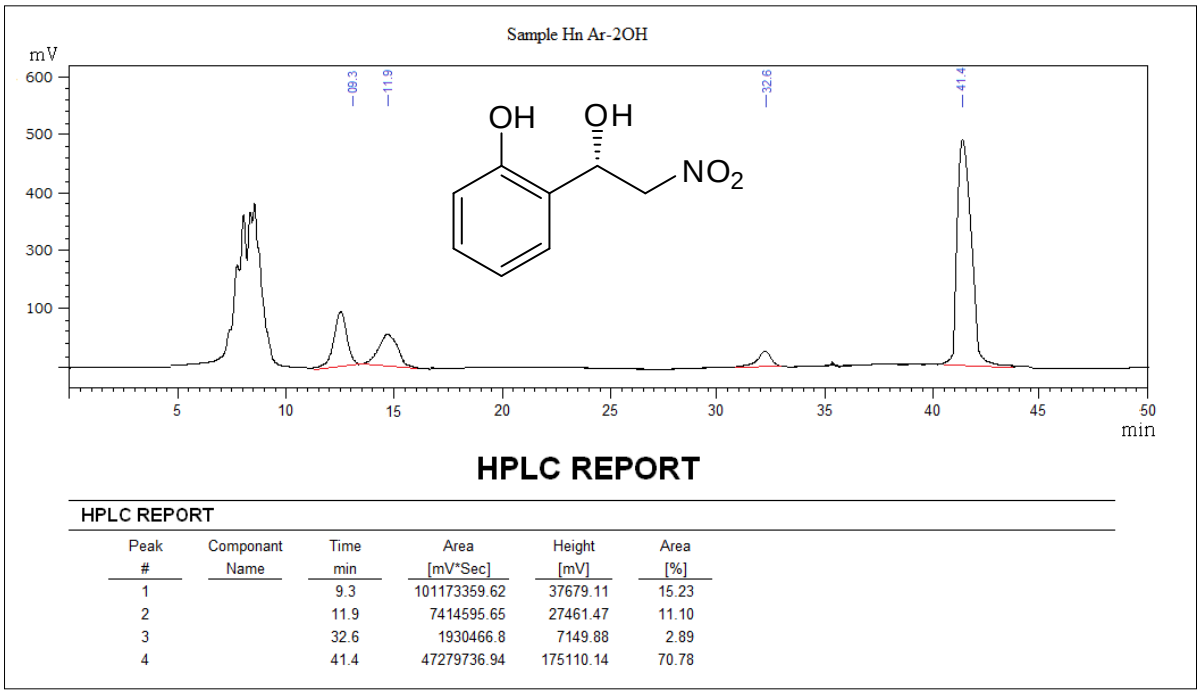


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		32.6	21124677.92	440097.46	38.57
2		41.4	33645034.08	700938.54	61.43

