Electronic Supplementary Material (ESI) for MedChemComm.

Synthesis and Biological Evaluation of Substituted N-alkylphenyl-3,5-dinitrobenzamide Analogs as Anti-TB Agents

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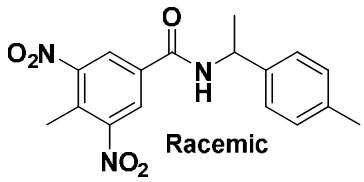
Part A: Chemistry

Experimental Section: General

All chemicals for this study were purchased from Sigma-Aldrich, USA. ^{1}HNMR recorded on 400 MHz or 500 MHz. Chemical data for protons are reported in parts per million (ppm, scale) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$: δ 7.26, DMSO-d_6: δ 2.5 or other solvents as mentioned). All the NMR spectra were processed in either MestReNova or Bruker software. Mass spectras were recorded with HRMS instrument. Chiral HPLC was performed on Agilent Technologies 1260 infinity series system using Astec CHIROBIOTIC T column with dimension 4.6 x 250 mm, particle size 5μm. Mobile phase used was (A) buffer having 10 mM ammonium acetate pH 4.0 adjusted with glacial acetic acid and (B) Acetonitrile. The experiment run on a gradient program as 0% B till 5 min then goes to 40 %B in 30 min, remain at 40%B for 5 min then return to 0 % B in 5 min and retained there for 5 min with a flow rate of 1 ml/min. UV recorded at 254 nm. Enantiomeric excess was calculated through area integration of enantiomers.

1. 4-methyl-3, 5-dinitro-N-(1-(*p*-tolyl)ethyl)benzamide (4b):

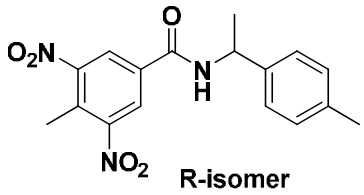


TLC (EtOAc/hexane, 2:8): R_f = 0.25; Light yellow solid; mp 124-125 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 2H), 7.26 (t, *J* = 4.0 Hz, 3H), 7.17 (d, *J* = 7.9 Hz, 2H), 6.53 (d, *J* = 6.8 Hz, 1H), 5.27 (p, *J* = 7.0 Hz, 1H), 2.60 (s, 3H), 2.34 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, Acetone-d_6) δ 162.59, 152.40, 141.72, 137.31, 135.68, 130.07, 129.81,

127.10, 126.98, 50.29, 50.18, 22.14, 20.99, 15.02; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 342.1089, found 342.1089.

(4b was a racemic mixture and it consists of *R-isomer*- 37.9%, *S-isomer*- 62.1%)

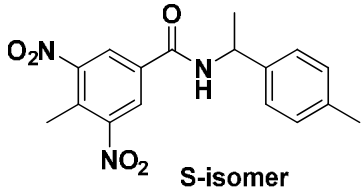
2. (*R*)-4-methyl-3, 5-dinitro-N-(1-(p-tolyl)ethyl)benzamide (7a):



R-isomer

TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 159-160 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 2H), 7.26 (t, *J* = 4.0 Hz, 3H), 7.17 (d, *J* = 7.9 Hz, 2H), 6.53 (d, *J* = 6.8 Hz, 1H), 5.27 (p, *J* = 7.0 Hz, 1H), 2.60 (s, 3H), 2.34 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, Acetone-d_6) δ 162.59, 152.40, 141.72, 137.31, 135.68, 130.07, 129.81, 127.10, 126.98, 50.29, 50.18, 22.14, 20.99, 15.02; $[\alpha]_D$ -52.7° (*c* 0.69, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 342.1089, found 342.1095.

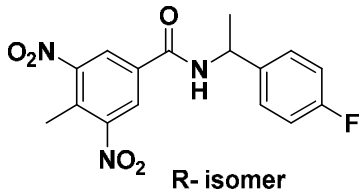
3. (*S*) - 4-methyl-3,5-dinitro-N-(1-(*p*-tolyl)ethyl)benzamide (7b):



S-isomer

TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 160-161 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 2H), 7.26 (t, *J* = 4.0 Hz, 3H), 7.17 (d, *J* = 7.9 Hz, 2H), 6.53 (d, *J* = 6.8 Hz, 1H), 5.27 (p, *J* = 7.0 Hz, 1H), 2.60 (s, 3H), 2.34 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, Acetone-d_6) δ 162.59, 152.40, 141.72, 137.31, 135.68, 130.07, 129.81, 127.10, 126.98, 50.29, 50.18, 22.14, 20.99, 15.02; $[\alpha]_D$ +56.9° (*c* 0.51, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 342.1089, found 342.1089.

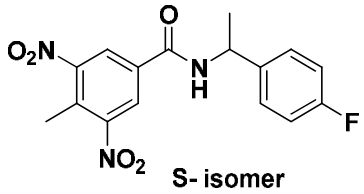
4. (*R*)-N-(1-(4-Fluorophenyl)ethyl)-4-methyl-3, 5-dinitrobenzamide (7c):



R- isomer

TLC (EtOAc:hexane 2:8): R_f = 0.30; Light yellow solid; mp 191-192 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 2H), 7.34 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.04 (t, *J* = 8.7 Hz, 2H), 6.61 (d, *J* = 6.1 Hz, 1H), 5.28 (p, *J* = 7.1 Hz, 1H), 2.60 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 162.69 (d, *J* = 243.08 Hz), 162.58, 152.41, 140.99 (d, *J* = 2.99 Hz), 135.49, 130.31, 129.13 (d, *J* = 8.09 Hz), 127.09, 115.84(d, *J* = 21.47 Hz), 50.00, 22.27, 15.17; $[\alpha]_D$ -52.0° (*c* 0.6, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 346.0839, found 346.0856.

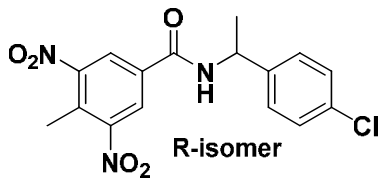
5. (*S*)-*N*-(1-(4-Fluorophenyl)ethyl)-4-methyl-3, 5-dinitrobenzamide (7d):



S- isomer

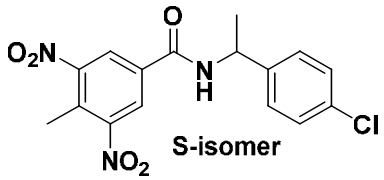
TLC (EtOAc:hexane 2:8): R_f = 0.30; Light yellow solid; mp 191.5-192.5 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 2H), 7.34 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.04 (t, *J* = 8.7 Hz, 2H), 6.61 (d, *J* = 6.1 Hz, 1H), 5.28 (p, *J* = 7.1 Hz, 1H), 2.60 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone-d_6) δ 162.69 (d, *J* = 243.08 Hz), 162.58, 152.41, 140.99 (d, *J* = 2.99 Hz), 135.49, 130.31, 129.13 (d, *J* = 8.09 Hz), 127.09, 115.84(d, *J* = 21.47 Hz), 50.00, 22.27, 15.17; $[\alpha]_D$ +55.7° (*c* 0.42, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 346.0839, found 346.0841.

6. (*R*)-*N*-(1-(4-Chlorophenyl)ethyl)-4-methyl-3, 5-dinitrobenzamide (7e):



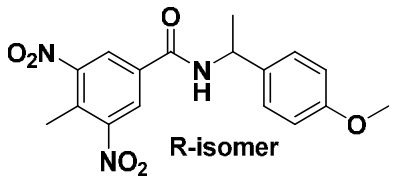
TLC (EtOAc:hexane 2:8): R_f = 0.15; Light yellow solid; mp 199-201 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 2H), 7.36 – 7.28 (m, 4H), 6.70 (d, *J* = 6.9 Hz, 1H), 5.32 – 5.21 (m, 1H), 2.61 (s, 3H), 1.62 (s, 3H); ^{13}C NMR (101 MHz, Acetone) δ 162.64, 152.43, 143.89, 135.47, 133.08, 130.29, 129.27, 128.98, 127.06, 50.15, 22.13, 15.16; $[\alpha]_D$ -59.47° (*c* 1.68, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 362.0544, found 362.0555.

7. (*S*)-*N*-(1-(4-Chlorophenyl)ethyl)-4-methyl-3, 5-dinitrobenzamide (7f):



TLC (EtOAc:hexane 2:8): R_f = 0.15; Light yellow solid; mp 200-201 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 2H), 7.29 – 7.17 (m, 5H), 6.55 (d, *J* = 7.0 Hz, 1H), 5.25 – 5.15 (m, 1H), 2.54 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (101 MHz, Acetone) δ 162.64, 152.43, 143.89, 135.47, 133.08, 130.29, 129.27, 128.98, 127.06, 50.15, 22.13, 15.16; $[\alpha]_D$ +63.18° (*c* 0.57, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 362.0544, found 362.0555.

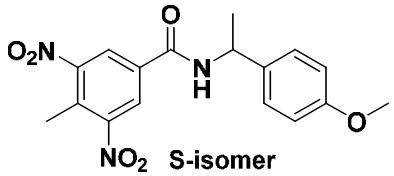
8. (*R*)-*N*-(1-(4-methoxyphenyl)ethyl)-4-methyl-3, 5-dinitrobenzamide (7g):



TLC (EtOAc:hexane 2:8): R_f = 0.20; Light yellow solid; mp 165-166 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 2H), 7.29 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.6 Hz, 2H), 6.57 (s, 1H),

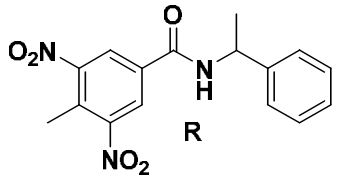
5.31 – 5.21 (m, 1H), 3.79 (s, 3H), 2.59 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.41, 159.77, 152.39, 136.66, 135.66, 130.20, 128.39, 127.06, 114.54, 55.51, 49.96, 22.17, 15.17; $[\alpha]_D$ -46.7° (*c* 0.82, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 358.1039, found 358.1047.

9. (*S*)-*N*-(1-(4-methoxyphenyl)ethyl)-4-methyl-3, 5-dinitrobenzamide (7h):



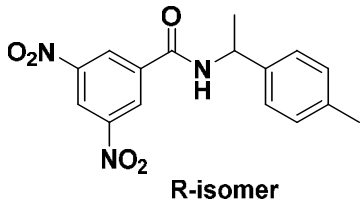
TLC (EtOAc:hexane 2:8): R_f = 0.20; Light yellow solid; mp 164-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.46 (d, *J* = 5.6 Hz, 1H), 5.28 (dd, *J* = 14.2, 7.3 Hz, 2H), 3.80 (s, 3H), 2.61 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.41, 159.77, 152.39, 136.66, 135.66, 130.20, 128.39, 127.06, 114.54, 55.51, 49.96, 22.17, 15.17; $[\alpha]_D$ +50.7° (*c* 0.76, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 358.1039, found 358.1047.

10. (*R*)-4-methyl-3, 5-dinitro-N-(1-phenylethyl)benzamide (7i):



TLC (EtOAc:hexane 2:8): R_f = 0.15; Light yellow solid; mp 171-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 2H), 7.36 (d, *J* = 4.3 Hz, 4H), 7.30 (dd, *J* = 8.2, 3.8 Hz, 1H), 6.59 (s, 1H), 5.37 – 5.24 (m, 1H), 2.60 (s, 3H), 1.63 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.59, 152.39, 144.82, 135.55, 130.27, 129.28, 127.91, 127.16, 127.11, 50.61, 22.29, 15.19; $[\alpha]_D$ -58.6° (*c* 0.44, Acetone), ee = 98.93%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 328.0933, found 328.0942.

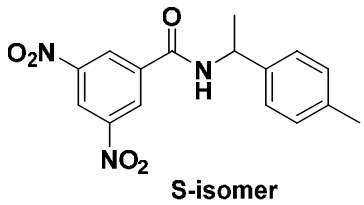
11. (*R*)-3, 5-Dinitro-*N*-(1-(*p*-tolyl)ethyl)benzamide (7j):



R-isomer

TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 184-185 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.0 Hz, 1H), 8.92 (d, *J* = 2.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.50 (d, *J* = 6.4 Hz, 1H), 5.36 – 5.28 (m, 1H), 2.35 (s, 3H), 1.66 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.67, 148.20, 139.63, 137.91, 136.73, 128.82, 127.44, 126.00, 120.34, 49.52, 21.05, 20.59, 12.94; $[\alpha]_D$ -46.5° (*c* 0.54, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M + H]^+$ 330.109, found 330.1083.

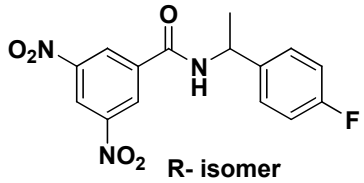
12. (*S*)-3,5-Dinitro-*N*-(1-(*p*-tolyl)ethyl)benzamide (7k):



S-isomer

TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 184-185 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.15 (t, *J* = 2.0 Hz, 1H), 8.92 (d, *J* = 2.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.50 (d, *J* = 6.4 Hz, 1H), 5.36 – 5.28 (m, 1H), 2.35 (s, 3H), 1.66 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.67, 148.20, 139.63, 137.91, 136.73, 128.82, 127.44, 126.00, 120.34, 49.52, 21.05, 20.59, 12.94; $[\alpha]_D$ +48.0° (*c* 0.36, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 328.0933, found 328.0940.

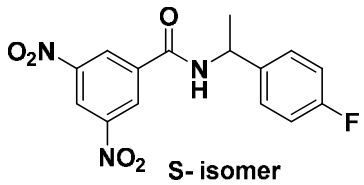
13. (*R*)-*N*-(1-(4-Fluorophenyl)ethyl)-3, 5-dinitrobenzamide (7l):



R- isomer

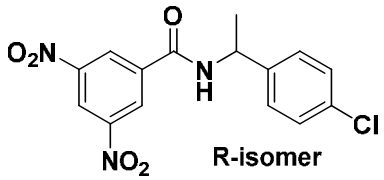
TLC (EtOAc:hexane 2:8): R_f = 0.20; Light yellow solid; mp 197-198 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.17 (t, *J* = 2.0 Hz, 1H), 8.93 (d, *J* = 2.0 Hz, 2H), 7.39 (dd, *J* = 8.7, 5.2 Hz, 2H), 7.08 (t, *J* = 8.6 Hz, 2H), 6.52 (d, *J* = 6.6 Hz, 1H), 5.39 – 5.30 (m, 1H), 1.68 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.73 (d, *J* = 243.07 Hz), 162.62, 162.55, 149.57, 138.69 (d, *J* = 3.89 Hz), 129.18 (d, *J* = 8.12 Hz), 128.38, 121.64, 115.86 (d, *J* = 21.42 Hz), 50.03, 22.12; $[\alpha]_D$ -42.23° (*c* 0.43, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 332.0682, found 332.06904.

14. (*S*)-*N*-(1-(4-fluorophenyl)ethyl)-3, 5-dinitrobenzamide (7m):



TLC (EtOAc:hexane 2:8): R_f = 0.20; Light yellow solid; mp 199-200 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.16 (t, *J* = 2.0 Hz, 1H), 8.94 (d, *J* = 0.7 Hz, 2H), 7.39 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.07 (t, *J* = 8.6 Hz, 2H), 6.57 (s, 1H), 5.35 (p, *J* = 7.0 Hz, 1H), 1.67 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.73 (d, *J* = 243.07 Hz), 162.62, 162.55, 149.57, 138.69 (d, *J* = 3.89 Hz), 129.18 (d, *J* = 8.12 Hz), 128.38, 121.64, 115.86 (d, *J* = 21.42 Hz), 50.03, 22.12; $[\alpha]_D$ +49.0° (*c* 0.4, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 332.0682, found 332.0695.

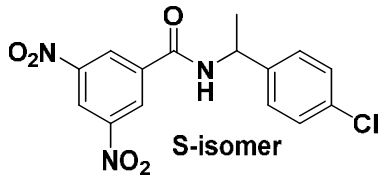
15. (*R*)-*N*-(1-(4-Chlorophenyl)ethyl)-3, 5-dinitrobenzamide (7n):



TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 177-178 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.16 (t, *J* = 3.5 Hz, 1H), 8.94 (d, *J* = 3.5 Hz, 2H), 7.36 – 7.31 (m, 4H), 6.67 (s, 1H), 5.35 – 5.26 (m, 1H), 1.66 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ

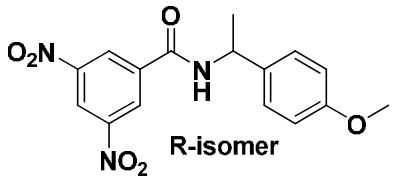
162.67, 149.55, 143.82, 138.57, 133.14, 129.29, 129.04, 128.40, 121.70, 50.28, 22.07; $[\alpha]_D$ -51.9° (*c* 0.67, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 348.0378, found 348.0397.

16. (*S*)-*N*-(1-(4-Chlorophenyl)ethyl)-3, 5-dinitrobenzamide (7o):



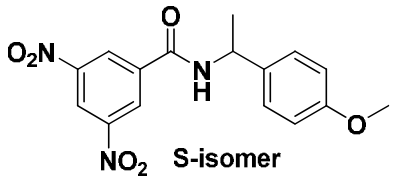
TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 180-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (t, *J* = 3.5 Hz, 1H), 8.94 (d, *J* = 3.5 Hz, 2H), 7.36 – 7.31 (m, 4H), 6.67 (s, 1H), 5.35 – 5.26 (m, 1H), 1.66 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.67, 149.55, 143.82, 138.57, 133.14, 129.29, 129.04, 128.40, 121.70, 50.28, 22.07; $[\alpha]_D$ +55.0° (*c* 0.68, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 348.0378, found 348.0398.

17. (*R*)-*N*-(1-(4-Methoxyphenyl)ethyl)-3,5-dinitrobenzamide (7p):



TLC (EtOAc:hexane 2:8): R_f = 0.15; Light yellow solid; mp 162-163 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.1 Hz, 1H), 8.92 (d, *J* = 2.0 Hz, 2H), 7.32 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.57 (d, *J* = 6.6 Hz, 1H), 5.30 (p, *J* = 7.1 Hz, 1H), 3.80 (s, 3H), 1.65 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.42, 159.80, 149.54, 138.85, 136.62, 128.45, 128.36, 121.56, 114.56, 55.51, 50.09, 22.09; $[\alpha]_D$ -36.99° (*c* 0.44, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 342.0882, found 342.0892.

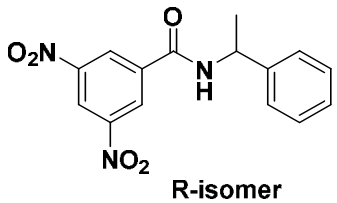
18. (*S*)-*N*-(1-(4-Methoxyphenyl)ethyl)-3,5-dinitrobenzamide (7q):



S-isomer

TLC (EtOAc:hexane 2:8): R_f = 0.15; Light yellow solid; mp 164-165 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.1 Hz, 1H), 8.92 (d, *J* = 2.0 Hz, 2H), 7.32 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.57 (d, *J* = 6.6 Hz, 1H), 5.30 (p, *J* = 7.1 Hz, 1H), 3.80 (s, 3H), 1.65 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.42, 159.80, 149.54, 138.85, 136.62, 128.45, 128.36, 121.56, 114.56, 55.51, 50.09, 22.09; $[\alpha]_D$ +35.5° (*c* 0.45, Acetone), ee = 99.29%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 342.0882, found 344.0892.

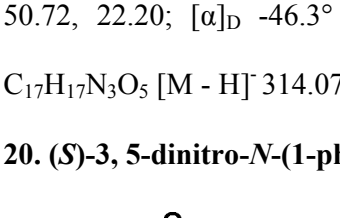
19. (*R*)-3, 5-Dinitro-*N*-(1-phenylethyl)benzamide (7r):



R-isomer

TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 157-158 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.13 (t, *J* = 2.1 Hz, 1H), 8.94 (d, *J* = 2.0 Hz, 2H), 7.40 – 7.28 (m, 5H), 6.75 (d, *J* = 6.9 Hz, 1H), 5.33 (dt, *J* = 14.1, 6.9 Hz, 1H), 1.67 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.56, 149.55, 144.78, 138.74, 129.30, 128.40, 127.96, 127.21, 121.63, 50.72, 22.20; $[\alpha]_D$ -46.3° (*c* 0.6, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 314.0776, found 314.0787.

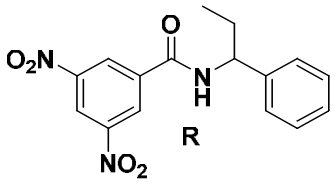
20. (*S*)-3, 5-dinitro-*N*-(1-phenylethyl)benzamide (7s):



S-isomer

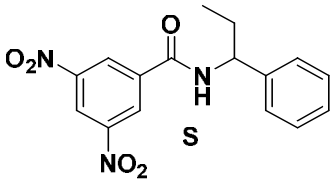
TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 156-157 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.0 Hz, 1H), 8.93 (d, *J* = 2.0 Hz, 2H), 7.43 – 7.29 (m, 5H), 6.66 (d, *J* = 7.9 Hz, 1H), 5.35 (dt, *J* = 14.3, 7.0 Hz, 1H), 1.67 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.56, 149.55, 144.78, 138.74, 129.30, 128.40, 127.96, 127.21, 121.63, 50.72, 22.20; $[\alpha]_D$ +54.7° (*c* 0.46, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 314.0776, found 314.0782.

21. (*R*)-3, 5-dinitro-*N*-(1-phenylpropyl)benzamide (7t):



TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 173-174 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.19 – 9.12 (m, 1H), 8.92 (d, *J* = 1.5 Hz, 2H), 7.38 – 7.32 (m, 3H), 7.32 – 7.27 (m, 2H), 6.66 (s, 1H), 5.08 (dd, *J* = 15.2, 7.6 Hz, 1H), 2.02 (dtd, *J* = 21.3, 14.0, 7.3 Hz, 2H), 0.98 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, Acetone) δ 204.24, 162.89, 149.57, 143.82, 138.82, 129.26, 128.36, 128.00, 127.74, 121.59, 57.14, 29.58, 11.75; $[\alpha]_D$ -30.59° (*c* 0.5, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 328.0933, found 328.0939.

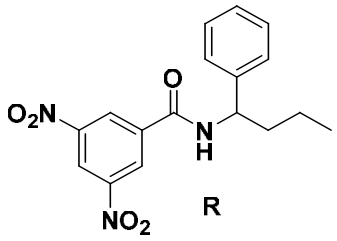
22. (*S*)-3, 5-dinitro-*N*-(1-phenylpropyl)benzamide (7u):



TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 175-176 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.17 – 9.12 (m, 1H), 8.93 (d, *J* = 2.1 Hz, 2H), 7.36 (d, *J* = 3.5 Hz, 4H), 7.33 – 7.28 (m, 1H), 6.66 (s, 1H), 5.09 (q, *J* = 7.6 Hz, 1H), 2.11 – 1.93 (m, 2H), 0.98 (t, *J* = 7.4 Hz,

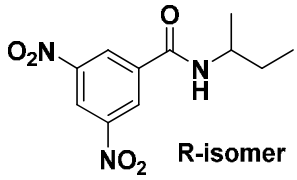
3H); ^{13}C NMR (101 MHz, Acetone) δ 204.24, 162.89, 149.57, 143.82, 138.82, 129.26, 128.36, 128.00, 127.74, 121.59, 57.14, 29.58, 11.75; $[\alpha]_D$ +35.8° (*c* 0.36, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 328.0933, found 328.0941.

23. (*R*)-3, 5-dinitro-*N*-(1-phenylbutyl)benzamide (7v):



TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 158-159 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 – 9.12 (m, 1H), 8.92 (d, *J* = 2.0 Hz, 2H), 7.36 (d, *J* = 4.3 Hz, 3H), 7.28 (dd, *J* = 10.6, 5.8 Hz, 2H), 6.60 (s, 1H), 5.18 (dd, *J* = 15.3, 7.6 Hz, 1H), 1.97 (dd, *J* = 15.9, 8.7 Hz, 2H), 1.39 – 1.25 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.81, 149.56, 144.11, 138.74, 129.29, 128.38, 127.98, 127.68, 121.73, 55.18, 38.96, 20.55, 14.06; $[\alpha]_D$ -32.4° (*c* 0.5, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 342.1089, found 342.1096.

24. (*R*)-*N*-(*sec*-Butyl)-3, 5-dinitrobenzamide (8a):



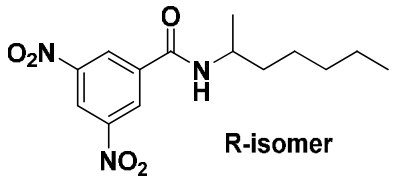
TLC (EtOAc:hexane 1:9): R_f = 0.15; Light yellow solid; mp 156-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (t, *J* = 2.1 Hz, 1H), 8.95 (d, *J* = 2.1 Hz, 2H), 6.10 (d, *J* = 6.6 Hz, 1H), 4.26 – 4.15 (m, 1H), 1.67 (ddd, *J* = 14.4, 7.3, 2.2 Hz, 2H), 1.33 (d, *J* = 6.6 Hz, 3H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.66, 149.55, 139.14, 128.23, 121.45, 48.73, ^{13}C NMR (126 MHz, Acetone) δ 162.66, 149.55, 139.14, 128.23, 121.45, 48.73,

29.98, 20.48, 11.05; $[\alpha]_D$ -22.7° (*c* 0.4, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 266.0776, found 266.0781.

25. (*S*)-*N*-(*sec*-butyl)-3, 5-dinitrobenzamide (8b):

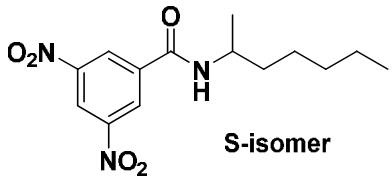
TLC (EtOAc:hexane 1:9): R_f = 0.15; Light yellow solid; mp 174-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (t, *J* = 2.0 Hz, 2H), 8.96 (d, *J* = 2.0 Hz, 5H), 6.13 (d, *J* = 7.5 Hz, 2H), 4.21 (tq, *J* = 13.4, 6.7 Hz, 3H), 1.68 (dtd, *J* = 14.3, 7.3, 2.3 Hz, 7H), 1.33 (d, *J* = 6.6 Hz, 8H), 1.03 (t, *J* = 7.4 Hz, 8H); ^{13}C NMR (126 MHz, Acetone) δ 162.66, 149.55, 139.14, 128.23, 121.45, 48.73, ^{13}C NMR (126 MHz, Acetone) δ 162.66, 149.55, 139.14, 128.23, 121.45, 48.73, 29.98, 20.48, 11.05; $[\alpha]_D$ +31.2° (*c* 0.41, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 266.0776, found 266.0788.

26. (*R*)-*N*-(Heptan-2-yl)-3, 5-dinitrobenzamide (8c):



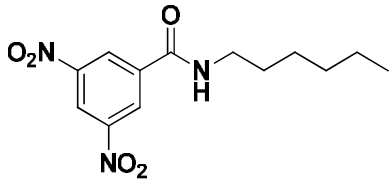
TLC (EtOAc:hexane 1:9): R_f = 0.20; Light yellow solid; mp 135-136 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.17 (t, *J* = 2.0 Hz, 1H), 8.94 (d, *J* = 2.0 Hz, 2H), 6.15 (d, *J* = 7.5 Hz, 1H), 4.30 – 4.20 (m, 1H), 1.68 – 1.54 (m, 5H), 1.44 – 1.28 (m, 6H), 0.90 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.55, 149.55, 139.15, 128.22, 121.44, 47.20, 37.16, 32.47, 26.75, 23.29, 21.02, 14.35; $[\alpha]_D$ -34.3° (*c* 0.94, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 308.1246, found 308.1251.

27. (*S*)-N-(Heptan-2-yl)-3, 5-dinitrobenzamide (8d):



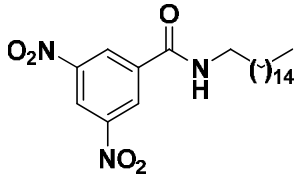
TLC (EtOAc:hexane 1:9): R_f = 0.20; Light yellow solid; mp 135-136 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.17 (t, *J* = 2.0 Hz, 1H), 8.94 (d, *J* = 2.0 Hz, 2H), 6.15 (d, *J* = 7.5 Hz, 1H), 4.30 – 4.20 (m, 1H), 1.68 – 1.54 (m, 5H), 1.44 – 1.28 (m, 6H), 0.90 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, Acetone) δ 162.55, 149.55, 139.15, 128.22, 121.44, 47.20, 37.16, 32.47, 26.75, 23.29, 21.02, 14.35; $[\alpha]_D$ +35.8° (*c* 0.73, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 308.1246, found 308.1254.

28. *N*-Hexyl-3, 5-dinitrobenzamide (8e):



TLC (EtOAc:hexane 1:9): R_f = 0.30; Light yellow solid; mp 90-91 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.16 (t, *J* = 2.0 Hz, 1H), 8.95 (d, *J* = 2.0 Hz, 2H), 6.48 (s, 1H), 3.53 (dd, *J* = 13.6, 6.6 Hz, 2H), 1.72 – 1.64 (m, 2H), 1.45 – 1.31 (m, 6H), 0.91 (t, *J* = 6.9 Hz, 3H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 294.1089, found 294.1090.

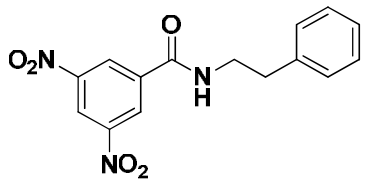
29. 3, 5-Dinitro-*N*-hexadecylbenzamide (8f):



TLC (EtOAc:hexane 1:9): R_f = 0.35; Light yellow solid; mp 102-103 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.0 Hz, 1H), 8.93 (d, *J* = 2.0 Hz, 2H), 6.38 (d, *J* = 1.9 Hz, 1H),

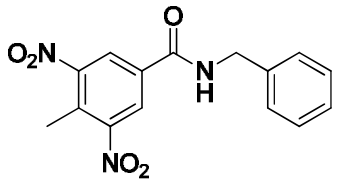
3.51 (dd, *J* = 13.2, 7.1 Hz, 2H), 1.66 (dt, *J* = 14.8, 7.4 Hz, 2H), 1.24 (m, 26H), 0.86 (t, *J* = 6.8 Hz, 3H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 434.2654, found 434.2661.

30. 3,5-Dinitro-*N*-phenethylbenzamide (9a):



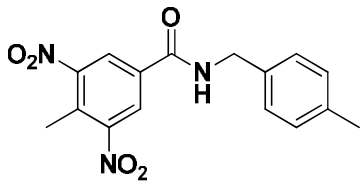
TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 148-149 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.0 Hz, 1H), 8.85 (d, *J* = 2.1 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.31 – 7.27 (m, 1H), 7.24 (d, *J* = 5.1 Hz, 2H), 6.32 (s, 1H), 3.80 (dd, *J* = 12.8, 6.8 Hz, 2H), 2.99 (dd, *J* = 12.5, 5.6 Hz, 2H); ^{13}C NMR (126 MHz, Acetone) δ 163.30, 149.56, 140.21, 138.84, 129.66, 129.33, 128.17, 127.18, 121.55, 42.57, 36.09, 11.79; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 314.0776, found 314.0780.

31. *N*-Benzyl-4-methyl-3, 5-dinitrobenzamide (9b):



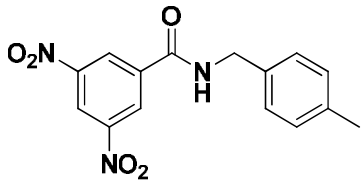
TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 180-181 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.46 – 7.30 (m, 3H), 6.55 (s, 2H), 4.66 (d, *J* = 5.6 Hz, 2H), 2.62 (s, 3H); ^{13}C NMR (126 MHz, Acetone) δ 163.30, 152.41, 139.59, 135.35, 130.33, 129.32, 128.73, 128.06, 127.08, 44.63, 15.03; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 314.0776, found 314.0787.

32. 4-Methyl-*N*-(4-methylbenzyl)-3, 5-dinitrobenzamide (9c):



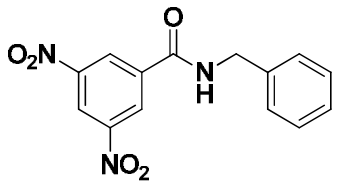
TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 197-198 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 2H), 7.18 – 7.21 (m, 4H), 6.51 (s, 1H), 4.61 (d, *J* = 5.4 Hz, 2H), 2.61 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (126 MHz, Acetone) δ 163.20, 152.46, 137.55, 136.60, 135.49, 130.33, 129.90, 128.70, 127.06, 44.22, 21.13, 15.19; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 328.0933, found 328.0943.

33. *N*-(4-Methylbenzyl)-3,5-dinitrobenzamide (9d):



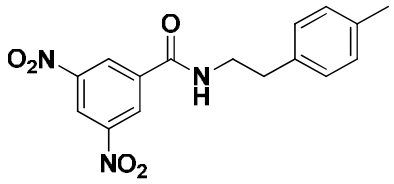
TLC (EtOAc:hexane 2:8): R_f = 0.25; Light yellow solid; mp 180-181 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.16 (t, *J* = 2.0 Hz, 1H), 8.95 (d, *J* = 2.0 Hz, 2H), 7.27 (d, *J* = 6.5 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.61 (s, 1H), 4.65 (d, *J* = 5.5 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (126 MHz, Acetone) δ 163.25, 149.59, 138.70, 137.60, 136.55, 129.91, 128.75, 128.33, 121.62, 44.36, 21.08; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 314.0776, found 314.0782.

34. *N*-Benzyl-3,5-dinitrobenzamide (9e):



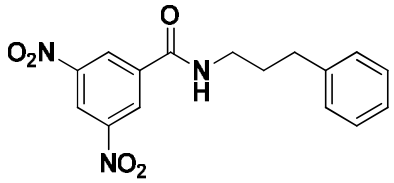
TLC (EtOAc:hexane 2:8): R_f = 0.20; Light yellow solid; mp 198.5-199.5 ^oC; ^1H NMR (400 MHz, Acetone) δ 9.15 (d, *J* = 2.0 Hz, 2H), 9.08 (t, *J* = 2.1 Hz, 1H), 8.94 (s, 1H), 7.42 (d, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 4.69 (d, *J* = 5.4 Hz, 2H); ^{13}C NMR (126 MHz, Acetone) δ 163.31, 149.63, 139.63, 138.67, 129.34, 128.72, 128.35, 128.11, 121.67, 44.57; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 300.0620, found 300.0626.

35. *N*-(4-Methylphenethyl)-3, 5-dinitrobenzamide (9f):



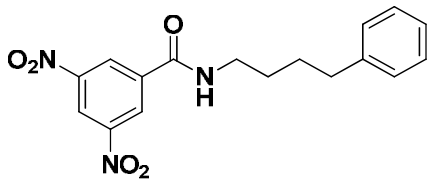
TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 175-176 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.14 (t, *J* = 2.0 Hz, 1H), 8.84 (d, *J* = 2.1 Hz, 2H), 7.15 (q, *J* = 8.0 Hz, 4H), 6.30 (s, 1H), 3.77 (dd, *J* = 12.8, 6.7 Hz, 2H), 2.95 (t, *J* = 6.8 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, Acetone) δ 163.28, 149.57, 138.89, 137.10, 136.43, 129.94, 129.56, 128.17, 121.53, 42.66, 35.67, 21.05; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 328.0933, found 328.0926.

36. 3,5-Dinitro-*N*-(3-phenylpropyl)benzamide (9g):



TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 120-121 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 3.3 Hz, 1H), 8.77 – 8.73 (m, 2H), 7.36 – 7.27 (m, 2H), 7.27 – 7.17 (m, 3H), 6.22 (s, 1H), 3.60 (tt, *J* = 10.1, 5.0 Hz, 2H), 2.78 (t, *J* = 7.0 Hz, 2H), 2.09 – 2.01 (m, 2H); ^{13}C NMR (126 MHz, Acetone) δ 163.26, 149.54, 142.71, 138.91, 129.24, 129.21, 128.21, 126.69, 121.50, 40.72, 33.88, 31.83; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 328.0933, found 328.0938.

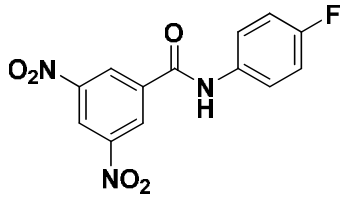
37. 3,5-Dinitro-*N*-(4-phenylbutyl)benzamide (9h):



TLC (EtOAc:hexane 2:8): R_f = 0.35; Light yellow solid; mp 160-161 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 9.15 (d, *J* = 2.0 Hz, 1H), 8.95 – 8.90 (m, 2H), 7.29 (d, *J* = 7.6 Hz, 2H), 7.19

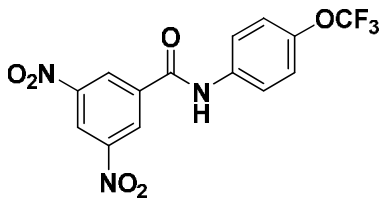
(t, *J* = 6.3 Hz, 3H), 6.43 (s, 1H), 3.63 – 3.46 (m, 2H), 2.69 (t, *J* = 6.9 Hz, 2H), 1.84 – 1.63 (m, 4H); ^{13}C NMR (126 MHz, Acetone) δ 163.15, 149.58, 143.23, 138.94, 129.25, 129.14, 128.19, 126.57, 121.48, 40.72, 36.09; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 342.1089, found 342.1095.

38. *N*-(4-Fluorophenyl)-3, 5-dinitrobenzamide (10a):



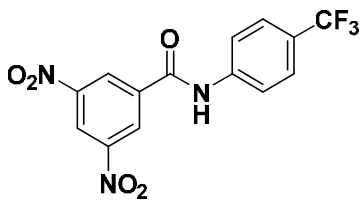
TLC (EtOAc:hexane 3:7): R_f = 0.25; Light yellow solid; mp 226-227 ^{o}C; ^{1}H NMR (400 MHz, Acetone) δ 10.31 (s, 3H), 9.20 (d, *J* = 1.9 Hz, 23H), 9.11 (t, *J* = 1.8 Hz, 9H), 7.86 (dd, *J* = 8.7, 4.9 Hz, 30H), 7.17 (t, *J* = 8.8 Hz, 28H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 304.0369, found 304.0380.

39. 3,5-Dinitro-*N*-(4-(trifluoromethoxy)phenyl)benzamide (10b):



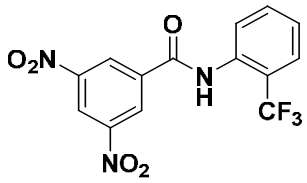
TLC (EtOAc:hexane 3:7): R_f = 0.35; Light yellow solid; mp 194-195 ^{o}C; ^{1}H NMR (400 MHz, Acetone) δ 10.40 (s, 1H), 9.22 (d, *J* = 2.0 Hz, 2H), 9.13 (t, *J* = 2.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 3H), 7.39 (d, *J* = 8.6 Hz, 3H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ [M - H]$^-$ 370.0286, found 370.0294.

40. 3,5-Dinitro-*N*-(4-(trifluoromethyl)phenyl)benzamide (10c):



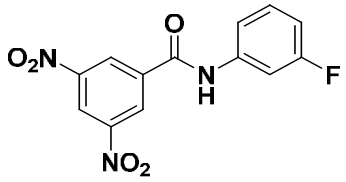
TLC (EtOAc:hexane 3:7): R_f = 0.35; Light yellow solid; mp 210-211 ^oC; ^1H NMR (400 MHz, Acetone) δ 9.23 (d, *J* = 2.1 Hz, 2H), 9.14 (t, *J* = 2.1 Hz, 1H), 8.08 (d, *J* = 8.5 Hz, 2H), 8.01 (s, 1H), 7.76 (d, *J* = 8.5 Hz, 2H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 354.0337, found 354.0345.

41. 3,5-Dinitro-*N*-(2-(trifluoromethyl)phenyl)benzamide (10d):



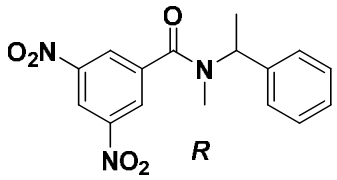
TLC (EtOAc:hexane 3:7): R_f = 0.15; Light yellow solid; mp 224-225 ^oC; ^1H NMR (400 MHz, Acetone) δ 9.20 (d, *J* = 2.1 Hz, 2H), 9.16 (t, *J* = 2.1 Hz, 1H), 8.01 (s, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.80 (d, *J* = 3.9 Hz, 2H), 7.61 (dt, *J* = 8.6, 4.5 Hz, 1H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 354.0337, found 354.0351.

42. *N*-(3-Fluorophenyl)-3, 5-dinitrobenzamide (10e):



TLC (EtOAc:hexane 3:7): R_f = 0.25; Light yellow solid; mp 197-198 ^oC; ^1H NMR (400 MHz, Acetone) δ 10.42 (s, 3H), 9.21 (d, *J* = 1.9 Hz, 20H), 9.13 (d, *J* = 1.8 Hz, 8H), 7.82 (d, *J* = 11.4 Hz, 11H), 7.58 (d, *J* = 8.1 Hz, 13H), 7.43 (dd, *J* = 14.9, 8.1 Hz, 13H), 6.97 (td, *J* = 8.4, 2.2 Hz, 11H); HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M - H]^-$ 304.0369, found 304.0385.

43. (*R*)-*N*-Methyl-3, 5-dinitro-*N*-(1-phenylethyl)benzamide (11a):



TLC (EtOAc:hexane 2:8): R_f = 0.35; Yellow viscous liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (d, *J* = 1.5 Hz, 1H), 8.61 (d, *J* = 1.8 Hz, 2H), 7.38 (dd, *J* = 22.2, 6.2 Hz, 5H), 6.15 (s, 1H), 2.67 (s, 3H), 1.68 (d, *J* = 7.0 Hz, 3H); $[\alpha]_D$ +83.2° (*c* 2.5, Acetone), ee = 100%; HRMS (ESI-TOF) calcd for $C_{17}H_{17}N_3O_5$ $[M + H]^+$ 330.109, found 330.1082.

Part B:

Pharmacokinetics studies of compounds 7a and 7d:

Discussion of *in vivo* PK for compound 7a:

The pharmacokinetics of compound **7a** was evaluated in Balb/C male mice following a single 2.5 mg/kg dose administration by intraperitoneal (IP) route and a 1 mg/kg dose by intravenous (IV) route in 5% DMSO, 5% Solutol : absolute alcohol (1:1, v/v) and 90% normal saline. Following IP administration maximum plasma concentration (C_{max}) of 60 ng/mL was achieved at 0.5 h (t_{max}). The terminal half life ($t_{1/2}$) was 0.9 h and the area under the curve (AUC) was 148 ng*h/mL and absolute intraperitoneal bioavailability (F%) of 49%. IV clearance was ~134 mL/min/Kg.

Plasma concentrations (ng/mL) of compound 7a in mice after 2.5 mg/kg IP dose:

Animal No.	Body Wt. (g)	Dose Vol. (mL)	Time point (h) / concentration in plasma (ng/mL)							
			0.25	0.5	1	2	4	8	10	24
1	28	0.30	50.3				11.7			
2	30	0.30	48.9				8.86			
3	27	0.25	67.7				17.0			
4	30	0.30		36.7				2.94		
5	27	0.25		96.2				BLQ		
6	32	0.30		49.5				1.69		
7	27	0.25			2.86 *				BLQ	
8	29	0.30			31.8				BLQ	
9	30	0.30			33.1				BLQ	
10	31	0.30				32.7				BLQ
11	29	0.30				31.9				BLQ
12	28	0.30				25.1				BLQ
Mean concentration (ng/mL)			55.6	60.8	32.5	29.9	12.5	2.31	NA	NA
SD			10.4	31.3	NA	4.20	4.12	NA	NA	NA
%CV			18.8	51.5	NA	14.0	33.0	NA	NA	NA

Plasma concentrations (ng/mL) of compound 7a in mice after 1 mg/kg IV dose:

Animal No.	Body Wt. (g)	Dose Vol. (mL)	Time point (h) / concentration in plasma (ng/mL)							
			0.12	0.25	0.5	1	2	4	8	24
1	31	0.30	279				16.6			
2	29	0.30	192				13.8			
3	26	0.25	221				10.4			
4	26	0.25		66.8				2.62		
5	30	0.30		108				3.02		
6	27	0.25		78.6				2.25		
7	29	0.30			23.4				BLQ	
8	25	0.25			58.4				BLQ	
9	29	0.30			48.5				BLQ	
10	30	0.30				19.3				BLQ
11	25	0.25				19.5				BLQ
12	29	0.30				33.0				BLQ
Mean concentration (ng/mL)			231	84.3	43.4	23.9	13.6	2.63	NA	NA
SD			44.7	21.0	18.0	7.87	3.09	0.38	NA	NA
%CV			19.4	24.9	41.5	32.9	22.7	14.6	NA	NA

NA: not applicable; BLQ: below limit of quantitation; *value not considered for calculation.

Parameter	Unit	Value
$t_{1/2, ß}$	(h)	0.93
C_{max}	ng/mL(nM)	231(672.8)
C_0	ng/mL (nM)	316(920.3)
AUC_{0-t}	ng·h/mL (nM·h)	121(352.42)
$AUC_{0-\infty}$	ng·h/mL (nM·h)	125(364.07)
CL	(mL/min/Kg)	134
V_d	(L/Kg)	10.7
V_{dss}	(L/Kg)	6.67
T_{last}	(h)	4.00
Time points considered for $t_{1/2, ß}$ calculation		1 – 4 h
C_0 calculated manually using initial 3 time points		

Table 5: Pharmacokinetic parameters of compound **7a** post IV dose at 1 mg/Kg to Balbc mice.

Parameter	Unit	Value
$t_{1/2,\beta}$	(h)	1.63
AUC_{0-t}	ng·h/mL (nM·h)	148 (431.06)
$AUC_{0-\infty}$	ng·h/mL(nM·h)	153(445.6)
C_{max}	ng/mL (nM)	60.8(177.08)
t_{max}	(h)	0.50
Bioavailability	(% F)	49
Time points considered for $t_{1/2,\beta}$ calculation:		2 - 8 h

$t_{1/2,\beta}$: terminal half life; AUC_{0-t}: the area under the plasma concentration-time curve from 0 to last measurable time point; $AUC_{0-\infty}$: area under the plasma concentration-time curve from time zero to infinity; C_{max}: maximum observed plasma concentration; t_{max}: time to the maximum observed plasma concentration; CL: clearance; V_d: volume of distribution; $V_{dss:}$ volume of distribution at steady state.

Table 6: Pharmacokinetic parameters of compound **7a** post IP dose at 2.5 mg/Kg to Balbc mice.

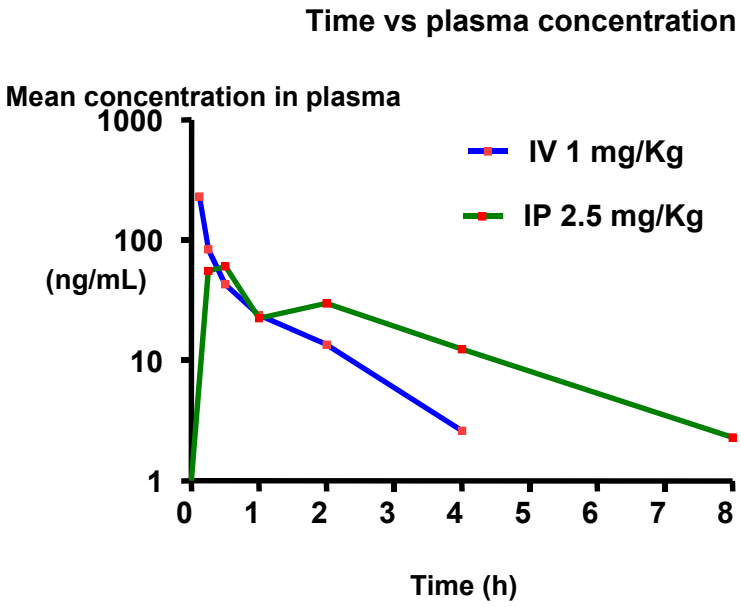


Fig 22: PK profile of compound 7a in Balb mice

Discussion of *in vivo* PK for compound 7d:

The pharmacokinetics of compound **7d** was evaluated in Balb/C male mice following a single 2.5 mg/kg dose administration by intraperitoneal (IP) route and a 1 mg/kg dose by intravenous (IV) route in 5% DMSO, 5% Solutol : absolute alcohol (1:1, v/v) and 90% normal saline. Following IP administration maximum plasma concentration (C_{max}) of 75 ng/mL was achieved at 0.25 h (t_{max}). The terminal half life ($t_{1/2}$) was 1.08 h and the area under the curve (AUC) was 122 ng*h/mL and absolute intraperitoneal bioavailability (F%) of 35%. IV clearance was ~111 mL/min/Kg.

Plasma concentrations (ng/mL) of compound 7d in mice after 2.5 mg/kg IP dose:

Animal No.	Body Wt. (g)	Dose Vol. (mL)	Time point (h) / concentration in plasma (ng/mL)							
			0.25	**0.5**	**1**	**2**	**4**	**8**	**10**	**24**
1	21	0.20	94.0				BLQ			
2	22	0.20	78.0				8.35			
3	24	0.25	53.6				6.38			
4	21	0.20		60.5				BLQ		
5	23	0.25		44.8				BLQ		
6	25	0.25		52.5				2.26 *		
7	26	0.25			36.9				BLQ	
8	24	0.25			65.4				BLQ	
9	23	0.25			65.2#				BLQ	
10	24	0.25				19.1				BLQ
11	25	0.25				27.2				BLQ
12	27	0.25				28.8				BLQ
Mean concentration (ng/mL)			75.2	52.6	51.1	25.0	7.36	NA	NA	NA
SD			20.4	7.85	NA	5.23	NA	NA	NA	NA
%CV			27.1	14.9	NA	20.9	NA	NA	NA	NA

Plasma concentrations (ng/mL) of compound 7d in mice after 1 mg/kg IV dose:

Animal No.	Body Wt. (g)	Dose Vol. (mL)	Time point (h) / concentration in plasma (ng/mL)							
			0.12	0.25	0.5	1	2	4	8	24
1	27	0.25	313				21.3			
2	28	0.30	177				10.6			
3	30	0.30	252				6.44[#]			
4	27	0.25		166				BLQ		
5	26	0.25		137				BLQ		
6	27	0.25		103				BLQ		
7	27	0.25			52.7				BLQ	
8	26	0.25			55.9				BLQ	
9	30	0.30			50.2				BLQ	
10	26	0.25				35.6				BLQ
11	30	0.30				25.8				BLQ
12	32	0.30				28.2				BLQ
Mean concentration (ng/mL)			247	135	53.0	29.9	16.0	NA	NA	NA
SD			68.2	31.2	2.88	5.11	NA	NA	NA	NA
%CV			27.6	23.1	5.43	17.1	NA	NA	NA	NA

NA: not applicable; BLQ: below limit of quantitation; *value not considered for calculation; [#]due to IS variation value was not considered for calculation.

