

**Synthesis and biological evaluation of polar functionalities containing
nitrodihydroimidazooxazoles as anti-TB agents**

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1. Experimental Section: General

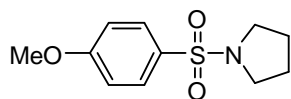
All chemicals for this study were purchased from Sigma-Aldrich, INDIA. ¹H-NMR recorded on 200 MHz or 400 MHz or 500 MHz and ¹³C-NMR recorded on 101 MHz or 126 MHz Bruker-Avance DPX FT-NMR instruments. Chemical data for protons are reported in parts per million (ppm, scale) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent (CDCl₃: 7.26, Acetone-*d*₆: 2.1, DMSO- *d*₆: 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 and LC-MS instrument. Melting points were recorded on digital melting point apparatus and are uncorrected. Purity of all final compounds (used for biological screening) was determined by using HPLC-Agilent Technologies 1260 infinity series system using following method; Coloumn RP-18e (Chromolith, 5µm, 4.6x250 mm) and the gradient mixture of water /methanol was used as a Mobile phase over 55 minutes with a flow rate of 0.8 ml/min. UV recorded at 254 nm.

General procedure for the preparation of compounds 3(a-g):

To a solution of substituted secondary amine **2** (3 mmol) in dichloromethane (10 ml) were added triethylamine (333 mg, 3.3 mmol), and a catalytic amount of 4-dimethylaminopyridine (DMAP). After stirring at room temperature for 15 min, a solution of 4-methoxy benzenesulfonyl chloride **1** (680 mg, 3.3 mmol) in 5 ml of dichloromethane was

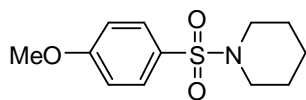
added slowly in dropwise manner. The reaction mixture was stirred at 40 °C under nitrogen atmosphere for 12 h. After complete conversion as indicated by TLC, the solvent was removed in vacuo, the residue was neutralized with saturated NaHCO₃ solution, and the aqueous layer was extracted with ethyl acetate, washed with water, and dried over anhydrous Na₂SO₄. The solvent was evaporated in vacuo and the compounds were purified by column chromatography.

1-((4-Methoxyphenyl)sulfonyl)pyrrolidine 3a:



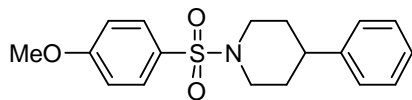
TLC (EtOAc:hexane 1:9): $R_f = 0.20$; Light yellow solid; Yield = 92%; ¹H NMR (200 MHz, CDCl₃) 7.72 (d, $J = 8.5$ Hz, 2H), 7.01 (d, $J = 8.5$ Hz, 2H), 3.82 (s, 3H), 3.18 – 3.16 (m, 4H), 1.72 – 1.70 (m, 4H); LC-MS (ESI+): m/z 242.08 [M + H]⁺.

1-((4-Methoxyphenyl)sulfonyl)piperidine 3b:



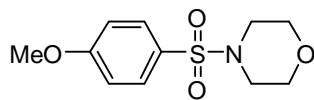
TLC (EtOAc:hexane 1:9): $R_f = 0.30$; Light yellow solid; Yield = 95%; ¹H NMR (500 MHz, CDCl₃) 7.62 (d, $J = 8.3$ Hz, 2H), 6.98 (d, $J = 8.4$ Hz, 2H), 3.85 (s, 3H), 2.99 – 2.96 (m, 4H), 1.64 – 1.62 (m, 4H), 1.42 (m, 1H). LC-MS (ESI+): m/z 256.1 [M + H]⁺.

1-((4-Methoxyphenyl)sulfonyl)-4-phenylpiperidine 3c:



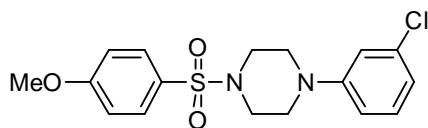
TLC (EtOAc:hexane 1:9): $R_f = 0.30$; Light yellow solid; Yield = 85%; ¹H NMR (400 MHz, CD₃OD) 7.92 (d, $J = 8.7$ Hz, 2H), 7.29 – 7.27 (m, 2H), 7.19 – 7.16 (m, 3H), 6.98 (d, $J = 8.8$ Hz, 2H), 3.89 (s, 3H), 3.87 – 3.85 (m, 2H), 2.50 – 2.45 (m, 3H), 1.88 – 1.82 (m, 4H); LC-MS (ESI+): m/z 332.1 [M + H]⁺.