HPLC Chromatograms of compound **10l**

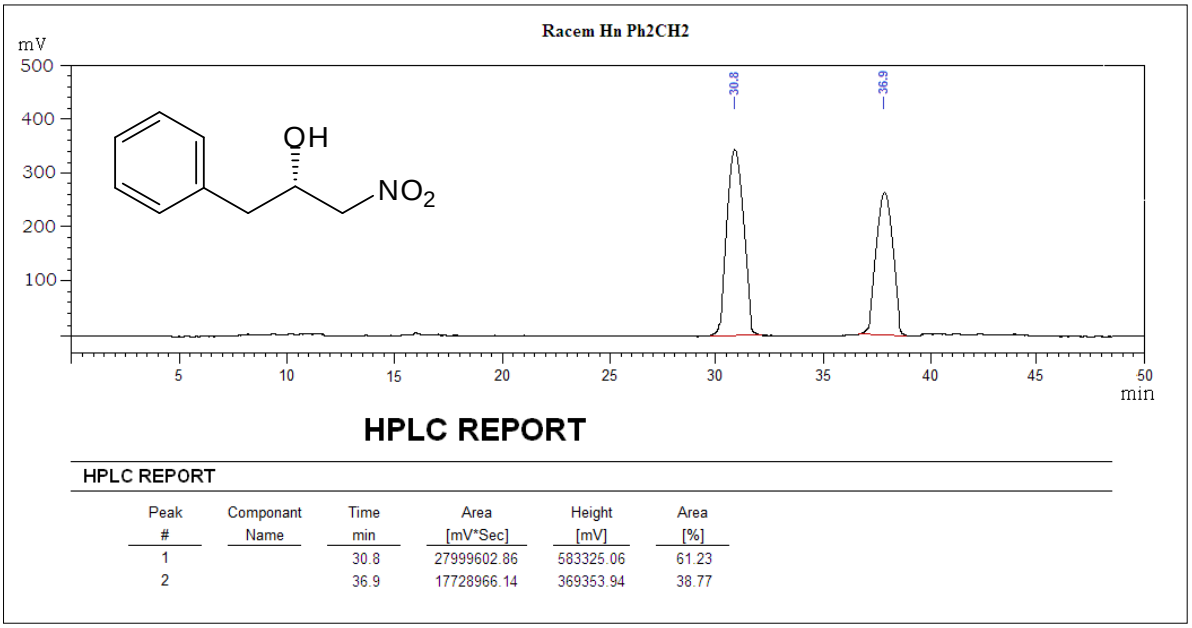


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		9.3	101173359.62	37679.11	15.23
2		11.9	7414595.65	27461.47	11.10
3		32.6	1930466.8	7149.88	2.89
4		41.4	47279736.94	175110.14	70.78

HPLC Chromatograms of Racemic compound **10m**

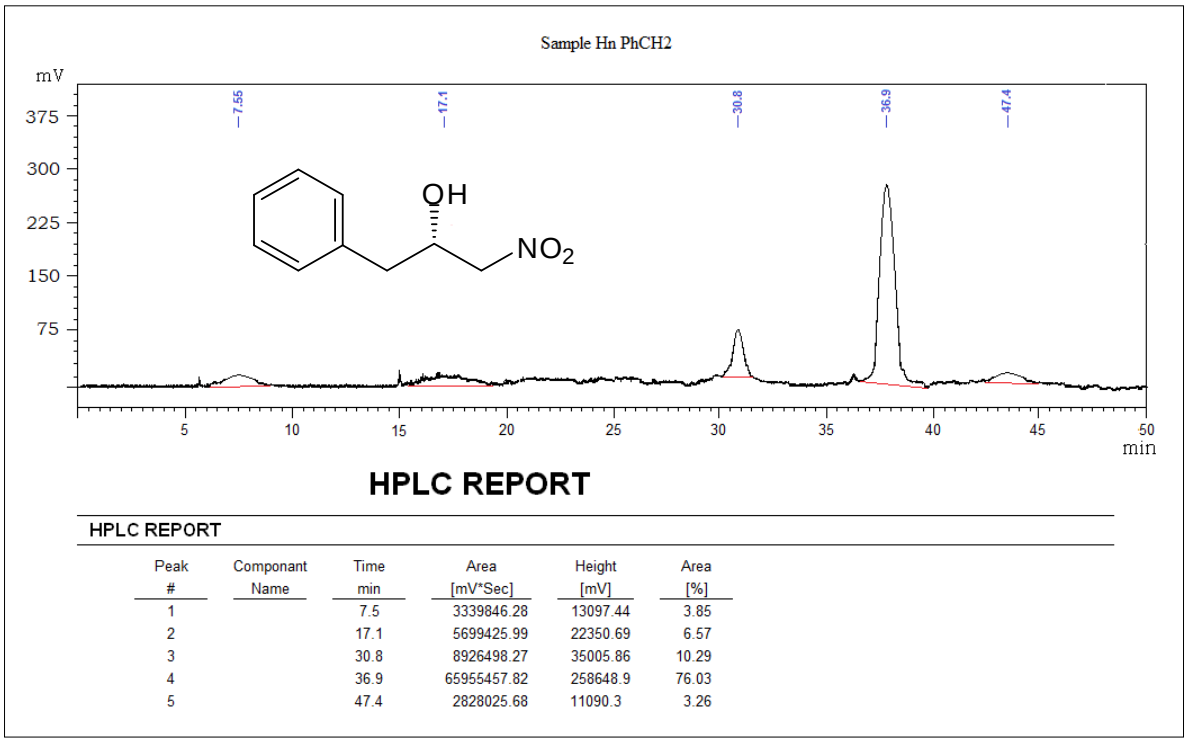


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		30.8	27999602.86	583325.06	61.23
2		36.9	17728966.14	369353.94	38.77

HPLC Chromatograms of compound **10m** [ref 5]