Parameter	Unit	Value
$t_{1/2, ß}$	(h)	0.90
C_{max}	ng/mL (nM)	247(711.1)
C_0	ng/mL (nM)	388(1117.1)
AUC_{0-t}	ng·h/mL (nM·h)	130(374.31)
$AUC_{0-\infty}$	ng·h/mL (nM·h)	151(434.78)
CL	(mL/min/Kg)	111
V_d	(L/Kg)	8.57
V_{dss}	(L/Kg)	5.57
T_{last}	(h)	2.00
Time points considered for $t_{1/2, ß}$ calculation		0.5 – 2 h
C_0 calculated manually using initial 3 time points		

Table 7: Pharmacokinetic parameters of compound **7d** post IV dose at 1 mg/Kg to Balbc mice:

Parameter	Unit	Value
$t_{1/2,\beta}$	(h)	1.08
AUC_{0-t}	ng·h/mL (nM·h)	122(351.27)
$AUC_{0-\infty}$	ng·h/mL (nM·h)	133(382.95)
C_{max}	ng/mL (nM)	75.2(216.5)
t_{max}	(h)	0.25
Bioavailability	(% F)	35
Time points considered for $t_{1/2,\beta}$ calculation:		1 - 4 h

$t_{1/2,\beta}$: terminal half life; AUC_{0-t}: the area under the plasma concentration-time curve from 0 to last measurable time point; $AUC_{0-\infty}$: area under the plasma concentration-time curve from time zero to infinity; C_{max}: maximum observed plasma concentration; t_{max}: time to the maximum observed plasma concentration; CL: clearance; V_d: volume of distribution; $V_{dss:}$ volume of distribution at steady state.

Table 8: Pharmacokinetic parameters of compound **7d** post IP dose at 2.5 mg/Kg to Balbc mice:

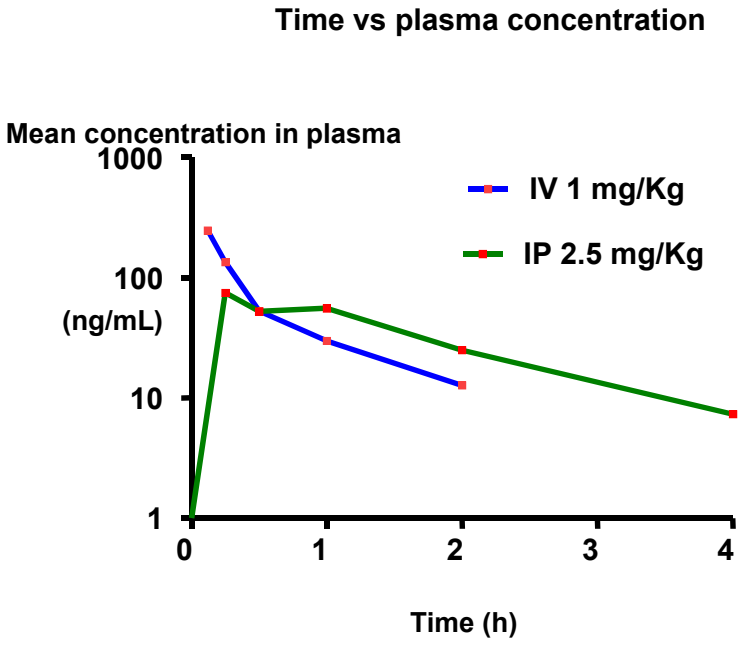
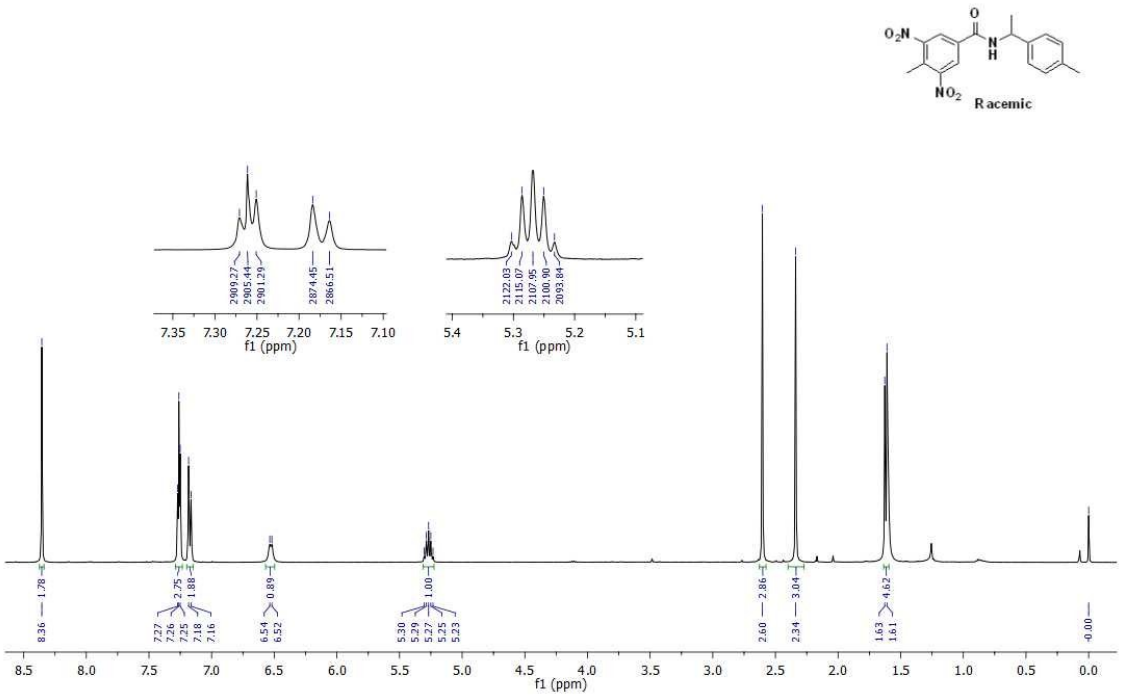


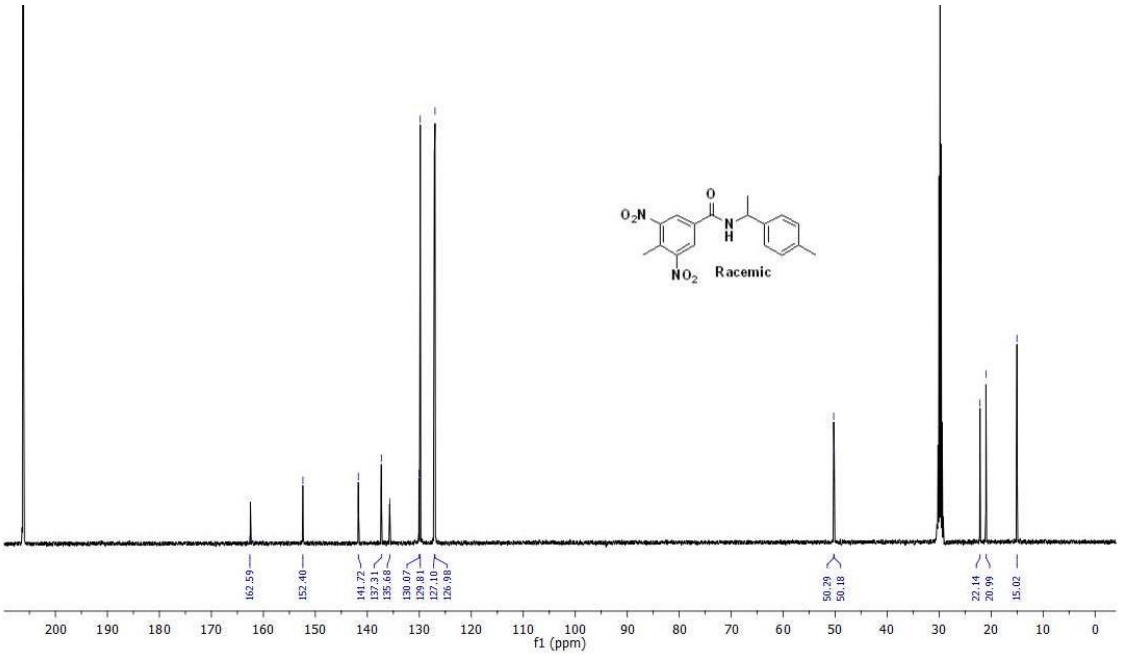
Fig 23: PK profile of compound 7d in Balb mice

Part E: Spectral data of synthesized DNB derivatives

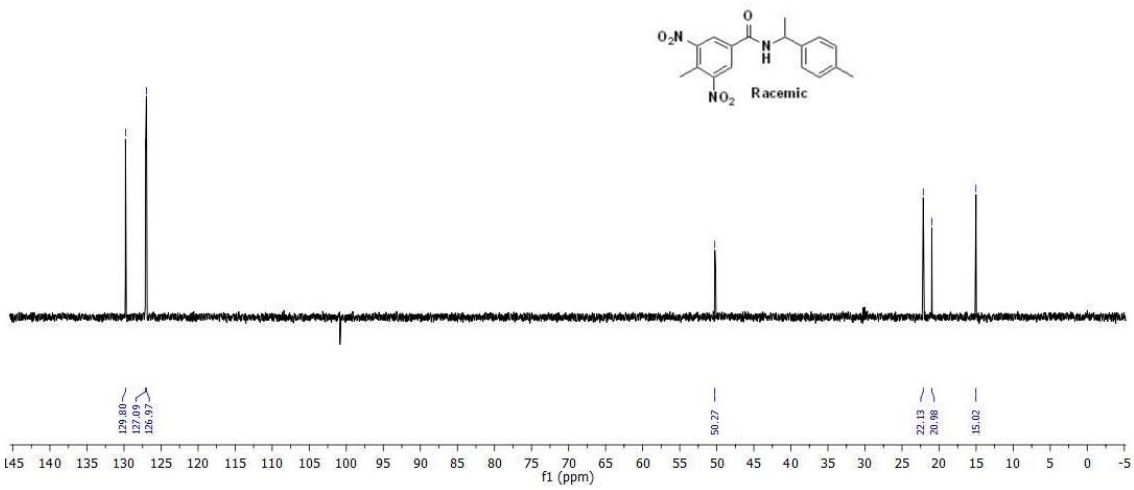
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4b:**



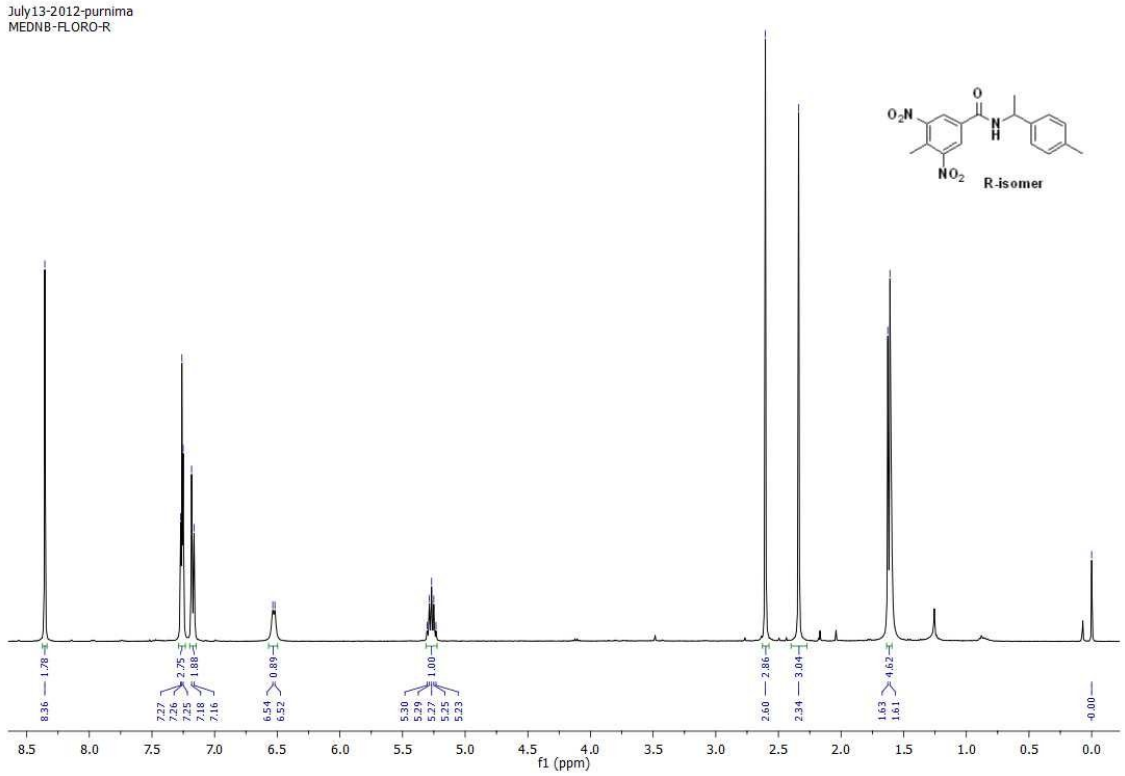
^{13}C NMR (101 MHz, Acetone-d_6) of compound **4b:**



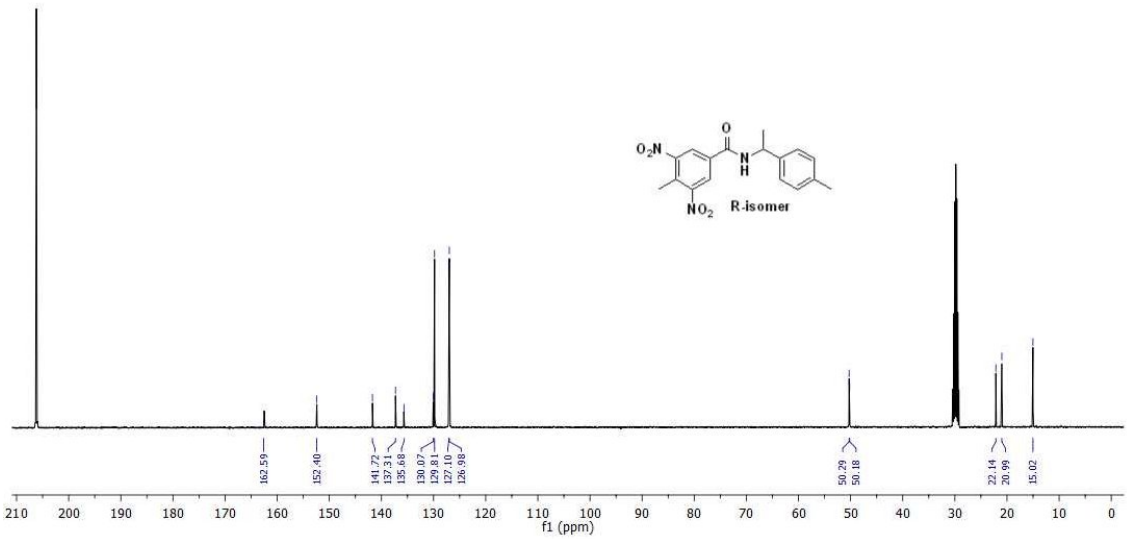
DEPT (101 MHz, Acetone-d_6) of compound **4b:**



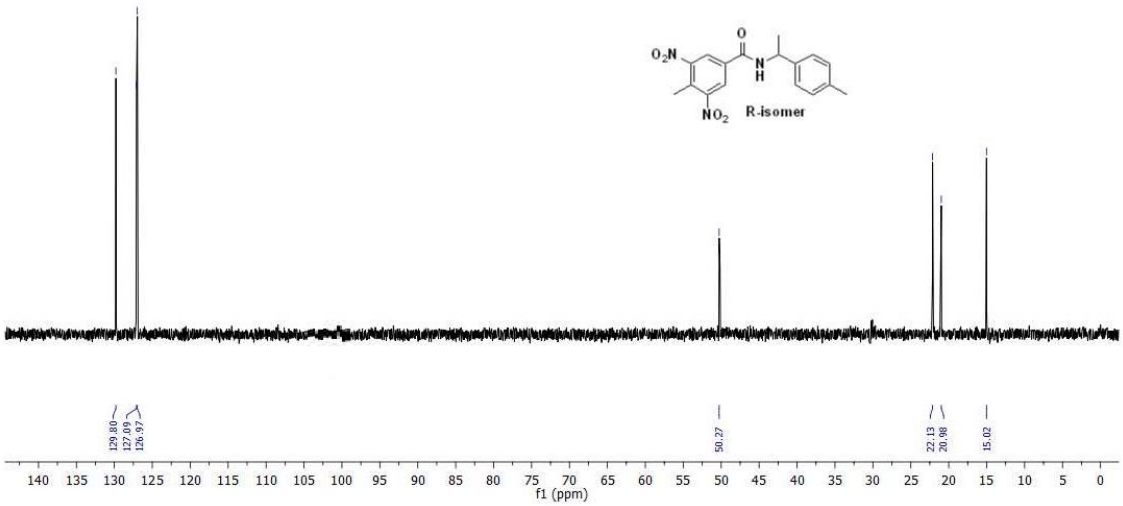
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7a:**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7a:**



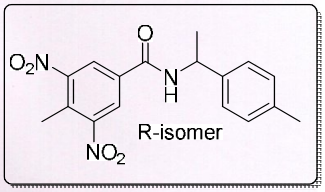
DEPT (101 MHz, Acetone-d_6) of compound **7a:**



HRMS (ESI-TOF) of compound **7a**:

Qualitative Compound Report

Data File	84.d	**Sample Name**	84
Sample Type	Sample	**Position**	Vial 38
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	28-07-2012 PM 03:14:11
IRM Calibration Status	Some Ions Missed	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

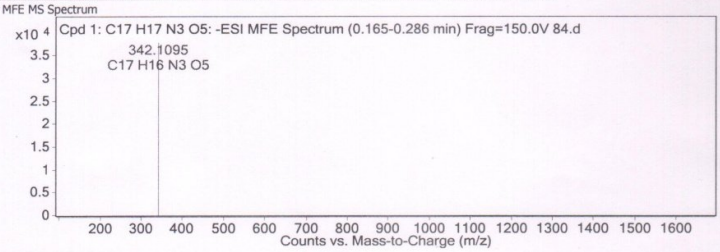


Compound Table

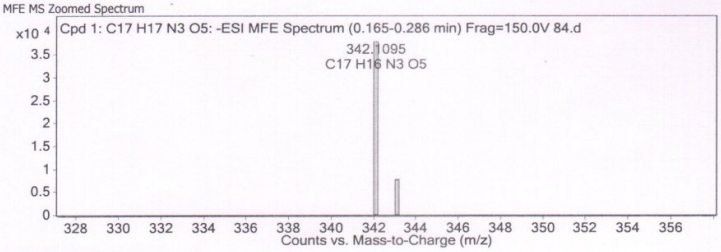
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C17 H17 N3 O5	0.213	343.1167	C17 H17 N3 O5	C17 H17 N3 O5	0.21	C17 H17 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C17 H17 N3 O5	342.1095	0.213	Find by Molecular Feature	343.1167

MFE MS Spectrum



MFE MS Zoomed Spectrum

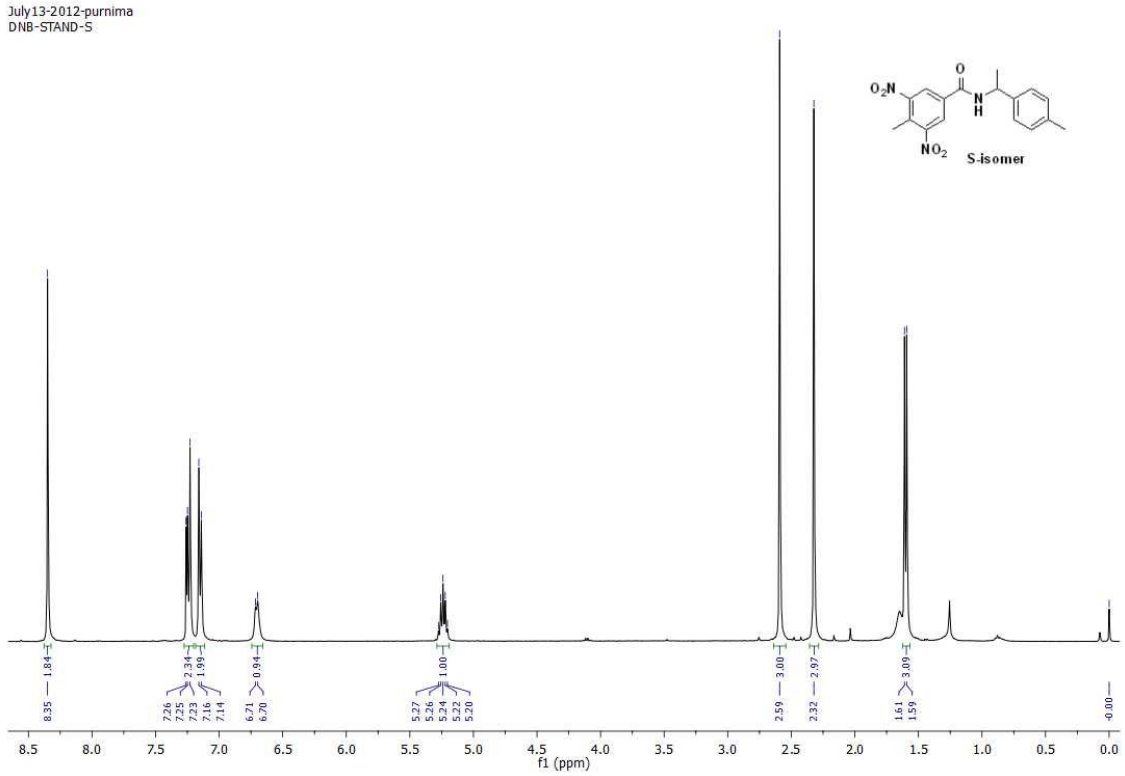


MS Spectrum Peak List

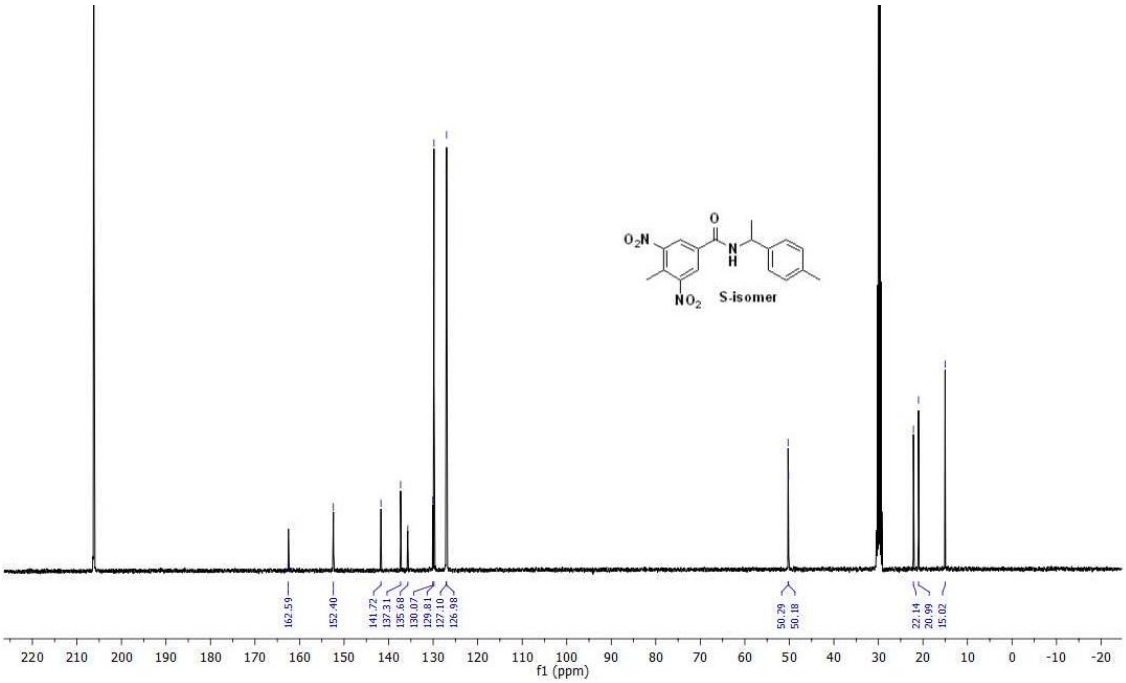
m/z	z	Abund	Formula	Ion
342.1095	-1	37748.9	C17 H16 N3 O5	(M-H)-
343.1128	-1	7585.8	C17 H16 N3 O5	(M-H)-

--- End Of Report ---

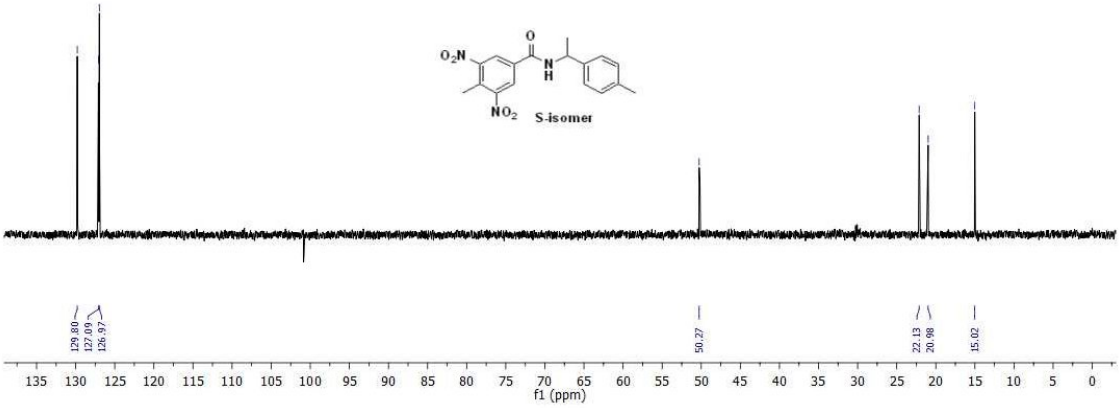
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7b:**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7b:**



DEPT (101 MHz, Acetone-d_6) of compound **7b:**

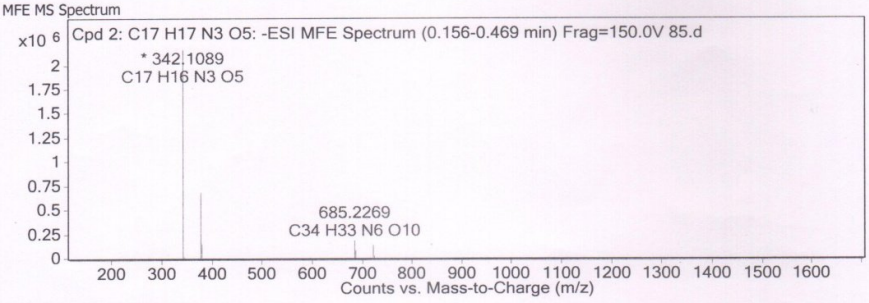


HRMS (ESI-TOF) of compound **7b**:

Qualitative Compound Report

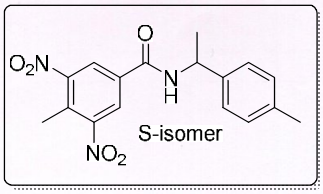
Data File	85.d	**Sample Name**	85
Sample Type	Sample	**Position**	Vial 39
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	27-07-2012 PM 05:31:43
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

MFE MS Spectrum



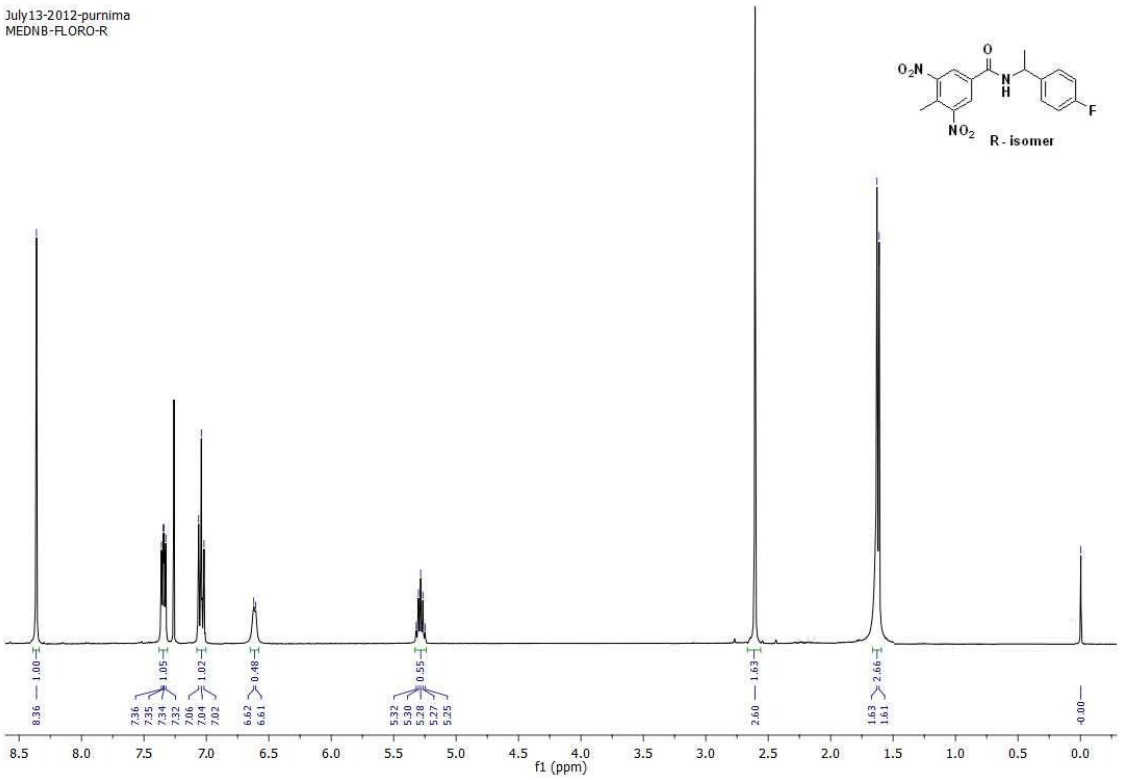
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
342.1089	-1	2162089.8	C17 H16 N3 O5	(M-H)-
343.1123	-1	310561.9	C17 H16 N3 O5	(M-H)-
378.0856	-1	678649.6	C17 H17 Cl N3 O5	(M+Cl)-
379.0897	-1	90943.6	C17 H17 Cl N3 O5	(M+Cl)-
380.0846	-1	142890	C17 H17 Cl N3 O5	(M+Cl)-
685.2269	-1	173803.8	C34 H33 N6 O10	(2M-H)-
686.2295	-1	78339.4	C34 H33 N6 O10	(2M-H)-
721.2034	-1	139284.7		(2M+Cl)-
722.2062	-1	64958.9		(2M+Cl)-
723.2023	-1	58238.7		(2M+Cl)-

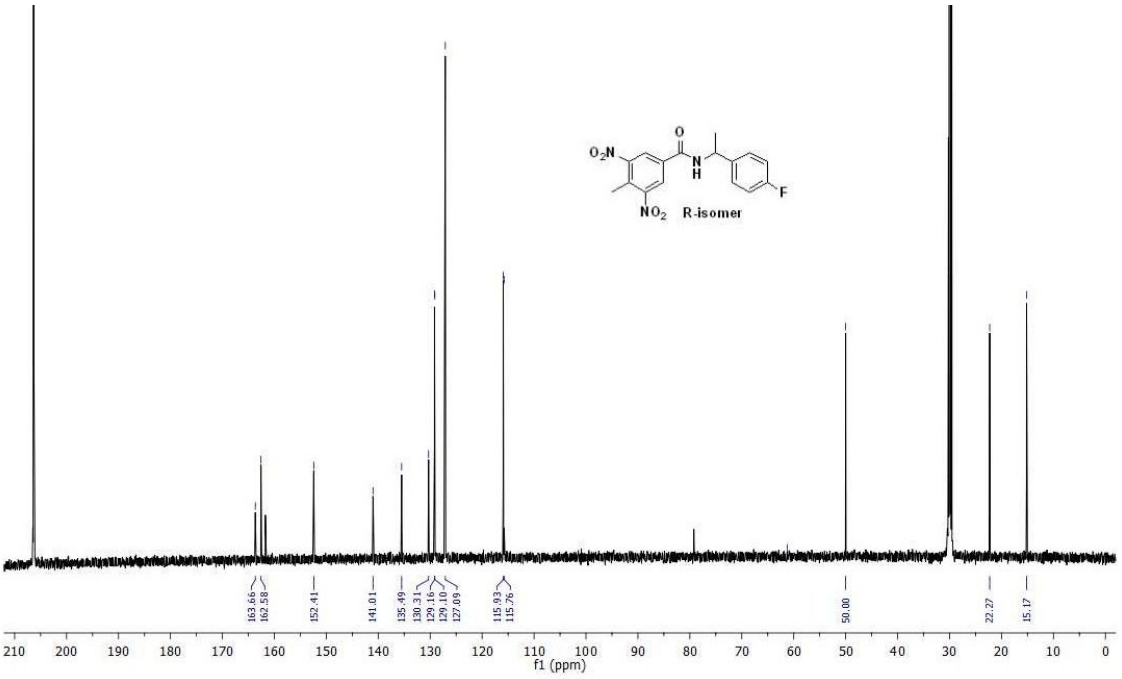


--- End Of Report ---

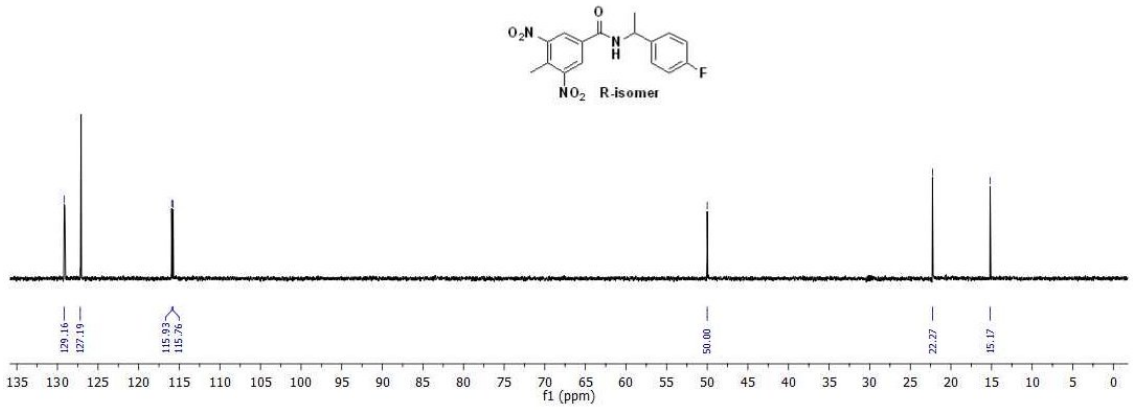
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7c:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7c:**



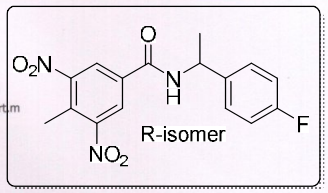
DEPT (126 MHz, Acetone-d_6) of compound **7c:**



HRMS (ESI-TOF) of compound **7c**:

Qualitative Compound Report

Data File	86.d	**Sample Name**	86
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	7/30/2012 10:11:53 AM
IRM Calibration Status	Some Ions Missed	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

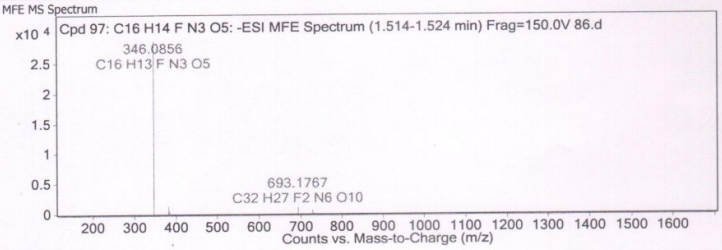


Compound Table

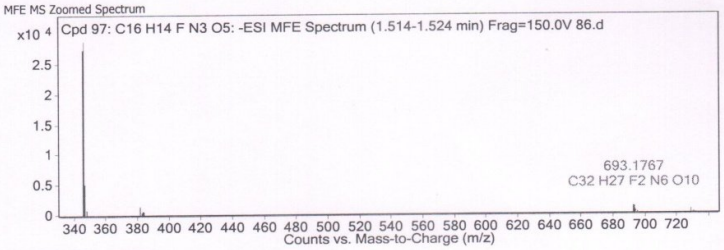
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 97: C16 H14 F N3 O5	1.519	347.0928	C16 H14 F N3 O5	C16 H14 F N3 O5	-3.14	C16 H14 F N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 97: C16 H14 F N3 O5	346.0856	1.519	Infusion Molecular Feature Extractor	347.0928

MFE MS Spectrum



MFE MS Zoomed Spectrum

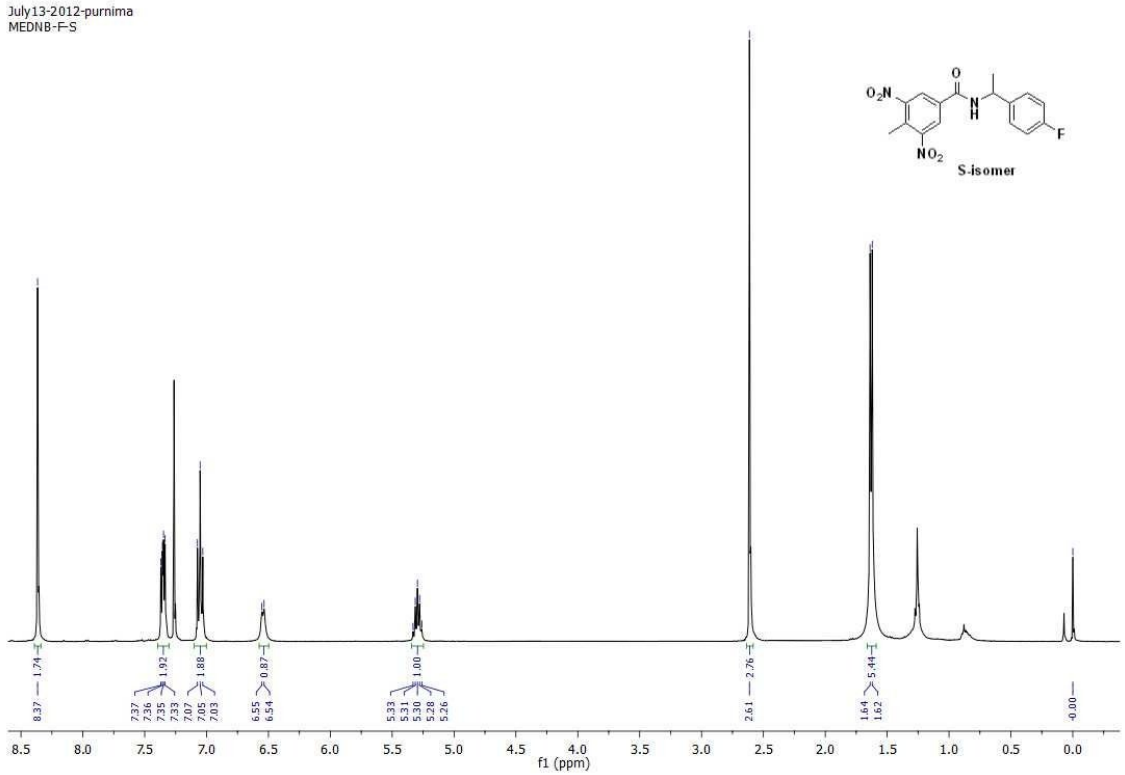


MS Spectrum Peak List

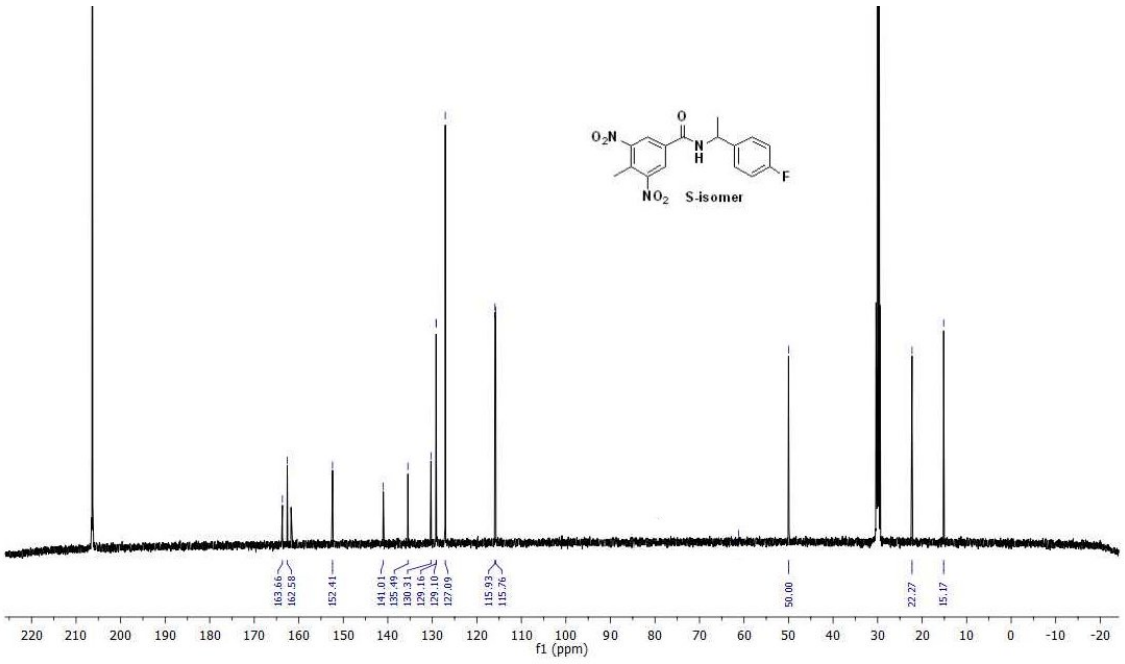
m/z	z	Abund	Formula	Ion
346.0856	-1	28685.4	C16 H13 F N3 O5	(M-H)-
347.0896	-1	3728.3	C16 H13 F N3 O5	(M-H)-
348.0918	-1	543.9	C16 H13 F N3 O5	(M-H)-
382.0627	-1	1382.9	C16 H14 Cl F N3 O5	(M+Cl)-
383.0613	-1	281.4	C16 H14 Cl F N3 O5	(M+Cl)-
384.0606	-1	450.9	C16 H14 Cl F N3 O5	(M+Cl)-
693.1767	-1	1096.1	C32 H27 F2 N6 O10	(2M-H)-
694.1802	-1	401.9	C32 H27 F2 N6 O10	(2M-H)-
729.1543	-1	520.2		(2M+Cl)-
730.1586	-1	200.8		(2M+Cl)-

--- End Of Report ---

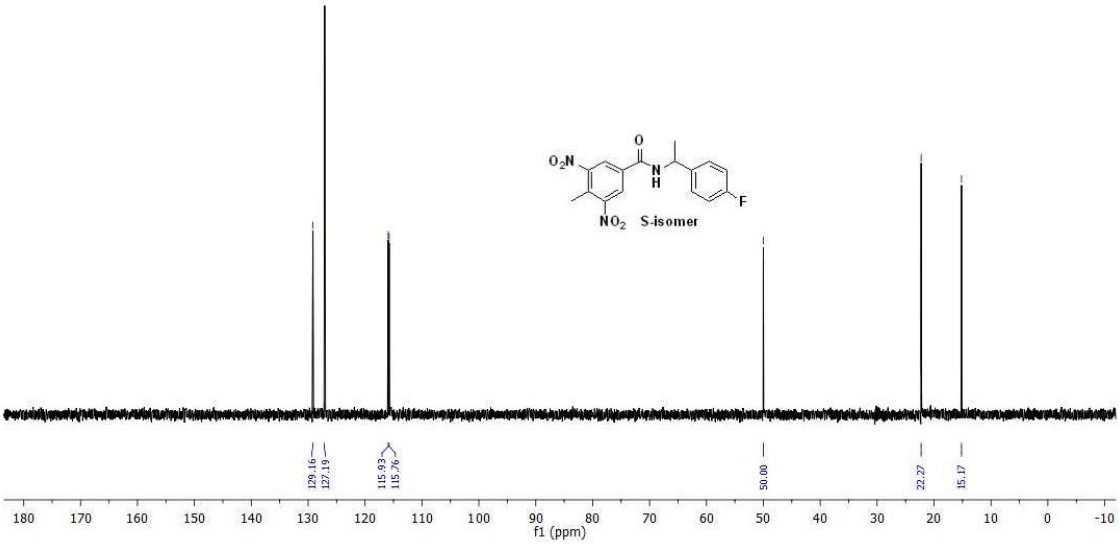
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7d:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7d:**



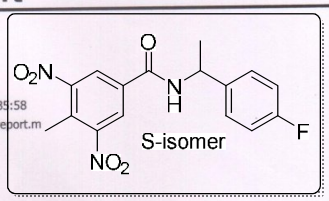
DEPT (126 MHz, Acetone-d_6) of compound **7d:**



HRMS (ESI-TOF) of compound **7d**:

Qualitative Compound Report

Data File	87.d	**Sample Name**	87
Sample Type	Sample	**Position**	Vial 41
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	28-07-2012 PM 03:35:58
IRM Calibration Status	Some Ions Missed	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

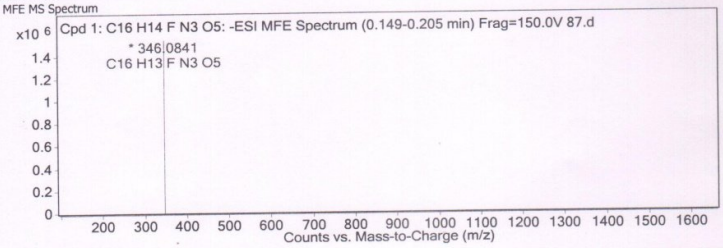


Compound Table

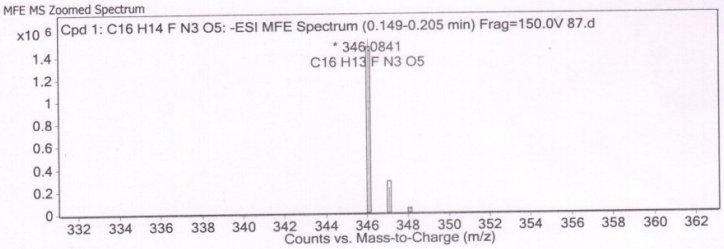
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C16 H14 F N3 O5	0.194	347.0913	C16 H14 F N3 O5	C16 H14 F N3 O5	1.17	C16 H14 F N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C16 H14 F N3 O5	346.0841	0.194	Find by Molecular Feature	347.0913

MFE MS Spectrum



MFE MS Zoomed Spectrum

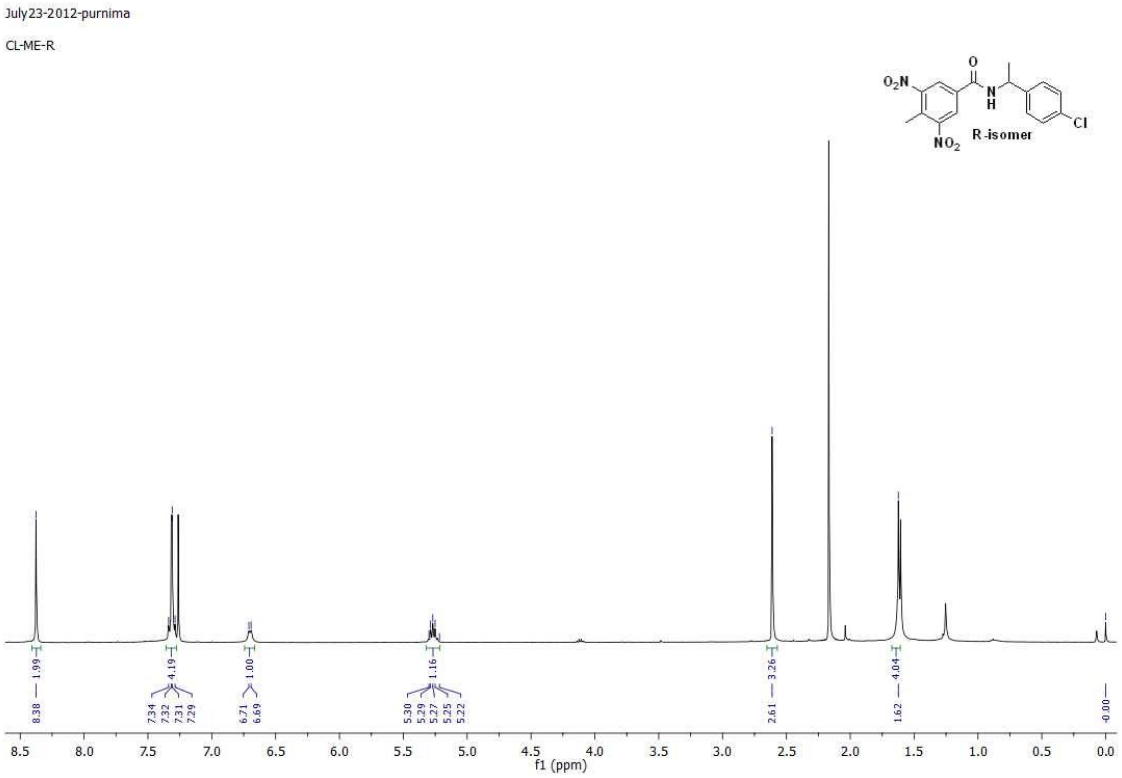


MS Spectrum Peak List

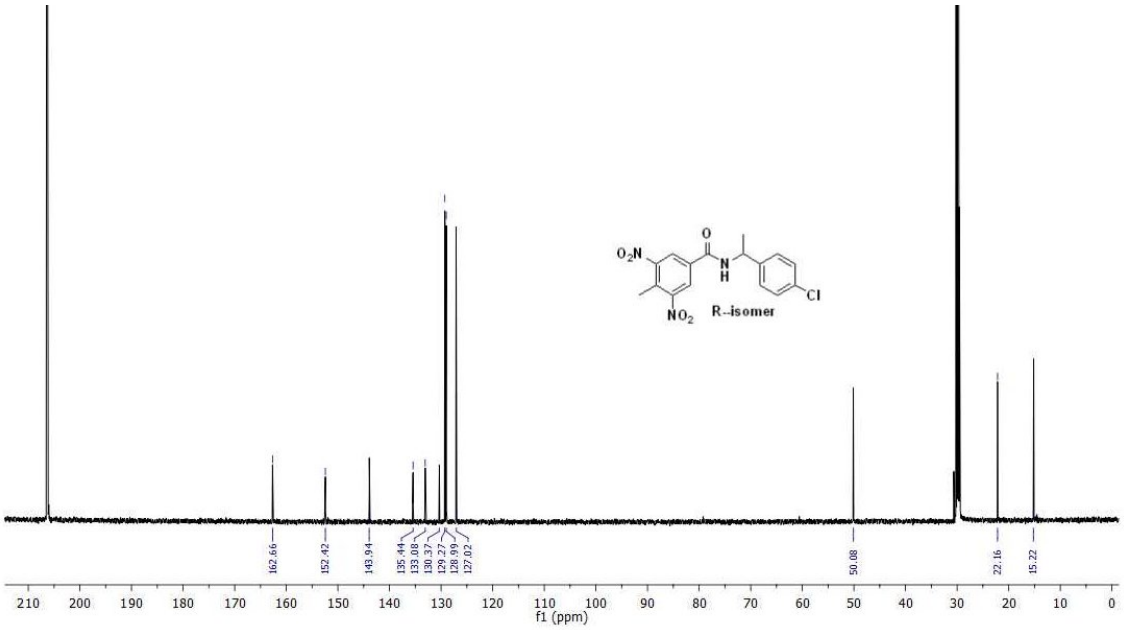
m/z	z	Abund	Formula	Ion
346.0841	-1	153927.0	C16 H13 F N3 O5	(M-H)-
347.0884	-1	222018.8	C16 H13 F N3 O5	(M-H)-
348.0905	-1	32530.2	C16 H13 F N3 O5	(M-H)-