4-((4-Methoxyphenyl)sulfonyl)morpholine 3d:

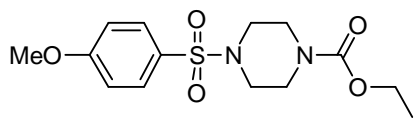


TLC (EtOAc:hexane 1:9): $R_f = 0.20$; White solid; Yield = 90%; ¹H NMR (400 MHz, CDCl₃) 7.58 (d, $J = 8.6$ Hz, 2H), 6.98 (d, $J = 8.7$ Hz, 2H), 3.86 (s, 3H), 3.85 – 3.75 (m, 4H), 3.07 – 3.02 (m, 4H); LC-MS (ESI+): m/z 258.1 [M + H]⁺.

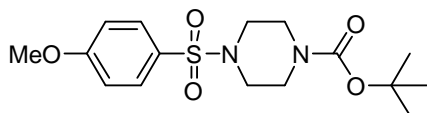
1-(3-Chlorophenyl)-4-((4-methoxyphenyl)sulfonyl)piperazine 3e:



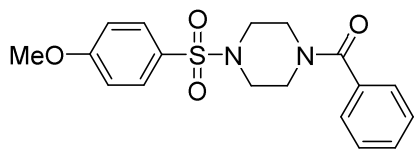
TLC (EtOAc:hexane 1:9): $R_f = 0.25$; Light yellow solid; Yield = 95%; ¹H NMR (200 MHz, CDCl₃) 7.72 (d, $J = 8.5$ Hz, 2H), 7.19 – 7.12 (m, 1H), 6.99 (d, $J = 8.5$ Hz, 2H), 6.86 – 6.71 (m, 3H), 3.82 (s, 3H), 3.25 – 3.15 (m, 8H); LC-MS (ESI+): m/z 367.1 [M + H]⁺.

Ethyl 4-((4-methoxyphenyl)sulfonyl)piperazine-1-carboxylate 3f:

TLC (EtOAc:hexane 1:9): $R_f = 0.25$; Light yellow solid; Yield = 88%; $^1\text{H NMR}$ (500 MHz, CDCl_3) 7.58 (d, $J = 8.8$ Hz, 2H), 6.91 (d, $J = 8.8$ Hz, 2H), 4.12 (q, $J = 7.2$ Hz, 2H), 3.82 (s, 3H), 3.65 – 3.55 (m, 4H), 3.01 – 2.93 (m, 4H), 1.23 (t, $J = 7.2$ Hz, 3H); LC-MS (ESI+): m/z 329.10 $[\text{M} + \text{H}]^+$.

tert-Butyl 4-((4-methoxyphenyl)sulfonyl)piperazine-1-carboxylate 3g:

TLC (EtOAc:hexane 1:9): $R_f = 0.20$; Light yellow solid; Yield = 88%; $^1\text{H NMR}$ (500 MHz, CDCl_3) 7.52 (d, $J = 8.6$ Hz, 2H), 6.95 (d, $J = 8.6$ Hz, 2H), 3.85 (s, 3H), 3.65 – 3.55 (m, 4H), 3.01 – 2.93 (m, 4H), 1.38 (s, 9H); LC-MS (ESI+): m/z 357.1 $[\text{M} + \text{H}]^+$.

(4-((4-Methoxyphenyl)sulfonyl)piperazin-1-yl)(phenyl)methanone 3h:

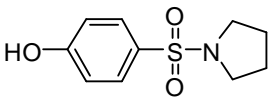
The compound **3g** (357 mg, 1 mmol) was dissolved in 20% TFA/DCM and the reaction mixture was stirred at room temperature for 2 h. Then the reaction mixture was evaporated in vacuo and the crude reaction mixture was dissolved in dichloromethane. The reaction mixture was added triethylamine (111.3 mg, 1.1 mmol), and a catalytic amount of 4-dimethylaminopyridine (DMAP). After stirring at room temperature for 15 min, a solution of benzoyl chloride (154 mg, 1.1 mmol) in 5 ml of dichloromethane was added slowly in dropwise manner. The reaction mixture was stirred at room temperature under nitrogen atmosphere for 3 h. After complete conversion as indicated by TLC, the solvent was removed in vacuo, the residue was neutralized with saturated NaHCO_3 solution, and the aqueous layer was extracted with ethyl acetate, washed with water, and dried over anhydrous Na_2SO_4 . The solvent was evaporated in vacuo and the compound was purified by column chromatography. TLC (EtOAc:hexane 1:9): $R_f = 0.30$; Light yellow solid; Yield: 90%; $^1\text{H NMR}$ (500 MHz, Acetone- d_6) 7.64 (d, $J = 8.74$ Hz, 2H), 7.45 – 7.35 (m, 5H) 7.04 (d, $J = 8.74$ Hz, 2H), 3.88 (s, 3H), 3.75 – 3.65 (m, 8H); LC-MS (ESI+): m/z 361.1 $[\text{M} + \text{H}]^+$.

General procedure for the preparation of compounds 4(a-g):

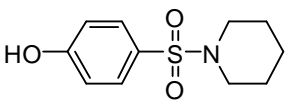
The appropriate 4-methoxy benzene sulphonamide compound **3(a-f)** and **3h** (1 mmol) was dissolved in 10 ml of dichloromethane. The reaction mixture was cooled to 0 °C and boron tribromide (1.8 mmol) was added slowly in dropwise. Then the reaction mixture was

stirred at room temperature for 12 h. The mixture was diluted with EtOAc, washed with water, dried with Na₂SO₄, and evaporated under vacuum and purified by column chromatography.

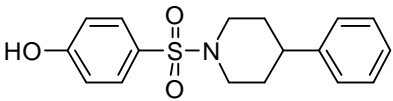
4-(Pyrrolidin-1-ylsulfonyl)phenol 4a:

 TLC (EtOAc:hexane 2:8): $R_f = 0.20$; Light yellow solid; Yield = 62%; ¹H NMR (200 MHz, CDCl₃) 7.72 (d, $J = 8.7$ Hz, 2H), 7.01 (d, $J = 8.7$ Hz, 2H), 3.22 – 3.20 (m, 4H), 1.75 – 1.72 (m, 4H); LC-MS (ESI+): m/z 228.06 [M + H]⁺.

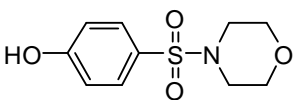
4-(Piperidin-1-ylsulfonyl)phenol 4b:

 TLC (EtOAc:hexane 2:8): $R_f = 0.30$; Light yellow solid; Yield = 60%; ¹H NMR (500 MHz, CDCl₃) 7.64 (d, $J = 8.6$ Hz, 2H), 6.95 (d, $J = 8.6$ Hz, 2H), 2.97 – 2.95 (m, 4H), 1.67 – 1.61 (m, 4H), 1.41 (m, 1H). LC-MS (ESI+): m/z 242.08 [M + H]⁺.

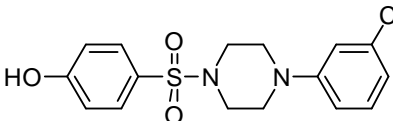
4-[(4-Phenylpiperidin-1-yl)sulfonyl]phenol 4c:

 TLC (EtOAc:hexane 2:8): $R_f = 0.30$; Light yellow solid; Yield = 80%; ¹H NMR (400 MHz, CD₃OD) 7.91 (d, $J = 8.8$ Hz, 2H), 7.29 – 7.25 (m, 2H), 7.19 – 7.15 (m, 3H), 6.98 (d, $J = 8.8$ Hz, 2H), 3.87 – 3.84 (m, 2H), 2.50 – 2.35 (m, 3H), 1.88 – 1.71 (m, 4H); LC-MS (ESI+): m/z 318.11 [M + H]⁺.

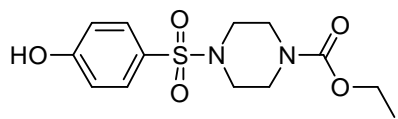
4-(Morpholinosulfonyl)phenol 4d:

 TLC (EtOAc:hexane 2:8): $R_f = 0.20$; Light yellow solid; Yield = 62%; ¹H NMR (400 MHz, CDCl₃) 7.68 (d, $J = 8.7$ Hz, 2H), 6.99 (d, $J = 8.8$ Hz, 2H), 3.83 – 3.75 (m, 4H), 3.07 – 2.98 (m, 4H); LC-MS (ESI+): m/z 244.06 [M + H]⁺.