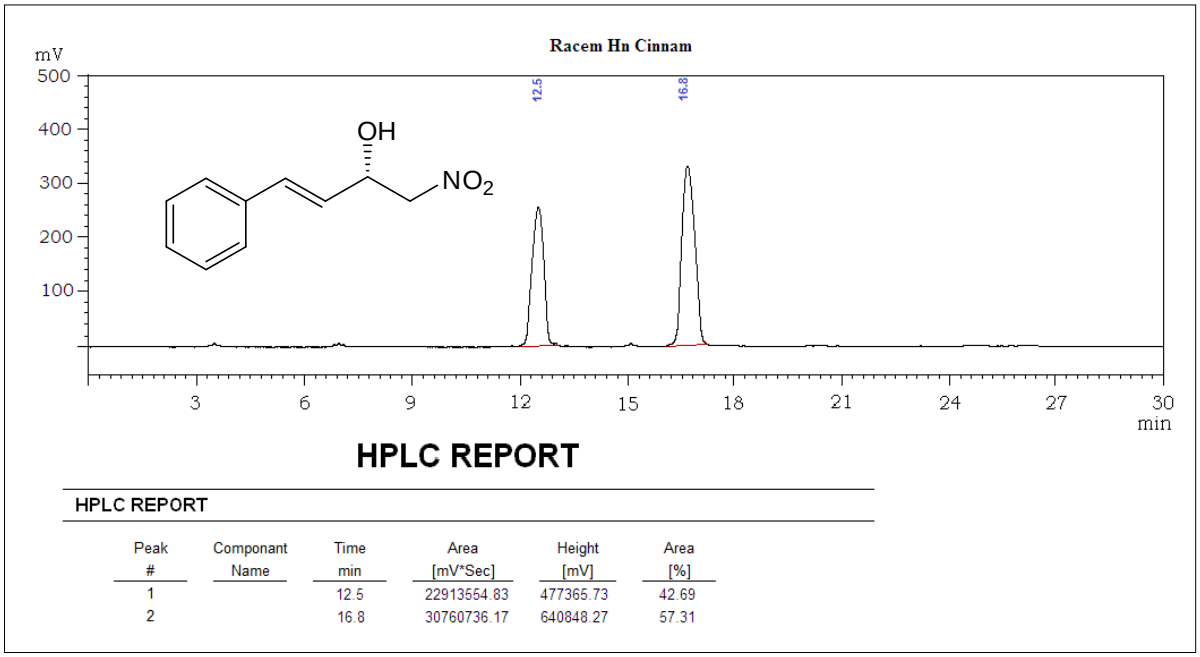


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		7.5	3339846.28	13097.44	3.85
2		17.1	5699425.99	22350.69	6.57
3		30.8	8926498.27	35005.86	10.29
4		36.9	65955457.82	258648.9	76.03
5		47.4	2828025.68	11090.3	3.26

HPLC Chromatograms of compound **10n**

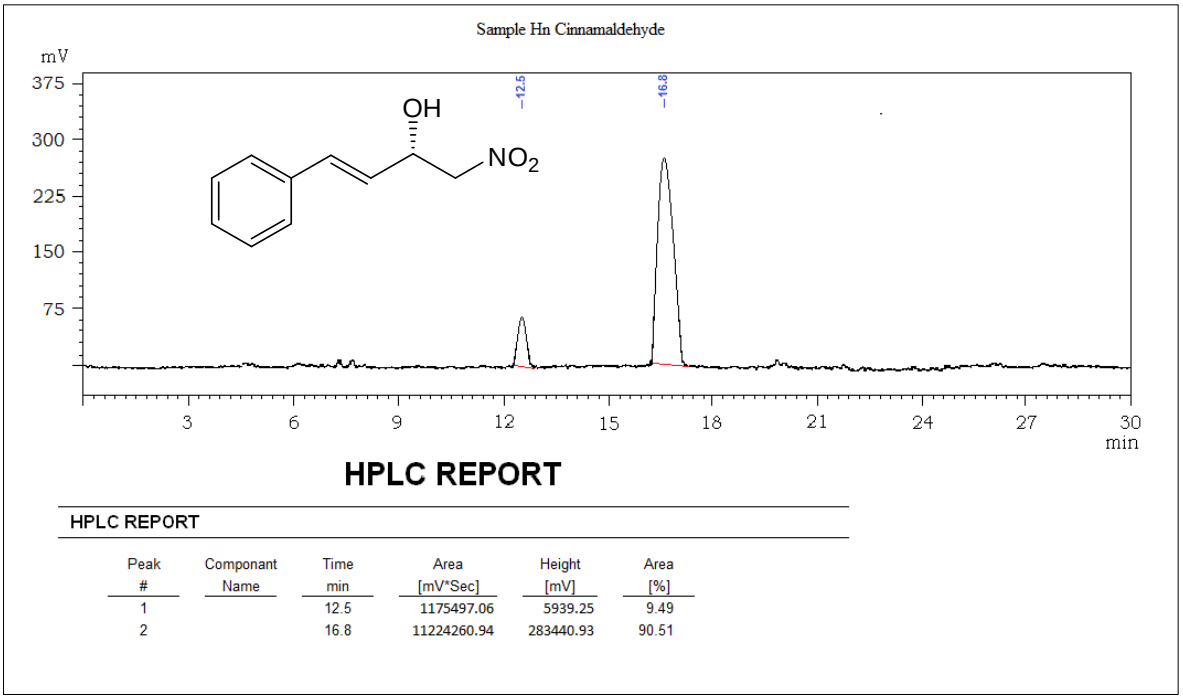


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		12.5	22913554.83	477365.73	42.69
2		16.8	30760736.17	640848.27	57.31