--- End Of Report ---

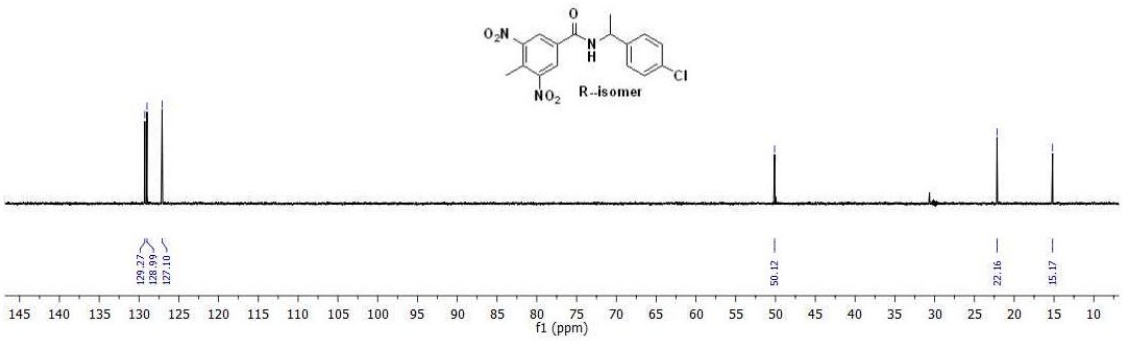
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7e:**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7e:**



DEPT (101 MHz, Acetone-d_6) of compound **7e:**

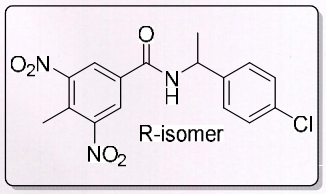


HRMS (ESI-TOF) of compound **7e**:

Qualitative Compound Report

Data File	106.d	**Sample Name**	107
Sample Type	Sample	**Position**	Vial 34
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 6:05:43
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

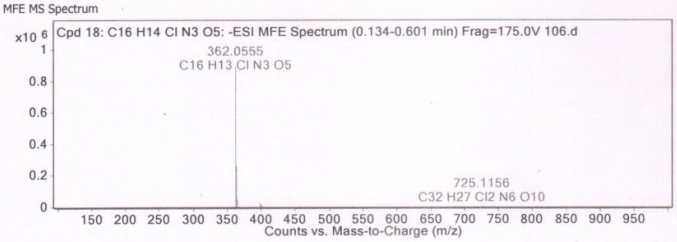


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C16 H14 Cl N3 O5	0.187	363.0627	C16 H14 Cl N3 O5	C16 H14 Cl N3 O5	-1.25	C16 H14 Cl N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C16 H14 Cl N3 O5	362.0555	0.187	Find by Molecular Feature	363.0627

MFE MS Spectrum



MS Spectrum Peak List

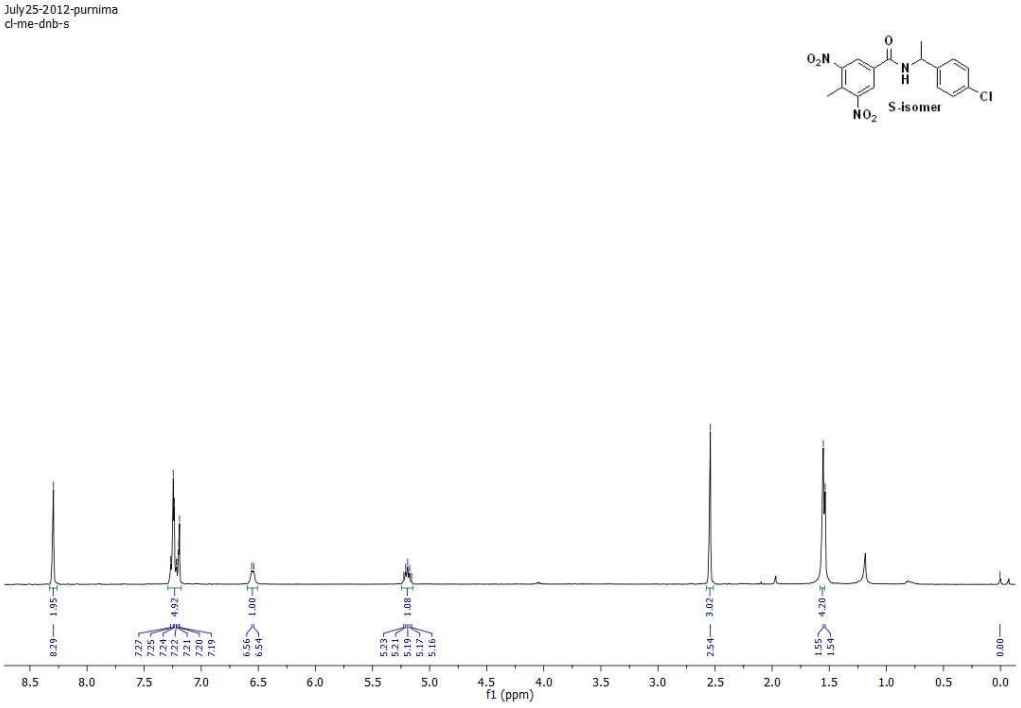
m/z	z	Abund	Formula	Ion
362.0555	-1	888825.13	C16 H13 Cl N3 O5	(M-H)-
363.0584	-1	146993.73	C16 H13 Cl N3 O5	(M-H)-
364.0529	-1	260138.05	C16 H13 Cl N3 O5	(M-H)-
365.0556	-1	45648.43	C16 H13 Cl N3 O5	(M-H)-
366.0582	-1	6131.97	C16 H13 Cl N3 O5	(M-H)-
398.0315	-1	24369.5	C16 H14 Cl2 N3 O5	(M+Cl)-
399.0341	-1	4515.21	C16 H14 Cl2 N3 O5	(M+Cl)-
400.029	-1	17215.26	C16 H14 Cl2 N3 O5	(M+Cl)-
725.1156	-1	6860.29	C32 H27 Cl2 N6 O10	(2M-H)-
727.1155	-1	5726.6	C32 H27 Cl2 N6 O10	(2M-H)-

Predicted Isotope Match Table

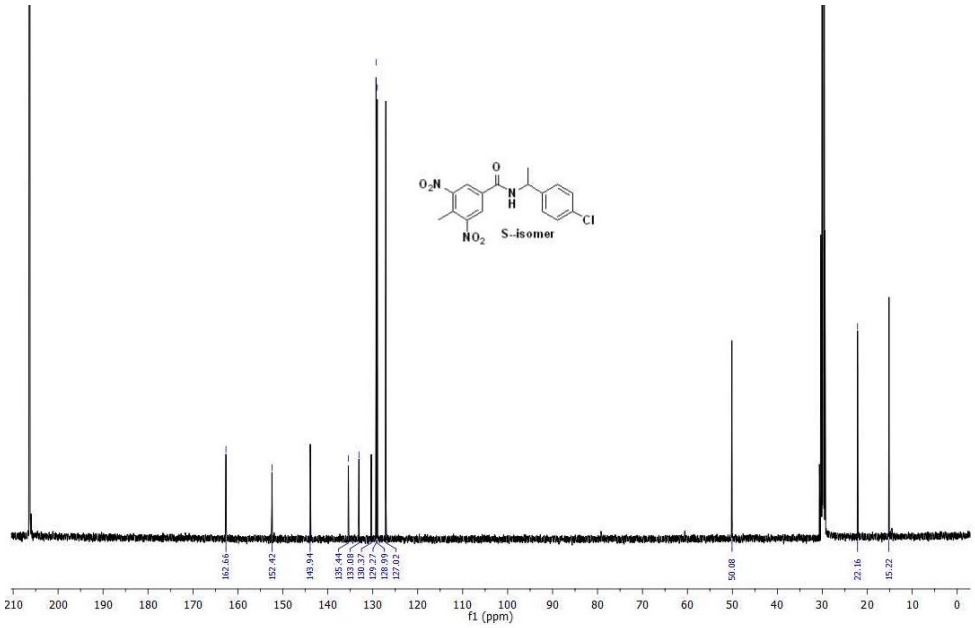
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	362.0555	362.0549	-1.46	100	100	65.92	62.23
2	363.0584	363.0579	-1.13	16.54	18.74	10.9	11.66
3	364.0529	364.0526	-0.67	29.27	34.68	19.29	21.59
4	365.0556	365.0553	-0.71	5.14	6.28	3.39	3.91
5	366.0582	366.0575	-1.76	0.69	0.88	0.45	0.55
6	367.0594	367.0599	1.41	0.08	0.09	0.05	0.06

--- End Of Report ---

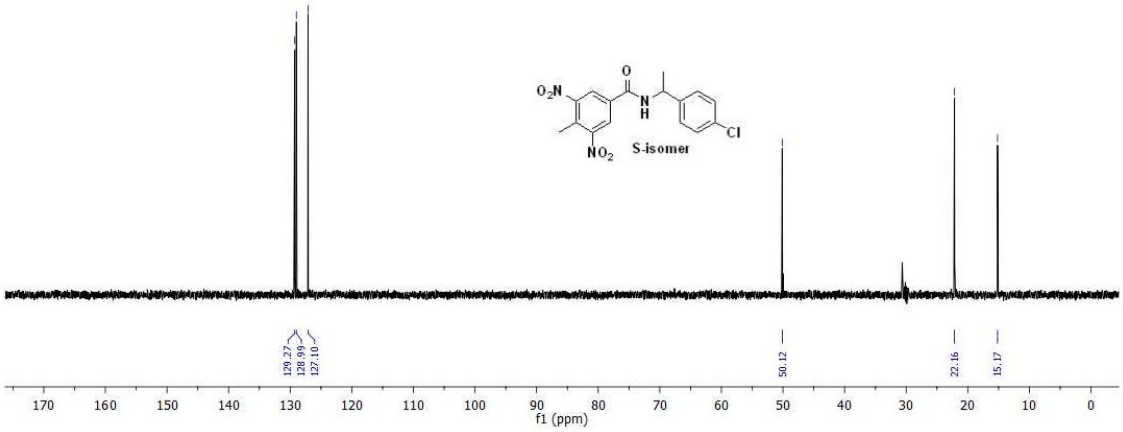
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7f:**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7f:**



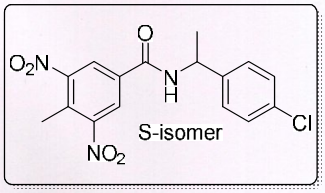
DEPT (101 MHz, Acetone-d_6) of compound **7f:**



HRMS (ESI-TOF) of compound **7f**:

Qualitative Compound Report

Data File	107.d	**Sample Name**	107
Sample Type	Sample	**Position**	Vial 34
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 6:05:43
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

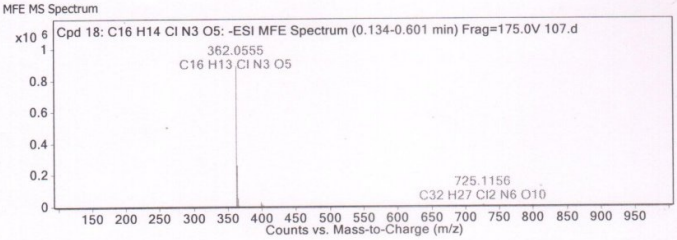


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C16 H14 Cl N3 O5	0.187	363.0627	C16 H14 Cl N3 O5	C16 H14 Cl N3 O5	-1.25	C16 H14 Cl N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C16 H14 Cl N3 O5	362.0555	0.187	Find by Molecular Feature	363.0627

MFE MS Spectrum



MS Spectrum Peak List

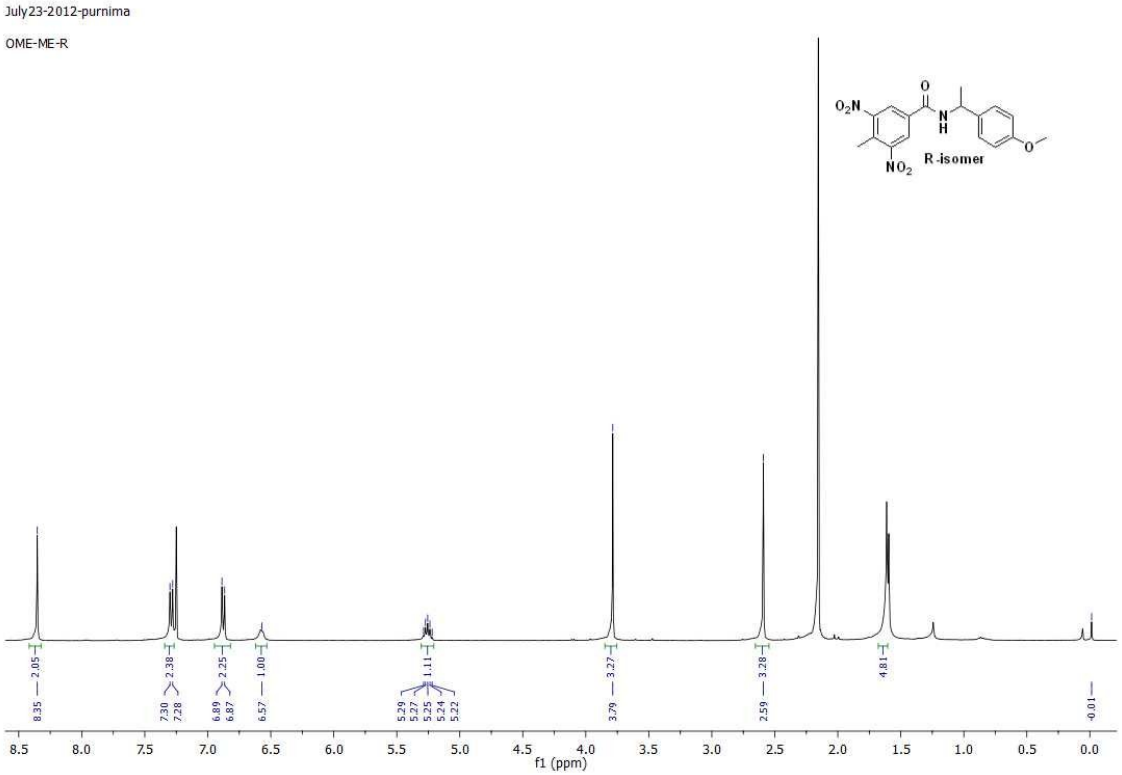
m/z	z	Abund	Formula	Ion
362.0555	-1	888825.13	C16 H13 Cl N3 O5	(M-H)-
363.0584	-1	146993.73	C16 H13 Cl N3 O5	(M-H)-
364.0529	-1	260138.05	C16 H13 Cl N3 O5	(M-H)-
365.0556	-1	45648.43	C16 H13 Cl N3 O5	(M-H)-
366.0582	-1	6131.97	C16 H13 Cl N3 O5	(M-H)-
398.0315	-1	24369.5	C16 H14 Cl2 N3 O5	(M+Cl)-
399.0341	-1	4515.21	C16 H14 Cl2 N3 O5	(M+Cl)-
400.029	-1	17215.26	C16 H14 Cl2 N3 O5	(M+Cl)-
725.1156	-1	6860.29	C32 H27 Cl2 N6 O10	(2M-H)-
727.1155	-1	5726.6	C32 H27 Cl2 N6 O10	(2M-H)-

Predicted Isotope Match Table

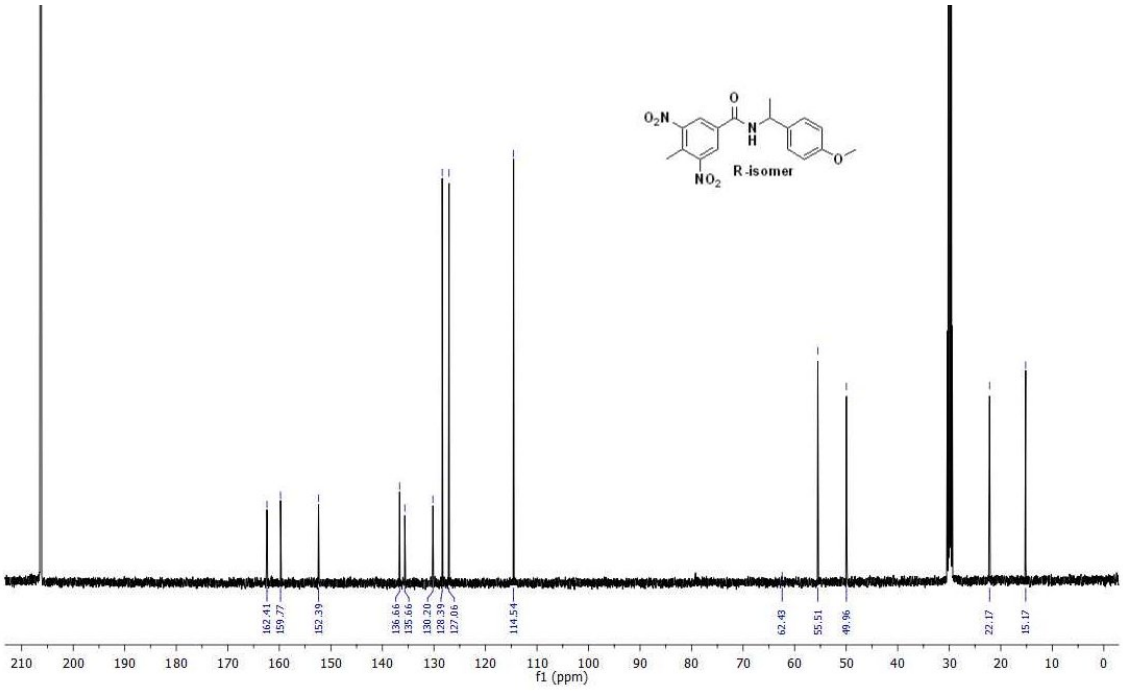
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	362.0555	362.0549	-1.46	100	100	65.92	62.23
2	363.0584	363.0579	-1.13	16.54	18.74	10.9	11.66
3	364.0529	364.0526	-0.67	29.27	34.68	19.29	21.59
4	365.0556	365.0553	-0.71	5.14	6.28	3.39	3.91
5	366.0582	366.0575	-1.76	0.69	0.88	0.45	0.55
6	367.0594	367.0599	1.41	0.08	0.09	0.05	0.06

--- End Of Report ---

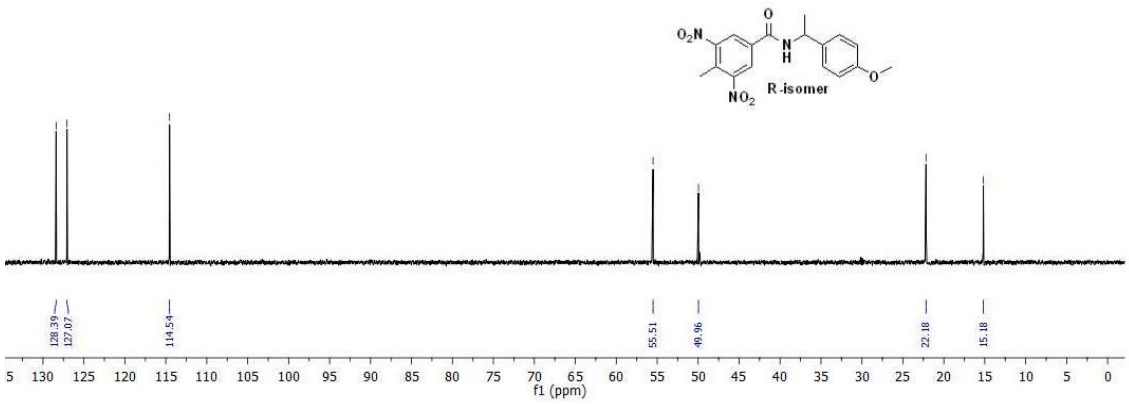
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7g:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7g:**



DEPT (126 MHz, Acetone-d_6) of compound **7g:**



HRMS (ESI-TOF) of compound **7g**:

Qualitative Compound Report

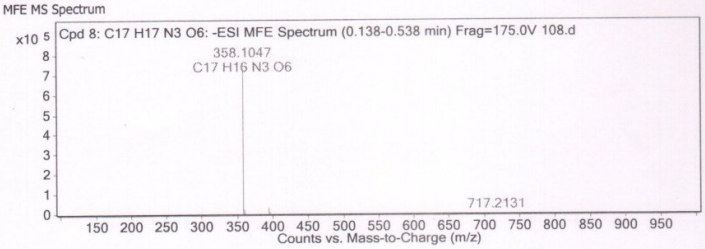
Data File	108.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment	Sample information is unavailable		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C17 H17 N3 O6	0.187	359.112	C17 H17 N3 O6	C17 H17 N3 O6	-0.68	C17 H17 N3 O6

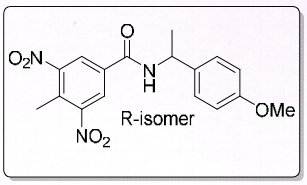
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C17 H17 N3 O6	358.1047	0.187	Find by Molecular Feature	359.112

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
358.1047	-1	730385	C17 H16 N3 O6	(M-H)-
359.1077	-1	130747.51	C17 H16 N3 O6	(M-H)-
360.11	-1	20668.91	C17 H16 N3 O6	(M-H)-
361.113	-1	2918.45	C17 H16 N3 O6	(M-H)-
394.0813	-1	29872.61	C17 H17 Cl N3 O6	(M+Cl)-
395.0845	-1	6219.38	C17 H17 Cl N3 O6	(M+Cl)-
396.0786	-1	8793.79	C17 H17 Cl N3 O6	(M+Cl)-
397.0814	-1	2150.94	C17 H17 Cl N3 O6	(M+Cl)-
717.2131	-1	853.04		(2M-H)-
718.2115	-1	458.15		(2M-H)-

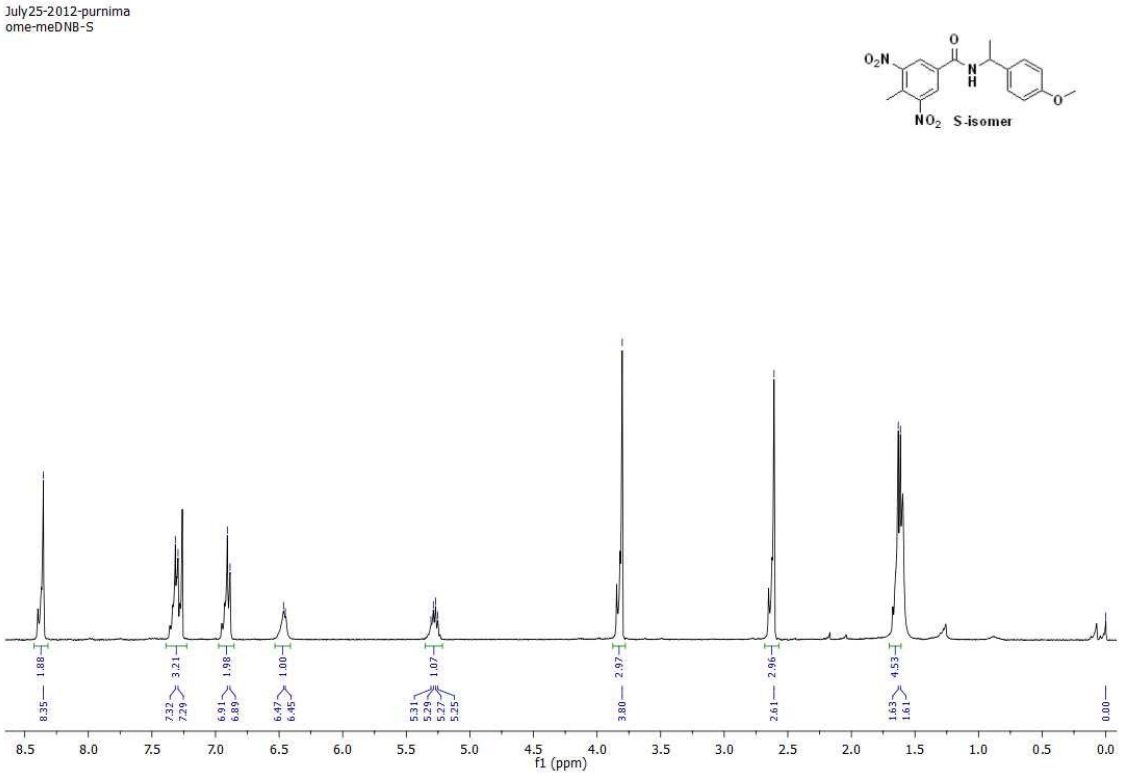


Predicted Isotope Match Table

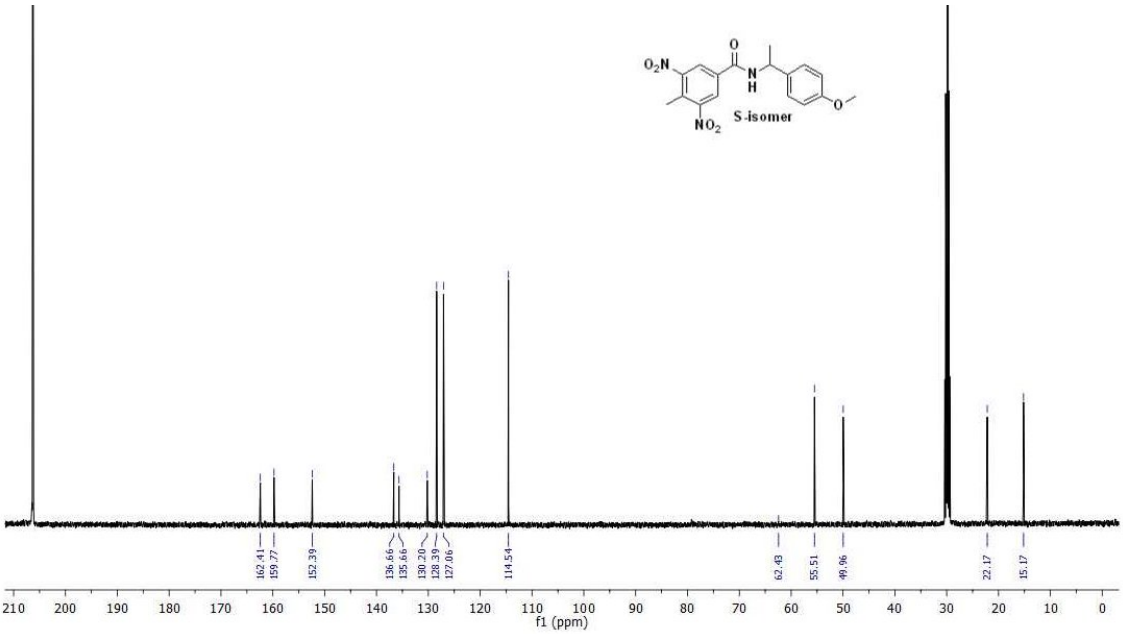
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	358.1047	358.1045	-0.7	100	100	82.56	81.06
2	359.1077	359.1075	-0.58	17.9	19.9	14.78	16.13
3	360.11	360.1098	-0.5	2.83	3.11	2.34	2.52
4	361.113	361.1123	-2.01	0.4	0.36	0.33	0.29

--- End Of Report ---

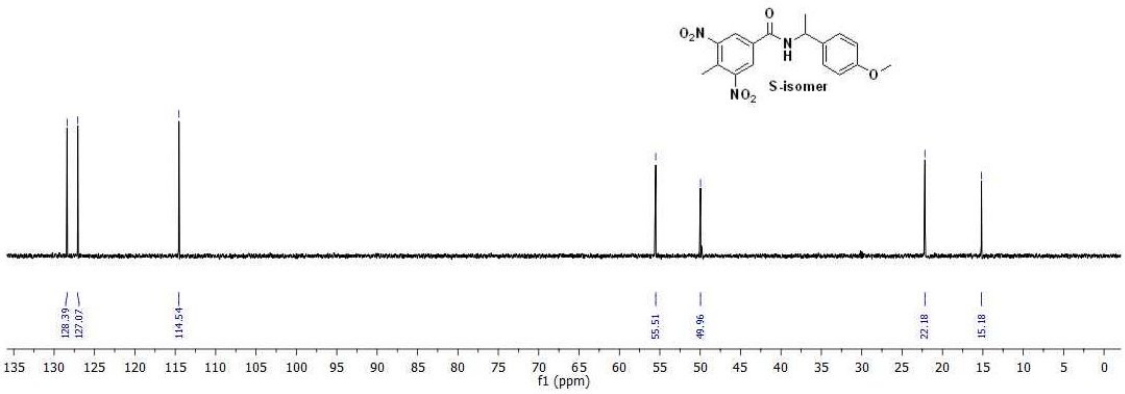
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7h:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7h:**



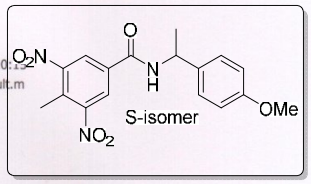
DEPT (126 MHz, Acetone-d_6) of compound **7h:**



HRMS (ESI-TOF) of compound **7h**:

Qualitative Compound Report

Data File	109.d	**Sample Name**	108
Sample Type	Sample	**Position**	Vial 35
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 6:10:12
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



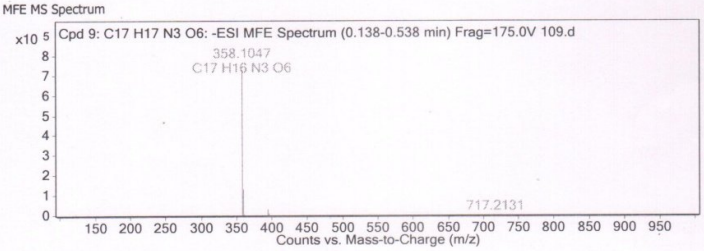
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C17 H17 N3 O6	0.187	359.112	C17 H17 N3 O6	C17 H17 N3 O6	-0.68	C17 H17 N3 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C17 H17 N3 O6	358.1047	0.187	Find by Molecular Feature	359.112

MFE MS Spectrum



MS Spectrum Peak List

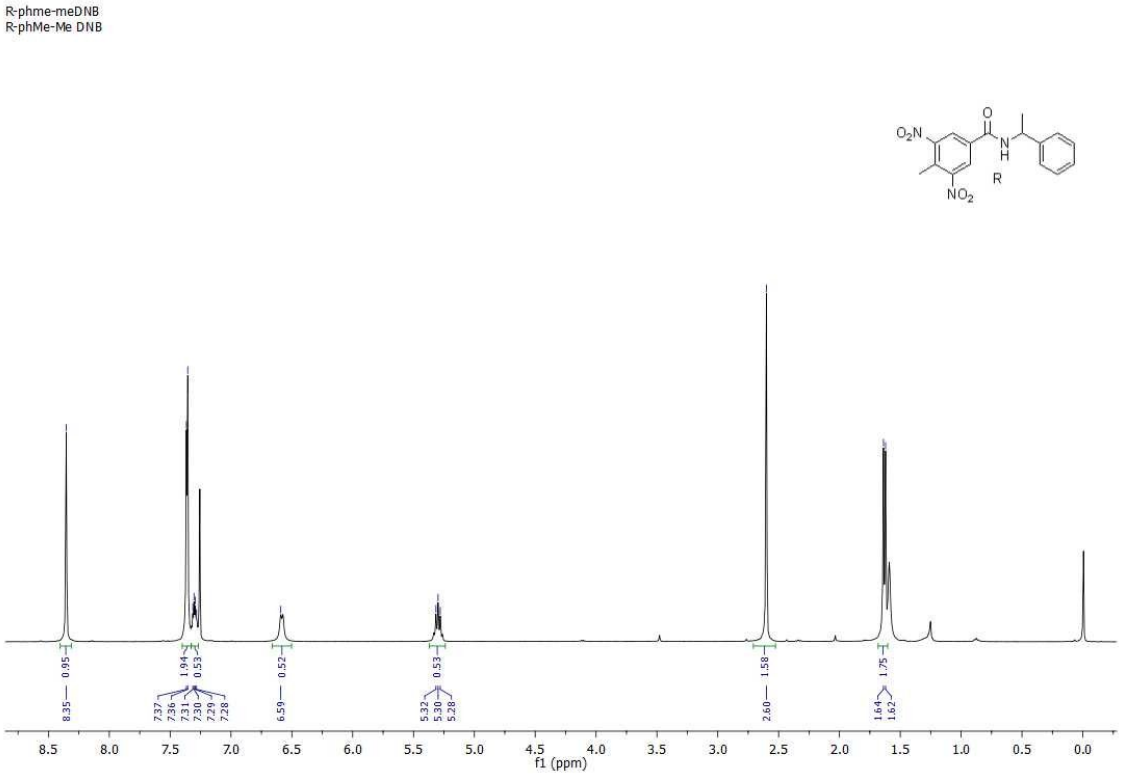
m/z	z	Abund	Formula	Ion
358.1047	-1	730537.94	C17 H16 N3 O6	(M-H)-
359.1077	-1	130747.51	C17 H16 N3 O6	(M-H)-
360.11	-1	20668.91	C17 H16 N3 O6	(M-H)-
361.113	-1	2918.45	C17 H16 N3 O6	(M-H)-
394.0813	-1	29872.61	C17 H17 Cl N3 O6	(M+Cl)-
395.0845	-1	6219.38	C17 H17 Cl N3 O6	(M+Cl)-
396.0786	-1	8793.79	C17 H17 Cl N3 O6	(M+Cl)-
397.0814	-1	2150.94	C17 H17 Cl N3 O6	(M+Cl)-
717.2131	-1	853.04		(2M-H)-
718.2115	-1	458.15		(2M-H)-

Predicted Isotope Match Table

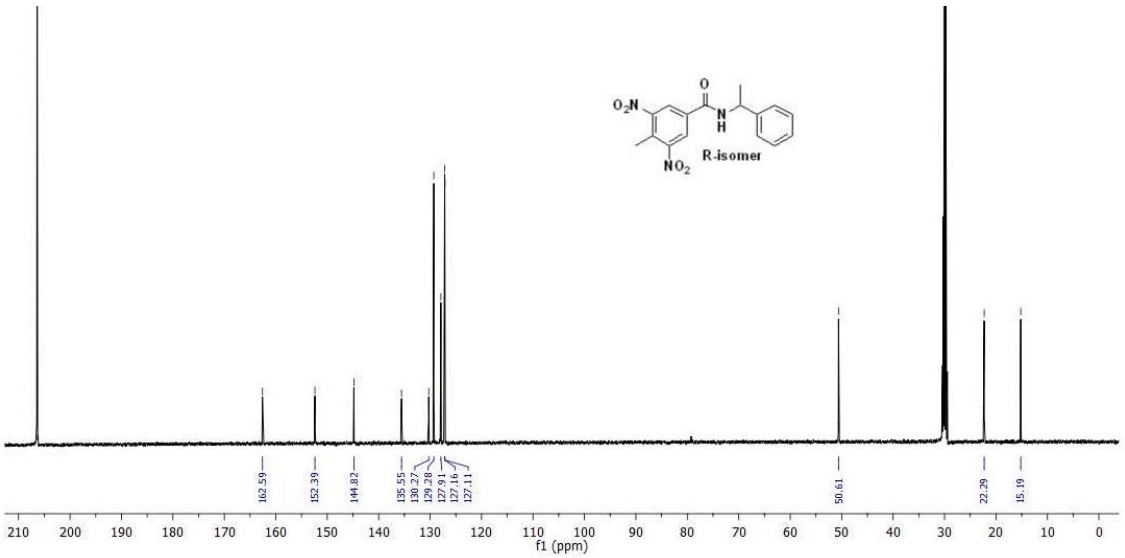
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	358.1047	358.1045	-0.7	100	100	82.56	81.06
2	359.1077	359.1075	-0.58	17.9	19.9	14.78	16.13
3	360.11	360.1098	-0.5	2.83	3.11	2.34	2.52
4	361.113	361.1123	-2.01	0.4	0.36	0.33	0.29

--- End Of Report ---

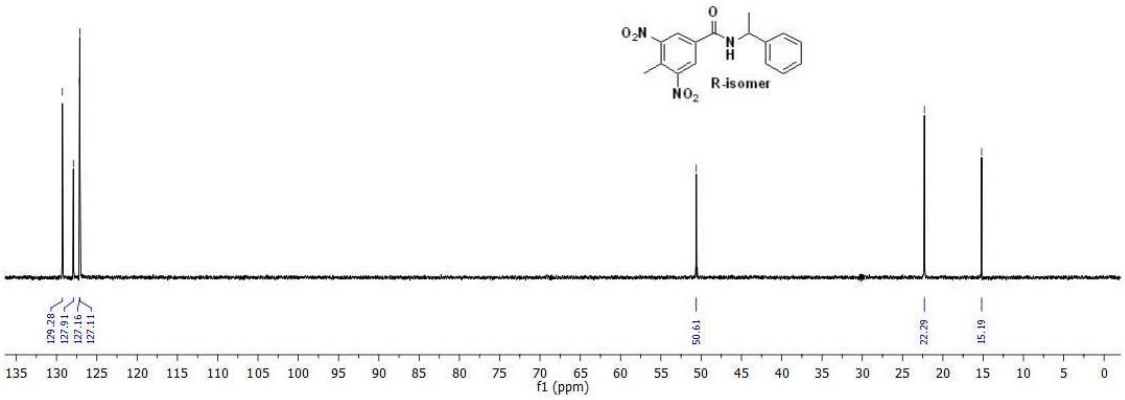
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7i:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7i:**



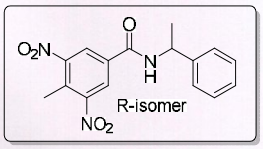
DEPT (126 MHz, Acetone-d_6) of compound **7i:**



HRMS (ESI-TOF) of compound **7i**:

Qualitative Compound Report

Data File	99.d	**Sample Name**	99
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 5:28:04
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



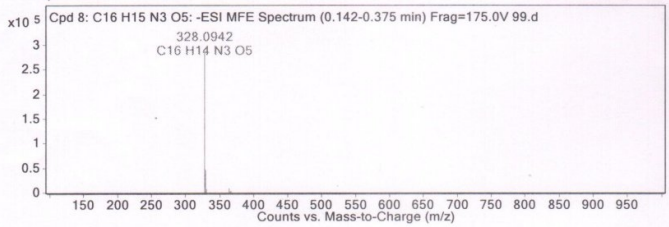
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C16 H15 N3 O5	0.19	329.1014	C16 H15 N3 O5	C16 H15 N3 O5	-0.8	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C16 H15 N3 O5	328.0942	0.19	Find by Molecular Feature	329.1014

MFE MS Spectrum



MS Spectrum Peak List

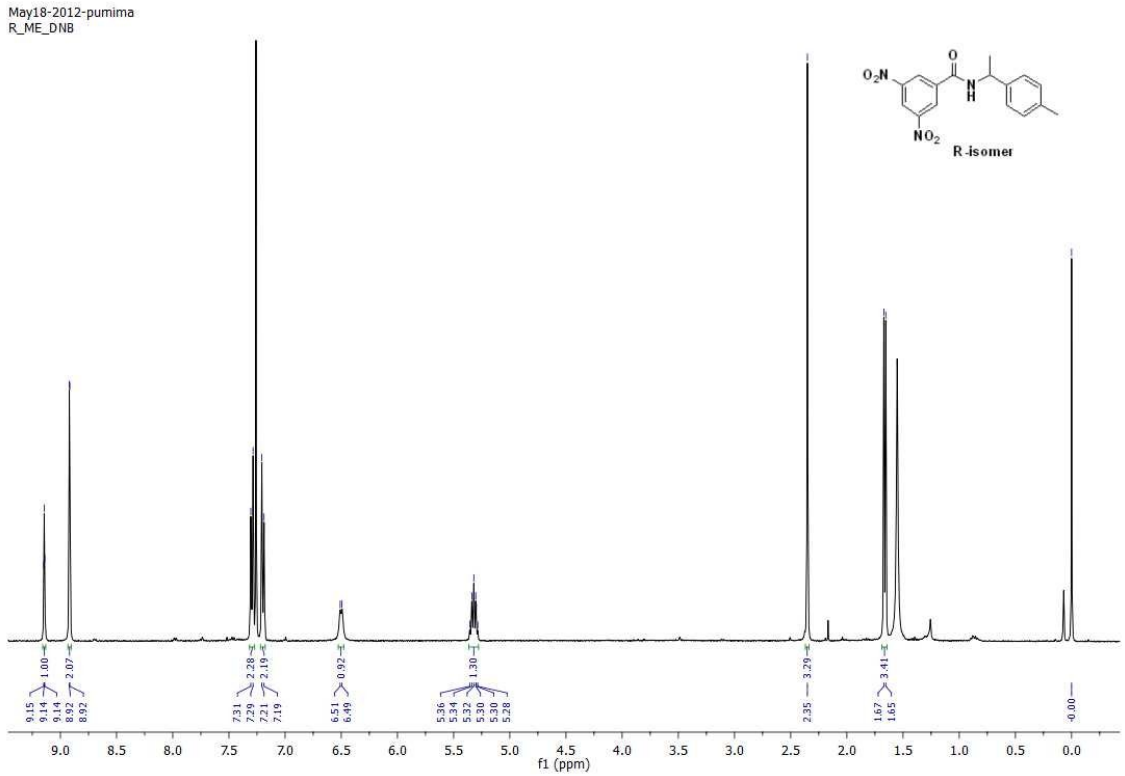
m/z	z	Abund	Formula	Ion
328.0942	-1	284907.25	C16 H14 N3 O5	(M-H)-
329.0971	-1	45430.21	C16 H14 N3 O5	(M-H)-
330.099	-1	7460.65	C16 H14 N3 O5	(M-H)-
331.1013	-1	1087.23	C16 H14 N3 O5	(M-H)-
364.0706	-1	7781.35	C16 H15 Cl N3 O5	(M+Cl)-
365.0733	-1	1039.23	C16 H15 Cl N3 O5	(M+Cl)-
366.0663	-1	2634.72	C16 H15 Cl N3 O5	(M+Cl)-
367.0704	-1	664.86	C16 H15 Cl N3 O5	(M+Cl)-
368.0825	-1	482.18	C16 H15 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

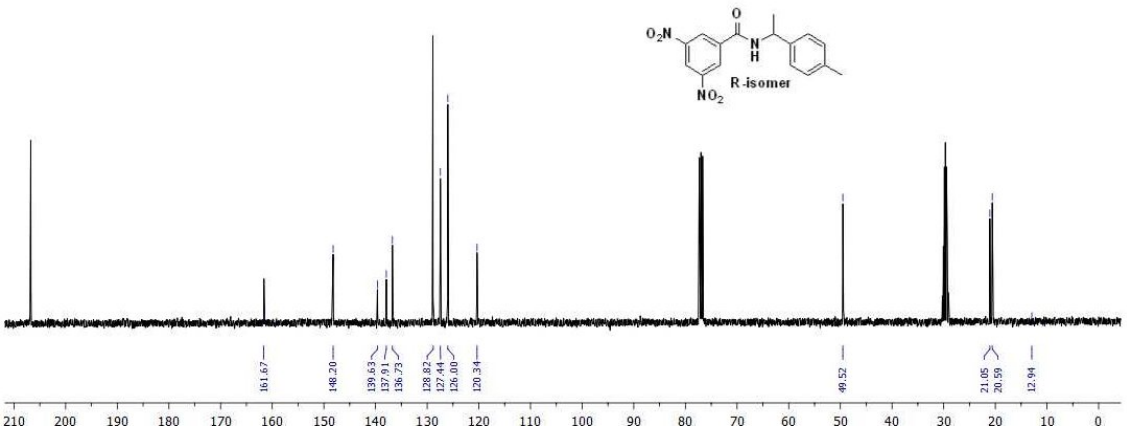
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.0942	328.0939	-0.88	100	100	84.07	82.15
2	329.0971	329.0969	-0.56	15.95	18.75	13.41	15.41
3	330.099	330.0992	0.57	2.62	2.69	2.2	2.21
4	331.1013	331.1017	1.27	0.38	0.28	0.32	0.23

--- End Of Report ---

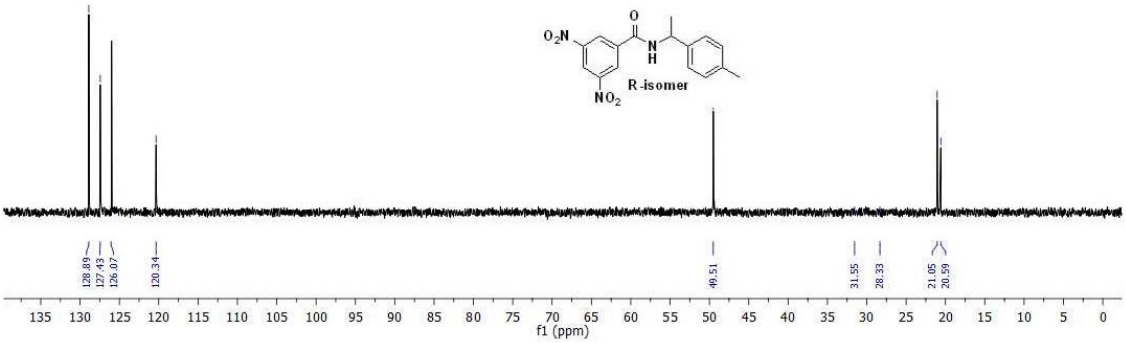
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7j**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7j:**



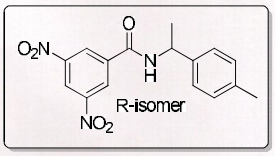
DEPT (101 MHz, Acetone-d_6) of compound **7j:**



HRMS (ESI-TOF) of compound **7j**:

Qualitative Compound Report

Data File	53.d	**Sample Name**	53
Sample Type	Sample	**Position**	Vial 29
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	01-04-2013 PM 5:32:21
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



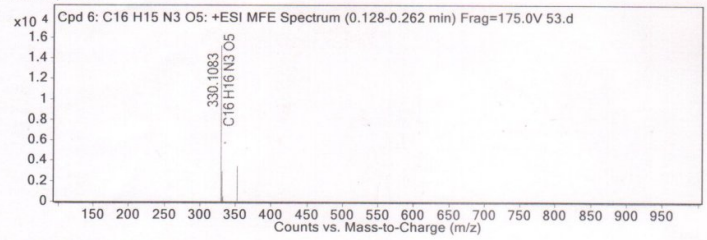
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C16 H15 N3 O5	0.186	329.1012	C16 H15 N3 O5	C16 H15 N3 O5	-0.1	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C16 H15 N3 O5	330.1083	0.186	Find by Molecular Feature	329.1012

MFE MS Spectrum



MS Spectrum Peak List

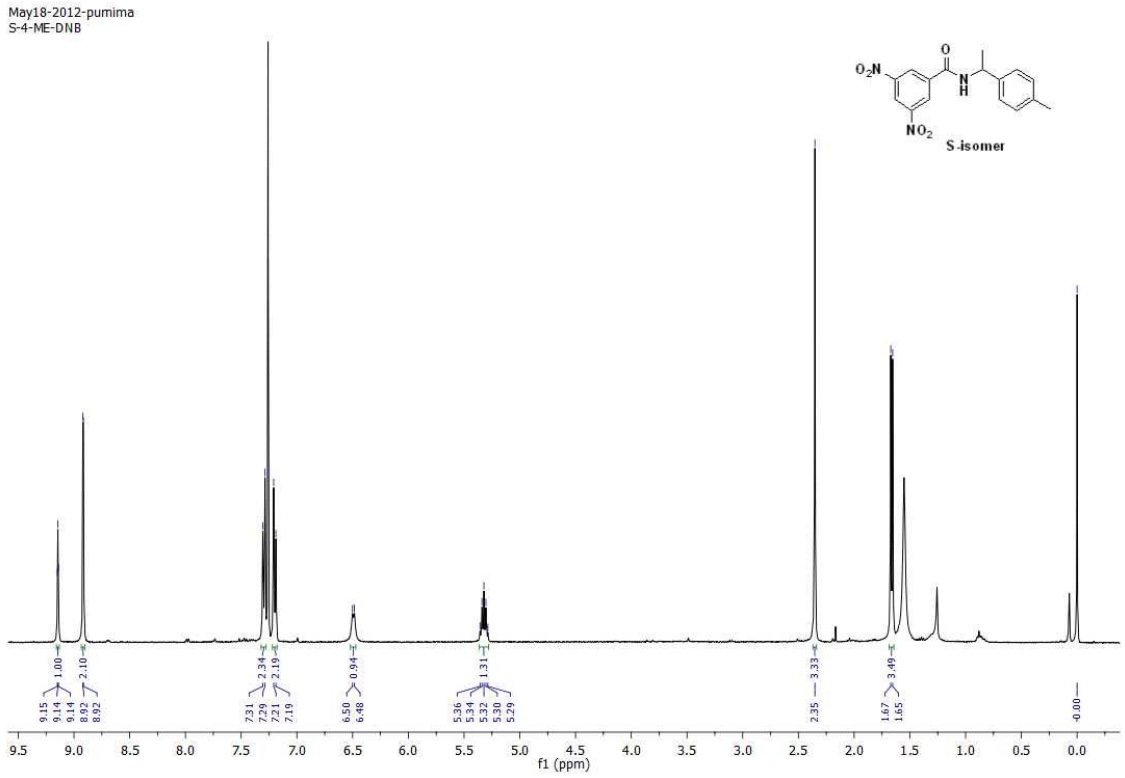
m/z	z	Abund	Formula	Ion
330.1083	1	15250.71	C16 H16 N3 O5	(M+H)+
331.1123	1	2926.61	C16 H16 N3 O5	(M+H)+
332.1133	1	511.6	C16 H16 N3 O5	(M+H)+
352.0899	1	3440.11	C16 H15 N3 Na O5	(M+Na)+
353.0946	1	582.13	C16 H15 N3 Na O5	(M+Na)+

Predicted Isotope Match Table

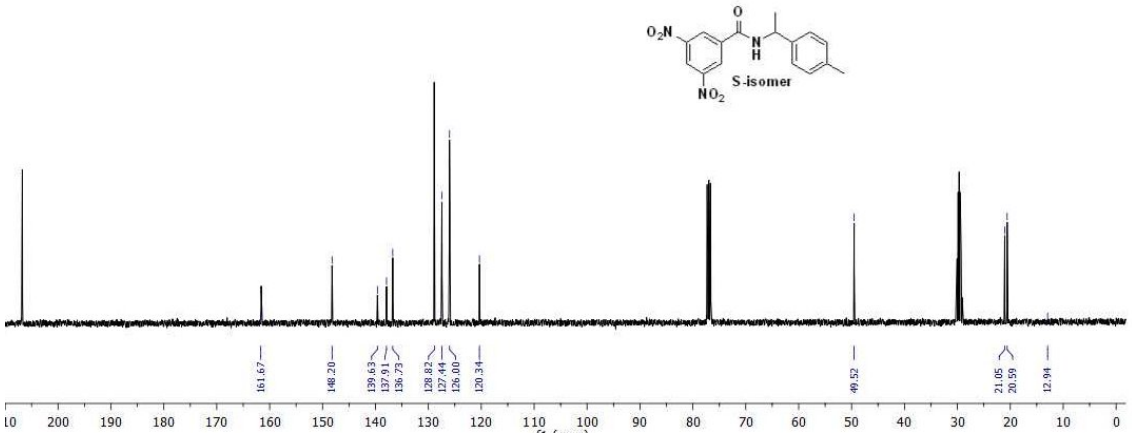
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	330.1083	330.1084	0.33	100	100	81.6	82.32
2	331.1123	331.1115	-2.56	19.19	18.78	15.66	15.46
3	332.1133	332.1138	1.39	3.35	2.69	2.74	2.22