4-[[4-(3-Chlorophenyl)piperazin-1-yl]sulfonyl]phenol 4e:

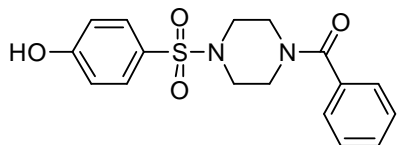
 TLC (EtOAc:hexane 2:8): $R_f = 0.25$; Light yellow solid; Yield = 75%; ¹H NMR (200 MHz, CDCl₃) 7.74 (d, $J = 8.5$ Hz, 2H), 7.19 – 7.12 (m, 1H), 6.98 (d, $J = 8.5$ Hz, 2H), 6.86 – 6.71 (m, 3H) 3.22 – 3.15 (m, 8H); LC-MS (ESI+): m/z 353.07 [M + H]⁺.

Ethyl 4-[(4-hydroxyphenyl)sulfonyl]piperazine-1-carboxylate 4f:



TLC (EtOAc:hexane 2:8): $R_f = 0.30$; Light yellow solid; Yield = 78%; $^1\text{H NMR}$ (500 MHz, CDCl_3) 7.60 (d, $J = 8.9$ Hz, 2H), 6.93 (d, $J = 8.8$ Hz, 2H), 4.11 (q, $J = 7.1$ Hz, 2H), 3.65 – 3.55 (m, 4H), 3.01 – 2.92 (m, 4H), 1.24 (t, $J = 7.1$ Hz, 3H); LC-MS (ESI+): m/z 315.1 $[\text{M} + \text{H}]^+$.

{4-[(4-Hydroxyphenyl)sulfonyl]piperazin-1-yl}phenyl methanone 4g:

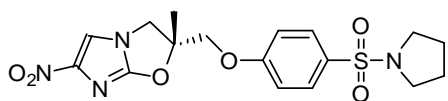


TLC (EtOAc:hexane 2:8): $R_f = 0.40$; Light yellow solid; Yield = 72%; $^1\text{H NMR}$ (500 MHz, Acetone- d_6) 7.64 (d, $J = 8.74$ Hz, 2H), 7.42 – 7.35 (m, 5H) 7.04 (d, $J = 8.74$ Hz, 2H), 3.75 – 3.65 (m, 8H); LC-MS (ESI+): m/z 347.10 $[\text{M} + \text{H}]^+$.

General procedure for the preparation of compounds 6(a-g):

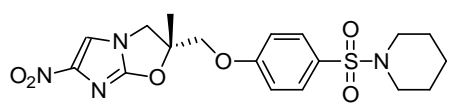
To a mixture of epoxide compound **5** (100 mg, 0.458 mmol) and phenolic compounds **4(a-g)** (0.458 mmol) in dry *N,N*-dimethylformamide (3 ml) was added 60% sodium hydride (33 mg, 1.376 mmol) at 0 °C portionwise. After the mixture was stirred at 50 °C for 12 h under a nitrogen atmosphere, the reaction mixture was cooled in an ice bath and carefully quenched with ethyl acetate (2.3 ml) and ice water (0.5 ml). The resultant reaction mixture was poured into water (30 ml) and extracted with ethylacetate twice washed with brine solution and dried under vacuo. This crude product was purified by silica gel column chromatography using a dichloromethane and ethyl acetate mixture as solvent.

(R)-2-Methyl-6-nitro-2-[4-(pyrrolidin-1-ylsulfonyl)phenoxy]methyl]-2,3-dihydroimidazo [2,1-*b*]oxazole 6a: IIM/MCD-033