HPLC Chromatograms of compound **10n** [ref2]

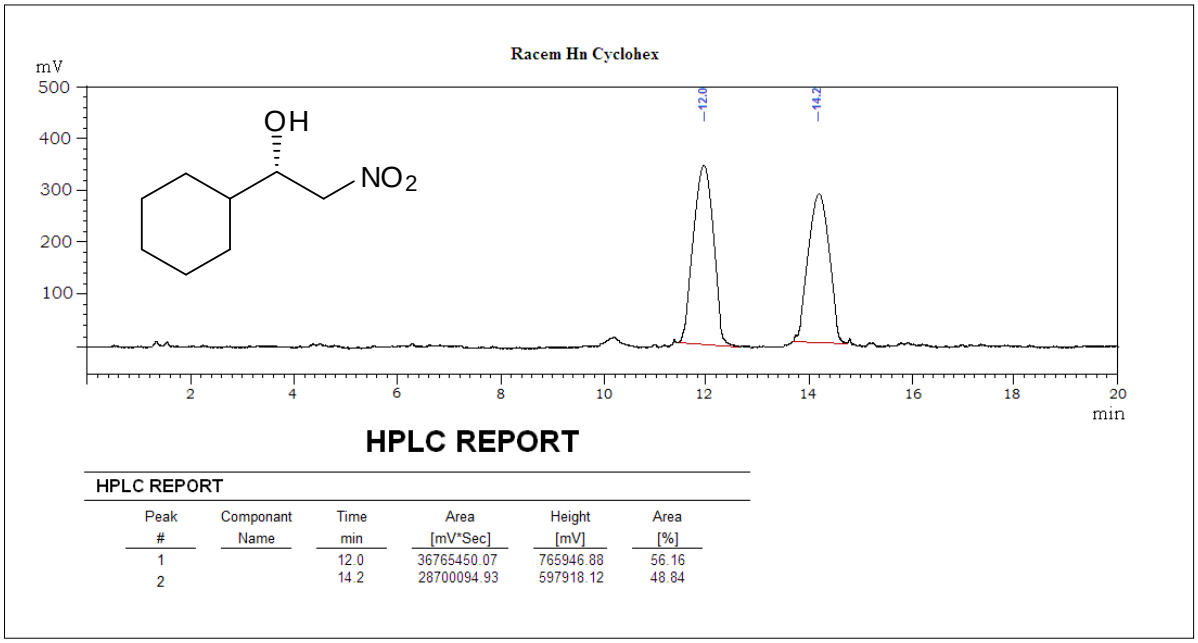


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		12.5	1175497.06	5939.25	9.49
2		16.8	11224260.94	283440.93	90.51