--- End Of Report ---

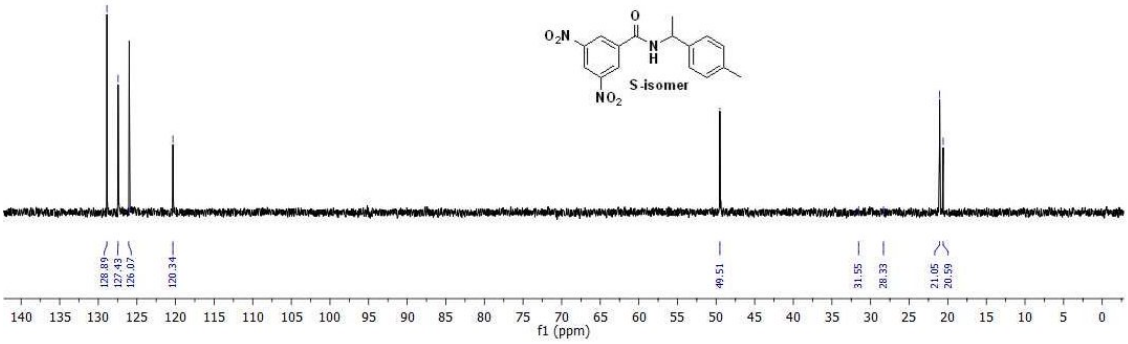
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7k**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7j:**



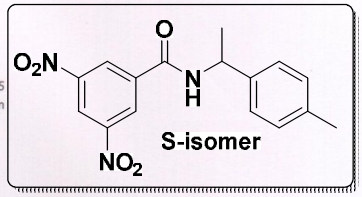
DEPT (101 MHz, Acetone-d_6) of compound **7j:**



HRMS (ESI-TOF) of compound **7k**:

Qualitative Compound Report

Data File	54.d	**Sample Name**	54
Sample Type	Sample	**Position**	Vial 19
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	04-03-2013 PM 3:32:15
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



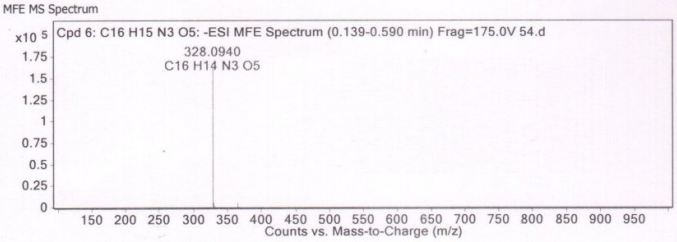
Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C16 H15 N3 O5	0.193	329.1012	C16 H15 N3 O5	C16 H15 N3 O5	-0.05	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C16 H15 N3 O5	328.094	0.193	Find by Molecular Feature	329.1012

MFE MS Spectrum



MS Spectrum Peak List

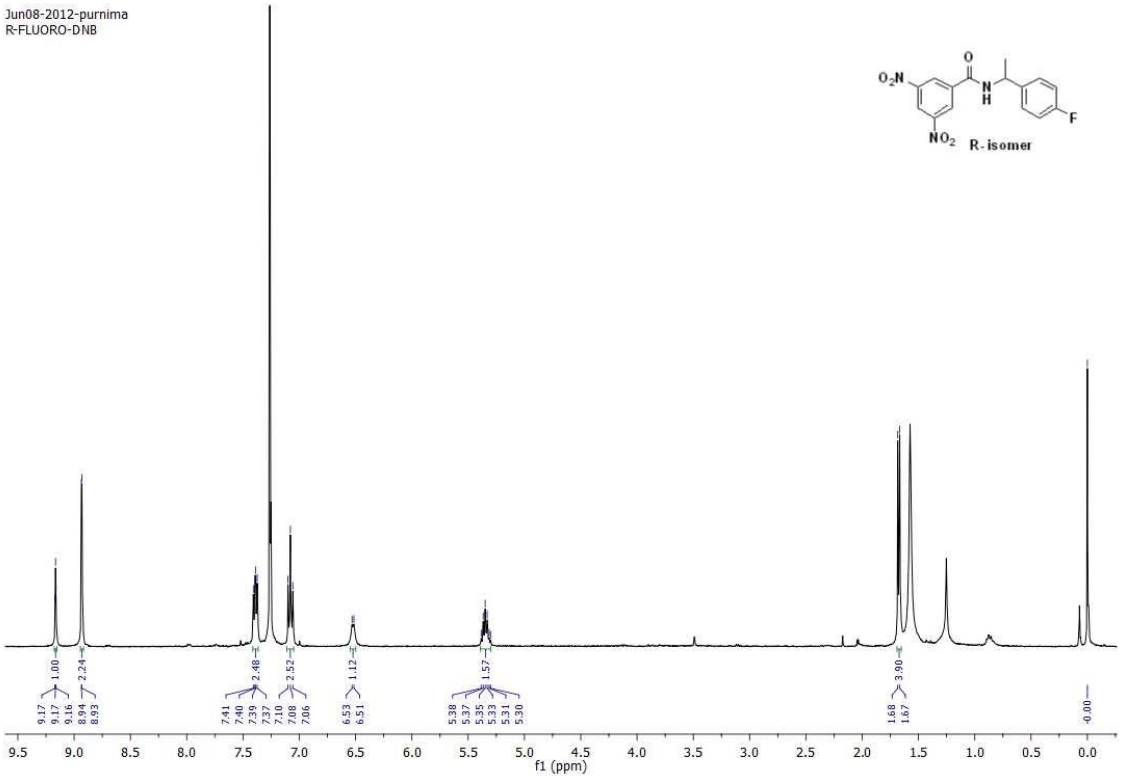
m/z	z	Abund	Formula	Ion
328.094	-1	162962.91	C16 H14 N3 O5	(M-H)-
329.0966	-1	28099.19	C16 H14 N3 O5	(M-H)-
330.0995	-1	4518.06	C16 H14 N3 O5	(M-H)-
331.1023	-1	853.26	C16 H14 N3 O5	(M-H)-
364.0692	-1	4930.71	C16 H15 Cl N3 O5	(M+Cl)-
365.0734	-1	1115.29	C16 H15 Cl N3 O5	(M+Cl)-
366.0665	-1	1143.32	C16 H15 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

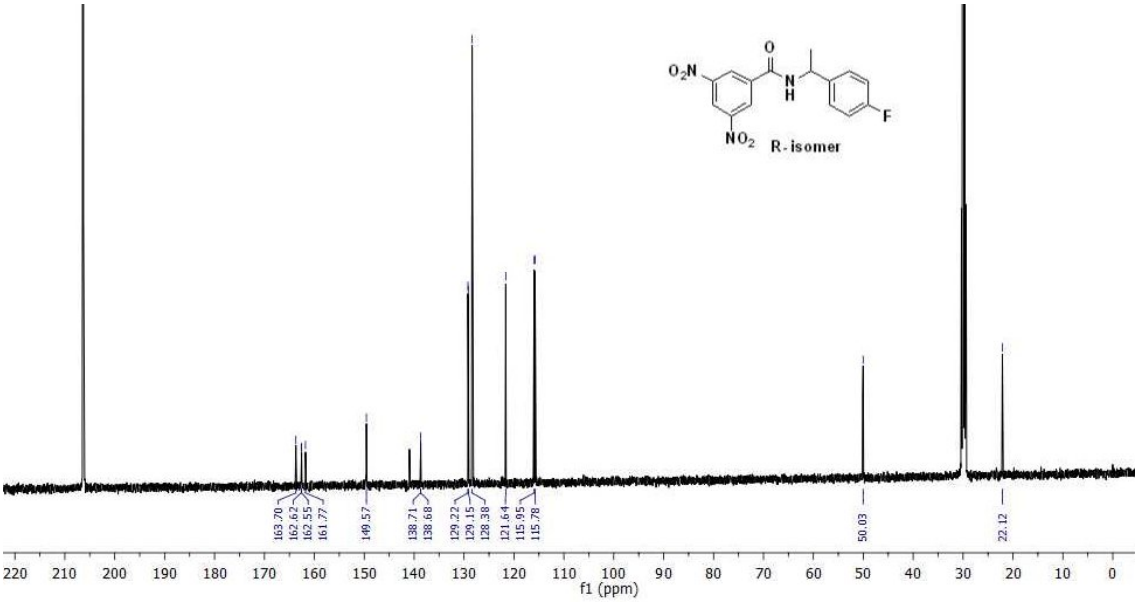
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.094	328.0939	-0.17	100	100	82.96	82.15
2	329.0966	329.0969	0.83	17.24	18.75	14.3	15.41
3	330.0995	330.0992	-0.83	2.77	2.69	2.3	2.21
4	331.1023	331.1017	-1.85	0.52	0.28	0.43	0.23

--- End Of Report ---

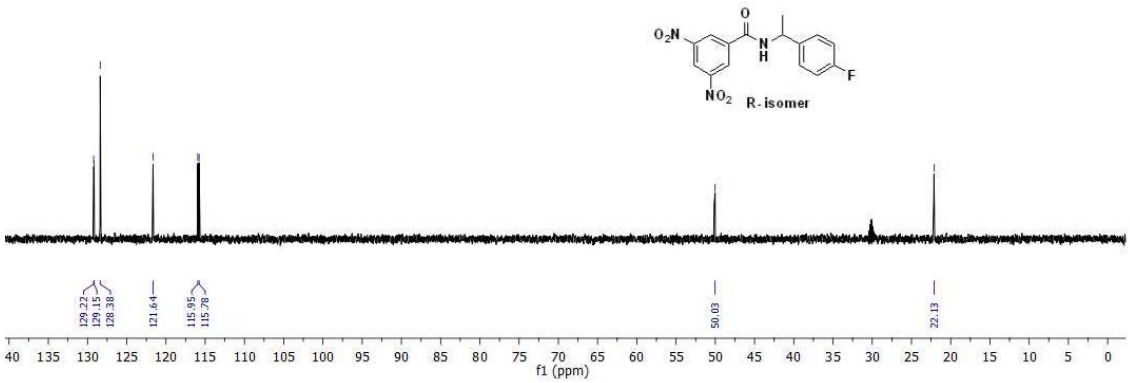
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7l:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7l:**



DEPT (126 MHz, Acetone-d_6) of compound **7l:**



HRMS (ESI-TOF) of compound **7l**:

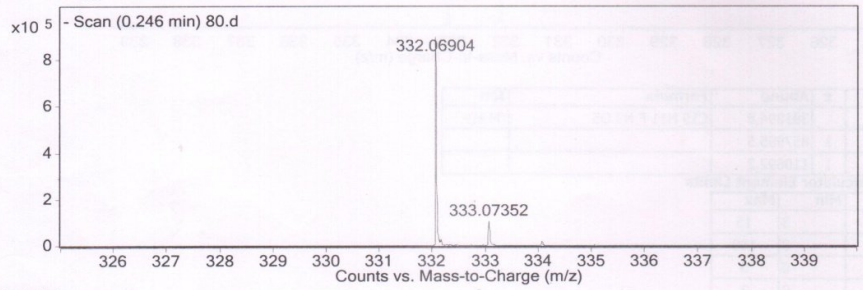
Qualitative Analysis Report

Data Filename	80.d	**Sample Name**	80
Sample Type	Sample	**Position**	Vial 10
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	7/30/2012 10:01:01 AM
IRM Calibration Status	Some Ions Missed	**DA Method**	2.m
Comment			

Sample Group **Info.**

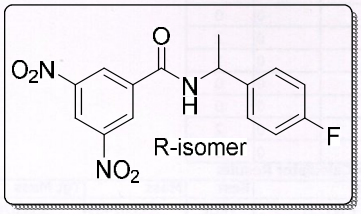
User Spectra

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund	Formula	Ion
332.06904	1	926404.9	C15 H11 F N3 O5	(M-H)-
333.07352	1	112971.7	C15 H11 F N3 O5	(M-H)-
446.06253	1	1538389.1		
447.06689	1	183653.6		



Formula Calculator Element Limits

Element	Min	Max
C	3	15
H	0	100
O	0	5
N	0	3
S	0	0
Cl	0	2
F	0	1
Na	0	0
P	0	0
Br	0	2
I	0	0

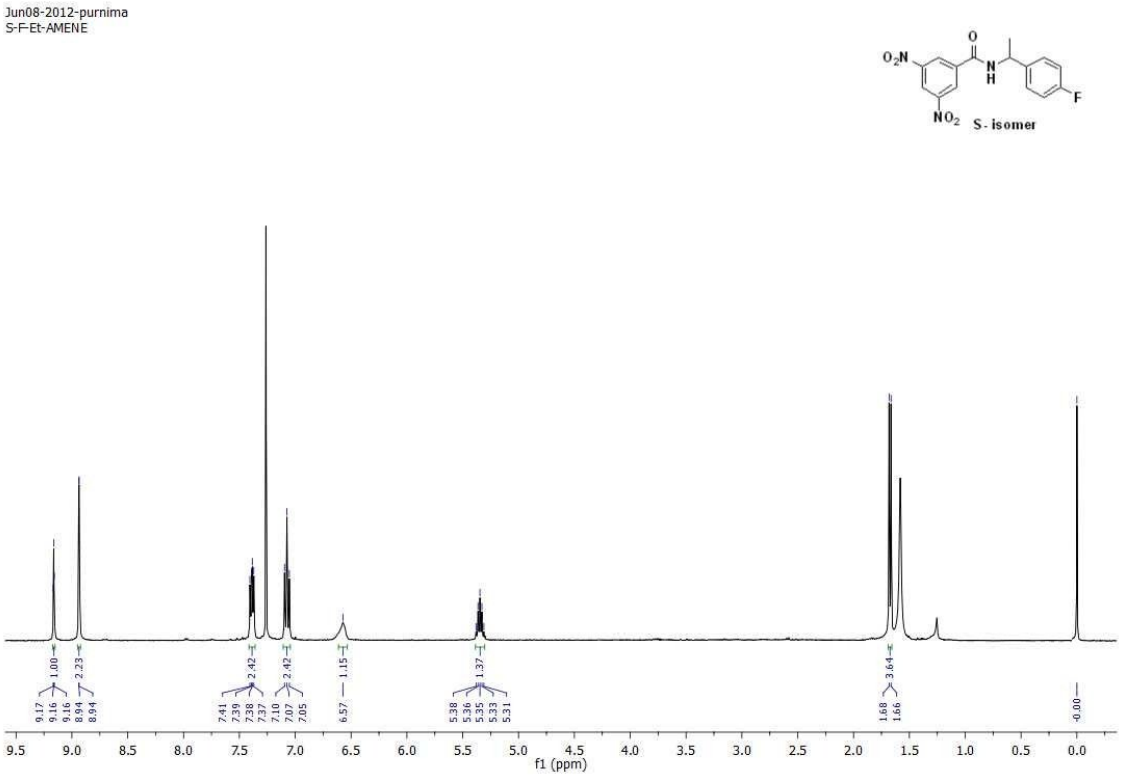
Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C15 H12 F N3 O5	TRUE	333.07632	333.0761	-0.65	C15 H11 F N3 O5	90.23

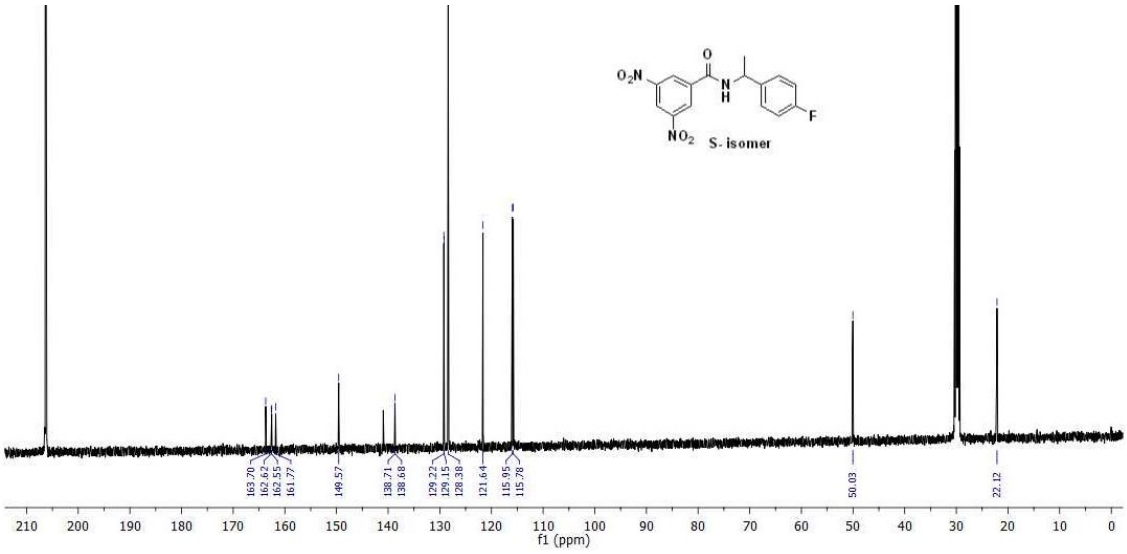
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

Agilent Technologies Page 1 of 2 Printed at: 10:47 AM on: 8/2/2012

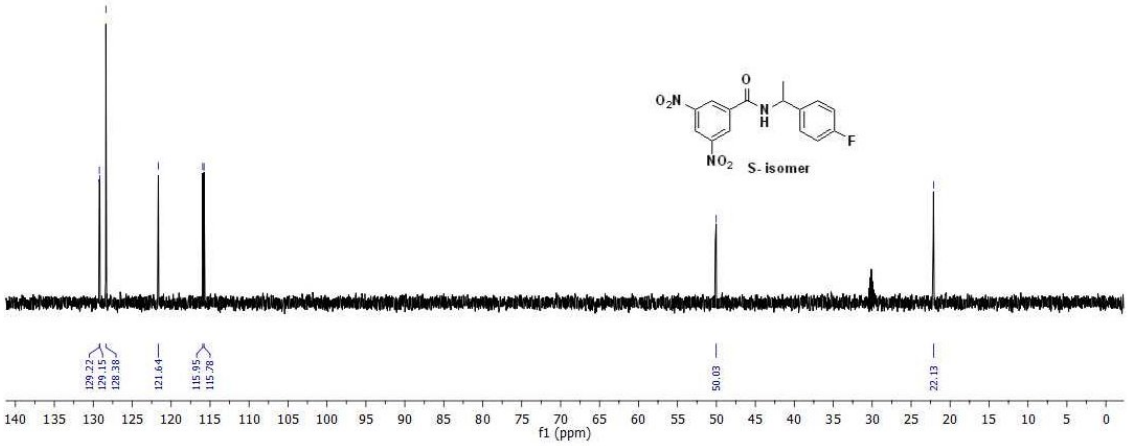
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7m:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7m:**



DEPT (126 MHz, Acetone-d_6) of compound **7m:**



HRMS (ESI-TOF) of compound **7m**:

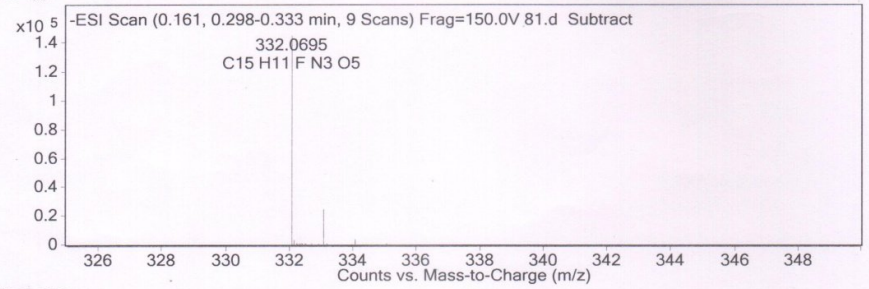
Qualitative Analysis Report

Data Filename	81.d	**Sample Name**	81
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	30-07-2012 AM 10:06:27
IRM Calibration Status	Some Ions Missed	**DA Method**	Vishal_Compound_report.m
Comment			

Sample Group **Info.**

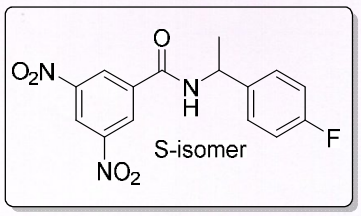
User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "- TIC Scan"	150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
332.0695	1	144836.4	C15 H11 F N3 O5	(M-H)-
333.0728	1	24628.8	C15 H11 F N3 O5	(M-H)-
446.0615	1	491475.2		
447.0656	1	61988.9		



Formula Calculator Element Limits

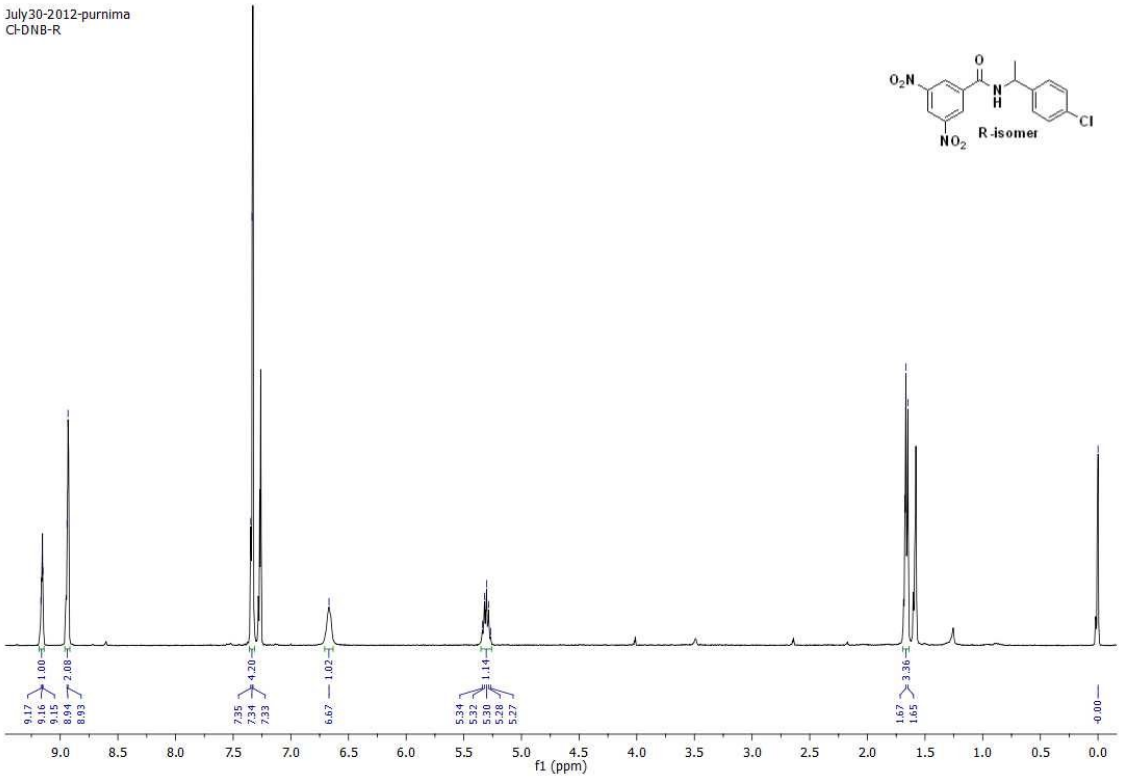
Element	Min	Max
C	3	80
H	0	120
O	0	10
N	0	10
F	0	10

Formula Calculator Results

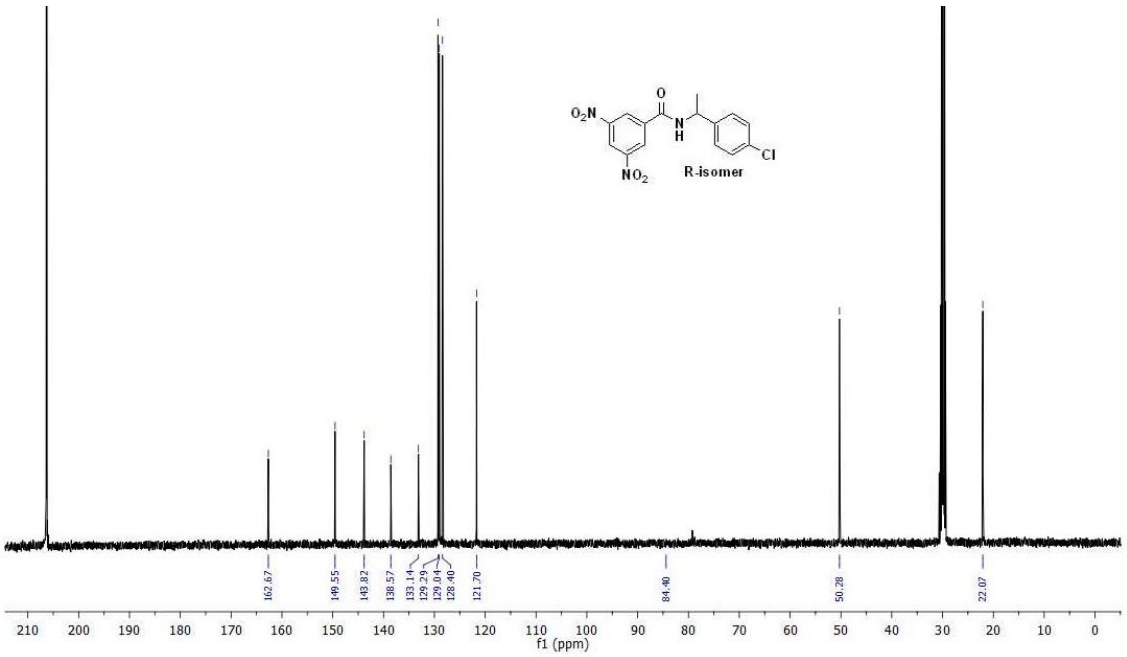
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C15 H12 F N3 O5	TRUE	333.0767	333.0761	-1.9	C15 H11 F N3 O5	98.47
C16 H9 F4 N4		333.0767	333.0763	-1.2	C16 H8 F4 N4	98.04
C17 H14 F O6		333.0767	333.0774	2.13	C17 H13 F O6	97.66
C13 H11 F8 N		333.0767	333.0764	-1.07	C13 H10 F8 N	97.5
C12 H13 F2 N3 O6		333.0767	333.0772	1.53	C12 H12 F2 N3 O6	97.18
C13 H10 F5 N4 O		333.0767	333.0775	2.23	C13 H9 F5 N4 O	97.1
C16 H8 F N7 O		333.0767	333.0774	2.11	C16 H7 F N7 O	95.45
C11 H8 F5 N7		333.0767	333.0761	-1.81	C11 H7 F5 N7	95.35
C12 H14 F5 O5		333.0767	333.0761	-1.77	C12 H13 F5 O5	95.33
C18 H11 F4 N O		333.0767	333.0777	2.84	C18 H10 F4 N O	94.95

--- End Of Report ---

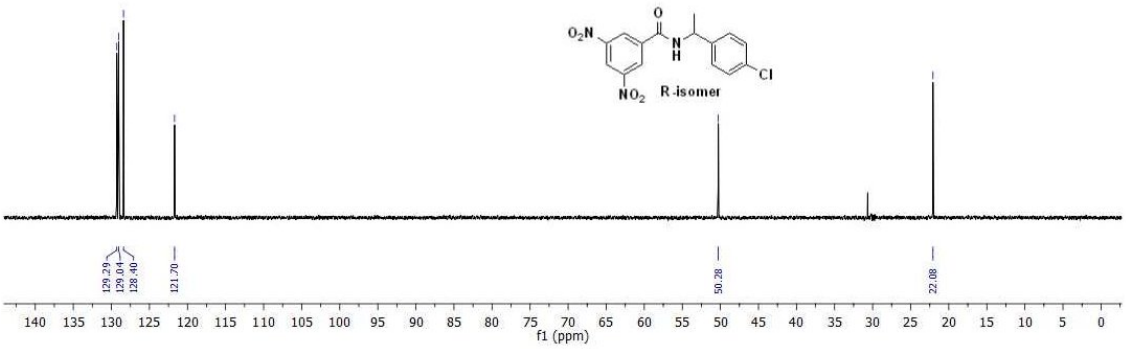
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7n:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7n:**



DEPT (126 MHz, Acetone-d_6) of compound **7n:**

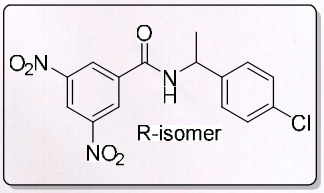


HRMS (ESI-TOF) of compound **7n**:

Qualitative Compound Report

Data File	102.d	**Sample Name**	102
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:19:34
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

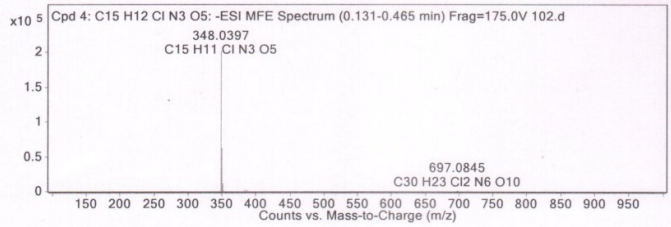


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C15 H12 Cl N3 O5	0.192	349.0469	C15 H12 Cl N3 O5	C15 H12 Cl N3 O5	-0.89	C15 H12 Cl N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C15 H12 Cl N3 O5	348.0397	0.192	Find by Molecular Feature	349.0469

MFE MS Spectrum



MS Spectrum Peak List

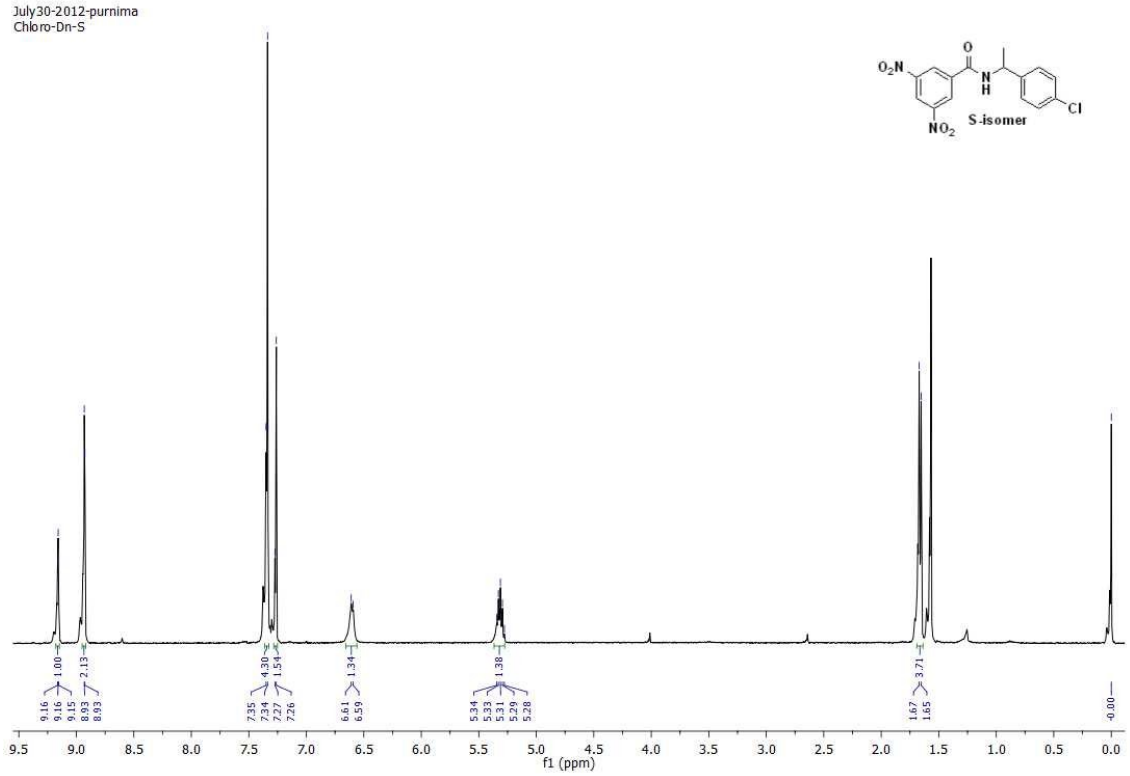
m/z	z	Abund	Formula	Ion
348.0397	-1	201861.14	C15 H11 Cl N3 O5	(M-H)-
349.0427	-1	33345.25	C15 H11 Cl N3 O5	(M-H)-
350.0368	-1	61505.89	C15 H11 Cl N3 O5	(M-H)-
351.0395	-1	12166.55	C15 H11 Cl N3 O5	(M-H)-
352.042	-1	1414.97	C15 H11 Cl N3 O5	(M-H)-
384.0156	-1	2660.78		(M+Cl)-
386.0129	-1	2425.72		(M+Cl)-
388.0127	-1	621.48		(M+Cl)-
697.0845	-1	1456.21	C30 H23 Cl2 N6 O10	(2M-H)-
699.0839	-1	1001.25	C30 H23 Cl2 N6 O10	(2M-H)-

Predicted Isotope Match Table

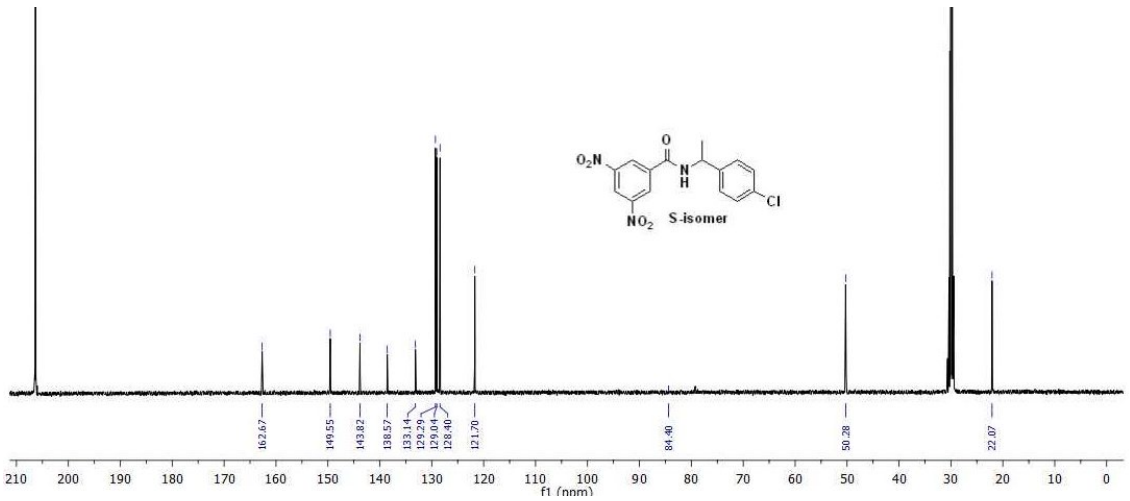
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	348.0397	348.0393	-1.25	100	100	65.05	62.95
2	349.0427	349.0423	-1.38	16.52	17.64	10.75	11.1
3	350.0368	350.0369	0.28	30.47	34.49	19.82	21.71
4	351.0395	351.0396	0.3	6.03	5.9	3.92	3.71
5	352.042	352.0418	-0.75	0.7	0.82	0.46	0.52

--- End Of Report ---

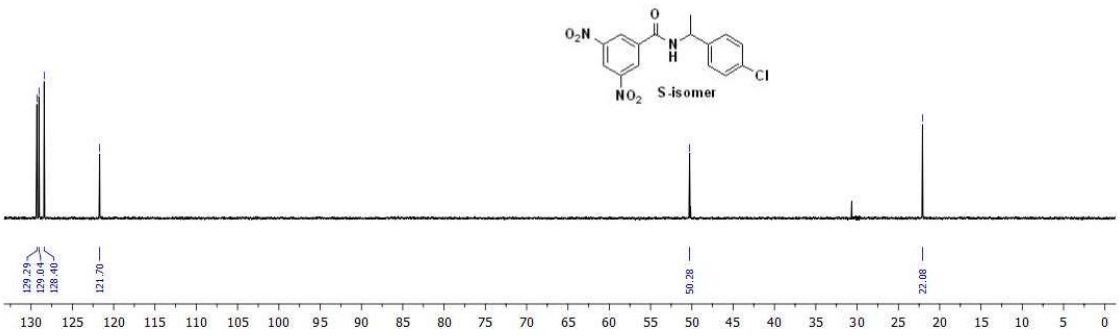
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7o:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7o:**



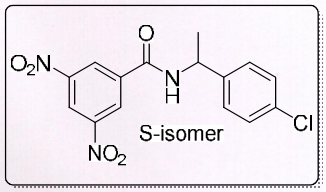
DEPT (126 MHz, Acetone-d_6) of compound **7o:**



HRMS (ESI-TOF) of compound **7o**:

Qualitative Compound Report

Data File	103.d	**Sample Name**	103
Sample Type	Sample	**Position**	Vial 31
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 5:47:34
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



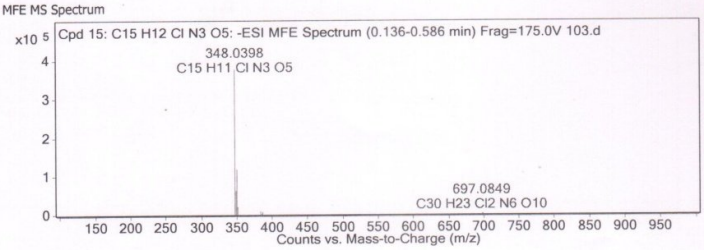
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C15 H12 Cl N3 O5	0.187	349.047	C15 H12 Cl N3 O5	C15 H12 Cl N3 O5	-1.31	C15 H12 Cl N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C15 H12 Cl N3 O5	348.0398	0.187	Find by Molecular Feature	349.047

MFE MS Spectrum



MS Spectrum Peak List

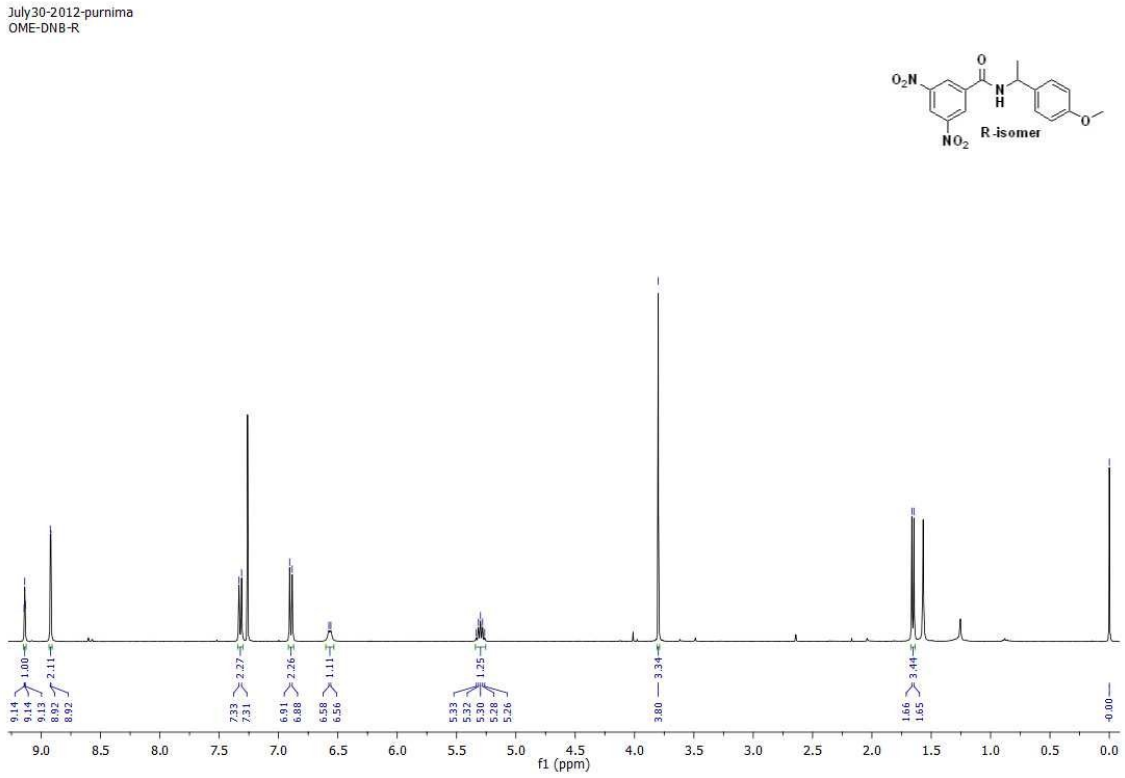
m/z	z	Abund	Formula	Ion
348.0398	-1	378520.44	C15 H11 Cl N3 O5	(M-H)-
349.0427	-1	63744.54	C15 H11 Cl N3 O5	(M-H)-
350.0372	-1	117417.26	C15 H11 Cl N3 O5	(M-H)-
351.0398	-1	20543.47	C15 H11 Cl N3 O5	(M-H)-
352.0418	-1	2998.3	C15 H11 Cl N3 O5	(M-H)-
384.0158	-1	8605.59	C15 H12 Cl2 N3 O5	(M+Cl)-
385.0204	-1	1134.21	C15 H12 Cl2 N3 O5	(M+Cl)-
386.0134	-1	6084.28	C15 H12 Cl2 N3 O5	(M+Cl)-
697.0849	-1	2429.62	C30 H23 Cl2 N6 O10	(2M-H)-
699.0807	-1	1937.37	C30 H23 Cl2 N6 O10	(2M-H)-

Predicted Isotope Match Table

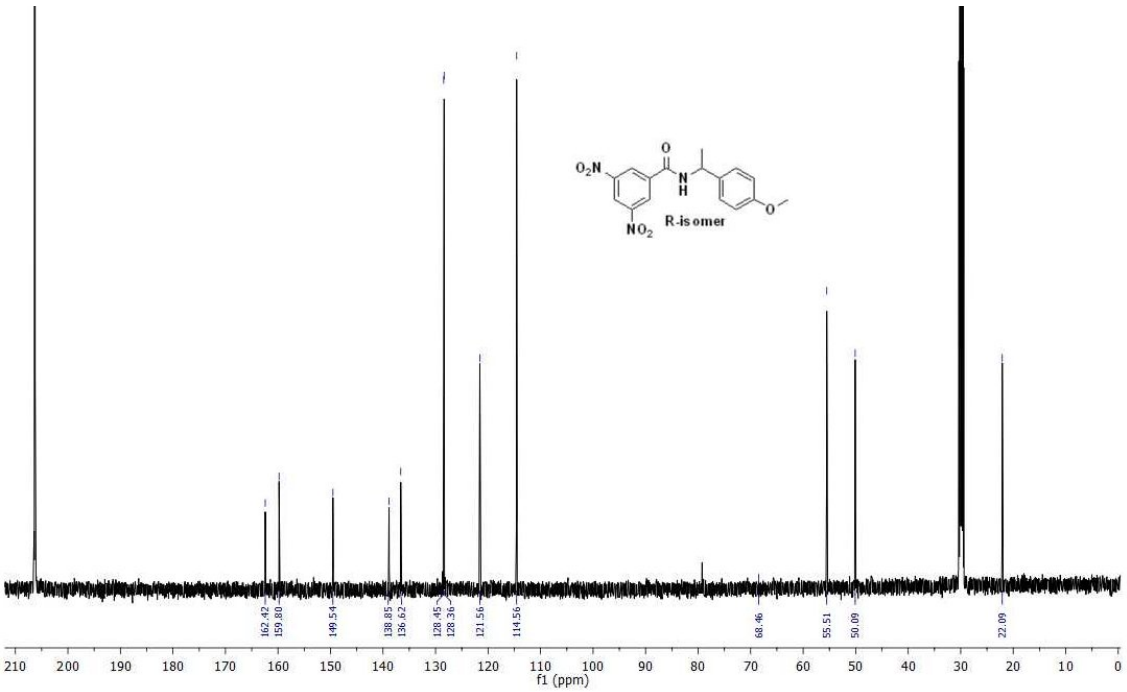
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	348.0398	348.0393	-1.57	100	100	64.86	62.92
2	349.0427	349.0423	-1.26	16.84	17.64	10.92	11.1
3	350.0372	350.0369	-0.7	31.02	34.49	20.12	21.7
4	351.0398	351.0396	-0.42	5.43	5.9	3.52	3.71
5	352.0418	352.0418	0	0.79	0.82	0.51	0.52
6	353.0418	353.0442	6.89	0.09	0.08	0.06	0.05

--- End Of Report ---

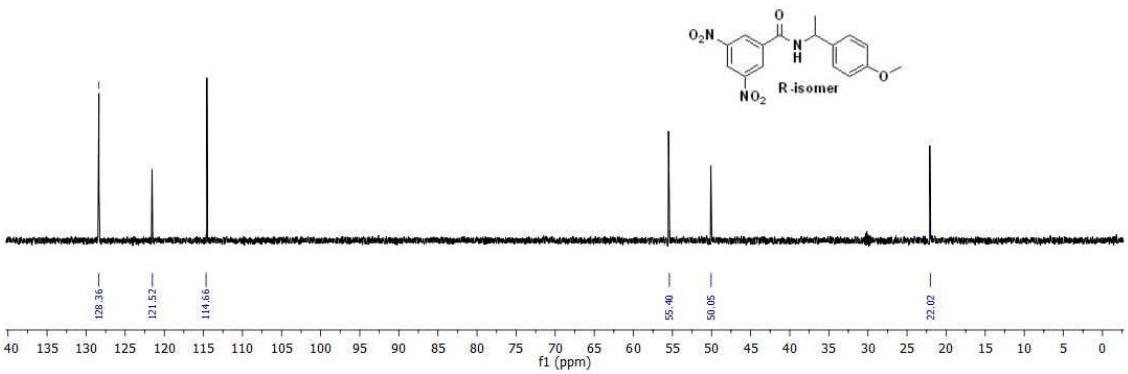
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7p:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7p:**



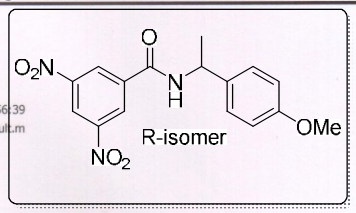
DEPT (126 MHz, Acetone-d_6) of compound **7p:**



HRMS (ESI-TOF) of compound **7p**:

Qualitative Compound Report

Data File	104.d	**Sample Name**	104
Sample Type	Sample	**Position**	Vial 32
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 5:56:39
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

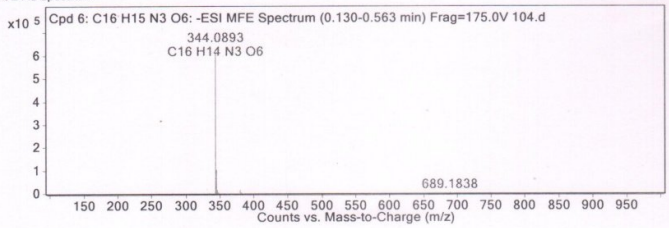


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C16 H15 N3 O6	0.186	345.0966	C16 H15 N3 O6	C16 H15 N3 O6	-1.37	C16 H15 N3 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C16 H15 N3 O6	344.0893	0.186	Find by Molecular Feature	345.0966

MFE MS Spectrum



MS Spectrum Peak List

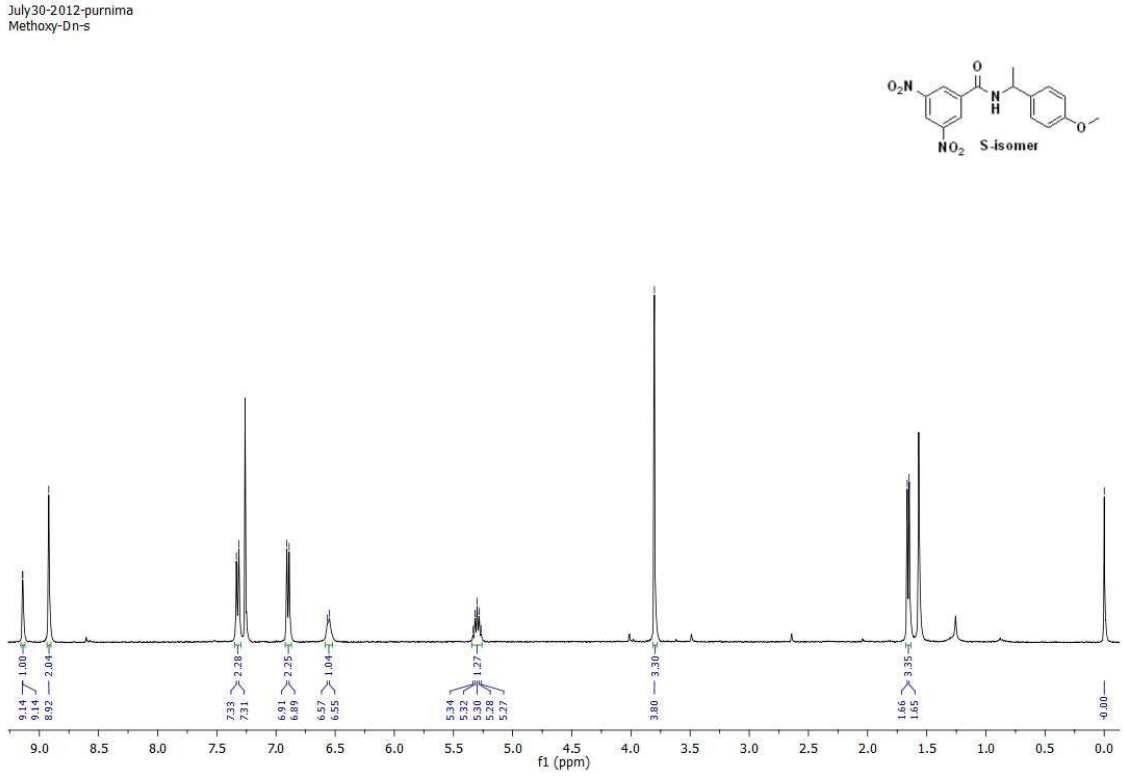
m/z	z	Abund	Formula	Ion
344.0893	-1	610876.81	C16 H14 N3 O6	(M-H)-
345.0921	-1	101181.52	C16 H14 N3 O6	(M-H)-
346.0941	-1	15975.81	C16 H14 N3 O6	(M-H)-
347.098	-1	2230.59	C16 H14 N3 O6	(M-H)-
380.065	-1	13910.89	C16 H15 Cl N3 O6	(M+Cl)-
381.0689	-1	2725.07	C16 H15 Cl N3 O6	(M+Cl)-
382.0634	-1	5227.45	C16 H15 Cl N3 O6	(M+Cl)-
383.0651	-1	889.7	C16 H15 Cl N3 O6	(M+Cl)-
689.1838	-1	2441.67		(2M-H)-
690.1868	-1	1336.17		(2M-H)-

Predicted Isotope Match Table

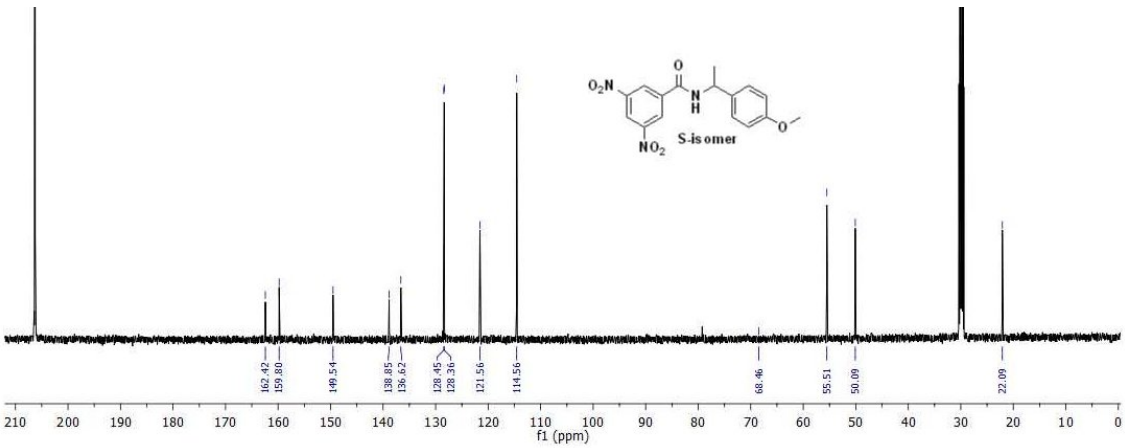
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	344.0893	344.0888	-1.48	100	100	83.65	81.96
2	345.0921	345.0918	-0.92	16.56	18.79	13.86	15.4
3	346.0941	346.0941	0.02	2.62	2.9	2.19	2.38
4	347.098	347.0966	-3.98	0.37	0.32	0.31	0.27

--- End Of Report ---

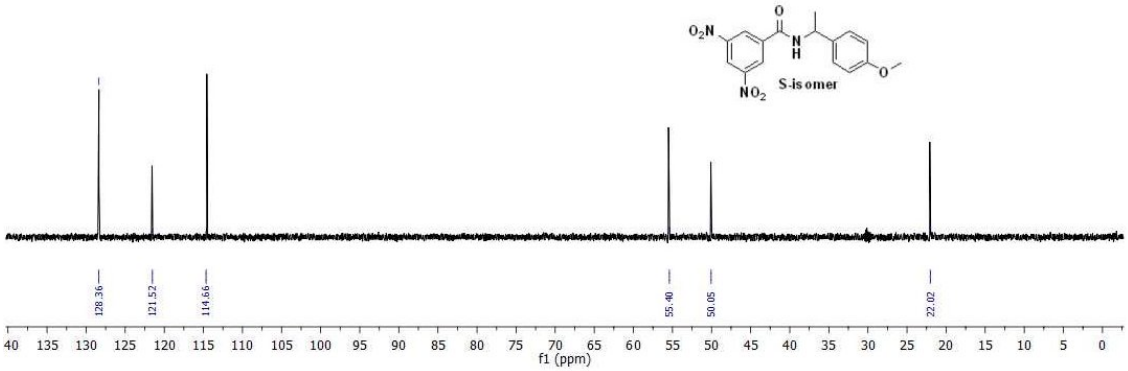
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7q:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7q:**



DEPT (126 MHz, Acetone-d_6) of compound **7q:**



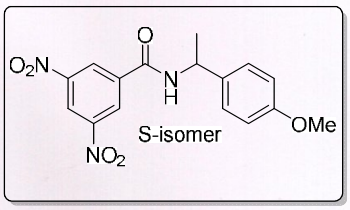
HRMS (ESI-TOF) of compound **7q**:

Qualitative Compound Report

Data File	105.d	**Sample Name**	105
Sample Type	Sample	**Position**	Vial 33
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 6:01:12
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Info.

Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

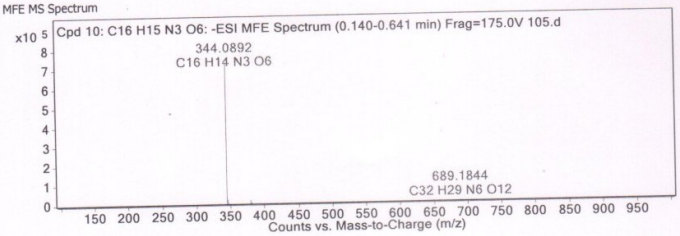


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C16 H15 N3 O6	0.187	345.0965	C16 H15 N3 O6	C16 H15 N3 O6	-1.14	C16 H15 N3 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C16 H15 N3 O6	344.0892	0.187	Find by Molecular Feature	345.0965

MFE MS Spectrum



MS Spectrum Peak List

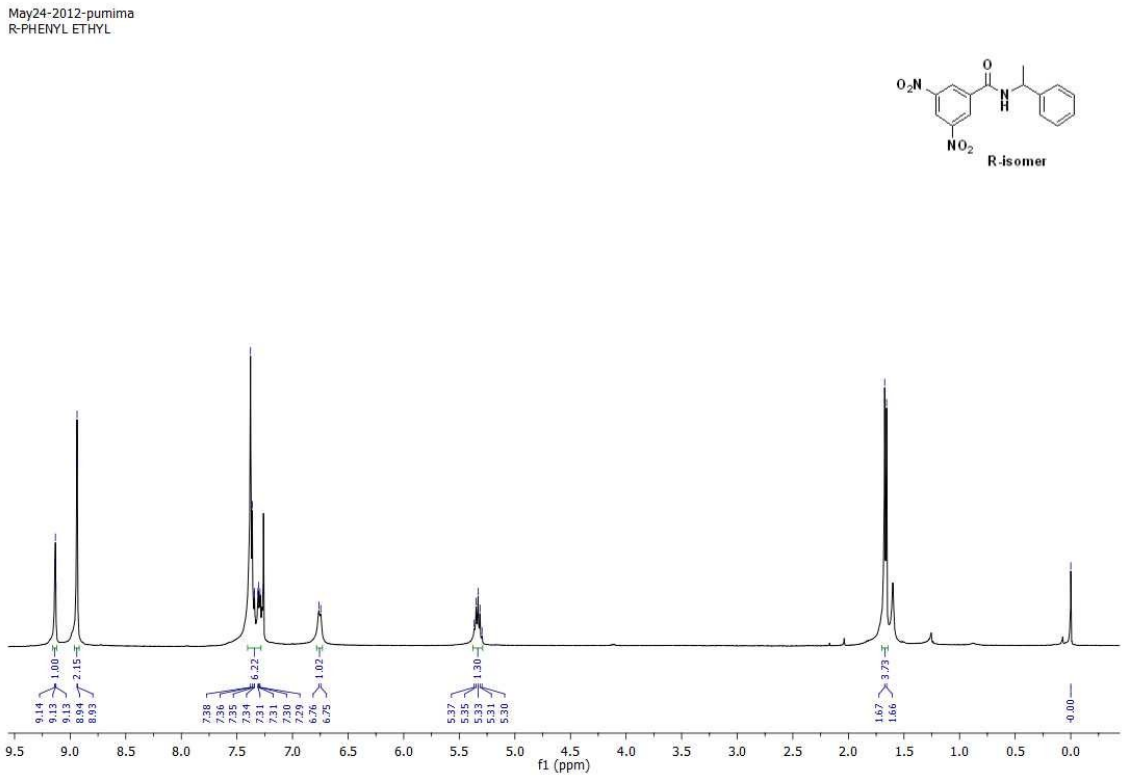
m/z	z	Abund	Formula	Ion
344.0892	-1	725897.63	C16 H14 N3 O6	(M-H)-
345.0923	-1	126956.16	C16 H14 N3 O6	(M-H)-
346.0948	-1	22641.56	C16 H14 N3 O6	(M-H)-
347.0964	-1	2493.41	C16 H14 N3 O6	(M-H)-
380.0654	-1	16197.67	C16 H15 Cl N3 O6	(M+Cl)-
381.0691	-1	3416.3	C16 H15 Cl N3 O6	(M+Cl)-
382.0635	-1	5541.72	C16 H15 Cl N3 O6	(M+Cl)-
689.1844	-1	3976.8	C32 H29 N6 O12	(2M-H)-
690.1833	-1	1040.4	C32 H29 N6 O12	(2M-H)-
691.1907	-1	466.38	C32 H29 N6 O12	(2M-H)-

Predicted Isotope Match Table

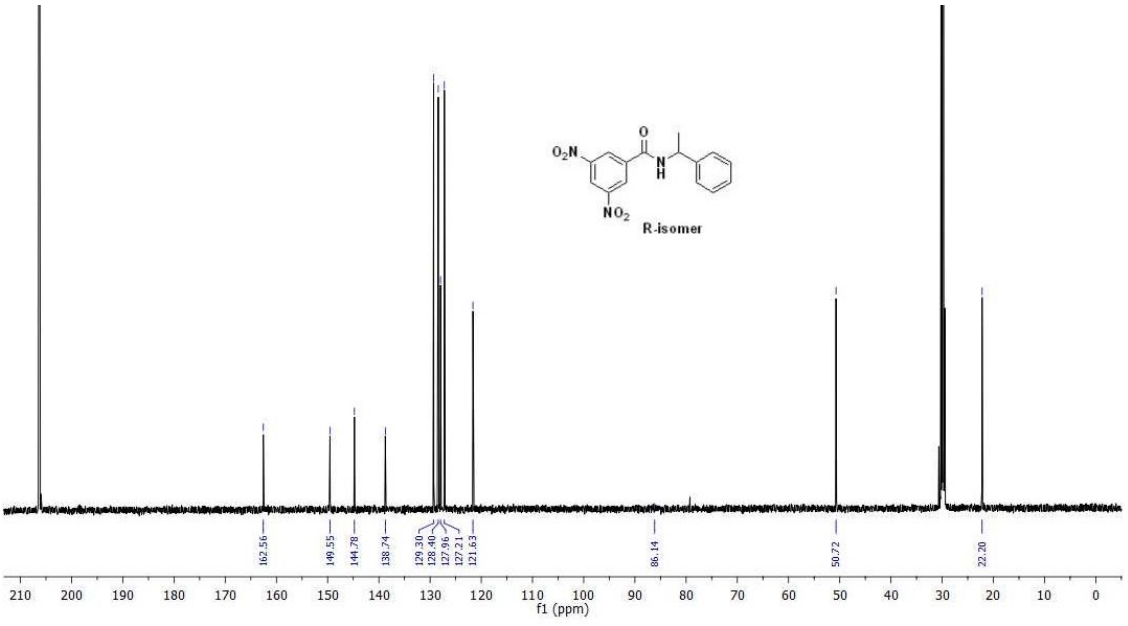
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	344.0892	344.0888	-1.08	100	100	82.68	81.96
2	345.0923	345.0918	-1.4	17.49	18.79	14.46	15.4
3	346.0948	346.0941	-2.08	3.12	2.9	2.58	2.38
4	347.0964	347.0966	0.48	0.34	0.32	0.28	0.27

--- End Of Report ---

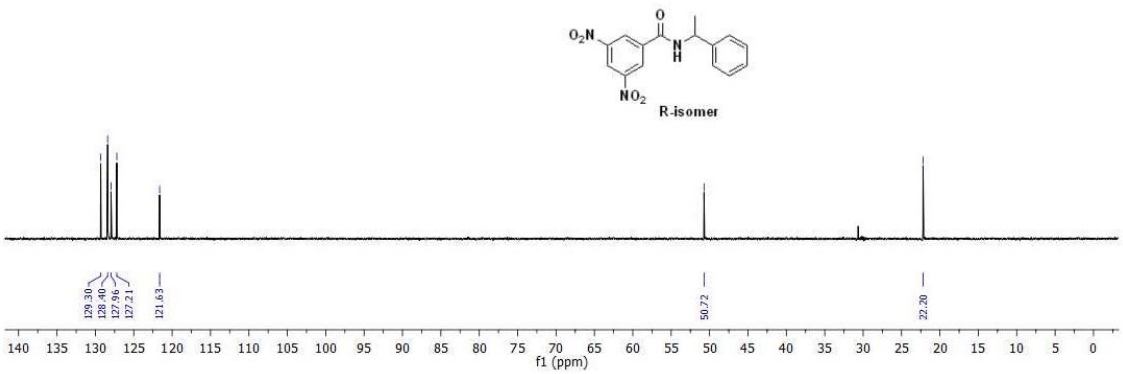
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7r:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7r:**



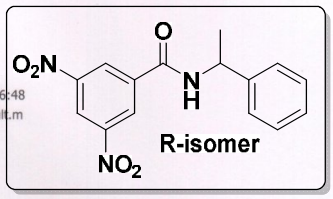
DEPT (126 MHz, Acetone-d_6) of compound **7r:**



HRMS (ESI-TOF) of compound **7r**:

Qualitative Compound Report

Data File	55.d	**Sample Name**	55
Sample Type	Sample	**Position**	Vial 20
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	04-03-2013 PM 3:36:48
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



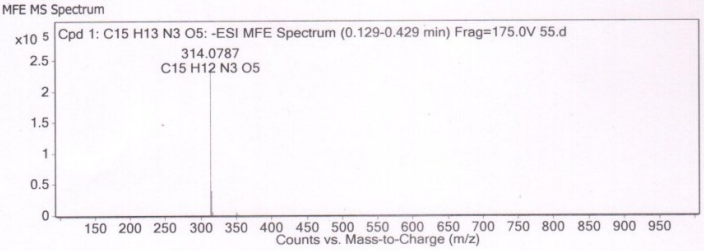
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C15 H13 N3 O5	0.191	315.086	C15 H13 N3 O5	C15 H13 N3 O5	-1.45	C15 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C15 H13 N3 O5	314.0787	0.191	Find by Molecular Feature	315.086

MFE MS Spectrum



MS Spectrum Peak List

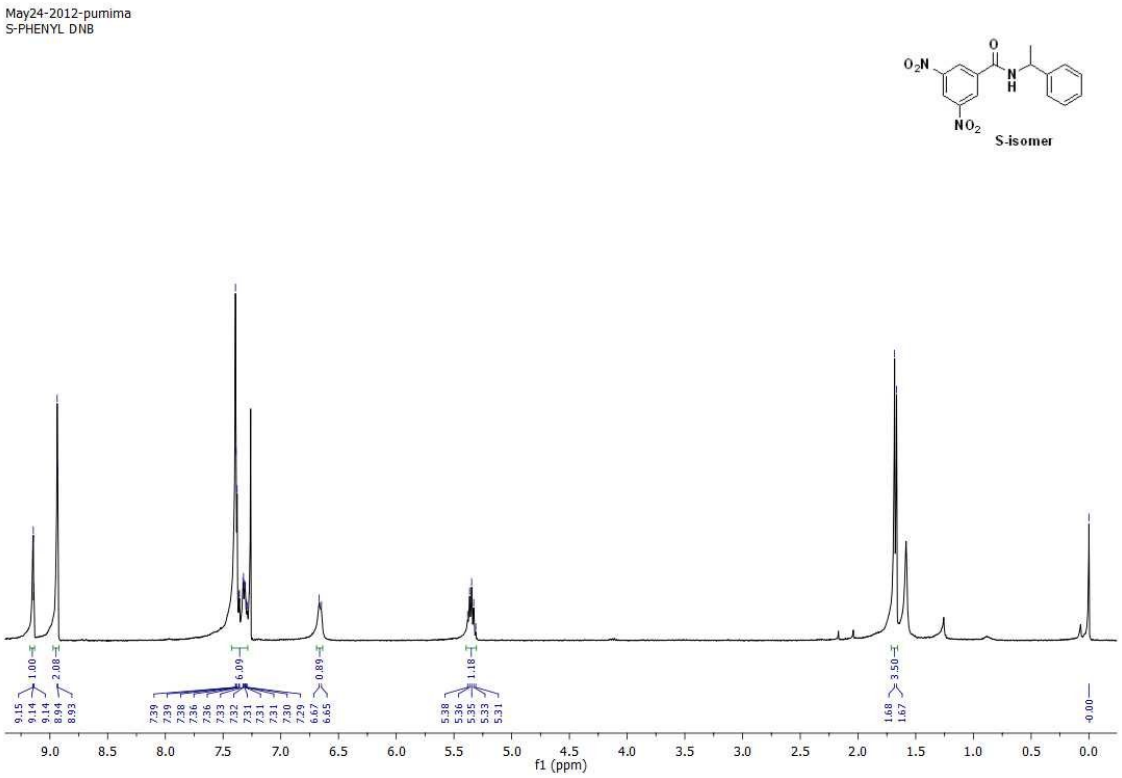
m/z	z	Abund	Formula	Ion
314.0787	-1	235398.56	C15 H12 N3 O5	(M-H)-
315.0818	-1	39925.2	C15 H12 N3 O5	(M-H)-
316.0844	-1	6107.2	C15 H12 N3 O5	(M-H)-
317.0857	-1	973.96	C15 H12 N3 O5	(M-H)-
350.0547	-1	4522.35	C15 H13 Cl N3 O5	(M+Cl)-
351.057	-1	1052.76	C15 H13 Cl N3 O5	(M+Cl)-
352.053	-1	1212.6	C15 H13 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

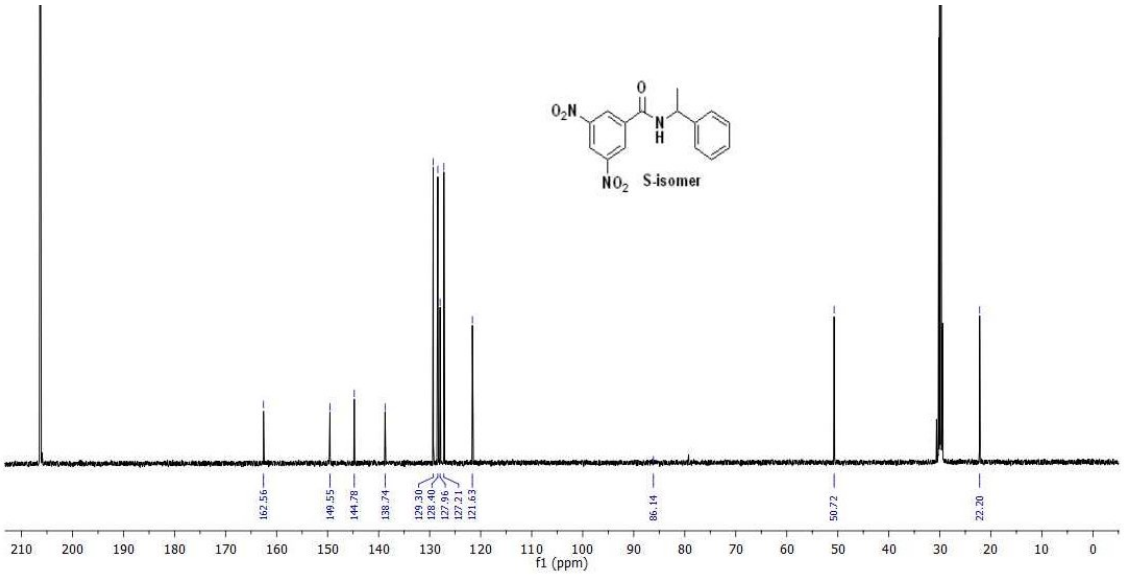
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	314.0787	314.0782	-1.38	100	100	83.35	83.06
2	315.0818	315.0812	-1.77	16.96	17.65	14.14	14.66
3	316.0844	316.0835	-2.7	2.59	2.49	2.16	2.07
4	317.0857	317.086	0.93	0.41	0.26	0.34	0.21

--- End Of Report ---

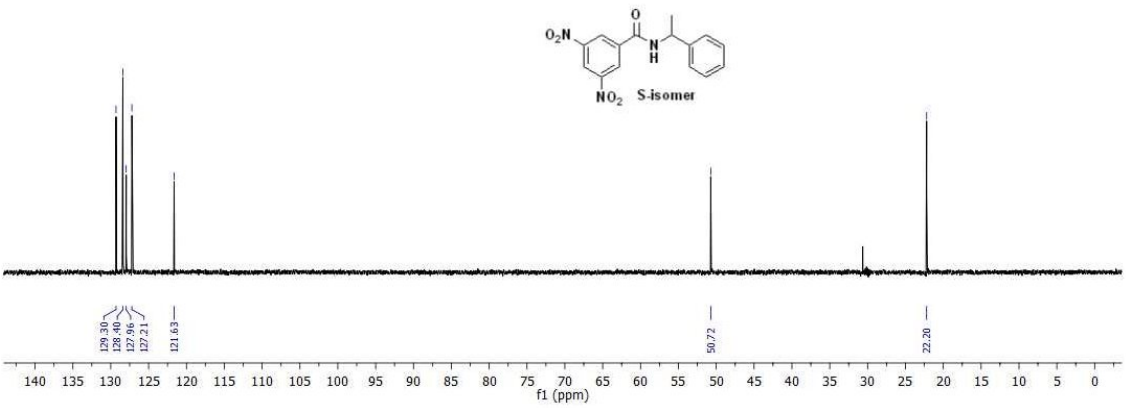
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7s:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7s:**



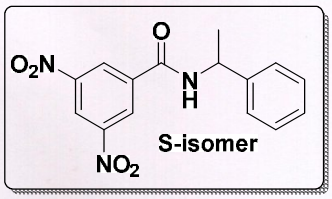
DEPT (126 MHz, Acetone-d_6) of compound **7s:**



HRMS (ESI-TOF) of compound **7s**:

Qualitative Compound Report

Data File	56.d	Sample Name	56
Sample Type	Sample	Position	Vial 21
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_neg12-01-13.m	Acquired Time	04-03-2013 PM 3:41:18
IRM Calibration Status	Success	DA Method	SamplePurity-Default.m
Comment			



Info.

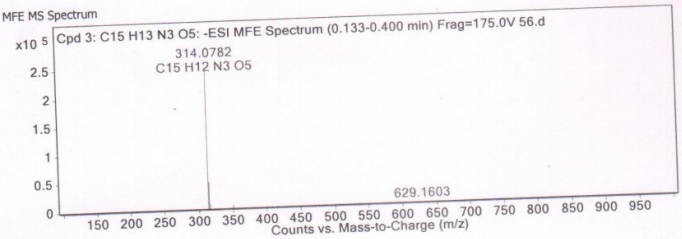
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C15 H13 N3 O5	0.194	315.0855	C15 H13 N3 O5	C15 H13 N3 O5	0.03	C15 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C15 H13 N3 O5	314.0782	0.194	Find by Molecular Feature	315.0855

MFE MS Spectrum



MS Spectrum Peak List

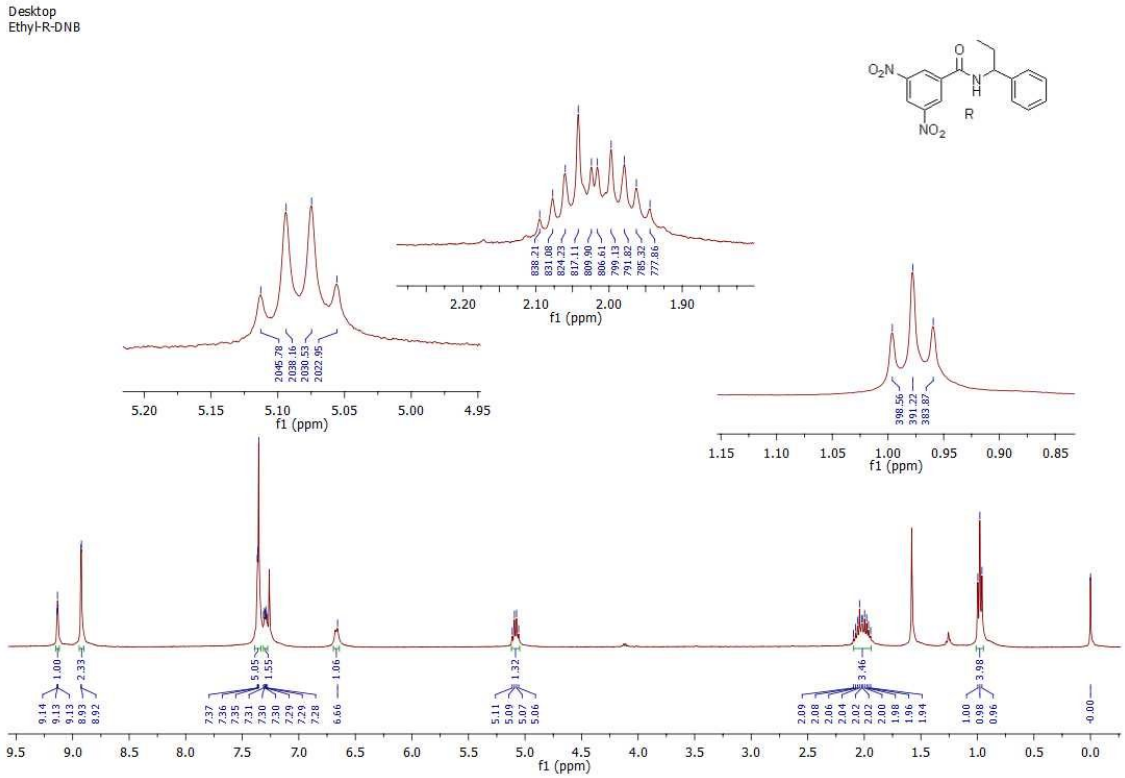
m/z	z	Abund	Formula	Ion
314.0782	-1	248029.78	C15 H12 N3 O5	(M-H)-
315.0813	-1	47317	C15 H12 N3 O5	(M-H)-
316.0831	-1	7160.78	C15 H12 N3 O5	(M-H)-
317.0886	-1	803.45	C15 H12 N3 O5	(M-H)-
350.0542	-1	4100.91	C15 H13 Cl N3 O5	(M+Cl)-
351.0565	-1	738.83	C15 H13 Cl N3 O5	(M+Cl)-
352.0505	-1	1277.92	C15 H13 Cl N3 O5	(M+Cl)-
629.1603	-1	392.7		(2M-H)-

Predicted Isotope Match Table

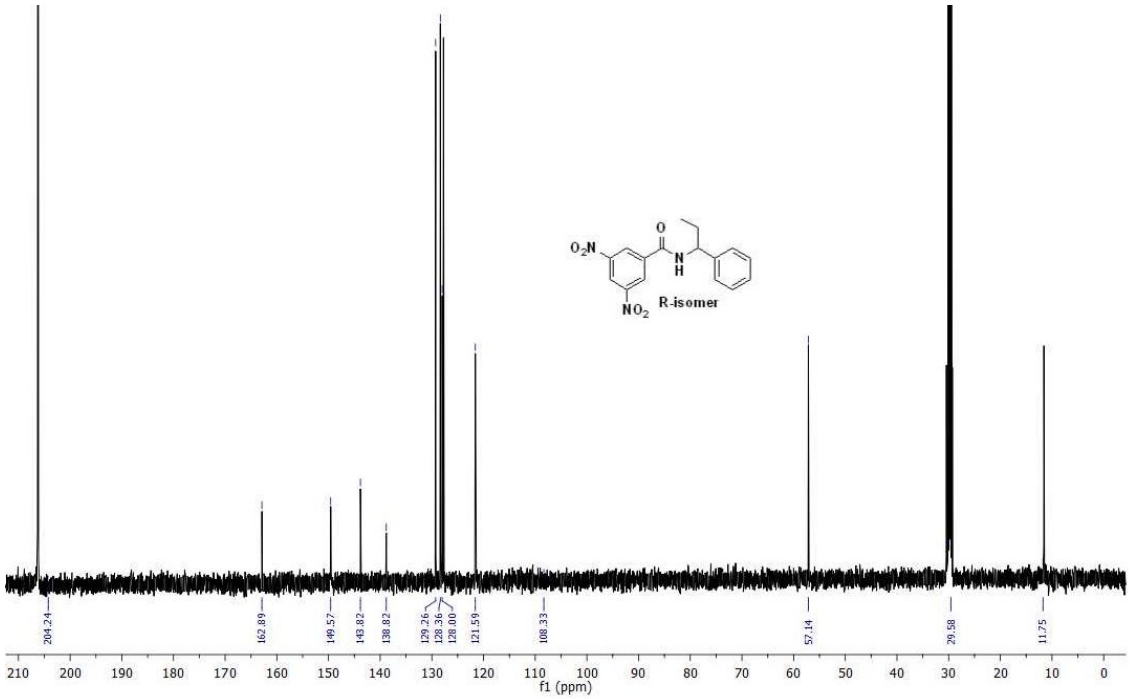
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	314.0782	314.0782	0.03	100	100	81.77	83.06
2	315.0813	315.0812	-0.05	19.08	17.65	15.6	14.66
3	316.0831	316.0835	1.33	2.89	2.49	2.36	2.07
4	317.0886	317.086	-8.14	0.32	0.26	0.26	0.21

--- End Of Report ---

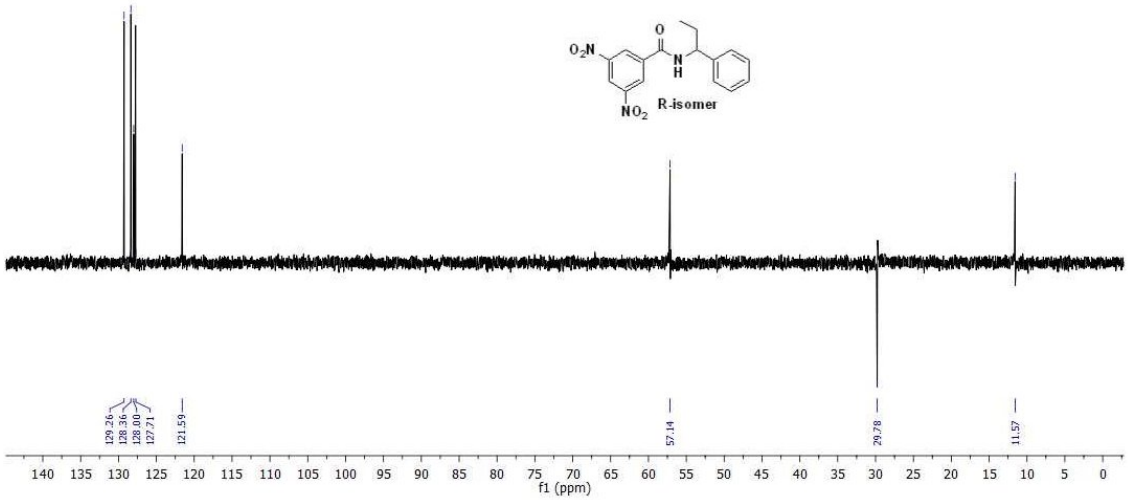
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7t:**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7t:**



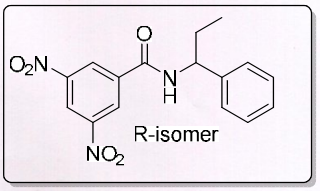
DEPT (101 MHz, Acetone-d_6) of compound **7t:**



HRMS (ESI-TOF) of compound **7t**:

Qualitative Compound Report

Data File	91.d	**Sample Name**	91
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 5:05:10
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



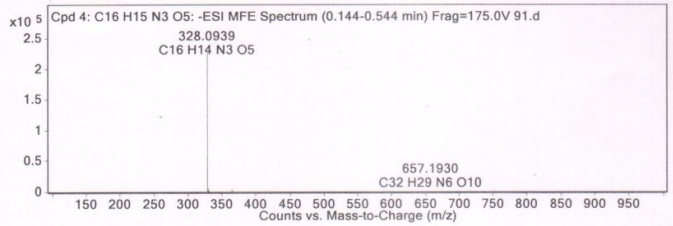
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C16 H15 N3 O5	0.195	329.1012	C16 H15 N3 O5	C16 H15 N3 O5	-0.1	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C16 H15 N3 O5	328.0939	0.195	Find by Molecular Feature	329.1012

MFE MS Spectrum



MS Spectrum Peak List

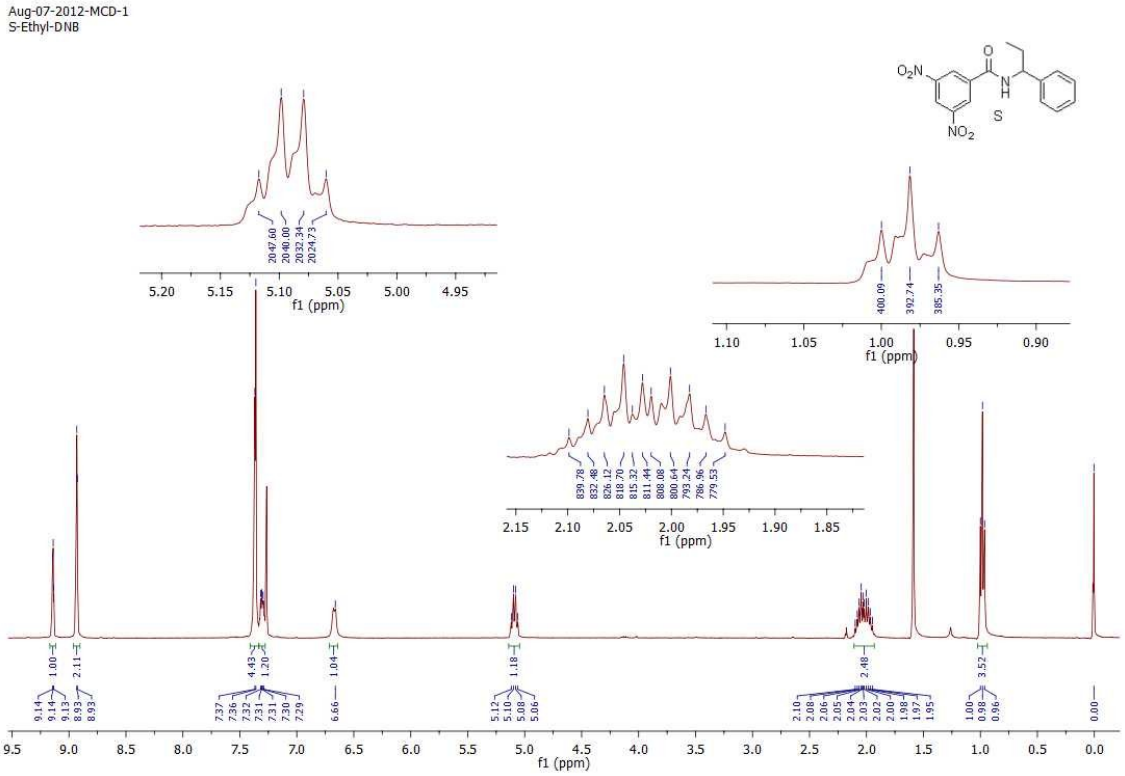
m/z	z	Abund	Formula	Ion
328.0939	-1	228341.8	C16 H14 N3 O5	(M-H)-
329.0971	-1	38304.57	C16 H14 N3 O5	(M-H)-
330.099	-1	5622.65	C16 H14 N3 O5	(M-H)-
331.1008	-1	908.66	C16 H14 N3 O5	(M-H)-
364.0702	-1	3475.63		(M+Cl)-
365.0717	-1	1136.71		(M+Cl)-
366.0661	-1	1777.39		(M+Cl)-
657.193	-1	350.78	C32 H29 N6 O10	(2M-H)-

Predicted Isotope Match Table

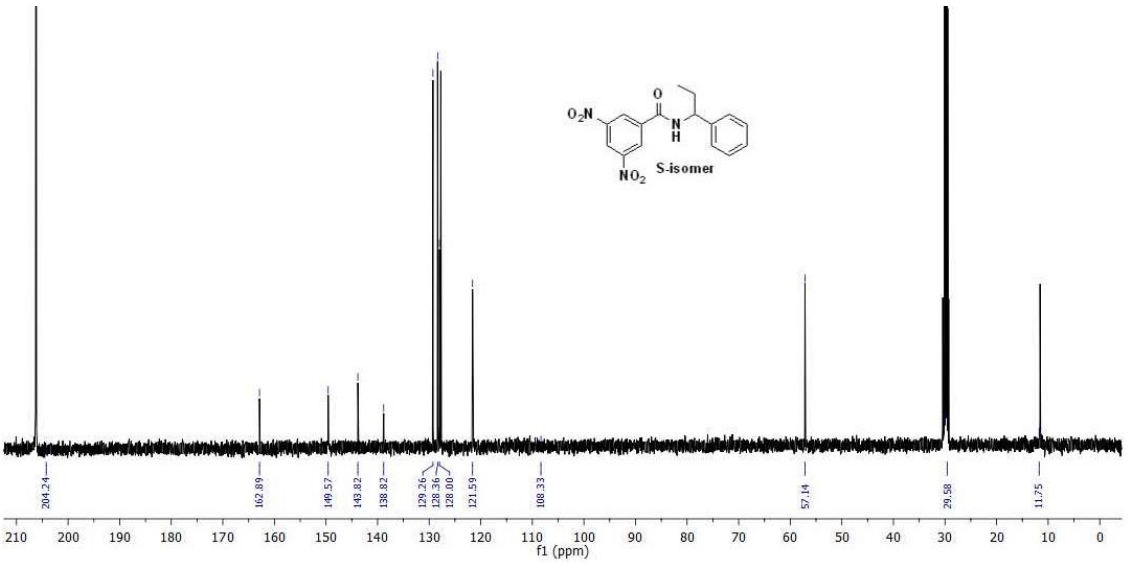
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.0939	328.0939	-0.07	100	100	83.59	82.15
2	329.0971	329.0969	-0.49	16.78	18.75	14.02	15.41
3	330.099	330.0992	0.84	2.46	2.69	2.06	2.21
4	331.1008	331.1017	2.84	0.4	0.28	0.33	0.23

--- End Of Report ---

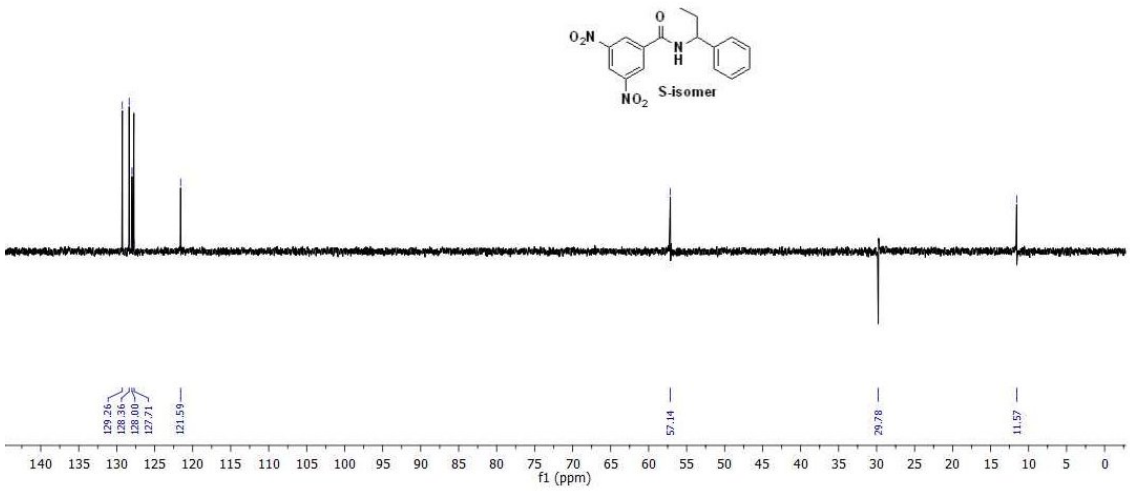
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7u:**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **7u:**



DEPT (101 MHz, Acetone-d_6) of compound **7u:**

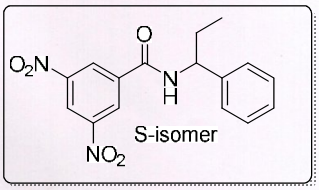


HRMS (ESI-TOF) of compound **7u**:

Qualitative Compound Report

Data File	92.d	**Sample Name**	92
Sample Type	Sample	**Position**	Vial 10
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:28:50
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

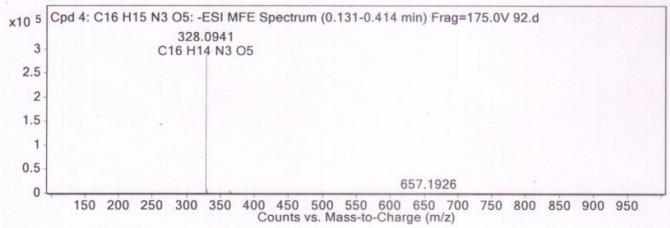


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C16 H15 N3 O5	0.195	329.1013	C16 H15 N3 O5	C16 H15 N3 O5	-0.53	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C16 H15 N3 O5	328.0941	0.195	Find by Molecular Feature	329.1013

MFE MS Spectrum



MS Spectrum Peak List

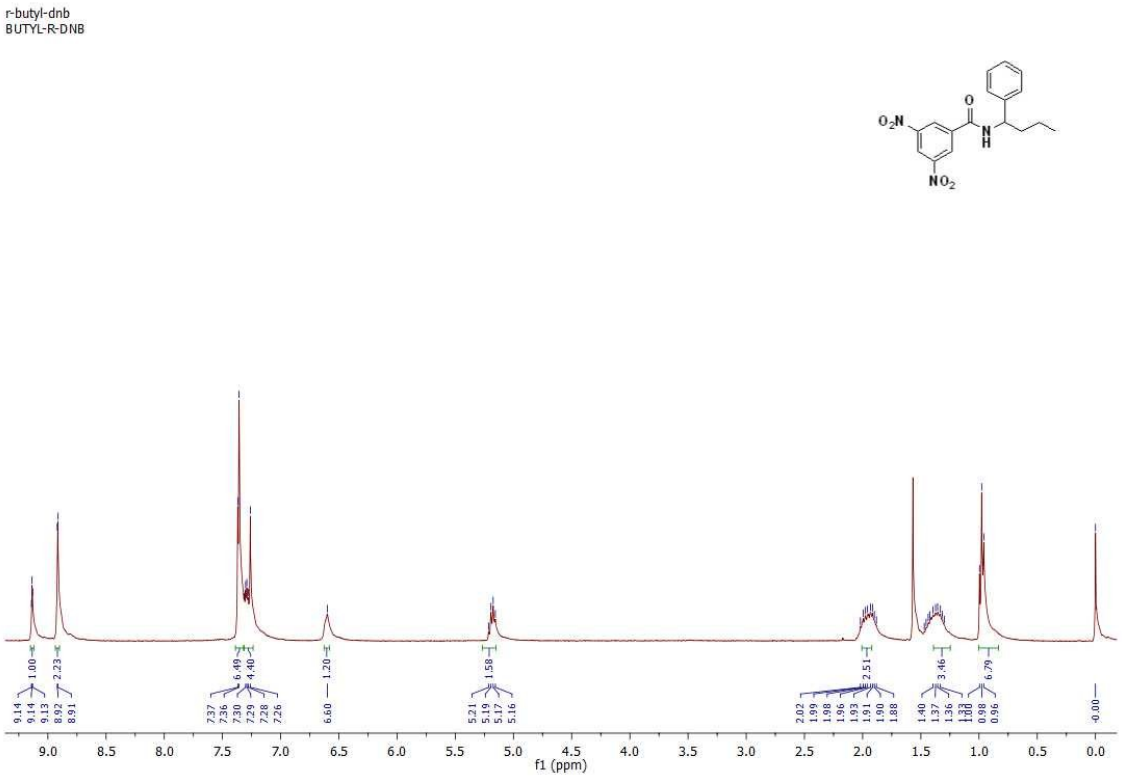
m/z	z	Abund	Formula	Ion
328.0941	-1	292619.28	C16 H14 N3 O5	(M-H)-
329.0969	-1	49689.63	C16 H14 N3 O5	(M-H)-
330.0997	-1	8497.9	C16 H14 N3 O5	(M-H)-
331.1004	-1	950.9	C16 H14 N3 O5	(M-H)-
364.0702	-1	5222.44	C16 H15 Cl N3 O5	(M+Cl)-
365.0733	-1	1114.89	C16 H15 Cl N3 O5	(M+Cl)-
366.0684	-1	1878.61	C16 H15 Cl N3 O5	(M+Cl)-
368.0832	-1	646.6	C16 H15 Cl N3 O5	(M+Cl)-
657.1926	-1	680.89		(2M-H)-
658.1966	-1	435.9		(2M-H)-

Predicted Isotope Match Table

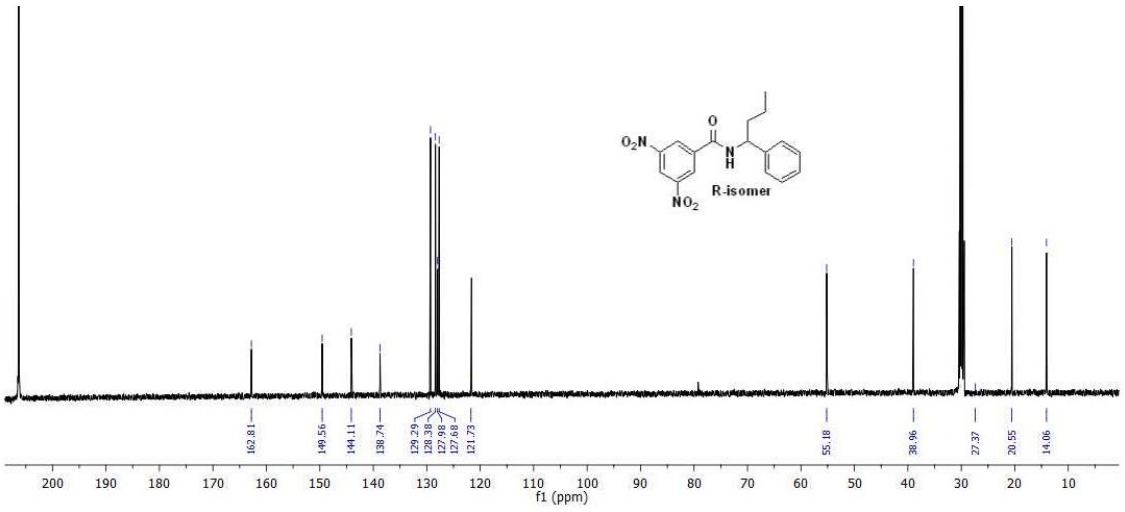
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.0941	328.0939	-0.61	100	100	83.19	82.15
2	329.0969	329.0969	-0.03	16.98	18.75	14.13	15.41
3	330.0997	330.0992	-1.36	2.9	2.69	2.42	2.21
4	331.1004	331.1017	3.94	0.32	0.28	0.27	0.23

--- End Of Report ---

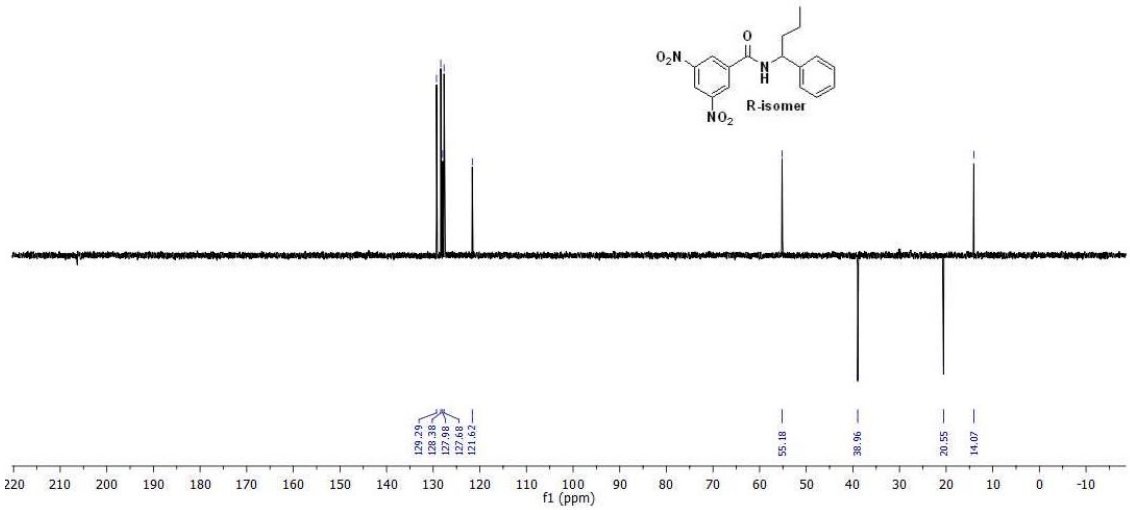
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7v:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **7v:**



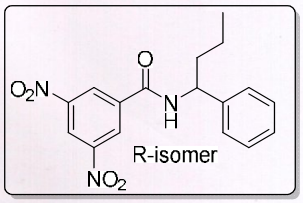
DEPT (126 MHz, Acetone-d_6) of compound **7v:**



HRMS (ESI-TOF) of compound **7v**:

Qualitative Compound Report

Data File	93.d	**Sample Name**	93
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:51:34
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



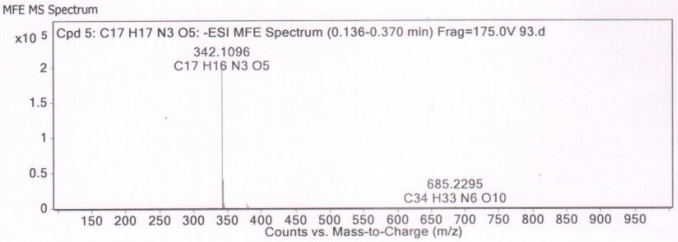
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C17 H17 N3 O5	0.192	343.1169	C17 H17 N3 O5	C17 H17 N3 O5	-0.17	C17 H17 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C17 H17 N3 O5	342.1096	0.192	Find by Molecular Feature	343.1169

MFE MS Spectrum



MS Spectrum Peak List

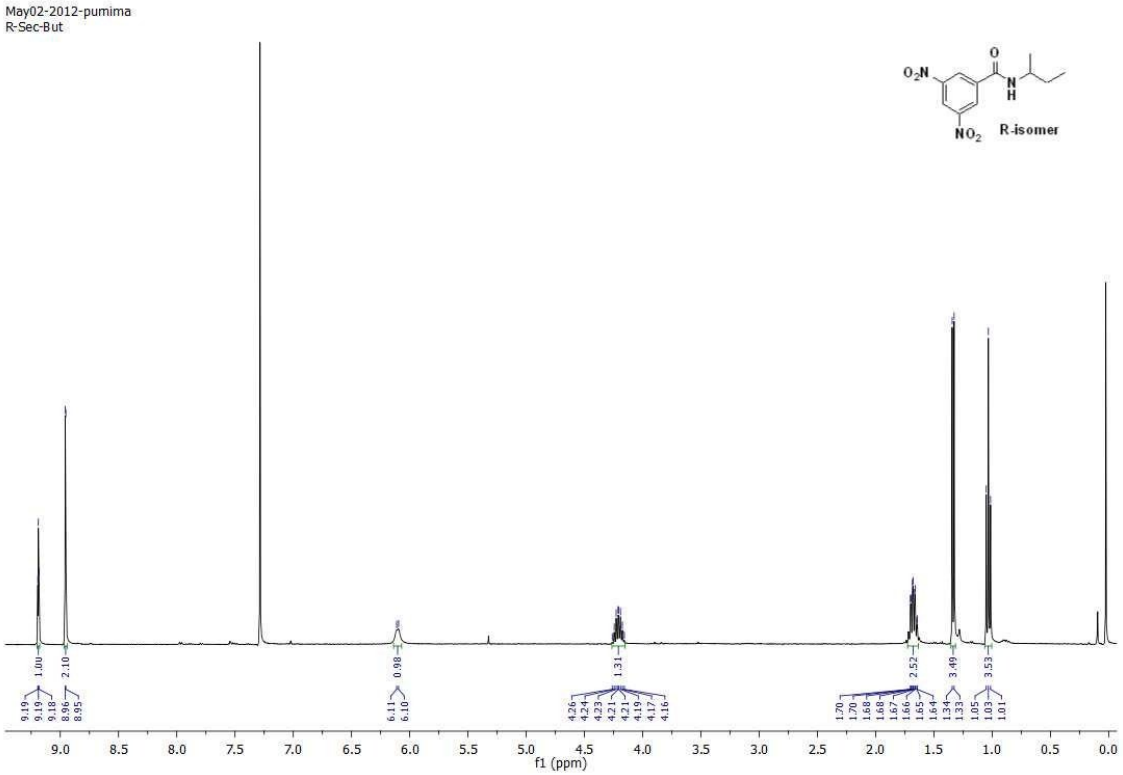
m/z	z	Abund	Formula	Ion
342.1096	-1	199693.44	C17 H16 N3 O5	(M-H)-
343.1126	-1	40620.65	C17 H16 N3 O5	(M-H)-
344.1146	-1	5707.66	C17 H16 N3 O5	(M-H)-
345.1157	-1	723.33	C17 H16 N3 O5	(M-H)-
378.0858	-1	5786.75	C17 H17 Cl N3 O5	(M+Cl)-
379.0865	-1	1078.57	C17 H17 Cl N3 O5	(M+Cl)-
380.083	-1	2086.93	C17 H17 Cl N3 O5	(M+Cl)-
381.0865	-1	463.38	C17 H17 Cl N3 O5	(M+Cl)-
685.2295	-1	672.09	C34 H33 N6 O10	(2M-H)-

Predicted Isotope Match Table

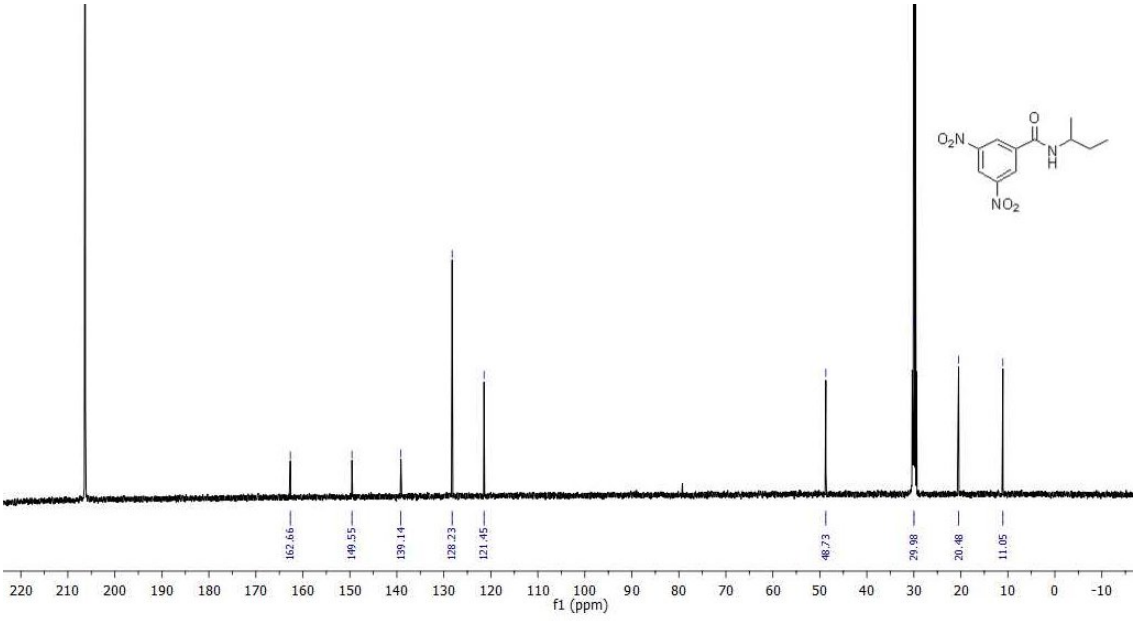
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	342.1096	342.1095	-0.24	100	100	80.93	81.25
2	343.1126	343.1126	-0.11	20.34	19.86	16.46	16.13
3	344.1146	344.115	1.19	2.86	2.9	2.31	2.35
4	345.1157	345.1175	5.03	0.36	0.31	0.29	0.26

--- End Of Report ---

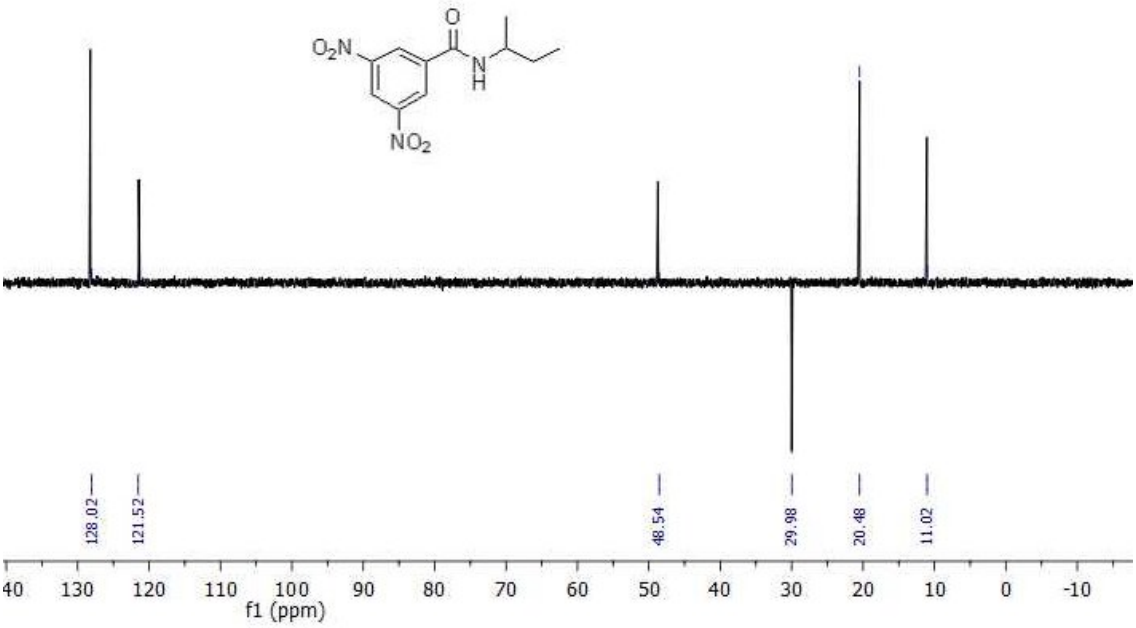
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8a:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **8a:**



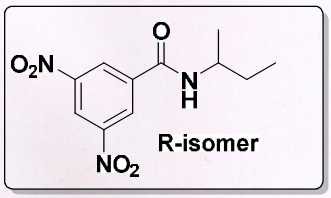
DEPT (126 MHz, Acetone-d_6) of compound **8a:**



HRMS (ESI-TOF) of compound **8a**:

Qualitative Compound Report

Data File	57.d	**Sample Name**	57
Sample Type	Sample	**Position**	Vial 22
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	04-03-2013 PM 3:45:46
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



Info.