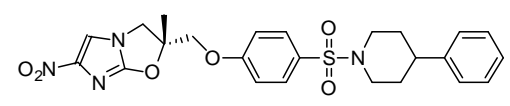


TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.5$; Light yellow solid; Yield = 32%; mp 184-186 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3 + 2 drops of Acetone- d_6) 7.75 (d, $J = 8.9$ Hz, 2H), 7.57 (s, 1H), 6.93 (d, $J = 8.9$ Hz, 2H), 4.52 (d, $J = 10.3$ Hz, 1H), 4.32 (d, $J = 10.2$ Hz, 1H), 4.16 (d, $J = 10.2$ Hz, 1H), 4.09 (d, $J = 10.3$ Hz, 1H), 3.20 (t, $J = 6.7$ Hz, 4H), 1.81 (s, 3H), 1.76 (t, $J = 6.7$ Hz, 4H). $^{13}\text{C NMR}$ (126 MHz, Acetone- d_6) 162.31, 156.85, 147.67, 130.62, 130.51, 115.85, 115.14, 94.38, 72.90, 52.06, 48.69, 25.73, 22.62; $[\alpha]_D -8.5^\circ$ (*c* 0.41, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{20}\text{N}_4\text{O}_6\text{S}$ $[\text{M} + \text{H}]^+$ 409.1182, found 409.1181; HPLC-purity 96.65%.

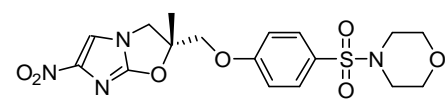
(R)-2-Methyl-6-nitro-2-[4-(piperidin-1-ylsulfonyl)phenoxy]methyl]-2,3-dihydroimidazo[2,1-b]oxazole 6b: IIIM/MCD-034/253

 TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.5$; Light yellow solid; Yield = 35%; mp 148-150 °C; ^1H NMR (500 MHz, CDCl_3) 7.66 (d, $J = 6.9$ Hz, 2H), 7.57 (s, 1H), 6.93 (d, $J = 7.2$ Hz, 2H), 4.52 (d, $J = 10.3$ Hz, 1H), 4.32 (d, $J = 10.1$ Hz, 1H), 4.16 (d, $J = 10.2$ Hz, 1H), 4.10 (d, $J = 10.3$ Hz, 1H), 2.94 (m, 4H), 1.81 (s, 3H), 1.64 – 1.60 (m, 4H), 1.44 – 1.41 (m, 2H); ^{13}C NMR (126 MHz, Acetone- d_6) 162.33, 156.85, 147.68, 130.72, 129.91, 115.82, 115.12, 94.36, 72.91, 52.06, 47.72, 25.92, 24.13, 22.63; $[\alpha]_D -15.67^\circ$ (c 1.33, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{18}\text{H}_{22}\text{N}_4\text{O}_6\text{S}$ $[\text{M} + \text{Na}]^+$ 423.1338, found 423.1303; HPLC-purity 97.95%.

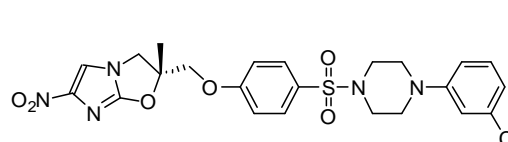
(R)-2-Methyl-6-nitro-2-[4-[(4-phenylpiperidin-1-yl)sulfonyl]phenoxy]methyl]-2,3-dihydroimidazo[2,1-b]oxazole 6c: IIIM/MCD-018

 TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.55$; Light yellow solid; Yield = 30%; mp 191-193 °C; ^1H NMR (400 MHz, CDCl_3) 7.81 (m, 2H), 7.55 (s, 1H), 7.23 (m, 3H), 6.82 (d, $J = 9.1$ Hz, 2H), 6.76 (d, $J = 9.1$ Hz, 2H), 4.47 (d, $J = 10.2$ Hz, 1H), 4.17 (d, $J = 10.2$ Hz, 1H), 4.02 (m, 2H), 3.15 (m, 8H), 2.08 (m, 1H), 1.76 (s, 3H); $[\alpha]_D -9.8^\circ$ (c 0.49, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_6\text{S}$ $[\text{M} + \text{Na}]^+$ 521.1471, found 521.1469; HPLC-purity 96.63%.