HPLC Chromatograms of Racemic compound **10o**

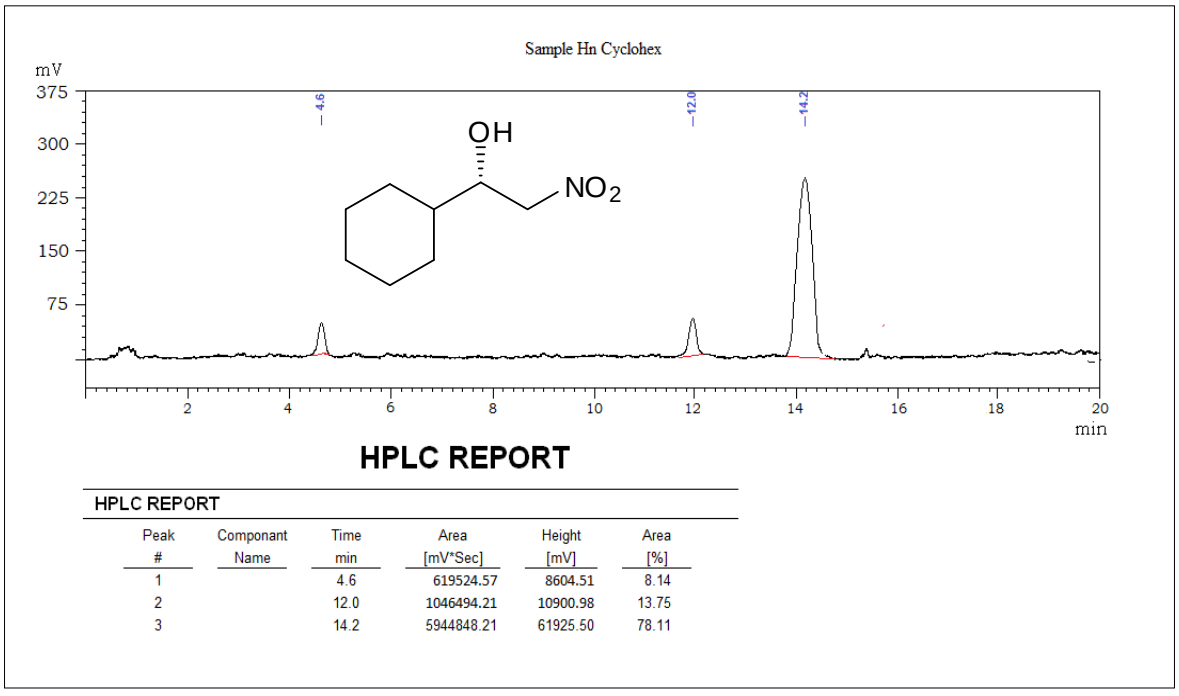


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		12.0	36765450.07	765946.88	56.16
2		14.2	28700094.93	597918.12	48.84

HPLC Chromatograms of compound **10o** [ref6]

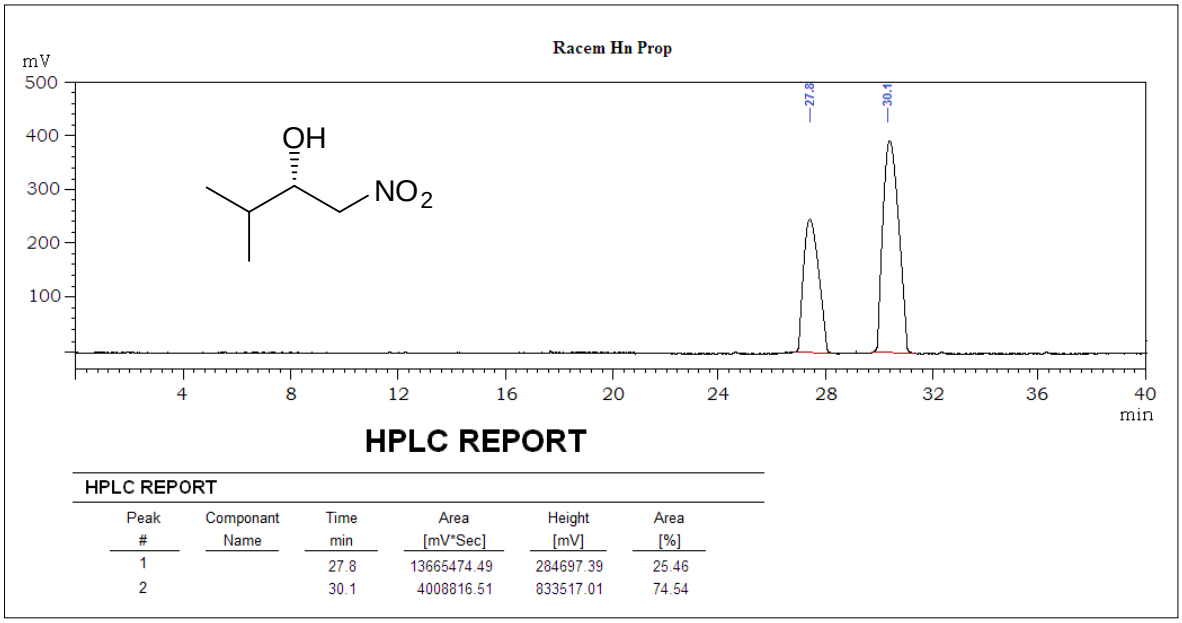


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		4.6	619524.57	8604.51	8.14
2		12.0	1046494.21	10900.98	13.75
3		14.2	5944848.21	61925.50	78.11