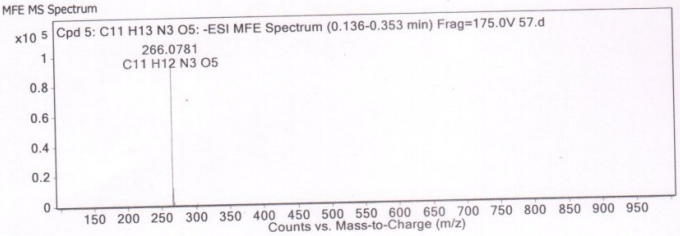
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C11 H13 N3 O5	0.187	267.0855	C11 H13 N3 O5	C11 H13 N3 O5	0.15	C11 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C11 H13 N3 O5	266.0781	0.187	Find by Molecular Feature	267.0855

MFE MS Spectrum



MS Spectrum Peak List

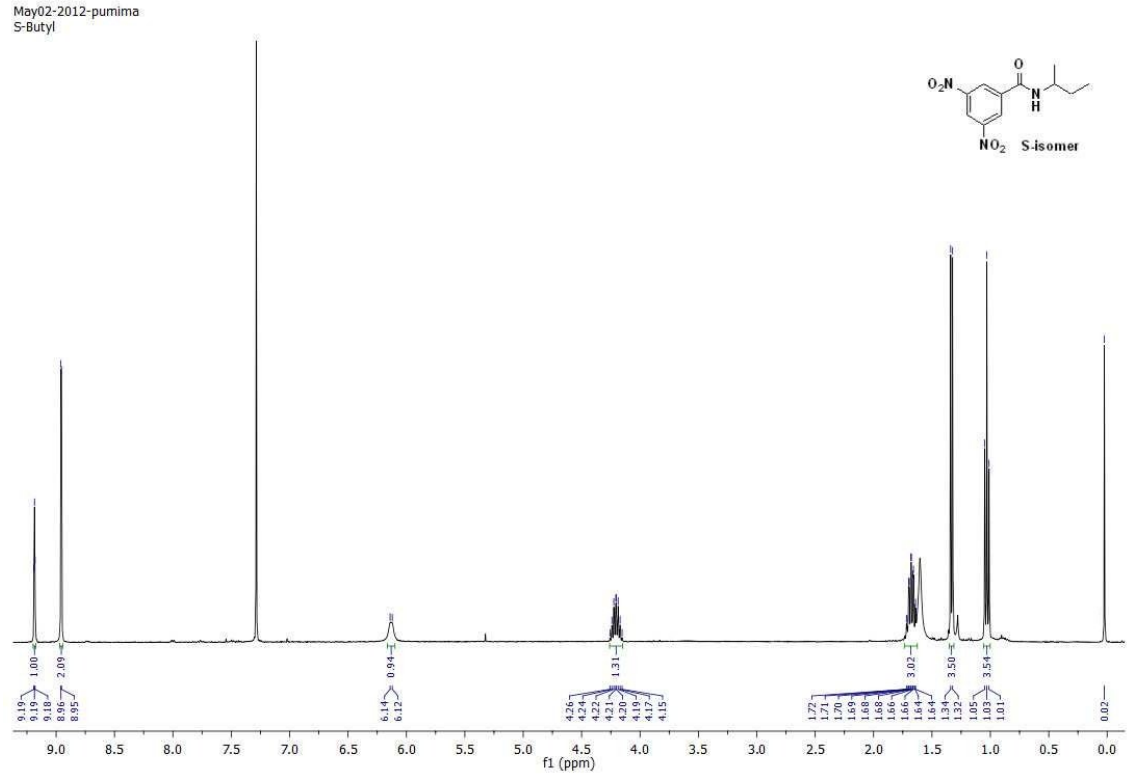
m/z	z	Abund	Formula	Ion
266.0781	-1	93970.29	C11 H12 N3 O5	(M-H)-
267.0814	-1	11795.6	C11 H12 N3 O5	(M-H)-
268.0839	-1	2285.53	C11 H12 N3 O5	(M-H)-
302.0545	-1	998.2	C11 H13 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

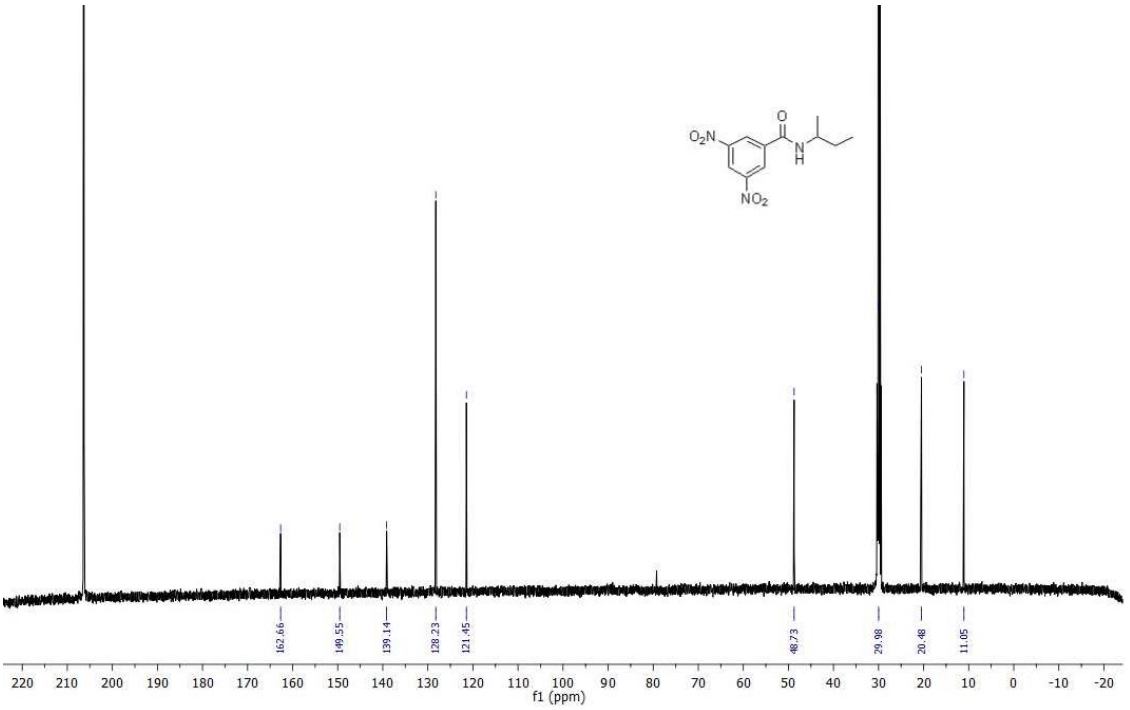
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	266.0781	266.0782	0.37	100	100	86.97	86.83
2	267.0814	267.0811	-1	12.55	13.32	10.92	11.57
3	268.0839	268.0831	-3.02	2.43	1.85	2.12	1.6

--- End Of Report ---

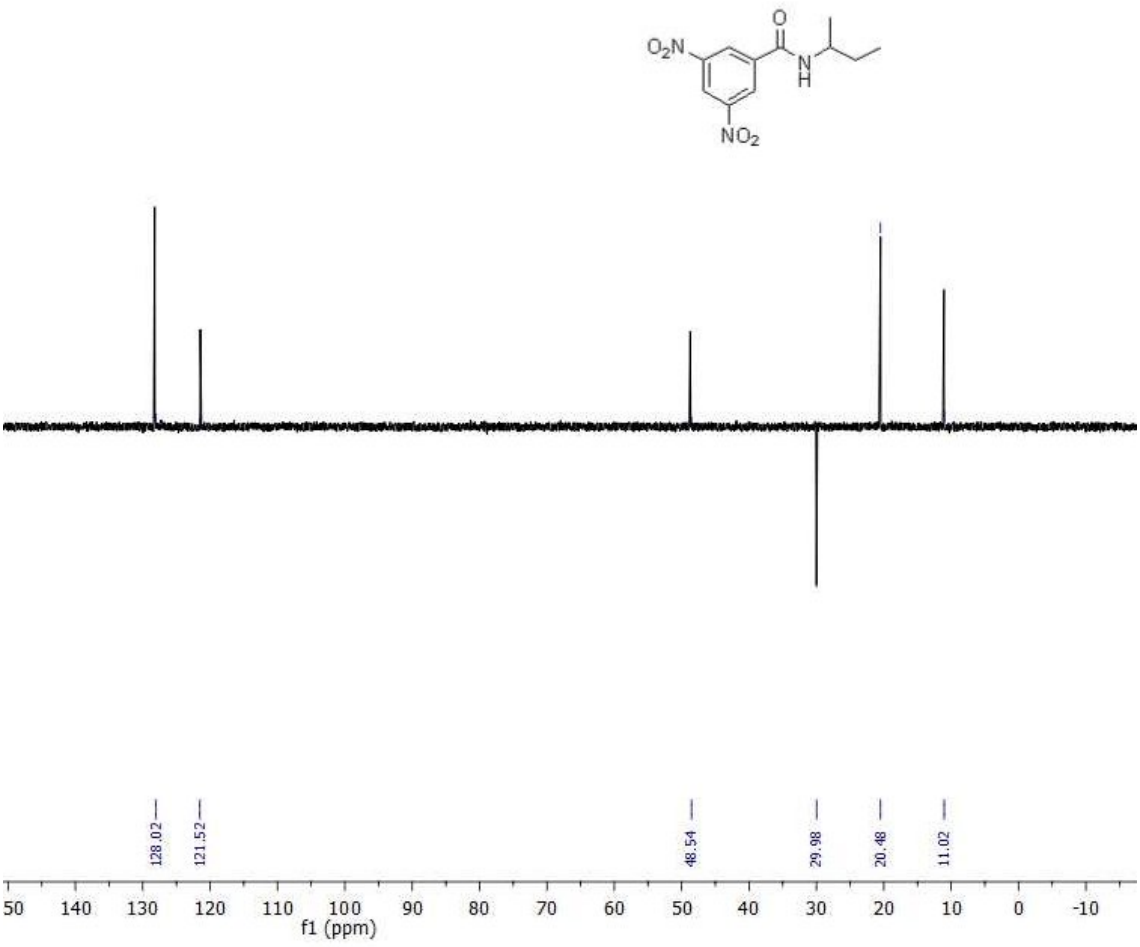
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8b:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **8b:**



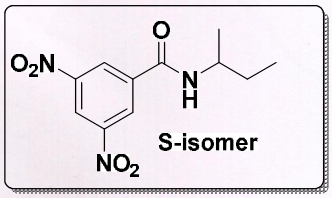
DEPT (126 MHz, Acetone-d_6) of compound **8b:**



HRMS (ESI-TOF) of compound **8b**:

Qualitative Compound Report

Data File	58.d	Sample Name	58
Sample Type	Sample	Position	Vial 23
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_neg12-01-13.m	Acquired Time	04-03-2013 PM 3:50:17
IRM Calibration Status	Success	DA Method	SamplePurity-Default.m
Comment			



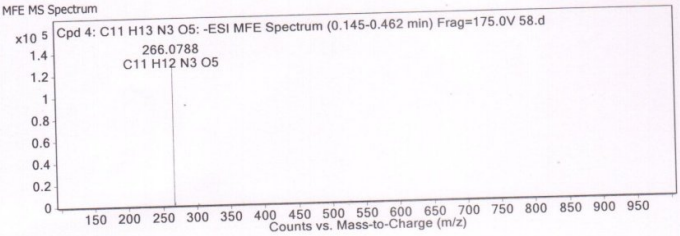
Info.	
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C11 H13 N3 O5	0.19	267.0861	C11 H13 N3 O5	C11 H13 N3 O5	-2.19	C11 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C11 H13 N3 O5	266.0788	0.19	Find by Molecular Feature	267.0861

MFE MS Spectrum



MS Spectrum Peak List

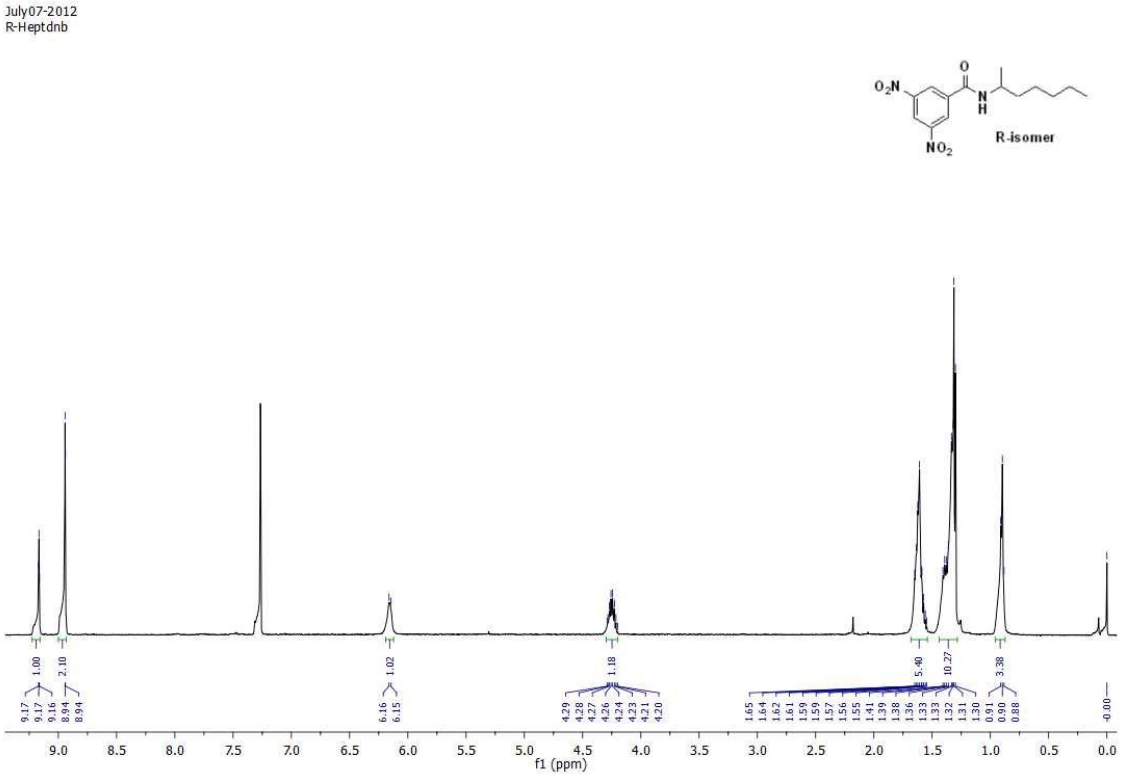
m/z	z	Abund	Formula	Ion
266.0788	-1	128660.33	C11 H12 N3 O5	(M-H)-
267.0818	-1	16763.63	C11 H12 N3 O5	(M-H)-
268.0835	-1	3442.76	C11 H12 N3 O5	(M-H)-
302.0545	-1	1417.69		(M+Cl)-
303.0554	-1	479.55		(M+Cl)-
304.0502	-1	545.05		(M+Cl)-

Predicted Isotope Match Table

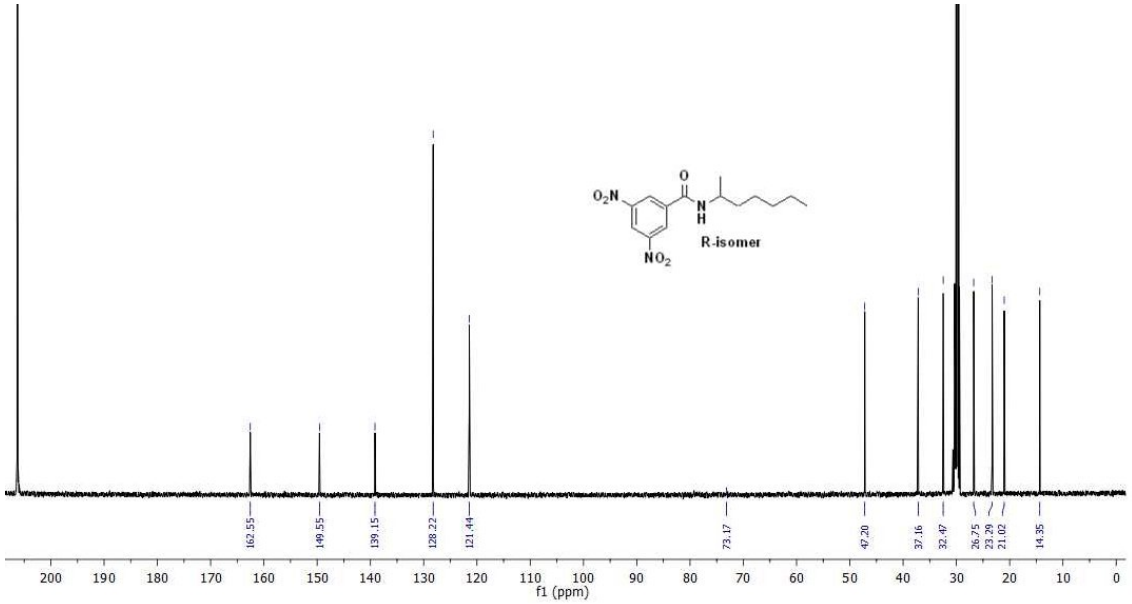
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	266.0788	266.0782	-2.17	100	100	86.43	86.83
2	267.0818	267.0811	-2.56	13.03	13.32	11.26	11.57
3	268.0835	268.0831	-1.45	2.68	1.85	2.31	1.6

--- End Of Report ---

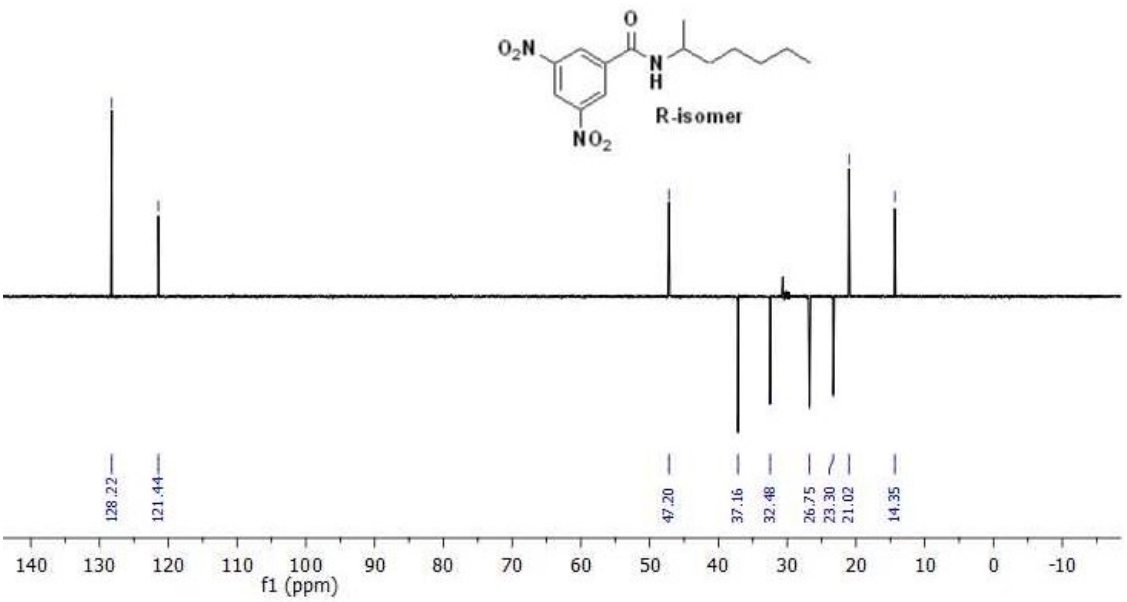
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8c:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **8c:**



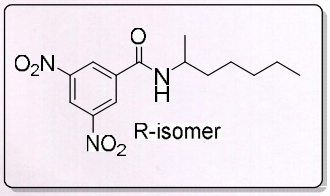
DEPT (126 MHz, Acetone-d_6) of compound **8c:**



HRMS (ESI-TOF) of compound **8c**:

Qualitative Compound Report

Data File	82.d	**Sample Name**	82
Sample Type	Sample	**Position**	Vial 36
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	28-07-2012 PM 03:03:17
IRM Calibration Status	Some Ions Missed	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

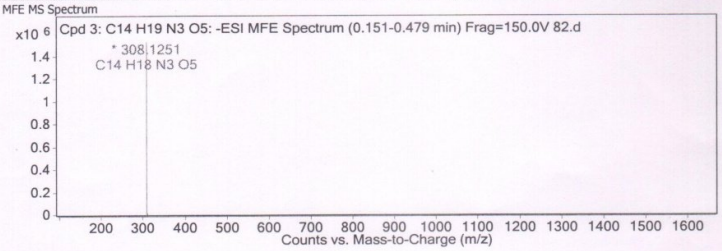


Compound Table

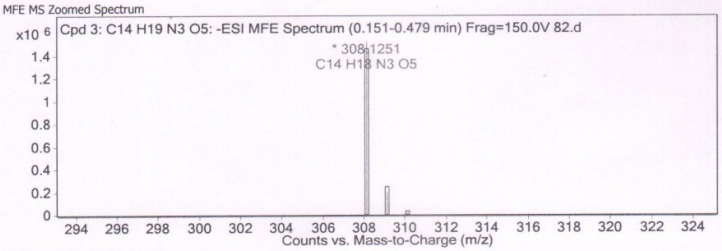
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C14 H19 N3 O5	0.212	309.1324	C14 H19 N3 O5	C14 H19 N3 O5	0.15	C14 H19 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C14 H19 N3 O5	308.1251	0.212	Find by Molecular Feature	309.1324

MFE MS Spectrum



MFE MS Zoomed Spectrum

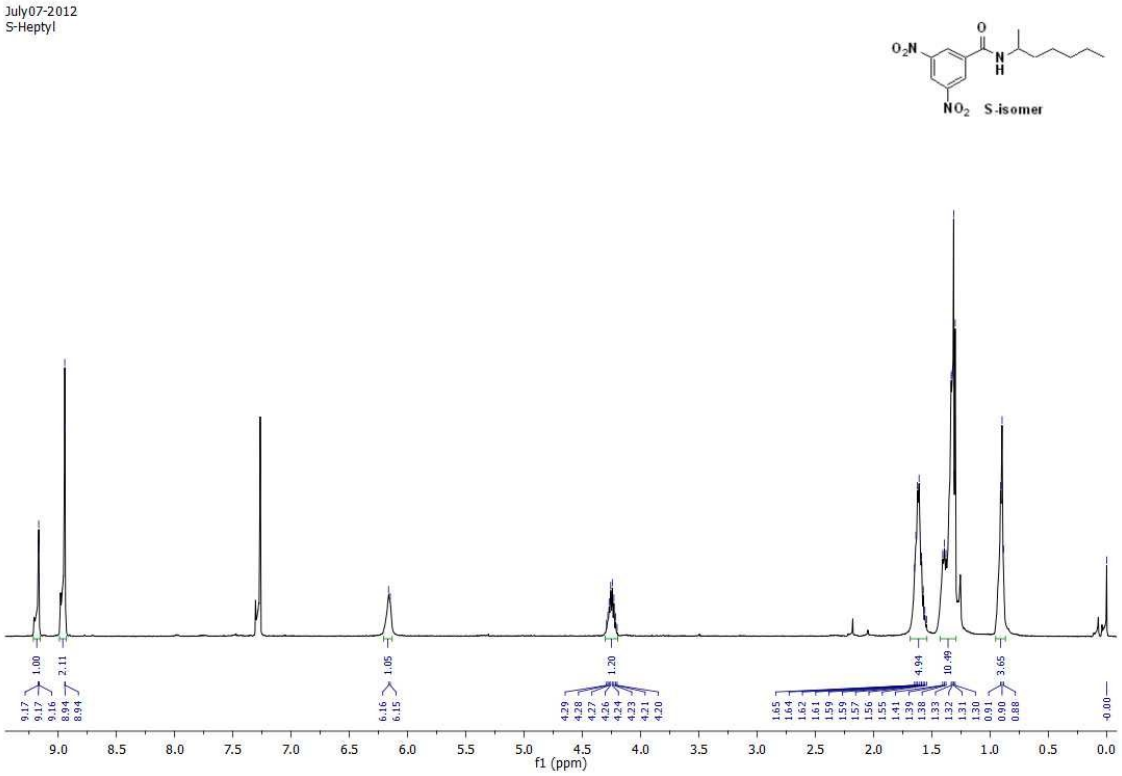


MS Spectrum Peak List

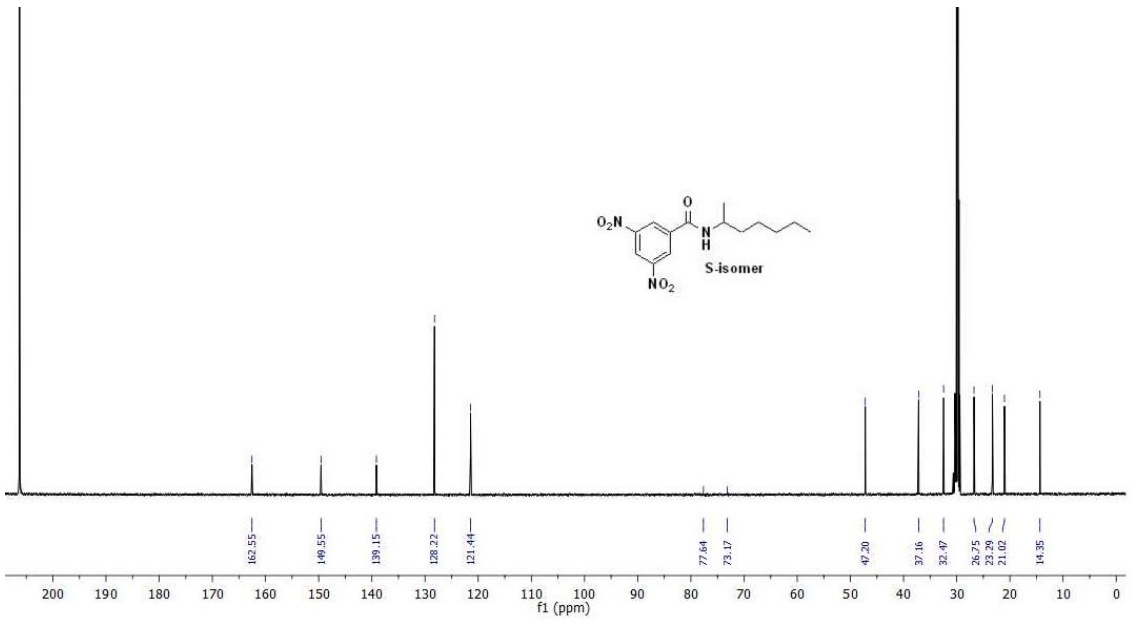
m/z	z	Abund	Formula	Ion
308.1251	-1	1525367.6	C14 H18 N3 O5	(M-H)-
309.1295	-1	200073	C14 H18 N3 O5	(M-H)-
310.1323	-1	16105.4	C14 H18 N3 O5	(M-H)-

--- End Of Report ---

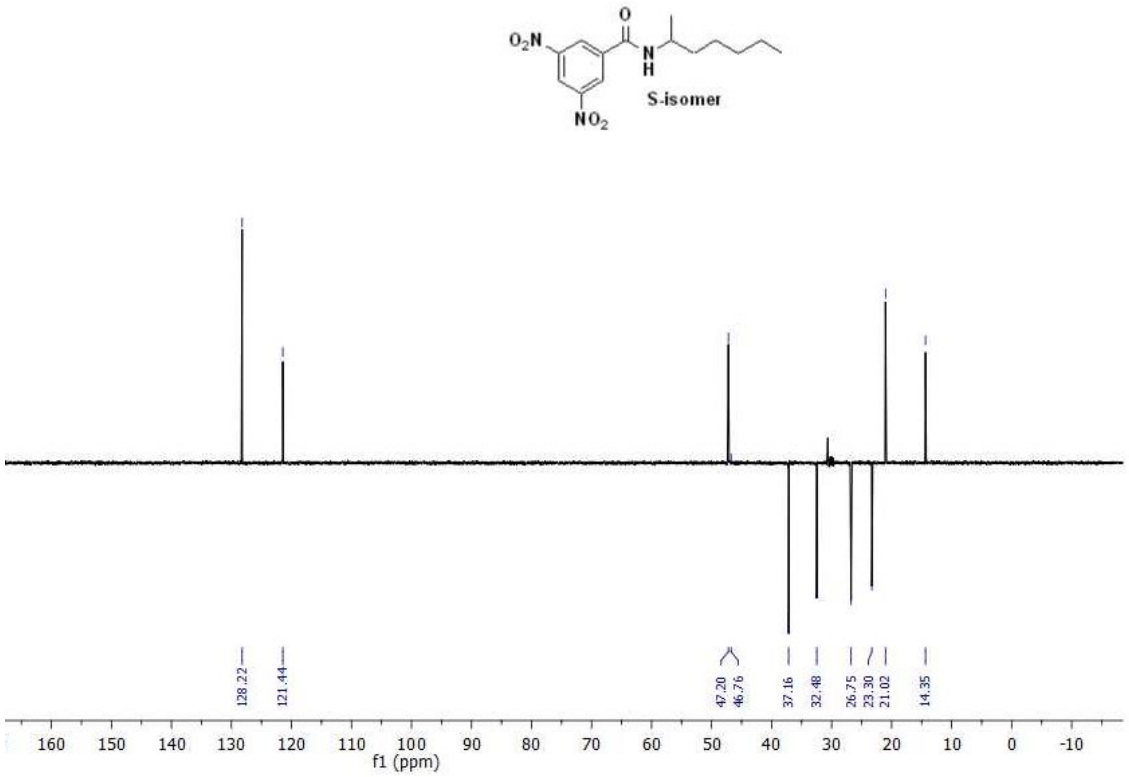
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8d:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **8d:**



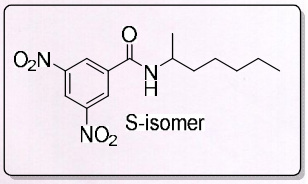
DEPT (126 MHz, Acetone-d_6) of compound **8d:**



HRMS (ESI-TOF) of compound **8d**:

Qualitative Compound Report

Data File	83.d	**Sample Name**	83
Sample Type	Sample	**Position**	Vial 37
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_Negative_mode.m	**Acquired Time**	28-07-2012 PM 03:08:43
IRM Calibration Status	Some Ions Missed	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

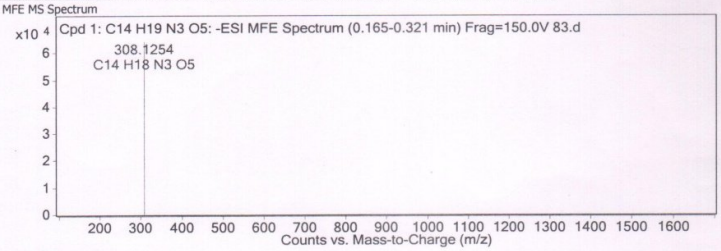


Compound Table

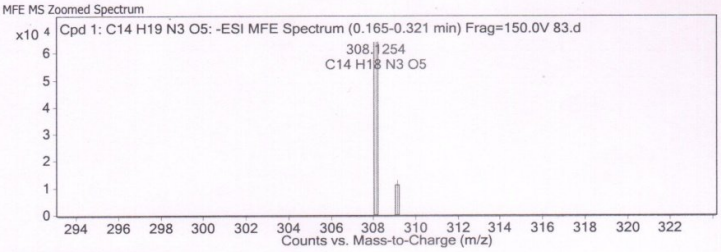
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C14 H19 N3 O5	0.212	309.1327	C14 H19 N3 O5	C14 H19 N3 O5	-0.7	C14 H19 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H19 N3 O5	308.1254	0.212	Find by Molecular Feature	309.1327

MFE MS Spectrum



MFE MS Zoomed Spectrum

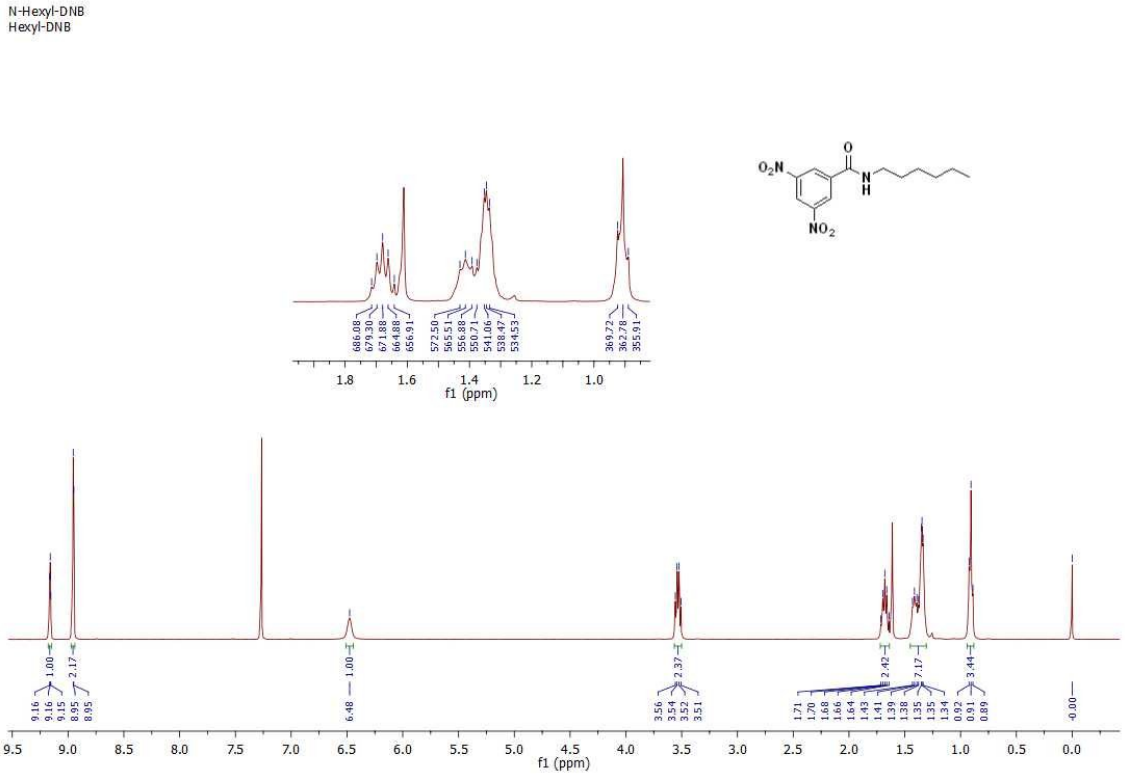


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
308.1254	-1	64050.7	C14 H18 N3 O5	(M-H)-
309.1287	-1	12739.6	C14 H18 N3 O5	(M-H)-

--- End Of Report ---

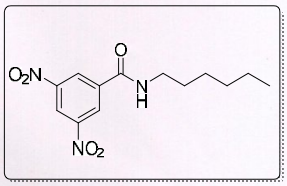
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8e:**



HRMS (ESI-TOF) of compound **8e**:

Qualitative Compound Report

Data File	94.d	**Sample Name**	94
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 5:14:18
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



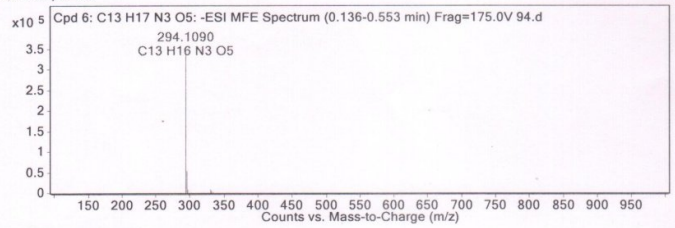
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C13 H17 N3 O5	0.194	295.1163	C13 H17 N3 O5	C13 H17 N3 O5	1.93	C13 H17 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C13 H17 N3 O5	294.109	0.194	Find by Molecular Feature	295.1163

MFE MS Spectrum



MS Spectrum Peak List

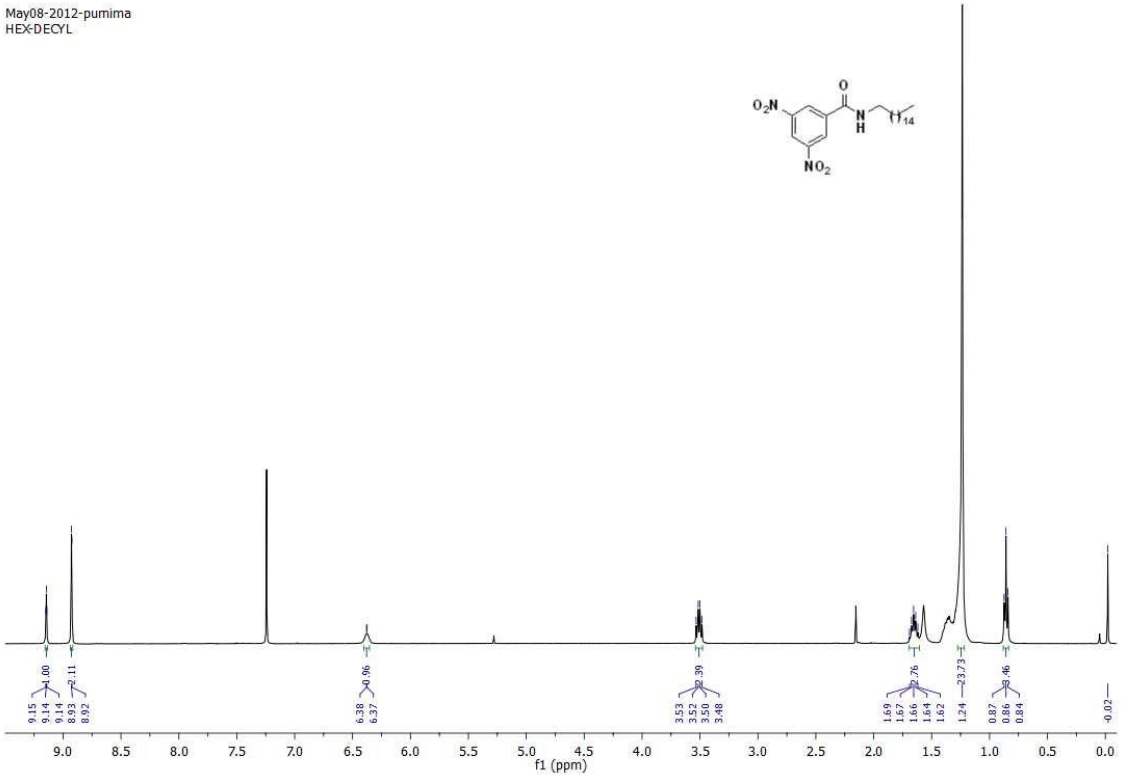
m/z	z	Abund	Formula	Ion
294.109	-1	341663.66	C13 H16 N3 O5	(M-H)-
295.1119	-1	52674.53	C13 H16 N3 O5	(M-H)-
296.1141	-1	7395.77	C13 H16 N3 O5	(M-H)-
297.1175	-1	824.31	C13 H16 N3 O5	(M-H)-
330.0852	-1	8844.18	C13 H17 Cl N3 O5	(M+Cl)-
331.0885	-1	1484.76	C13 H17 Cl N3 O5	(M+Cl)-
332.0828	-1	3362.59	C13 H17 Cl N3 O5	(M+Cl)-
333.0839	-1	371.07	C13 H17 Cl N3 O5	(M+Cl)-
334.0988	-1	1427.12	C13 H17 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	294.109	294.1095	1.94	100	100	84.87	84.82
2	295.1119	295.1125	1.98	15.42	15.53	13.08	13.17
3	296.1141	296.1146	1.68	2.16	2.16	1.84	1.83
4	297.1175	297.1171	-1.14	0.24	0.21	0.2	0.18

--- End Of Report ---

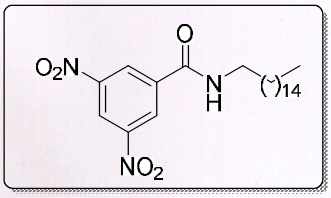
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8f:**



HRMS (ESI-TOF) of compound **8f**:

Qualitative Compound Report

Data File	59.d	**Sample Name**	59
Sample Type	Sample	**Position**	Vial 37
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 6:14:48
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



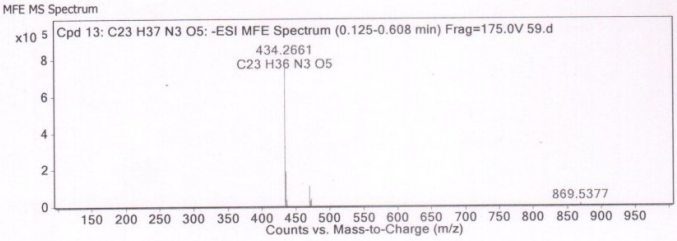
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C23 H37 N3 O5	0.19	435.2735	C23 H37 N3 O5	C23 H37 N3 O5	-0.33	C23 H37 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C23 H37 N3 O5	434.2661	0.19	Find by Molecular Feature	435.2735

MFE MS Spectrum



MS Spectrum Peak List

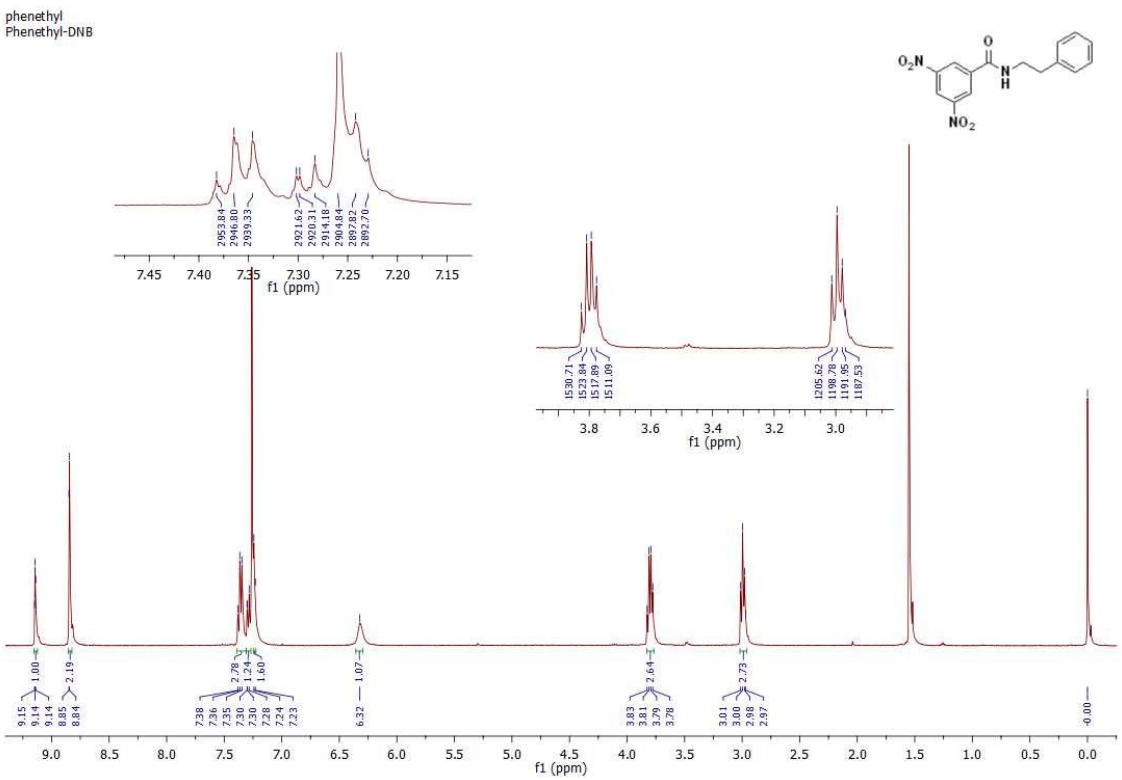
m/z	z	Abund	Formula	Ion
434.2661	-1	764667.69	C23 H36 N3 O5	(M-H)-
435.2694	-1	186249.17	C23 H36 N3 O5	(M-H)-
436.2724	-1	29959.85	C23 H36 N3 O5	(M-H)-
437.2761	-1	4755.93	C23 H36 N3 O5	(M-H)-
470.2425	-1	109277.3	C23 H37 Cl N3 O5	(M+Cl)-
471.2455	-1	29304.59	C23 H37 Cl N3 O5	(M+Cl)-
472.2405	-1	37263.44	C23 H37 Cl N3 O5	(M+Cl)-
473.2435	-1	9328.33	C23 H37 Cl N3 O5	(M+Cl)-
869.5377	-1	7317.81		(2M-H)-
870.5405	-1	5897.85		(2M-H)-