(R)-2-Methyl-6-nitro-2-[4-(morpholin-4-ylsulfonyl)phenoxy]methyl]-2,3-dihydroimidazo[2,1-b]oxazole 6d: IIIM/MCD-017/248

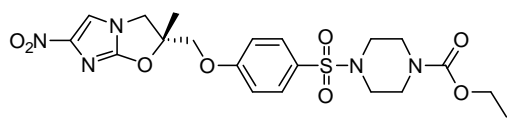
 TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.45$; Light yellow solid; Yield = 28%; mp 160-162 °C; ^1H NMR (400 MHz, CDCl_3) 7.70 (d, $J = 8.8$ Hz, 2H), 7.57 (s, 1H), 6.98 (d, $J = 8.8$ Hz, 2H), 4.50 (d, $J = 10.3$ Hz, 1H), 4.33 (d, $J = 10.1$ Hz, 1H), 4.17 (d, $J = 10.1$ Hz, 1H), 4.10 (d, $J = 10.3$ Hz, 1H), 3.78 – 3.71 (m, 4H), 2.99 – 2.96 (m, 4H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) 161.11, 155.77, 147.19, 130.05, 128.26, 115.04, 112.76, 92.77, 71.66, 66.03, 51.39, 46.03, 23.04; $[\alpha]_D -6.5^\circ$ (c 0.41, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{20}\text{N}_4\text{O}_7\text{S}$ $[\text{M} + \text{Na}]^+$ 447.0951, found 447.0958; HPLC-purity 98.64%.

(R)-2-Methyl-6-nitro-2-[4-[(3-chlorophenyl)piperazin-1-yl)sulfonyl]phenoxy]methyl]-2,3-dihydroimidazo[2,1-b]oxazole 6e: IIIM/MCD-036/250

 TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.35$; Light yellow solid; Yield = 32%; mp 189-191 °C; ^1H

NMR (500 MHz, CDCl₃) 7.73 (d, *J* = 8.9 Hz, 2H), 7.58 (s, 1H), 7.15 (t, *J* = 8.1 Hz, 1H), 6.98 (d, *J* = 8.9 Hz, 2H), 6.86 – 6.80 (m, 2H), 6.72 (dd, *J* = 8.6, 2.0 Hz, 1H), 4.50 (d, *J* = 10.3 Hz, 1H), 4.32 (d, *J* = 10.1 Hz, 1H), 4.17 (d, *J* = 10.1 Hz, 1H), 4.09 (d, *J* = 10.3 Hz, 1H), 3.27 – 3.23 (m, 4H), 3.15 – 3.10 (m, 4H), 1.82 (s, 3H); ¹³C NMR (126 MHz, Acetone-*d*₆) 162.67, 156.84, 153.02, 147.69, 135.31, 131.25, 130.98, 128.98, 120.17, 116.70, 116.02, 115.43, 115.12, 94.29, 72.94, 52.06, 48.92, 46.85, 22.63; [α]_D -18.3° (*c* 1.0, Acetone); HRMS (ESI-TOF) calcd for C₂₃H₂₄ClN₅O₆S [M + H]⁺ 534.1214, found 534.1224; HPLC-purity 96.90%.

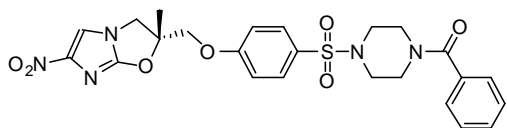
(R)-Methyl4-[[4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-*b*]oxazol-2-yl)methoxy)phenyl]sulfonyl]piperazine-1-carboxylate 6f: IIIM/MCD-037/251



TLC (EtOAc:DCM 0.5:9.5): *R*_f = 0.45; Light yellow solid; Yield = 35%; mp 158-160 °C; ¹H NMR (400 MHz, CDCl₃+ 2 drops of Acetone-*d*₆)

7.67 (d, *J* = 8.9 Hz, 2H), 7.57 (s, 1H), 6.96 (d, *J* = 8.9 Hz, 2H), 4.50 (d, *J* = 10.3 Hz, 1H), 4.32 (d, *J* = 10.2 Hz, 1H), 4.17 (d, *J* = 10.2 Hz, 1H), 4.12 – 4.05 (m, 3H), 3.58 – 3.53 (m, 4H), 2.95 (s, 4H), 1.82 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (126 MHz, Acetone-*d*₆) 162.66, 156.84, 155.43, 147.68, 130.90, 129.04, 116.03, 115.92, 115.14, 94.30, 72.93, 61.93, 52.06, 46.80, 22.63, 14.88; [α]_D -10.95° (*c* 2.66, Acetone); HRMS (ESI-TOF) calcd for C₂₀H₂₅N₅O₈S [M + Na]⁺ 518.1322, found 518.1329; HPLC-purity 96.26%.