HPLC Chromatograms of Racemic compound **10p**

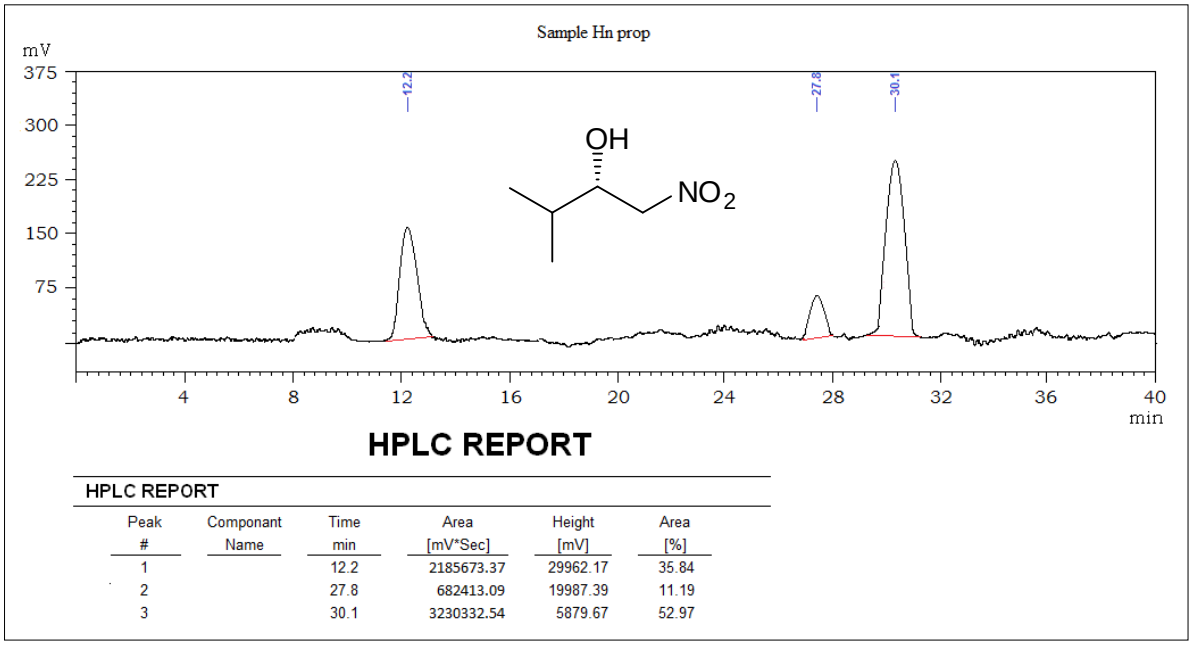


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		27.8	13665474.49	284697.39	25.46
2		30.1	4008816.51	833517.01	74.54

HPLC Chromatograms of compound **10p** [ref6]

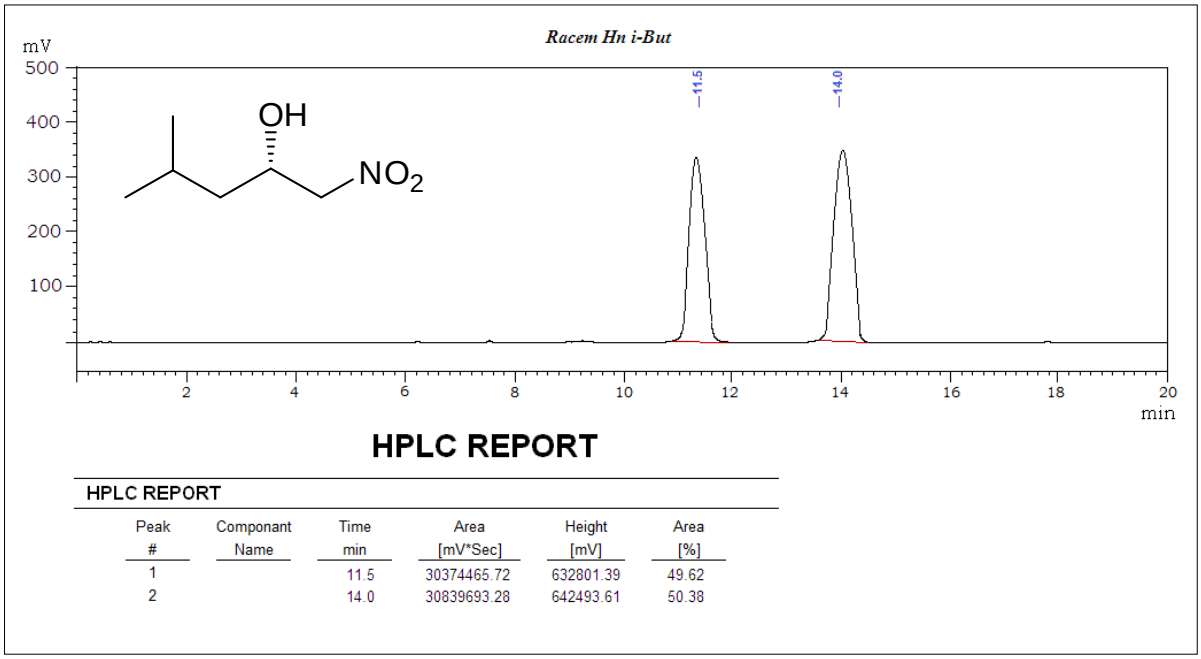


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		12.2	2185673.37	29962.17	35.84
2		27.8	682413.09	19987.39	11.19
3		30.1	3230332.54	5879.67	52.97