Predicted Isotope Match Table

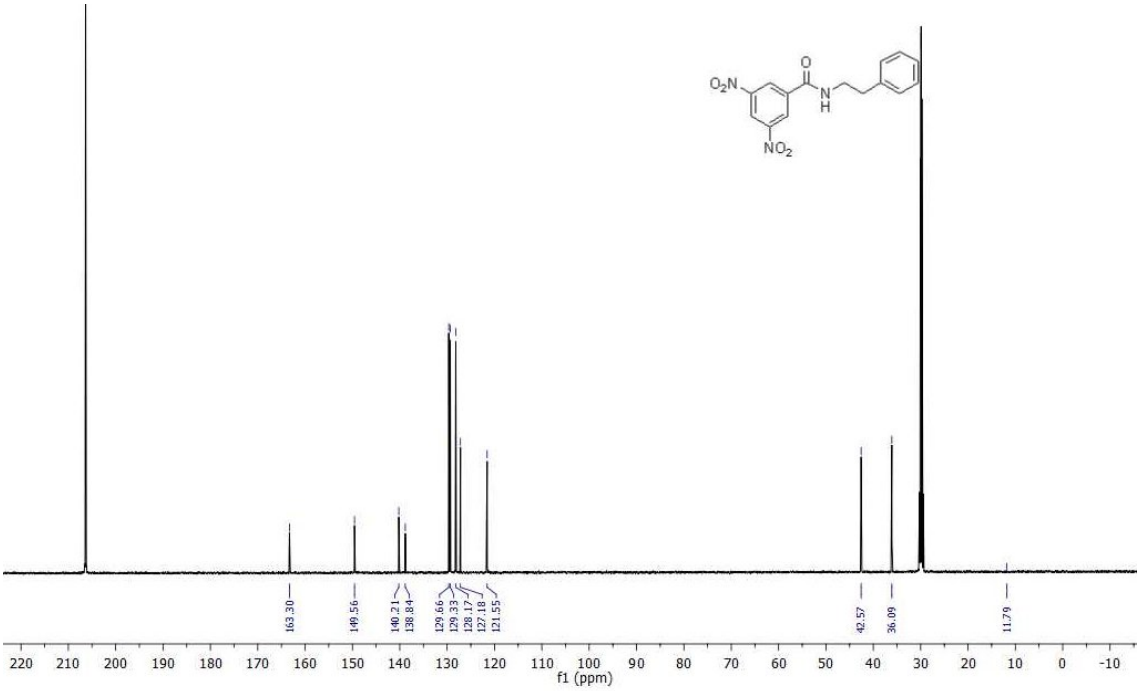
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	434.2661	434.266	-0.2	100	100	77.54	75.99
2	435.2694	435.2692	-0.59	24.36	26.58	18.89	20.19
3	436.2724	436.2719	-1.31	3.92	4.42	3.04	3.36
4	437.2761	437.2745	-3.77	0.62	0.55	0.48	0.42
5	438.2779	438.277	-2.05	0.07	0.06	0.05	0.04

--- End Of Report ---

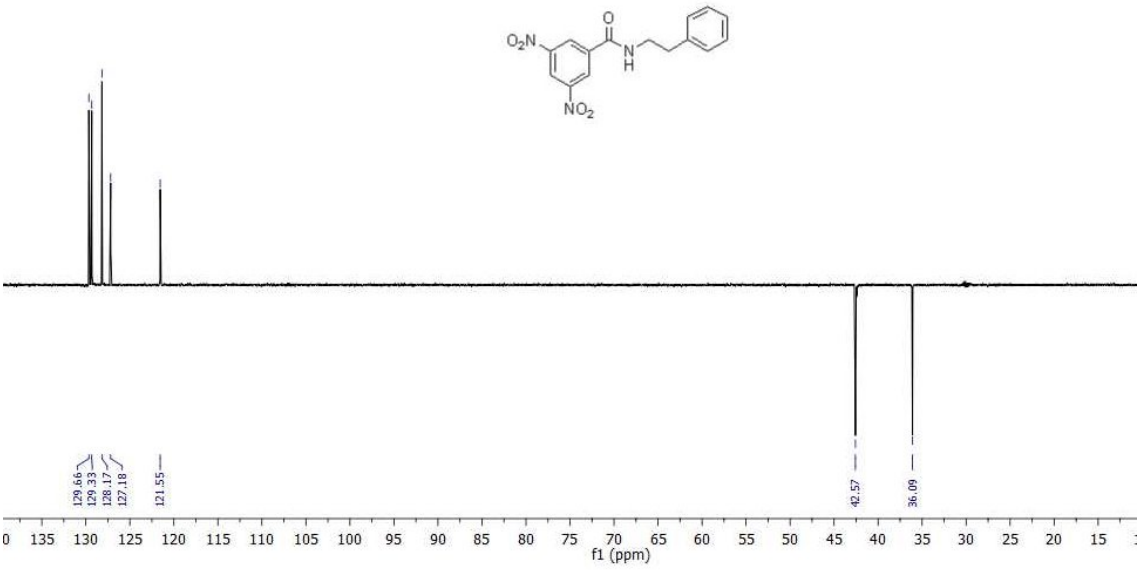
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9a:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9a:**



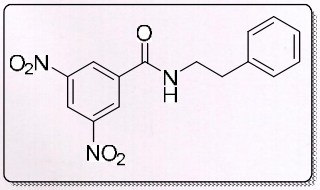
DEPT (126 MHz, Acetone-d_6) of compound **9a:**



HRMS (ESI-TOF) of compound **9a**:

Qualitative Compound Report

Data File	89.d	**Sample Name**	89
Sample Type	Sample	**Position**	Vial 13
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:47:02
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

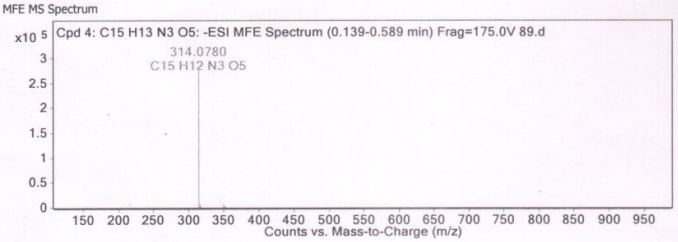


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C15 H13 N3 O5	0.193	315.0853	C15 H13 N3 O5	C15 H13 N3 O5	0.84	C15 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C15 H13 N3 O5	314.078	0.193	Find by Molecular Feature	315.0853

MFE MS Spectrum



MS Spectrum Peak List

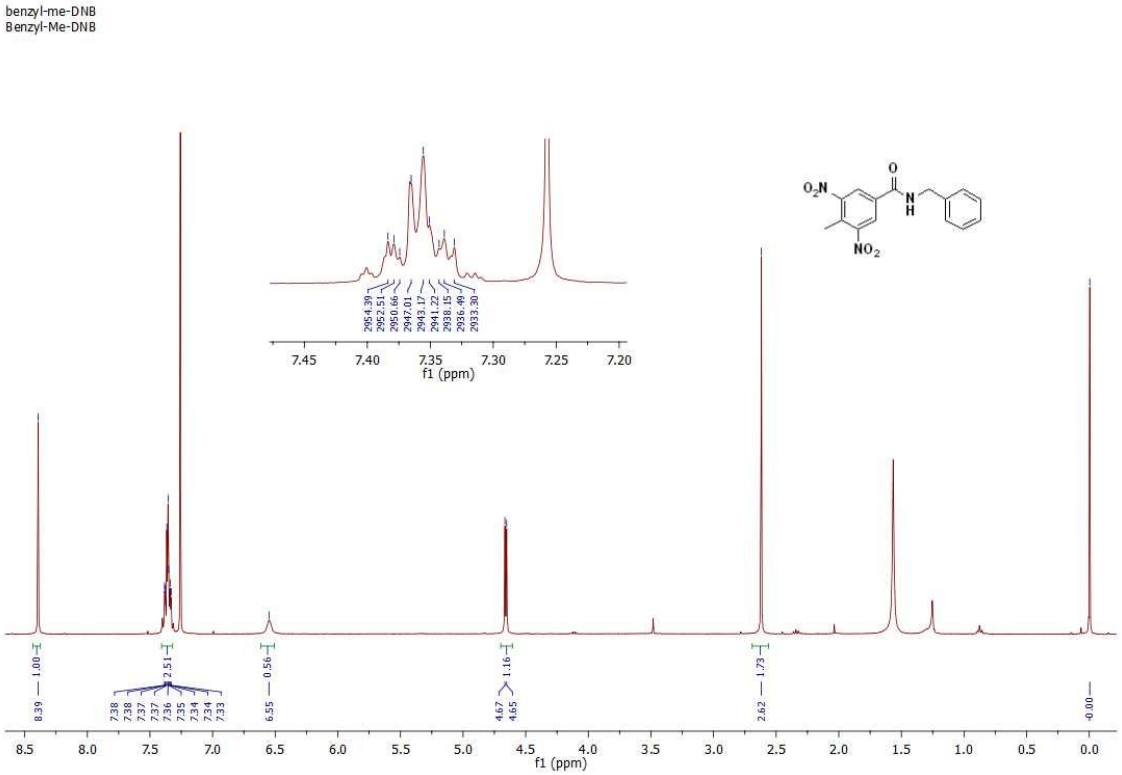
m/z	z	Abund	Formula	Ion
314.078	-1	282142.03	C15 H12 N3 O5	(M-H)-
315.0807	-1	46531.81	C15 H12 N3 O5	(M-H)-
316.0834	-1	7398.45	C15 H12 N3 O5	(M-H)-
317.0845	-1	915.71	C15 H12 N3 O5	(M-H)-
350.0543	-1	6271.39	C15 H13 Cl N3 O5	(M+Cl)-
351.0567	-1	918.49	C15 H13 Cl N3 O5	(M+Cl)-
352.0518	-1	2316.99	C15 H13 Cl N3 O5	(M+Cl)-
353.0533	-1	587.3	C15 H13 Cl N3 O5	(M+Cl)-
354.0681	-1	819.36	C15 H13 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

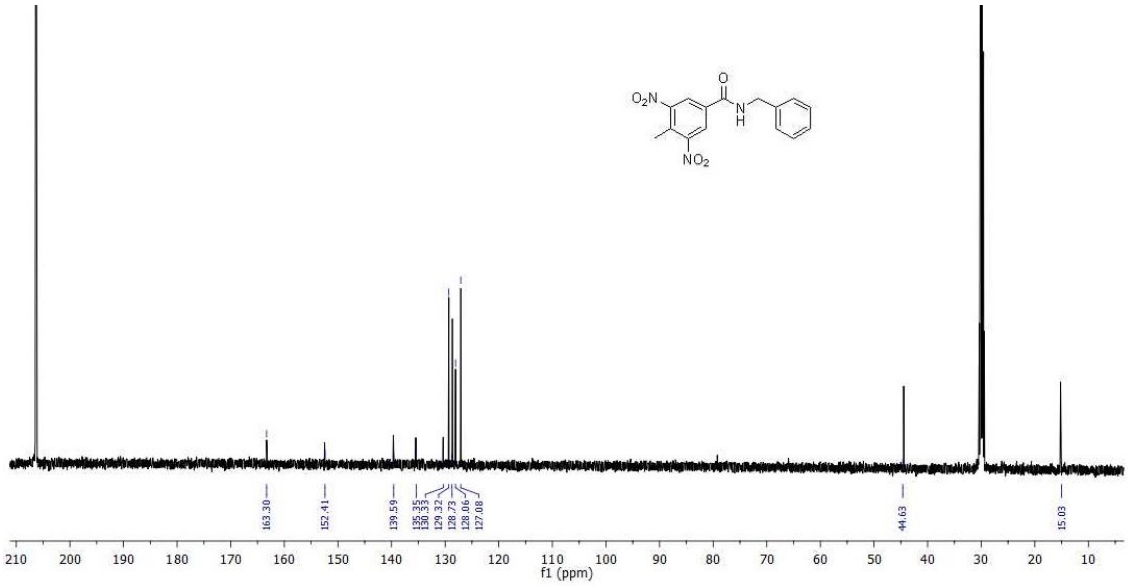
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	314.078	314.0782	0.69	100	100	83.72	83.06
2	315.0807	315.0812	1.74	16.49	17.65	13.81	14.66
3	316.0834	316.0835	0.38	2.62	2.49	2.2	2.07
4	317.0845	317.086	4.72	0.32	0.26	0.27	0.21

--- End Of Report ---

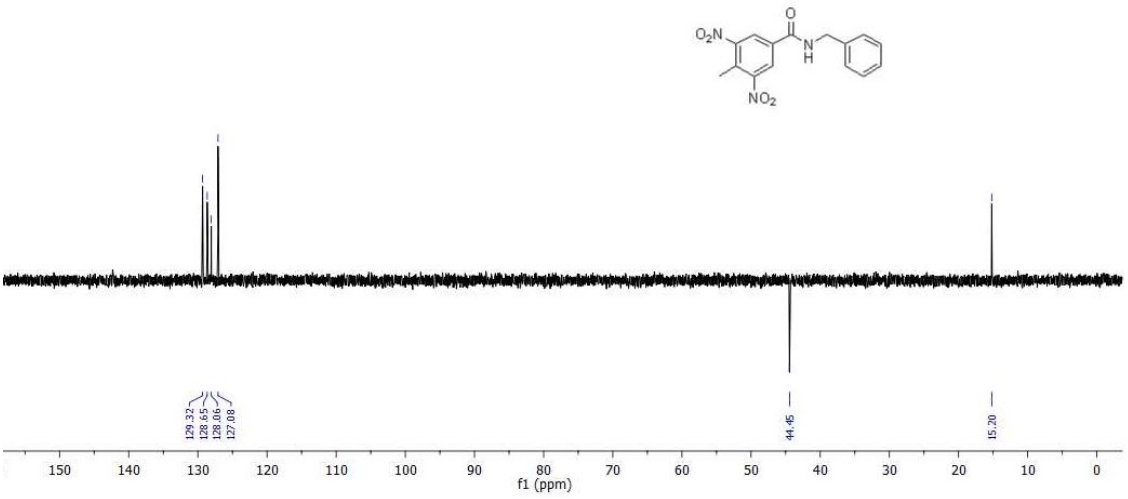
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9b:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9b:**



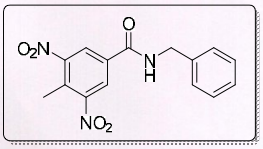
DEPT (126 MHz, Acetone-d_6) of compound **9b:**



HRMS (ESI-TOF) of compound **9b**:

Qualitative Compound Report

Data File	100.d	**Sample Name**	100
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:33:24
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



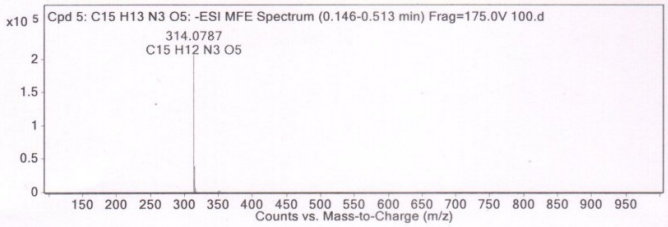
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C15 H13 N3 O5	0.193	315.0859	C15 H13 N3 O5	C15 H13 N3 O5	-1.2	C15 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C15 H13 N3 O5	314.0787	0.193	Find by Molecular Feature	315.0859

MFE MS Spectrum



MS Spectrum Peak List

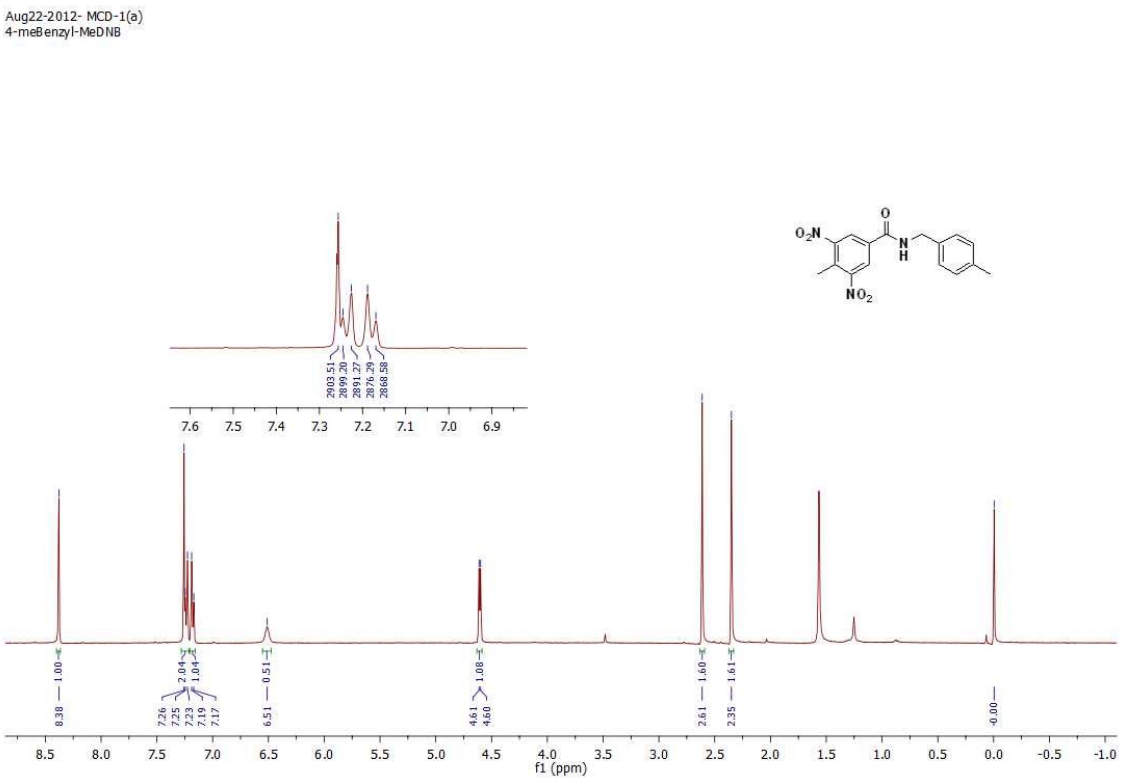
m/z	z	Abund	Formula	Ion
314.0787	-1	211157.81	C15 H12 N3 O5	(M-H)-
315.0815	-1	38568.73	C15 H12 N3 O5	(M-H)-
316.0838	-1	5885.88	C15 H12 N3 O5	(M-H)-
317.0835	-1	1286	C15 H12 N3 O5	(M-H)-
350.0554	-1	3078.83		(M+Cl)-
351.0578	-1	1302.27		(M+Cl)-
352.0514	-1	1904.36		(M+Cl)-

Predicted Isotope Match Table

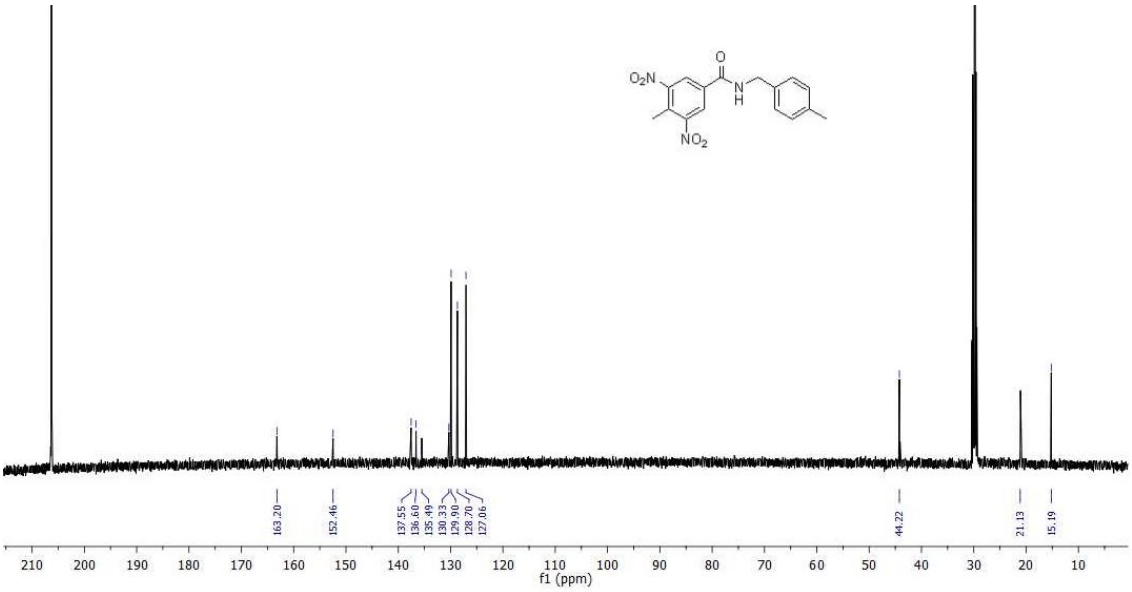
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	314.0787	314.0782	-1.33	100	100	82.2	83.06
2	315.0815	315.0812	-0.87	18.27	17.65	15.01	14.66
3	316.0838	316.0835	-0.91	2.79	2.49	2.29	2.07
4	317.0835	317.086	7.91	0.61	0.26	0.5	0.21

--- End Of Report ---

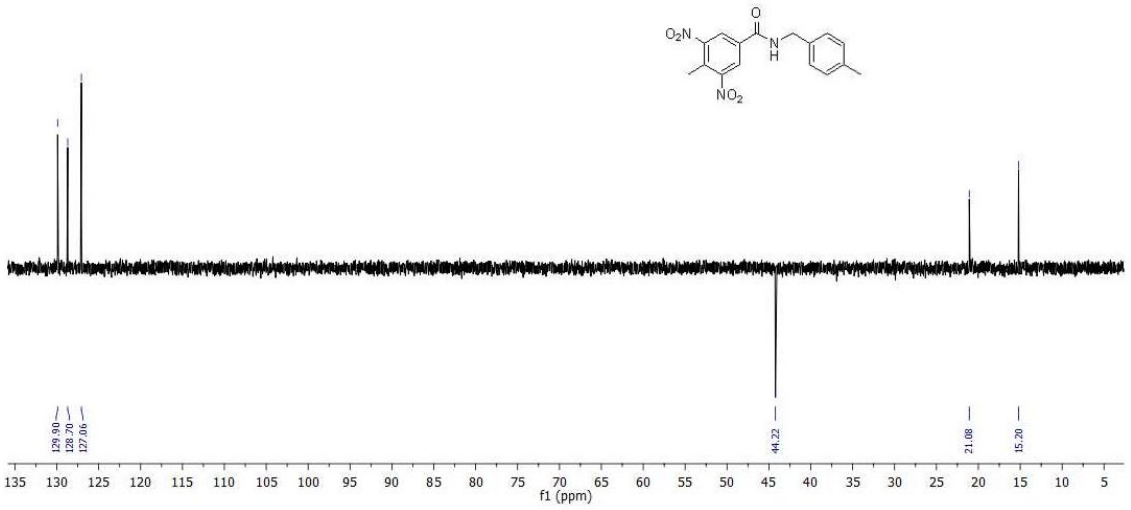
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9c:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9c:**



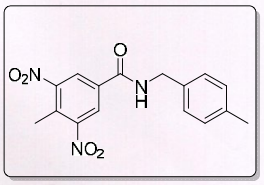
DEPT (126 MHz, Acetone-d_6) of compound **9c:**



HRMS (ESI-TOF) of compound **9c**:

Qualitative Compound Report

Data File	97.d	**Sample Name**	97
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:40:55
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



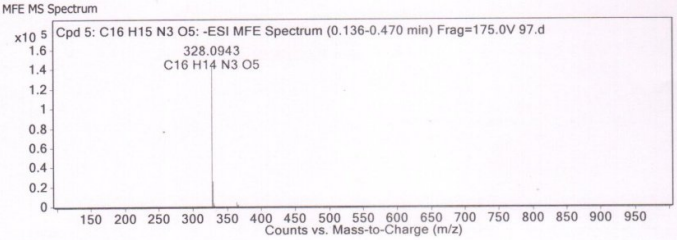
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C16 H15 N3 O5	0.189	329.1016	C16 H15 N3 O5	C16 H15 N3 O5	-1.16	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C16 H15 N3 O5	328.0943	0.189	Find by Molecular Feature	329.1016

MFE MS Spectrum



MS Spectrum Peak List

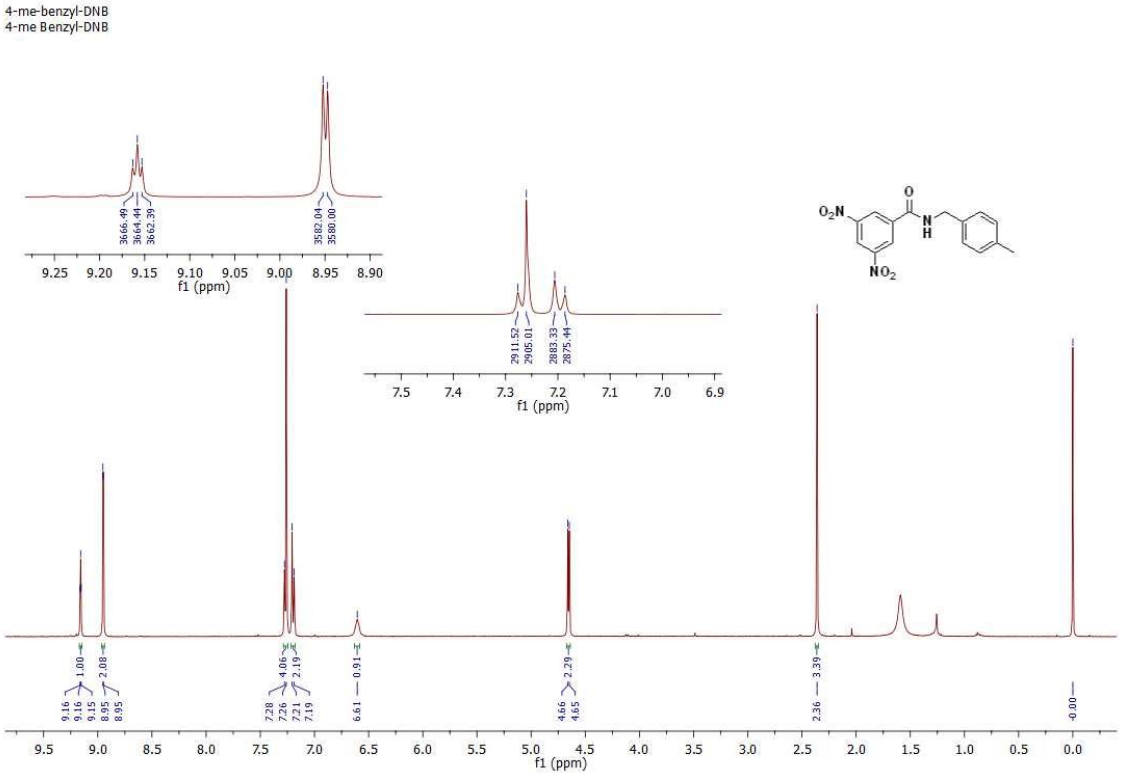
m/z	z	Abund	Formula	Ion
328.0943	-1	143199.56	C16 H14 N3 O5	(M-H)-
329.0973	-1	25317.36	C16 H14 N3 O5	(M-H)-
330.0989	-1	3646.56	C16 H14 N3 O5	(M-H)-
331.0982	-1	577.49	C16 H14 N3 O5	(M-H)-
364.0709	-1	3867.98		(M+Cl)-
365.0769	-1	1321.15		(M+Cl)-
366.0681	-1	1429.23		(M+Cl)-

Predicted Isotope Match Table

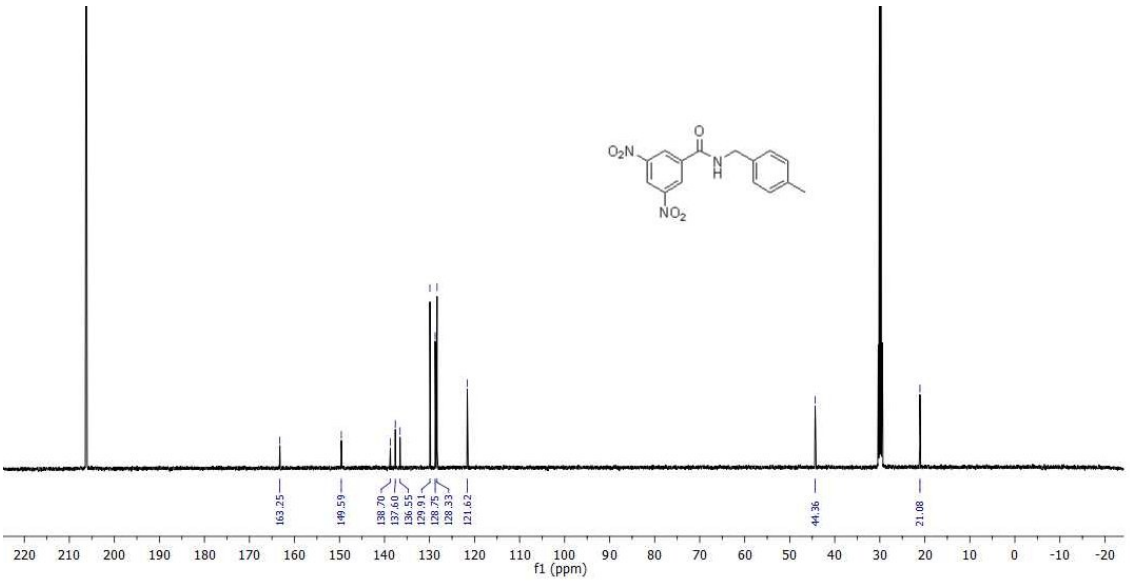
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.0943	328.0939	-1.26	100	100	82.9	82.15
2	329.0973	329.0969	-1.21	17.68	18.75	14.66	15.41
3	330.0989	330.0992	0.99	2.55	2.69	2.11	2.21
4	331.0982	331.1017	10.73	0.4	0.28	0.33	0.23

--- End Of Report ---

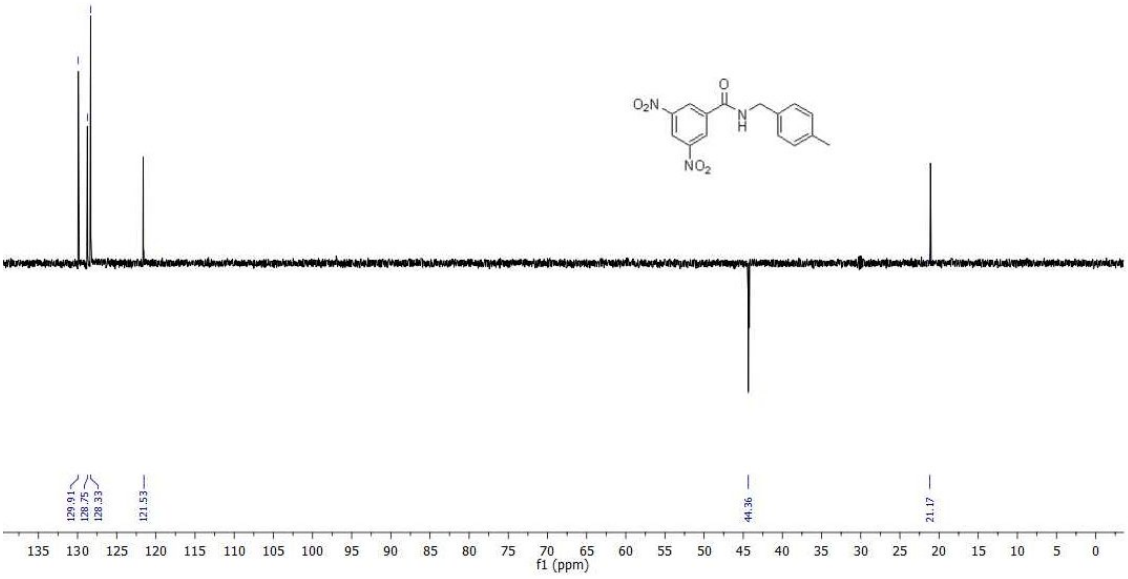
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9d:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9d:**



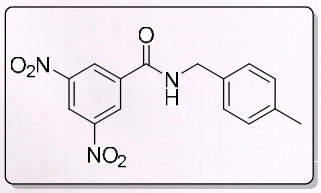
DEPT (126 MHz, Acetone-d_6) of compound **9d:**



HRMS (ESI-TOF) of compound **9d**:

Qualitative Compound Report

Data File	90.d	**Sample Name**	90
Sample Type	Sample	**Position**	Vial 16
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 5:00:38
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



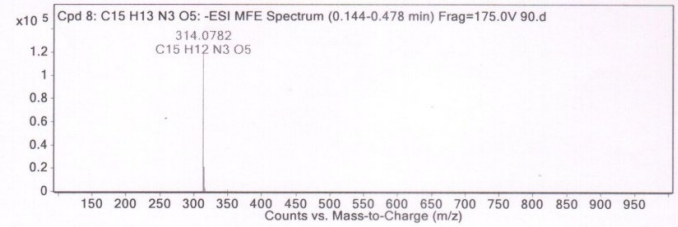
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C15 H13 N3 O5	0.191	315.0854	C15 H13 N3 O5	C15 H13 N3 O5	0.28	C15 H13 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C15 H13 N3 O5	314.0782	0.191	Find by Molecular Feature	315.0854

MFE MS Spectrum



MS Spectrum Peak List

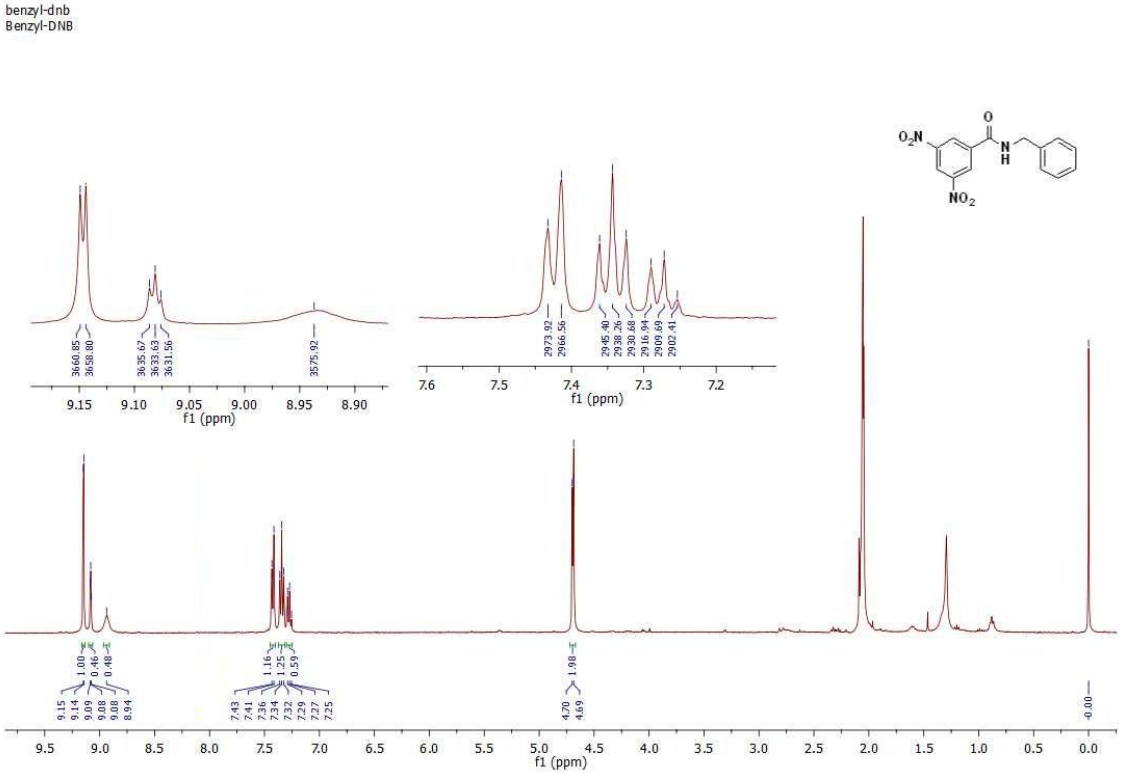
m/z	z	Abund	Formula	Ion
314.0782	-1	120876.75	C15 H12 N3 O5	(M-H)-
315.0811	-1	21042.51	C15 H12 N3 O5	(M-H)-
316.0836	-1	2708.79	C15 H12 N3 O5	(M-H)-
317.0866	-1	318.94	C15 H12 N3 O5	(M-H)-
350.0539	-1	1799.25	C15 H13 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

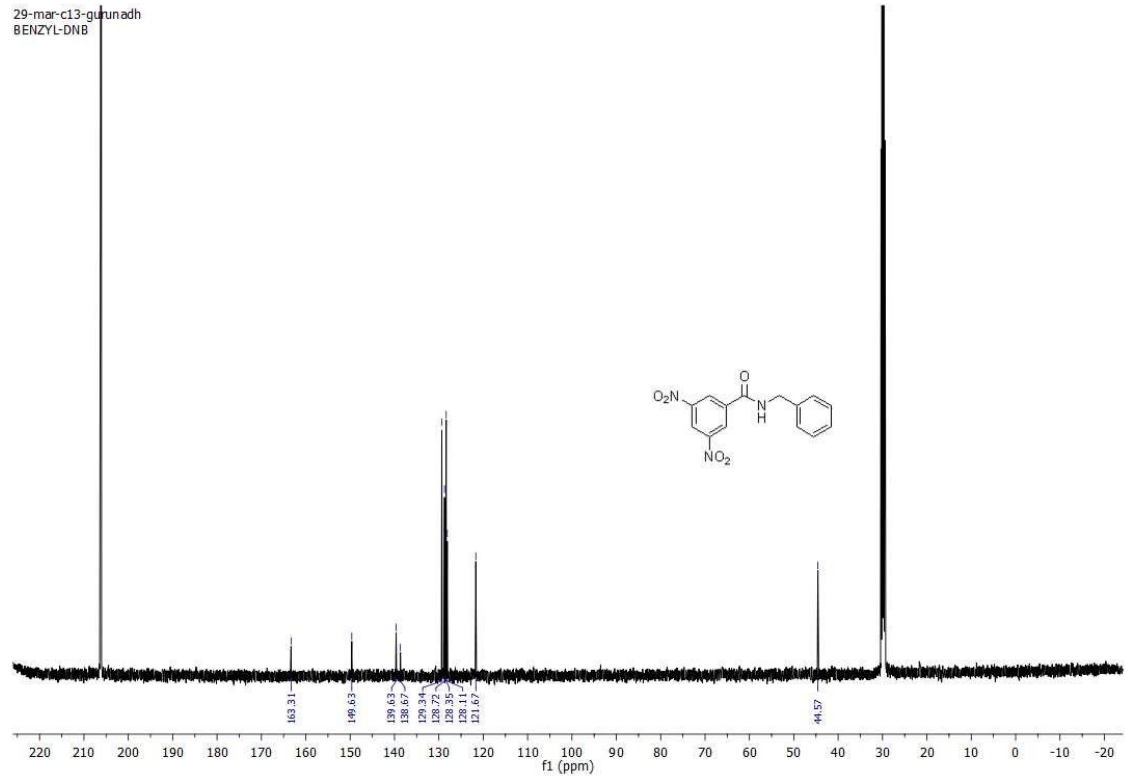
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	314.0782	314.0782	0.24	100	100	83.39	83.06
2	315.0811	315.0812	0.57	17.41	17.65	14.52	14.66
3	316.0836	316.0835	-0.19	2.24	2.49	1.87	2.07
4	317.0866	317.086	-2.01	0.26	0.26	0.22	0.21

--- End Of Report ---

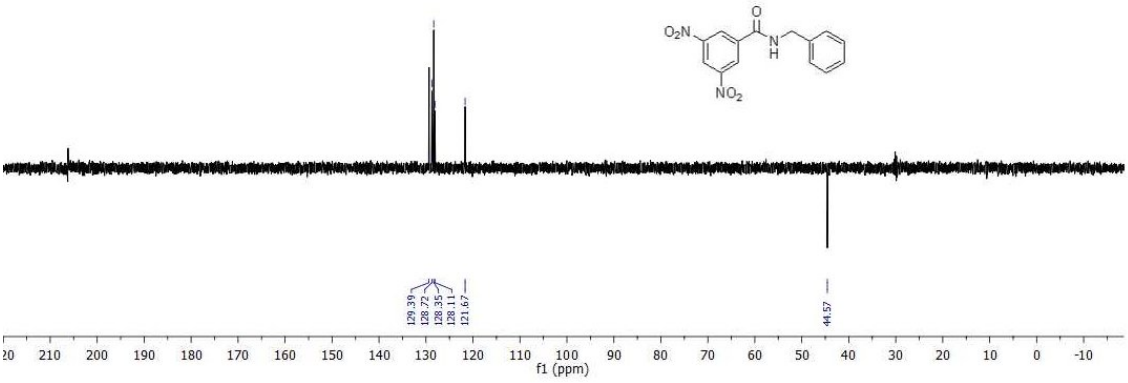
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9e:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9e:**



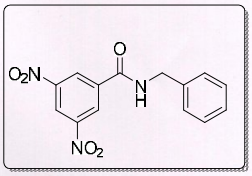
DEPT (126 MHz, Acetone-d_6) of compound **9e:**



HRMS (ESI-TOF) of compound **9e**:

Qualitative Compound Report

Data File	95.d	**Sample Name**	95
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:56:06
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

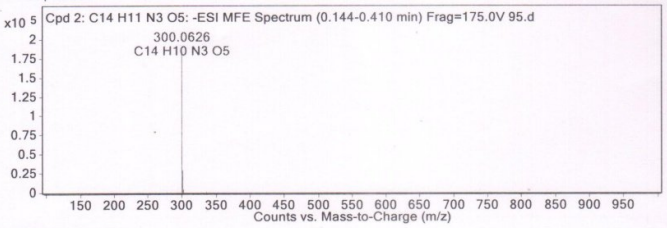


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C14 H11 N3 O5	0.192	301.0699	C14 H11 N3 O5	C14 H11 N3 O5	0	C14 H11 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C14 H11 N3 O5	300.0626	0.192	Find by Molecular Feature	301.0699

MFE MS Spectrum



MS Spectrum Peak List

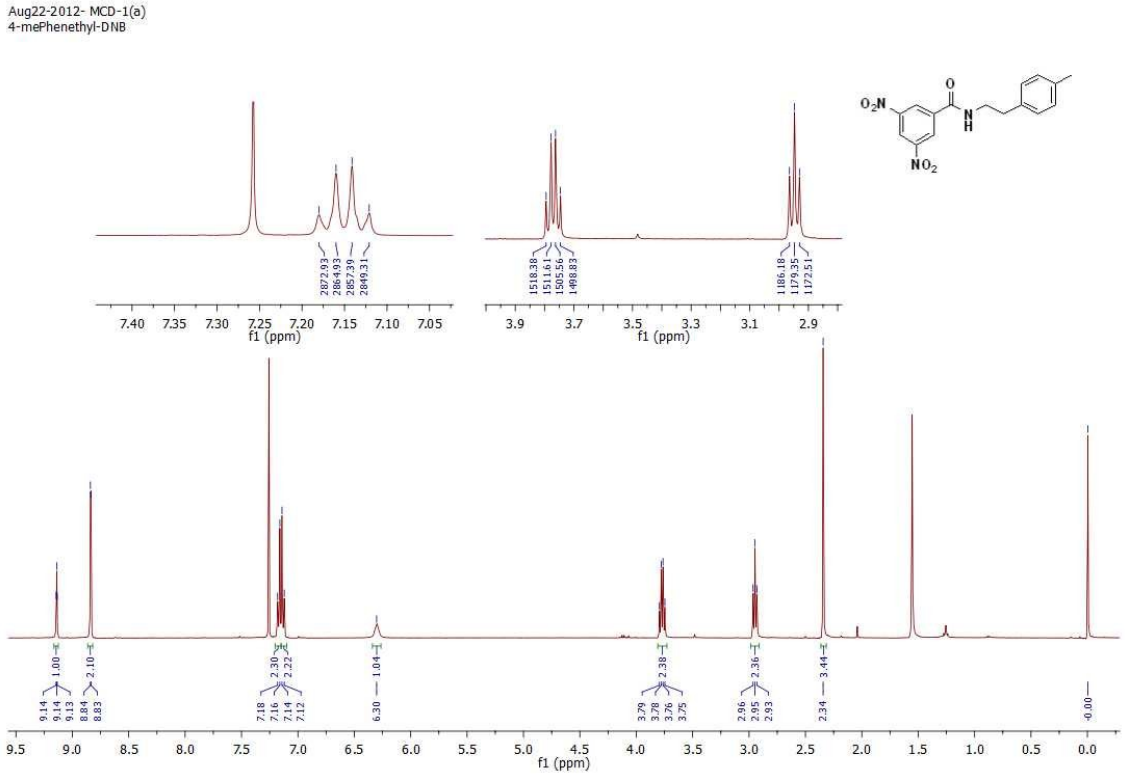
m/z	z	Abund	Formula	Ion
300.0626	-1	182599.19	C14 H10 N3 O5	(M-H)-
301.0655	-1	29832.1	C14 H10 N3 O5	(M-H)-
302.0675	-1	4209.35	C14 H10 N3 O5	(M-H)-
303.0685	-1	532.24	C14 H10 N3 O5	(M-H)-
336.0382	-1	1083.18	C14 H11 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

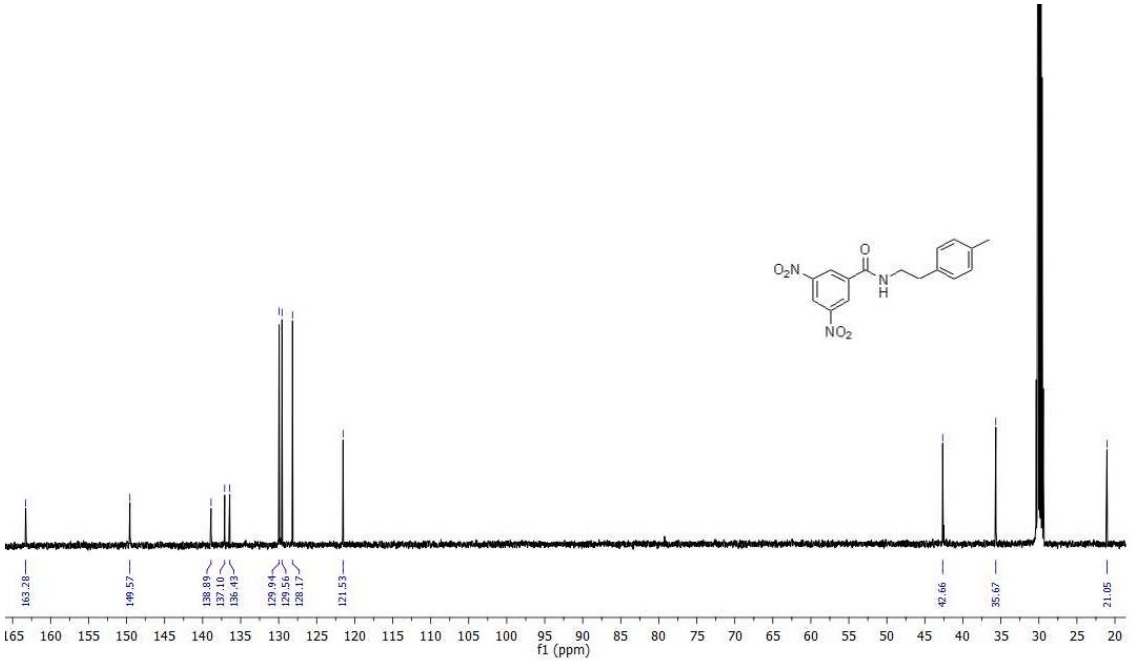
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	300.0626	300.0626	-0.06	100	100	84.08	83.97
2	301.0655	301.0656	0.16	16.34	16.54	13.74	13.89
3	302.0675	302.0678	0.73	2.31	2.31	1.94	1.94
4	303.0685	303.0702	5.85	0.29	0.23	0.25	0.19

--- End Of Report ---

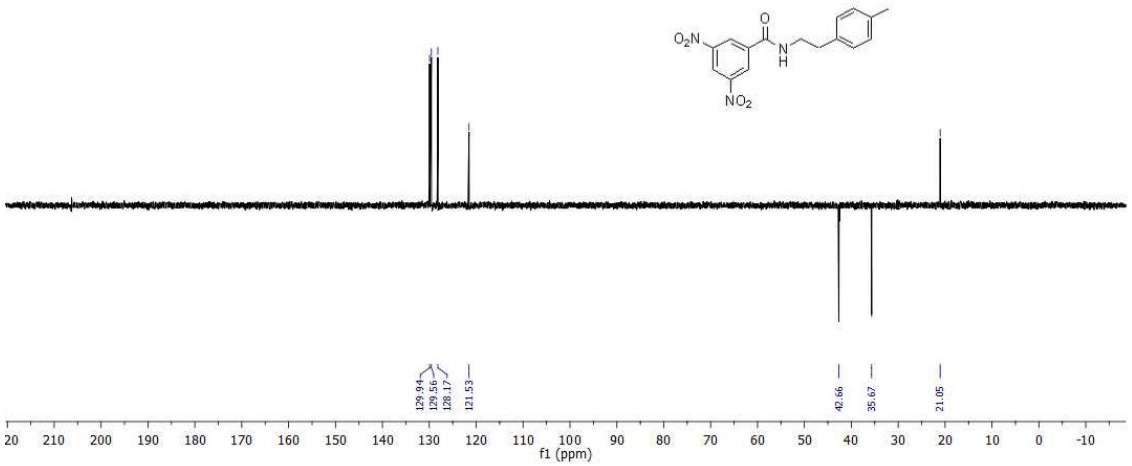
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9f:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9f:**



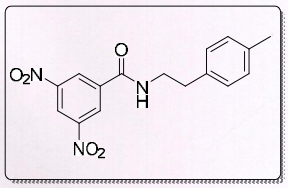
DEPT (126 MHz, Acetone-d_6) of compound **9f:**



HRMS (ESI-TOF) of compound **9f**:

Qualitative Compound Report

Data File	101.d	**Sample Name**	101
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 4:15:02
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

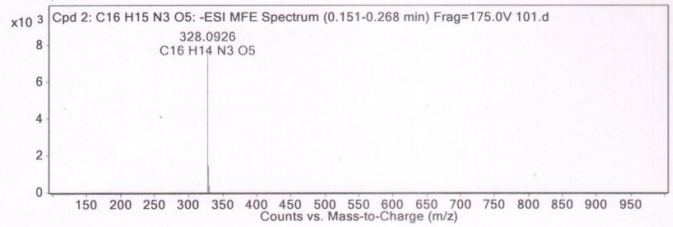


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C16 H15 N3 O5	0.191	329.0999	C16 H15 N3 O5	C16 H15 N3 O5	3.74	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C16 H15 N3 O5	328.0926	0.191	Find by Molecular Feature	329.0999