HPLC Chromatograms of Racemic compound **10q**

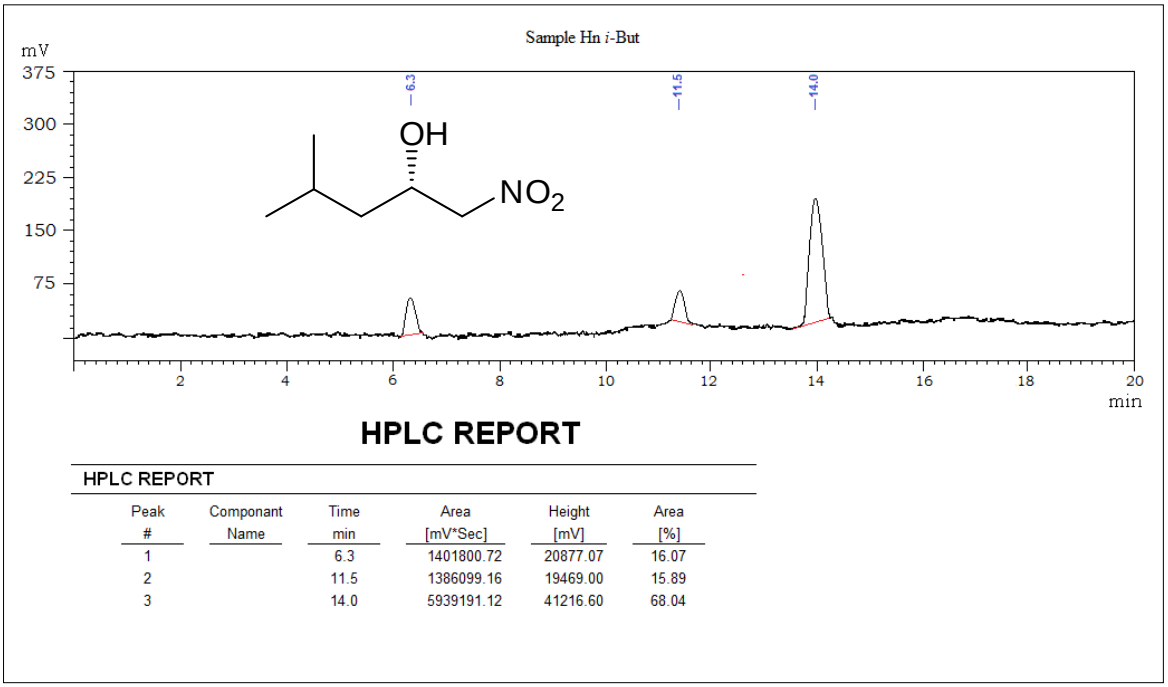


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		11.5	30374465.72	632801.39	49.62
2		14.0	30839693.28	642493.61	50.38

HPLC Chromatograms of compound **10q** [ref1]

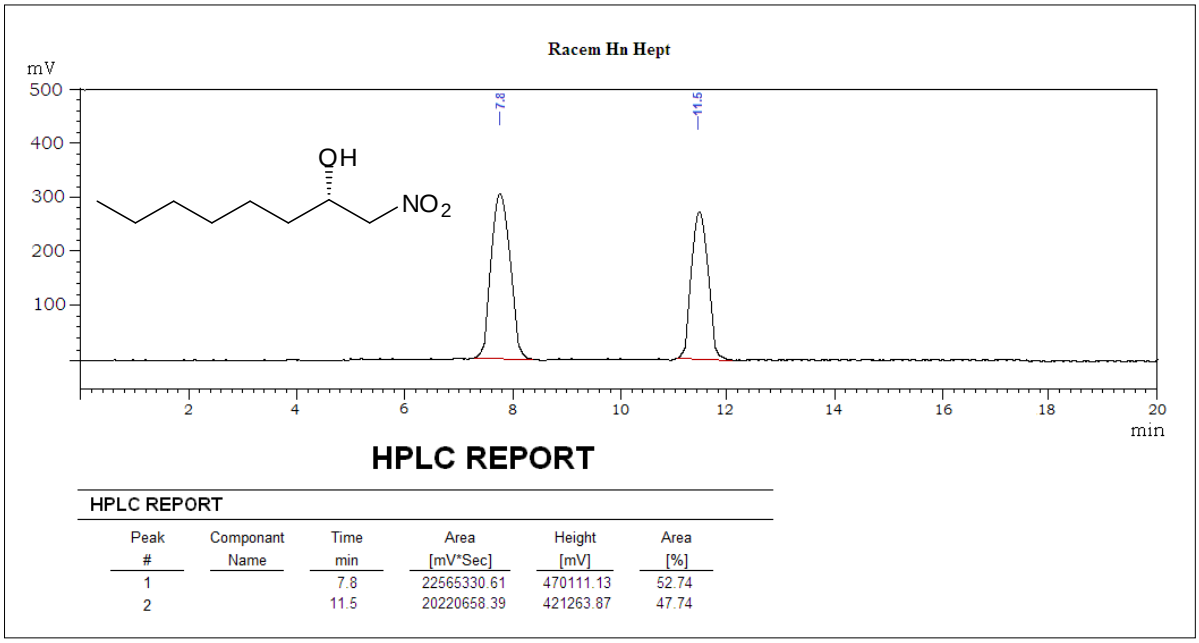


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		6.3	1401800.72	20877.07	16.07
2		11.5	1386099.16	19469.00	15.89
3		14.0	5939191.12	41216.60	68.04

HPLC Chromatograms of Racemic compound **10r**

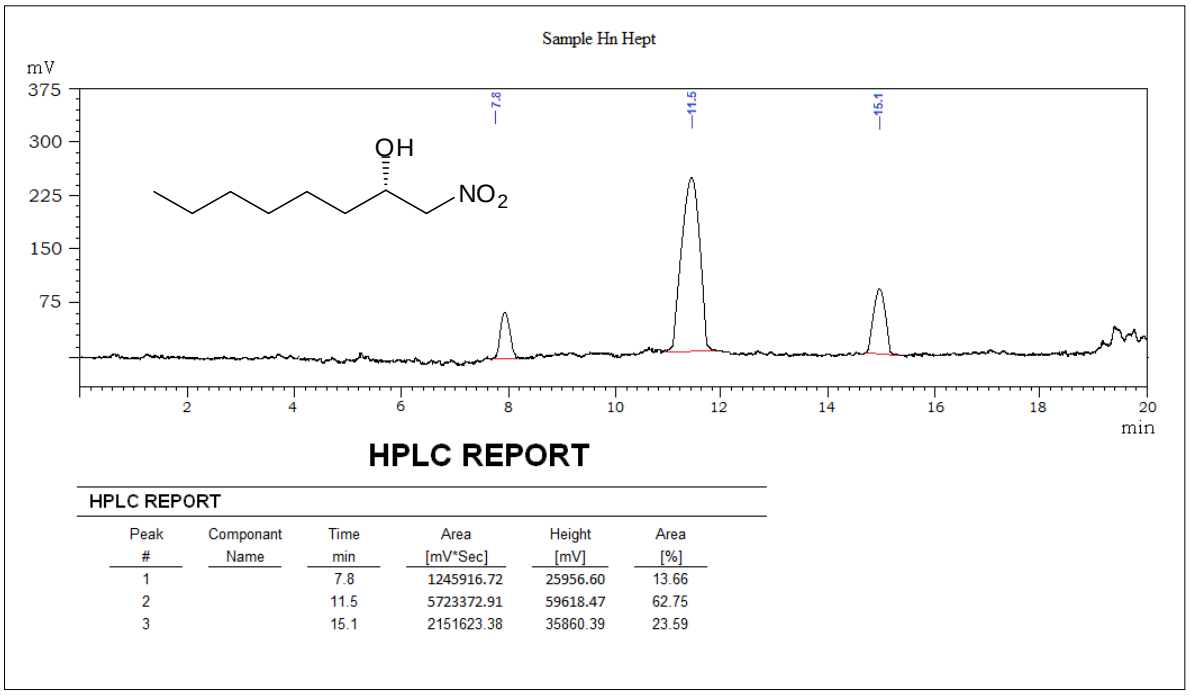


HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		7.8	22565330.61	470111.13	52.74
2		11.5	20220658.39	421263.87	47.74

HPLC Chromatograms of compound **10r** [ref3c]



HPLC REPORT

HPLC REPORT

Peak #	Componant Name	Time min	Area [mV*Sec]	Height [mV]	Area [%]
1		7.8	1245916.72	25956.60	13.66
2		11.5	5723372.91	59618.47	62.75
3		15.1	2151623.38	35860.39	23.59

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