MFE MS Spectrum



MS Spectrum Peak List

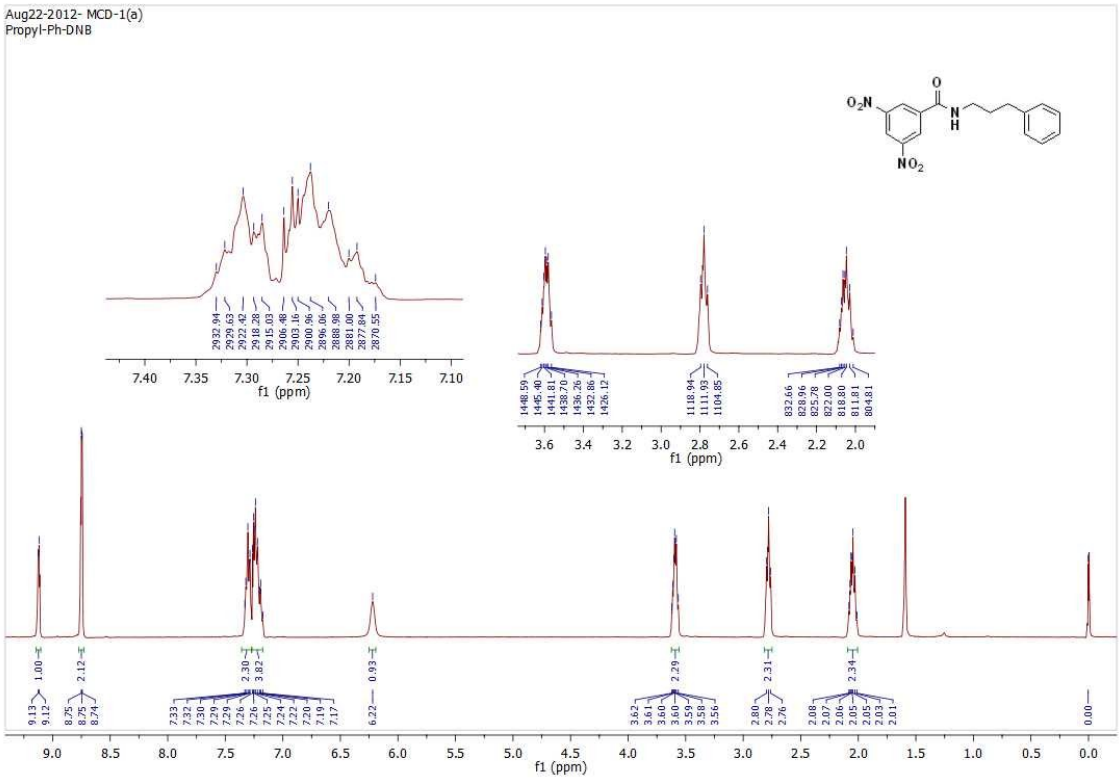
m/z	z	Abund	Formula	Ion
328.0926	-1	7630.13	C16 H14 N3 O5	(M-H)-
329.0963	-1	1446.84	C16 H14 N3 O5	(M-H)-
330.0972	-1	347.64	C16 H14 N3 O5	(M-H)-

Predicted Isotope Match Table

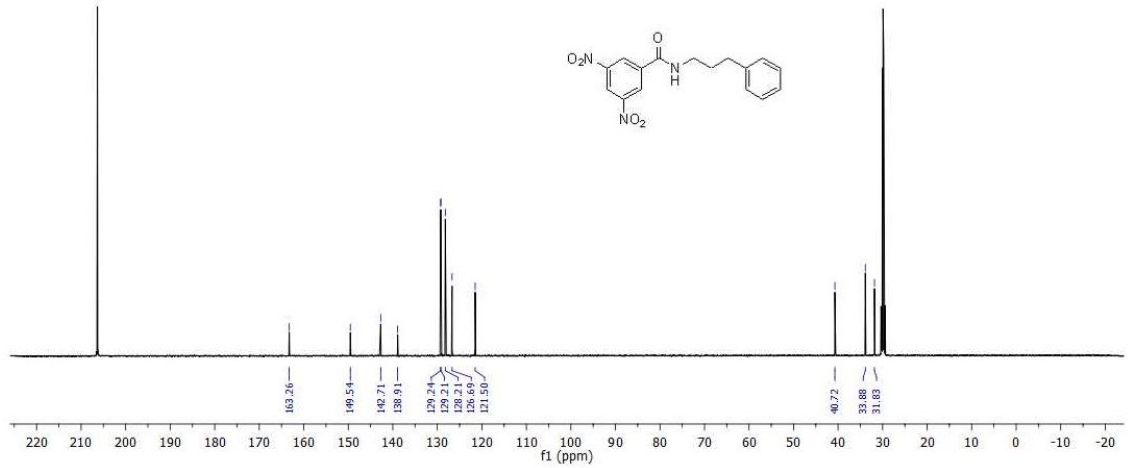
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.0926	328.0939	4.02	100	100	80.96	82.34
2	329.0963	329.0969	1.76	18.96	18.75	15.35	15.44
3	330.0972	330.0992	6.21	4.56	2.69	3.69	2.22

--- End Of Report ---

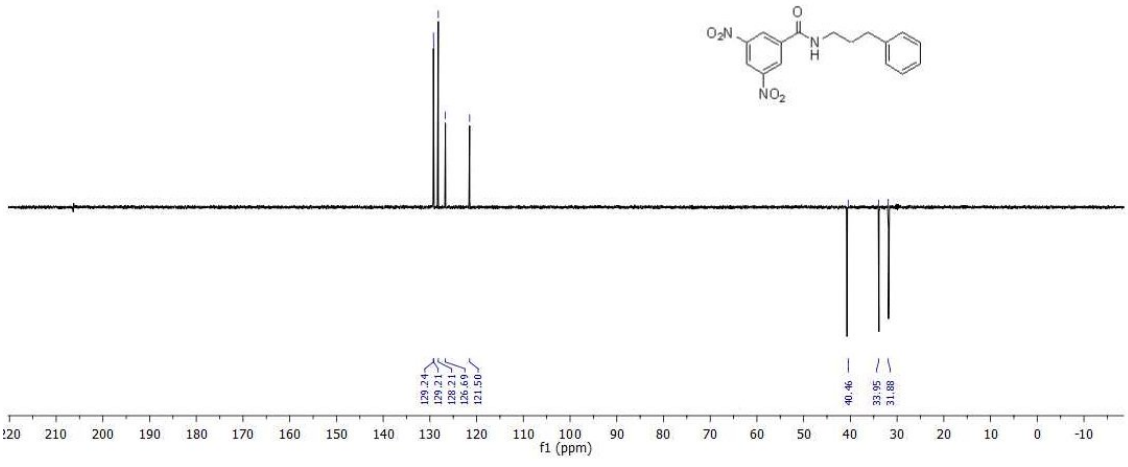
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9g:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9g:**



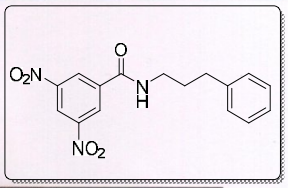
DEPT (126 MHz, Acetone-d_6) of compound **9g:**



HRMS (ESI-TOF) of compound **9g**:

Qualitative Compound Report

Data File	96.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment	Sample information is unavailable		

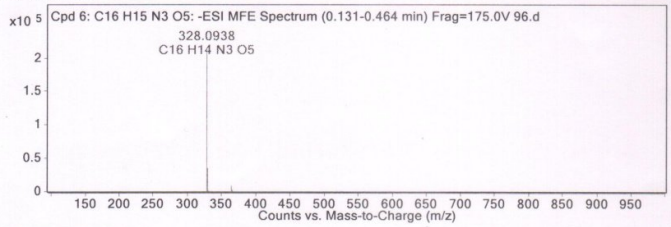


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C16 H15 N3 O5	0.19	329.1011	C16 H15 N3 O5	C16 H15 N3 O5	0.26	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C16 H15 N3 O5	328.0938	0.19	Find by Molecular Feature	329.1011

MFE MS Spectrum



MS Spectrum Peak List

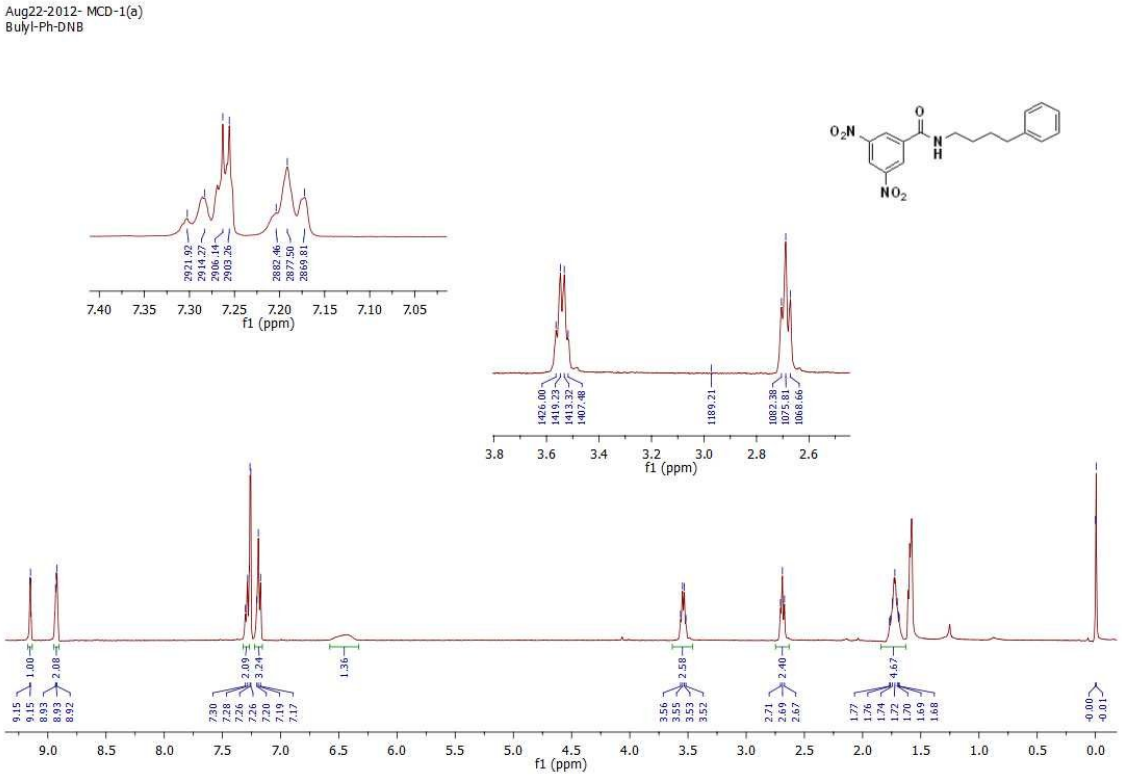
m/z	z	Abund	Formula	Ion
328.0938	-1	209791.05	C16 H14 N3 O5	(M-H)-
329.0969	-1	34655.51	C16 H14 N3 O5	(M-H)-
330.0999	-1	5948.92	C16 H14 N3 O5	(M-H)-
331.1015	-1	742.01	C16 H14 N3 O5	(M-H)-
364.0704	-1	8729.43	C16 H15 Cl N3 O5	(M+Cl)-
365.0728	-1	2112.05	C16 H15 Cl N3 O5	(M+Cl)-
366.0681	-1	2267.78	C16 H15 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

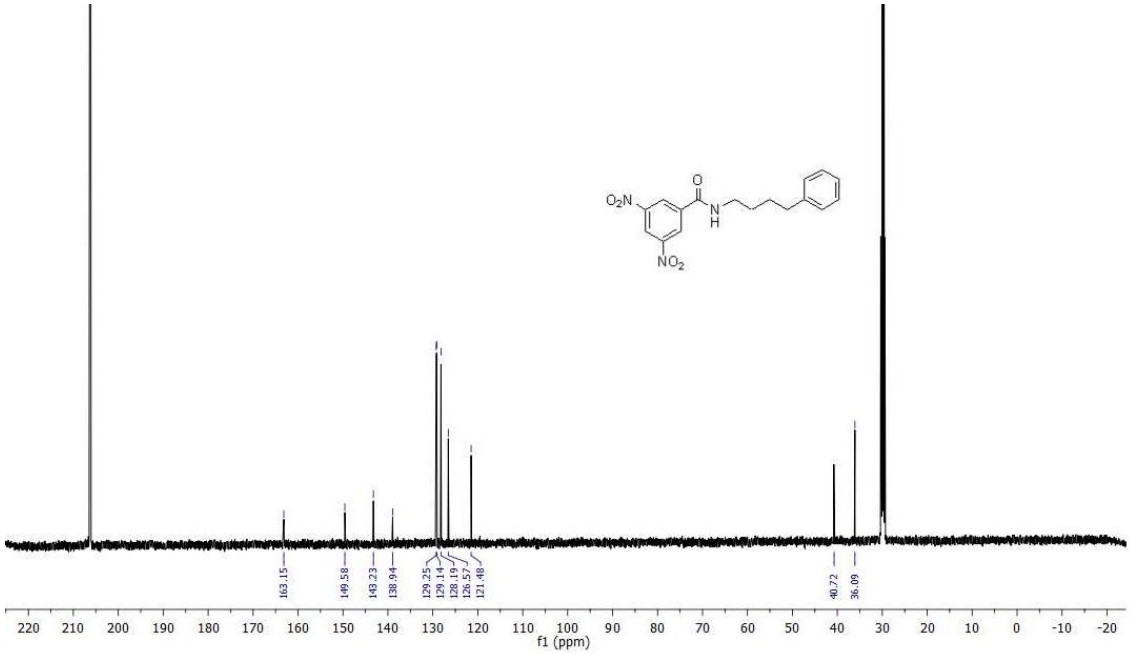
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	328.0938	328.0939	0.36	100	100	83.54	82.15
2	329.0969	329.0969	0.07	16.52	18.75	13.8	15.41
3	330.0999	330.0992	-2.04	2.84	2.69	2.37	2.21
4	331.1015	331.1017	0.79	0.35	0.28	0.3	0.23

--- End Of Report ---

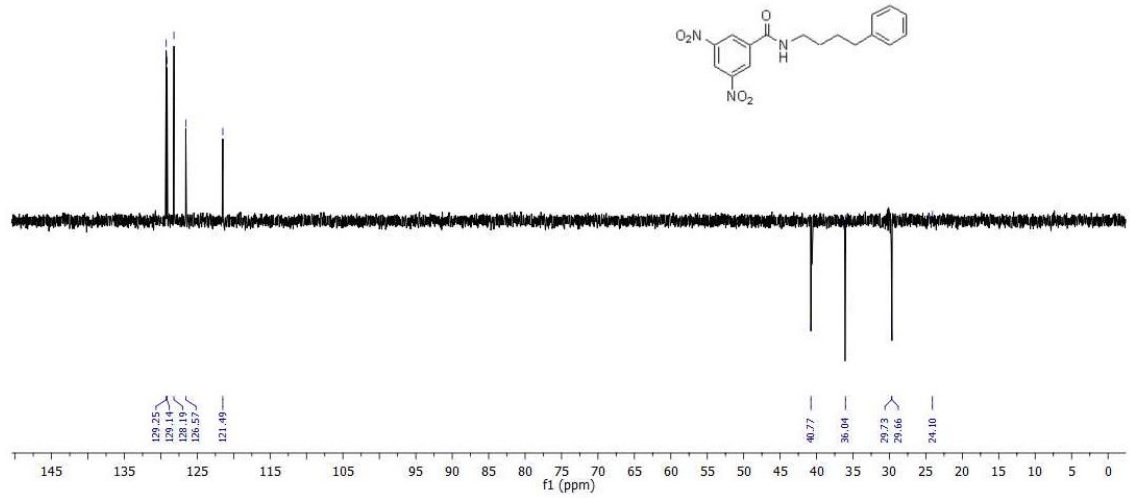
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9h:**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **9h:**



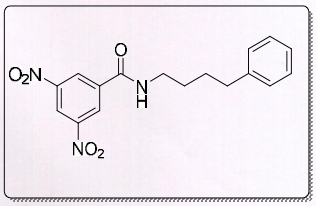
DEPT (126 MHz, Acetone-d_6) of compound **9h:**



HRMS (ESI-TOF) of compound **9h**:

Qualitative Compound Report

Data File	98.d	**Sample Name**	98
Sample Type	Sample	**Position**	Vial 20
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	06-03-2013 PM 5:23:31
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

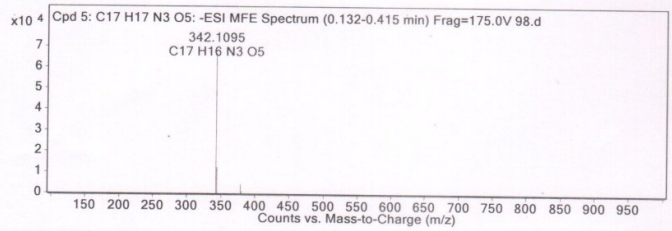


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C17 H17 N3 O5	0.192	343.1168	C17 H17 N3 O5	C17 H17 N3 O5	-0.08	C17 H17 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C17 H17 N3 O5	342.1095	0.192	Find by Molecular Feature	343.1168

MFE MS Spectrum



MS Spectrum Peak List

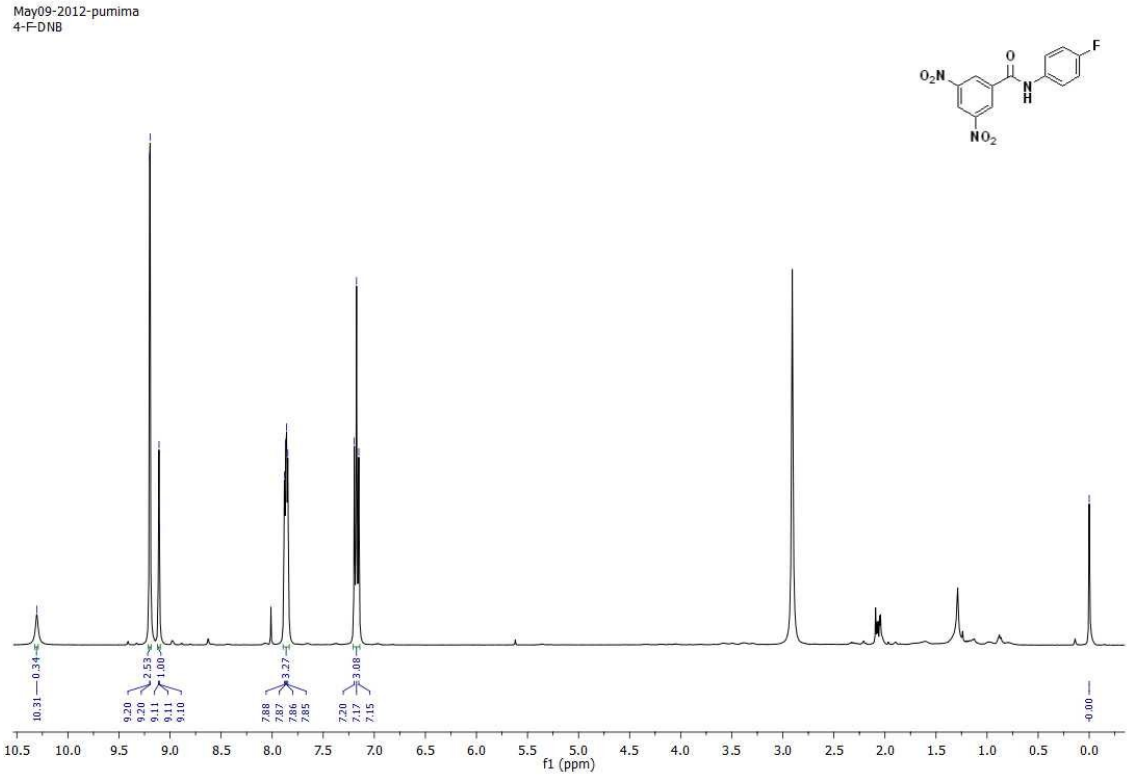
m/z	z	Abund	Formula	Ion
342.1095	-1	66890.43	C17 H16 N3 O5	(M-H)-
343.1129	-1	12550.85	C17 H16 N3 O5	(M-H)-
344.116	-1	1956.42	C17 H16 N3 O5	(M-H)-
378.0859	-1	4526.63	C17 H17 Cl N3 O5	(M+Cl)-
379.0903	-1	817	C17 H17 Cl N3 O5	(M+Cl)-
380.0839	-1	1149.73	C17 H17 Cl N3 O5	(M+Cl)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	342.1095	342.1095	0.17	100	100	82.18	81.46
2	343.1129	343.1126	-0.94	18.76	19.86	15.42	16.18
3	344.116	344.115	-2.89	2.92	2.9	2.4	2.36

--- End Of Report ---

^{1}H NMR (400 MHz, $CDCl_3$) of compound **10a:**

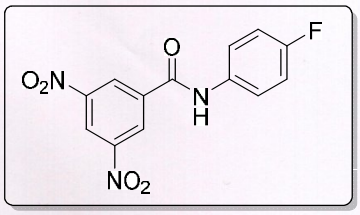


HRMS (ESI-TOF) of compound **10a**:

Qualitative Compound Report

Data File	60.d	**Sample Name**	60
Sample Type	Sample	**Position**	Vial 24
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	04-03-2013 PM 3:54:47
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

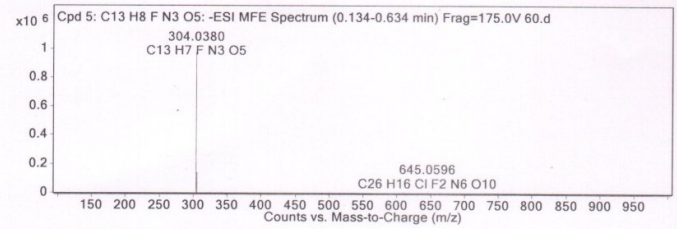


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C13 H8 F N3 O5	0.194	305.0453	C13 H8 F N3 O5	C13 H8 F N3 O5	-1.56	C13 H8 F N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C13 H8 F N3 O5	304.038	0.194	Find by Molecular Feature	305.0453

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
304.038	-1	975104.75	C13 H7 F N3 O5	(M-H)-
305.0411	-1	140109.38	C13 H7 F N3 O5	(M-H)-
306.043	-1	18894.85	C13 H7 F N3 O5	(M-H)-
307.0466	-1	2044.24	C13 H7 F N3 O5	(M-H)-
340.0146	-1	6072.72	C13 H8 Cl F N3 O5	(M+Cl)-
342.012	-1	2337.86	C13 H8 Cl F N3 O5	(M+Cl)-
609.0827	-1	4074.4	C26 H15 F2 N6 O10	(2M-H)-
645.0596	-1	5595.32	C26 H16 Cl F2 N6 O10	(2M+Cl)-
646.0627	-1	1941.91	C26 H16 Cl F2 N6 O10	(2M+Cl)-
647.0562	-1	1559.75	C26 H16 Cl F2 N6 O10	(2M+Cl)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	304.038	304.0375	-1.5	100	100	85.83	84.91
2	305.0411	305.0405	-1.99	14.37	15.43	12.33	13.1
3	306.043	306.0426	-1.41	1.94	2.14	1.66	1.82
4	307.0466	307.0451	-4.93	0.21	0.21	0.18	0.18

--- End Of Report ---

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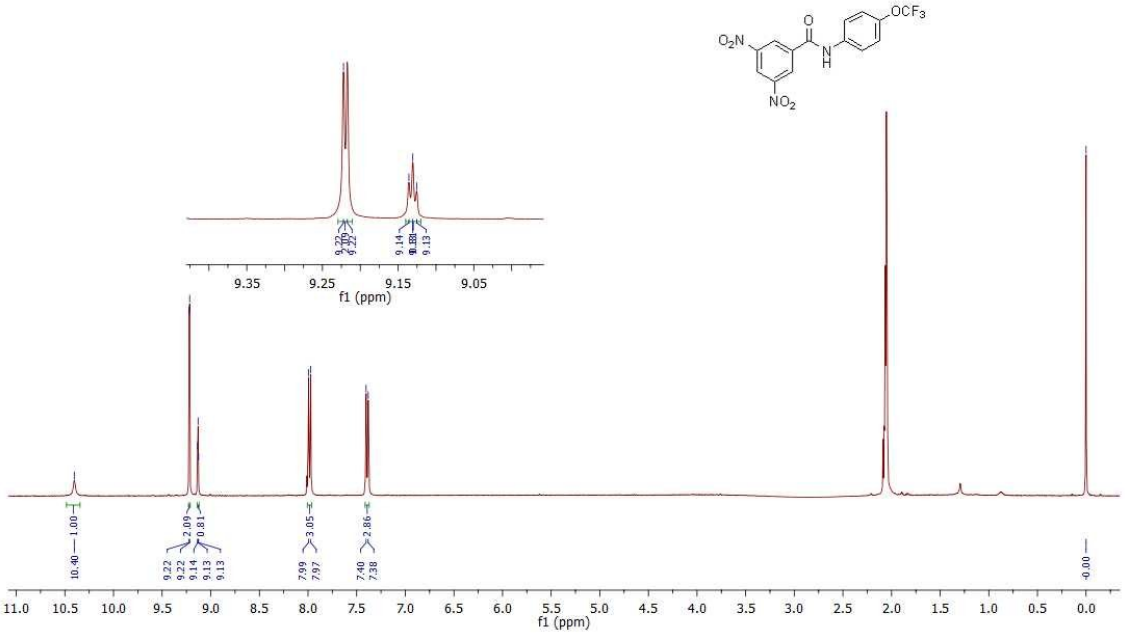
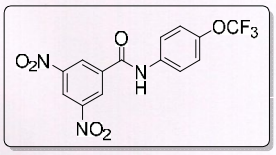
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10b:**



HRMS (ESI-TOF) of compound **10b**:

Qualitative Compound Report

Data File	110.d	**Sample Name**	110
Sample Type	Sample	**Position**	Vial 27
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 5:29:25
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



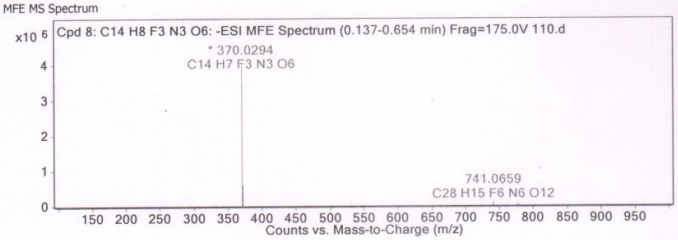
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C14 H8 F3 N3 O6	0.189	371.0368	C14 H8 F3 N3 O6	C14 H8 F3 N3 O6	-0.73	C14 H8 F3 N3 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C14 H8 F3 N3 O6	370.0294	0.189	Find by Molecular Feature	371.0368

MFE MS Spectrum



MS Spectrum Peak List

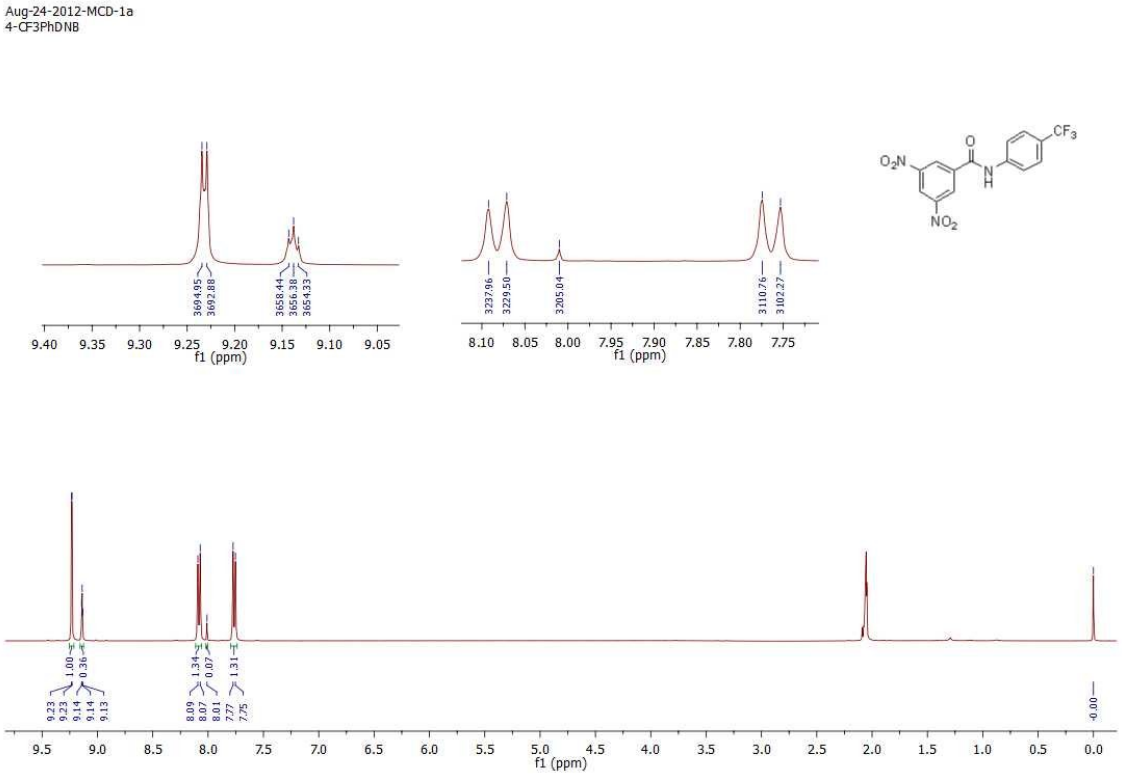
m/z	z	Abund	Formula	Ion
370.0294	-1	3980783	C14 H7 F3 N3 O6	(M-H)-
371.0332	-1	600660.69	C14 H7 F3 N3 O6	(M-H)-
372.035	-1	85941.88	C14 H7 F3 N3 O6	(M-H)-
373.0372	-1	8095.59	C14 H7 F3 N3 O6	(M-H)-
406.0066	-1	8499.77	C14 H8 Cl F3 N3 O6	(M+Cl)-
741.0659	-1	93075.37	C28 H15 F6 N6 O12	(2M-H)-
742.0688	-1	30319.69	C28 H15 F6 N6 O12	(2M-H)-
777.0421	-1	55560.52		(2M+Cl)-
778.0451	-1	18611.9		(2M+Cl)-
779.0409	-1	20188.72		(2M+Cl)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	370.0294	370.0292	-0.41	100	100	85.14	83.78
2	371.0332	371.0322	-2.68	15.09	16.55	12.85	13.86
3	372.035	372.0343	-1.81	2.16	2.52	1.84	2.11
4	373.0372	373.0368	-1.03	0.2	0.27	0.17	0.22
5	374.0383	374.0391	1.97	0.01	0.02	0	0.02

--- End Of Report ---

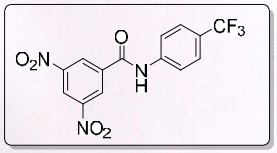
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10c:**



HRMS (ESI-TOF) of compound **10c**:

Qualitative Compound Report

Data File	111.d	**Sample Name**	111
Sample Type	Sample	**Position**	Vial 28
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 5:33:56
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



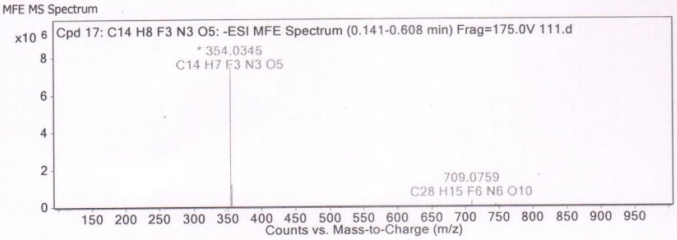
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 17: C14 H8 F3 N3 O5	0.192	355.0418	C14 H8 F3 N3 O5	C14 H8 F3 N3 O5	-0.62	C14 H8 F3 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 17: C14 H8 F3 N3 O5	354.0345	0.192	Find by Molecular Feature	355.0418

MFE MS Spectrum



MS Spectrum Peak List

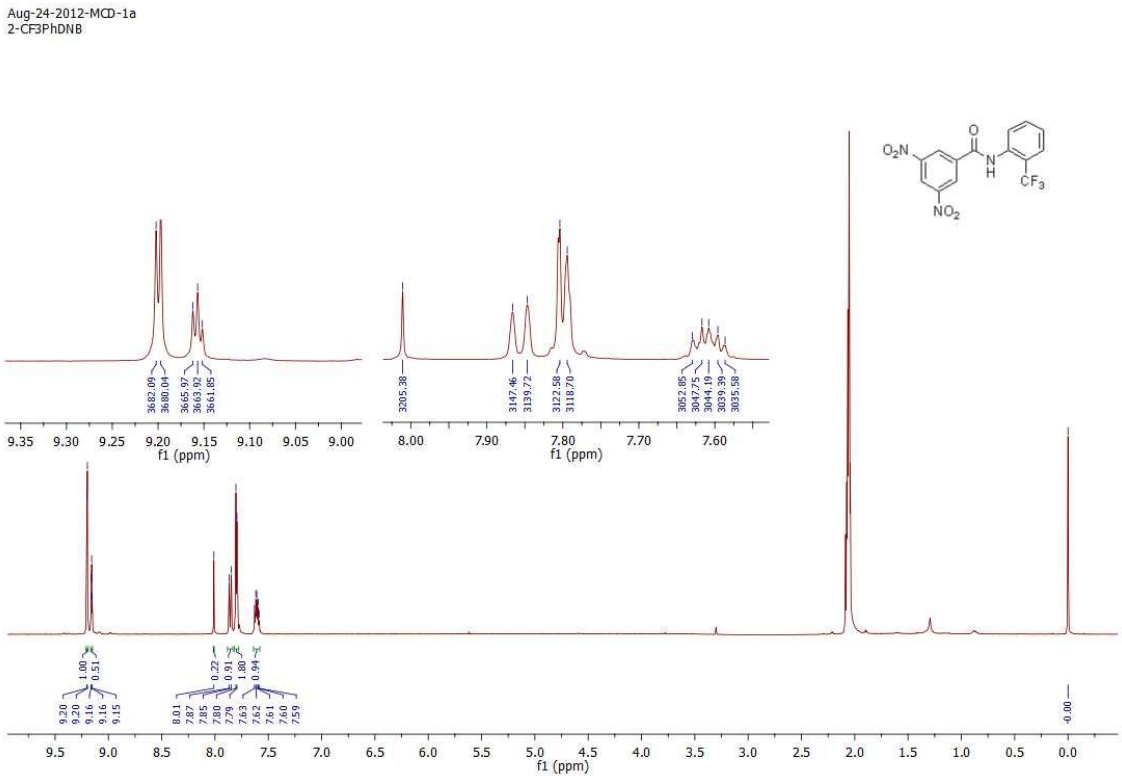
m/z	z	Abund	Formula	Ion
354.0345	-1	7531740.5	C14 H7 F3 N3 O5	(M-H)-
355.0379	-1	1153634.5	C14 H7 F3 N3 O5	(M-H)-
356.0402	-1	161538.94	C14 H7 F3 N3 O5	(M-H)-
390.0111	-1	12965.01	C14 H8 Cl F3 N3 O5	(M+Cl)-
709.0759	-1	261669.72	C28 H15 F6 N6 O10	(2M-H)-
710.0788	-1	87459.38	C28 H15 F6 N6 O10	(2M-H)-
711.0806	-1	18530.51	C28 H15 F6 N6 O10	(2M-H)-
745.0525	-1	103022.52	C28 H16 Cl F6 N6 O10	(2M+Cl)-
746.0549	-1	32834.59	C28 H16 Cl F6 N6 O10	(2M+Cl)-
747.0515	-1	37311.26	C28 H16 Cl F6 N6 O10	(2M+Cl)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	354.0345	354.0343	-0.44	100	100	85.01	83.99
2	355.0379	355.0373	-1.6	15.32	16.51	13.02	13.87
3	356.0402	356.0395	-2.11	2.14	2.31	1.82	1.94
4	357.0424	357.042	-1.29	0.16	0.23	0.14	0.19
5	358.045	358.0443	-2.1	0.01	0.02	0.01	0.02

--- End Of Report ---

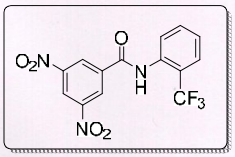
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10d:**



HRMS (ESI-TOF) of compound **10d**:

Qualitative Compound Report

Data File	112.d	**Sample Name**	112
Sample Type	Sample	**Position**	Vial 29
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	07-03-2013 PM 5:38:27
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			



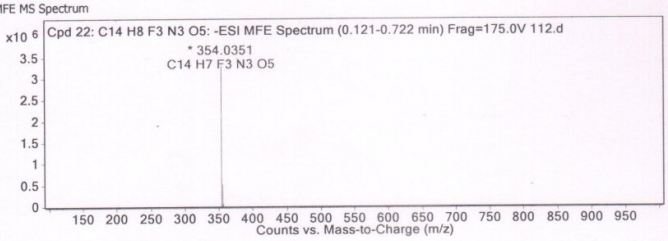
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C14 H8 F3 N3 O5	0.189	355.0424	C14 H8 F3 N3 O5	C14 H8 F3 N3 O5	-2.28	C14 H8 F3 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C14 H8 F3 N3 O5	354.0351	0.189	Find by Molecular Feature	355.0424

MFE MS Spectrum



MS Spectrum Peak List

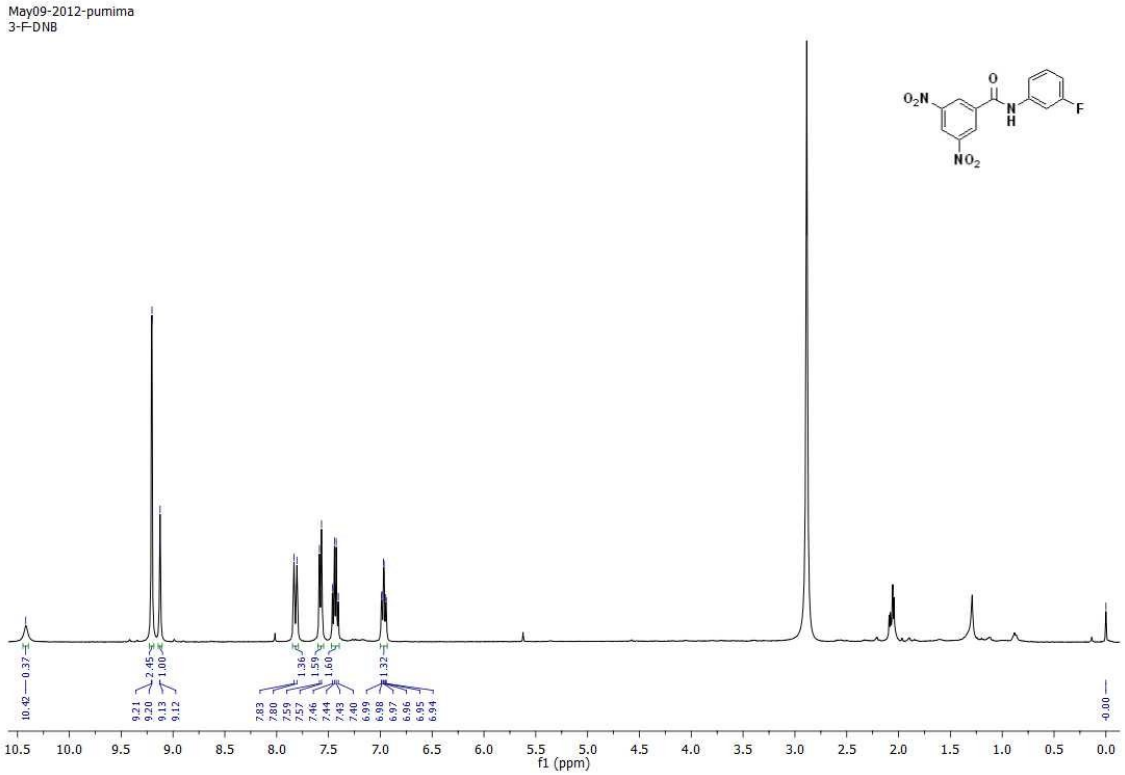
m/z	z	Abund	Formula	Ion
354.0351	-1	3299008	C14 H7 F3 N3 O5	(M-H)-
355.0386	-1	518787.34	C14 H7 F3 N3 O5	(M-H)-
356.0403	-1	59826.64	C14 H7 F3 N3 O5	(M-H)-
357.0427	-1	6142.26	C14 H7 F3 N3 O5	(M-H)-
358.0445	-1	263.01	C14 H7 F3 N3 O5	(M-H)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	354.0351	354.0343	-2.05	100	100	84.94	83.99
2	355.0386	355.0373	-3.81	15.73	16.51	13.36	13.87
3	356.0403	356.0395	-2.26	1.81	2.31	1.54	1.94
4	357.0427	357.042	-2	0.19	0.23	0.16	0.19
5	358.0445	358.0443	-0.56	0.01	0.02	0.01	0.02

--- End Of Report ---

^{1}H NMR (400 MHz, $CDCl_3$) of compound **10e:**

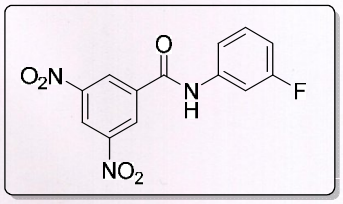


HRMS (ESI-TOF) of compound **10e**:

Qualitative Compound Report

Data File	61.d	**Sample Name**	60
Sample Type	Sample	**Position**	Vial 24
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_neg12-01-13.m	**Acquired Time**	04-03-2013 PM 3:54:47
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

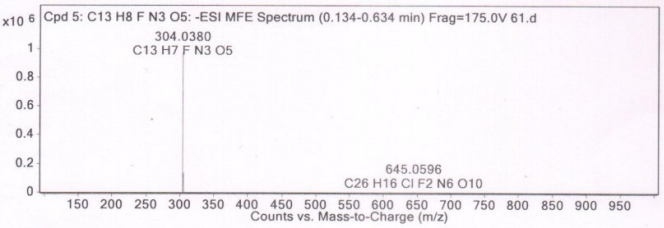


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C13 H8 F N3 O5	0.194	305.0453	C13 H8 F N3 O5	C13 H8 F N3 O5	-1.56	C13 H8 F N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C13 H8 F N3 O5	304.038	0.194	Find by Molecular Feature	305.0453

MFE MS Spectrum



MS Spectrum Peak List

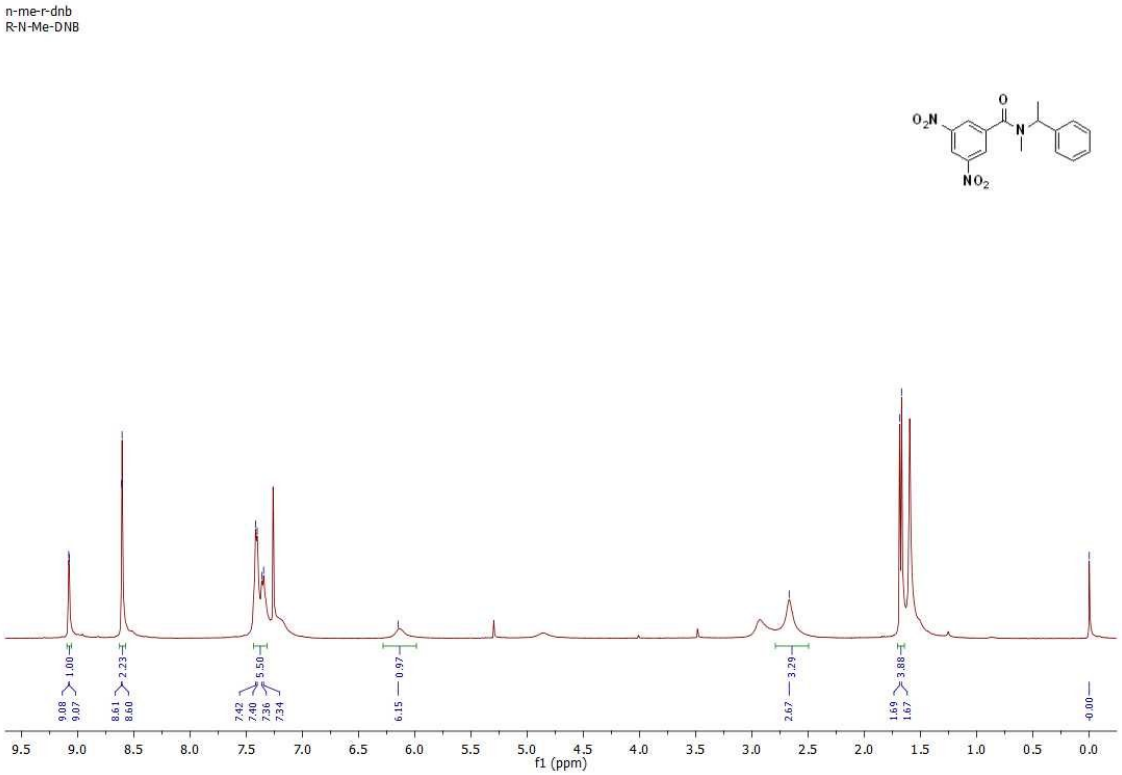
m/z	z	Abund	Formula	Ion
304.038	-1	975104.75	C13 H7 F N3 O5	(M-H)-
305.0411	-1	140109.38	C13 H7 F N3 O5	(M-H)-
306.043	-1	18894.85	C13 H7 F N3 O5	(M-H)-
307.0466	-1	2044.24	C13 H7 F N3 O5	(M-H)-
340.0146	-1	6072.72	C13 H8 Cl F N3 O5	(M+Cl)-
342.012	-1	2337.86	C13 H8 Cl F N3 O5	(M+Cl)-
609.0827	-1	4074.4	C26 H15 F2 N6 O10	(2M-H)-
645.0596	-1	5595.32	C26 H16 Cl F2 N6 O10	(2M+Cl)-
646.0627	-1	1941.91	C26 H16 Cl F2 N6 O10	(2M+Cl)-
647.0562	-1	1559.75	C26 H16 Cl F2 N6 O10	(2M+Cl)-

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	304.038	304.0375	-1.5	100	100	85.83	84.91
2	305.0411	305.0405	-1.99	14.37	15.43	12.33	13.1
3	306.043	306.0426	-1.41	1.94	2.14	1.66	1.82
4	307.0466	307.0451	-4.93	0.21	0.21	0.18	0.18

--- End Of Report ---

^{1}H NMR (400 MHz, $CDCl_3$) of compound **11a:**

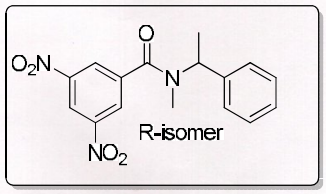


HRMS (ESI-TOF) of compound **10d**:

Qualitative Compound Report

Data File	113.d	**Sample Name**	113
Sample Type	Sample	**Position**	Vial 28
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	01-04-2013 PM 5:27:48
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

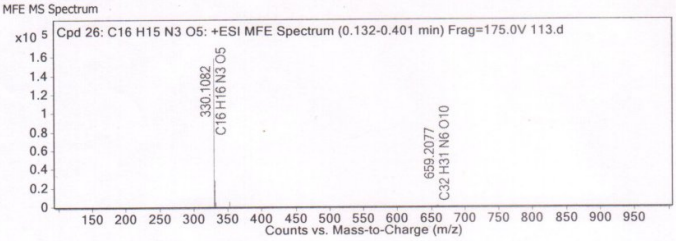


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 26: C16 H15 N3 O5	0.187	329.1009	C16 H15 N3 O5	C16 H15 N3 O5	0.7	C16 H15 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 26: C16 H15 N3 O5	330.1082	0.187	Find by Molecular Feature	329.1009

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
330.1082	1	158467.95	C16 H16 N3 O5	(M+H)+
331.1113	1	27377.96	C16 H16 N3 O5	(M+H)+
332.1142	1	4201.93	C16 H16 N3 O5	(M+H)+
333.1168	1	431.09	C16 H16 N3 O5	(M+H)+
352.09	1	5081.64	C16 H15 N3 Na O5	(M+Na)+
353.094	1	734	C16 H15 N3 Na O5	(M+Na)+
354.096	1	369.34	C16 H15 N3 Na O5	(M+Na)+
659.2077	1	1299.82	C32 H31 N6 O10	(2M+H)+
660.2087	1	550.95	C32 H31 N6 O10	(2M+H)+
681.1884	1	399.1	C32 H30 N6 Na O10	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	330.1082	330.1084	0.77	100	100	83.19	82.13
2	331.1113	331.1115	0.6	17.28	18.78	14.37	15.42
3	332.1142	332.1138	-1.17	2.65	2.69	2.21	2.21
4	333.1168	333.1163	-1.52	0.27	0.29	0.23	0.23

--- End Of Report ---

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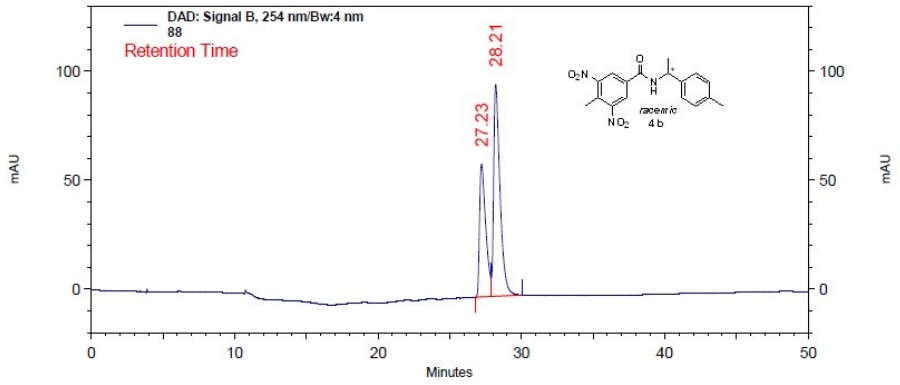
Chiral HPLC analysis of **4b**, **7a** and **7b**:

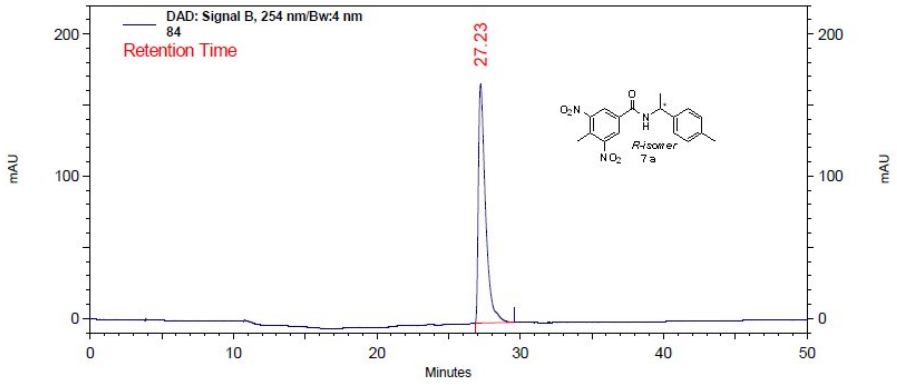
HPLC graph of compound **4b** (racemic):



DAD: Signal B, 254 nm/Bw:4 nm Results

Retention Time	Area	Height	Area %
27.23	3834175	127791	37.90
28.21	6282791	203805	62.10
Totals	10116966	331596	100.00

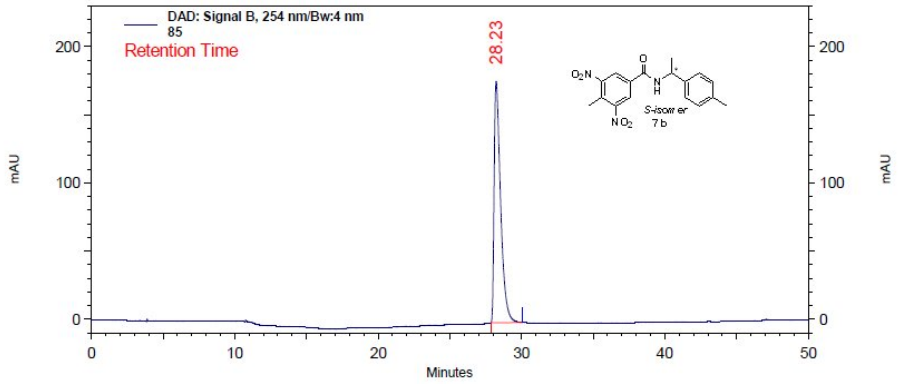
HPLC graph of compound **7a** (**R**-enantiomer):



DAD: Signal B, 254 nm/Bw:4 nm Results

Retention Time	Area	Height	Area %
27.23	12195694	352105	100.00
Totals	12195694	352105	100.00

HPLC graph of compound **7b** (*S*-enantiomer):



DAD: Signal B, 254 nm/Bw:4 nm Results

Retention Time	Area	Height	Area %
28.23	11627387	371417	100.00
Totals	11627387	371417	100.00