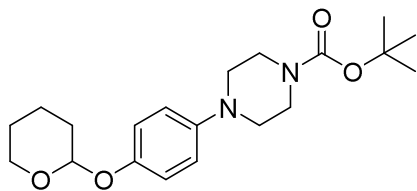
(R)-2-Methyl-6-nitro-2-{4-[(4-benzoylpiperazin-1-yl)sulfonyl]phenoxy}methyl}-2,3-dihydroimidazo[2,1-*b*]oxazole 6g: IIIM/MCD-035/249



TLC (EtOAc:DCM 0.5:9.5): *R*_f = 0.30; Light yellow solid; Yield = 25%; mp 176-178 °C; ¹H NMR (500 MHz, CDCl₃) 7.68 (d, *J* = 8.8 Hz,

2H), 7.58 (s, 1H), 7.44 -7.37 (m, 3H), 7.32 (d, *J* = 7.9 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 4.51 (d, *J* = 10.3 Hz, 1H), 4.34 (d, *J* = 10.2 Hz, 1H), 4.18 (d, *J* = 10.2 Hz, 1H), 4.11 (d, *J* = 10.3 Hz, 1H), 3.88 – 3.84 (m, 2H), 3.58 – 3.53 (m, 2H), 3.05 – 2.99 (m, 4H), 1.83 (s, 3H); ¹³C NMR (126 MHz, Acetone-*d*₆) 170.39, 162.66, 156.85, 147.67, 136.67, 130.92, 130.57, 129.25, 129.13, 128.09, 116.07, 115.17, 94.34, 72.95, 52.07, 22.63; [α]_D -18.2° (*c* 2.0, Acetone); HRMS (ESI-TOF) calcd for C₂₄H₂₅N₅O₇S [M + H]⁺ 528.1553, found 528.1558; HPLC-purity 98.18%.

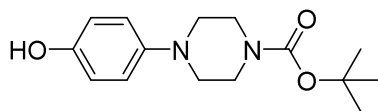
***tert*-Butyl 4-(4-((tetrahydro-2H-pyran-2-yl)oxy)phenyl)piperazine-1-carboxylate 9:**



A mixture of N-Boc piperazine **8** (3.72 g, 20 mmol) and 2-(4-bromophenoxy)-tetrahydropyran **7** (5.12 g, 20 mmol) in the presence of palladium acetate (0.12 g, 0.6 mmol), rac-2,2-bis-(diphenylphosphino)-1,1-binaphthyl (0.74 g, 1.2 mmol), and cesium carbonate

(9.77 g, 30 mmol) in toluene (50 ml) was refluxed under a nitrogen atmosphere for 30 min. The reaction mixture was allowed to cool to room temperature, and ethyl acetate and water were added. The thus-obtained mixture was filtered through Celite. The organic layer was separated, washed with brine, dried over magnesium sulfate, and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give **9**. TLC (EtOAc:hexane 2:8): $R_f = 0.40$; Yellow solid; Yield = 65%; $^1\text{H NMR}$ (200 MHz, CDCl_3) 6.85 (d, $J = 8.7$ Hz, 2H), 6.78 (d, $J = 8.8$ Hz, 2H), 5.32 – 5.29 (m, 1H) 3.66 – 3.44 (m, 4H), 3.10 – 2.85 (m, 4H), 3.42 – 3.38 (m, 2H), 2.04 – 1.64 (m, 4H), 1.59 – 1.56 (m, 2H), 1.48 (s, 9H). LC-MS (ESI+): m/z 363.22 $[\text{M} + \text{H}]^+$.

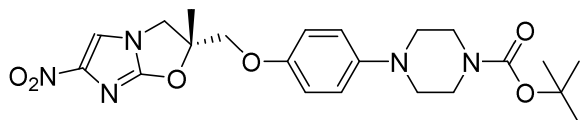
***tert*-Butyl 4-(4-hydroxyphenyl)piperazine-1-carboxylate **10**:**



A mixture of **9** (3.63 g, 10 mmol) and pyridinium *p*-toluenesulfonate (0.75 g, 3 mmol) in ethanol (75 ml) was heated at 70 °C for 24 h. The reaction mixture was

allowed to cool to room temperature and concentrated under reduced pressure. Saturated sodium hydrogen carbonate aqueous solution was added to the residue, which was extracted with dichloromethane. The organic layer was washed with brine, dried over magnesium sulfate, and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by silica gel column chromatography. TLC (EtOAc:hexane 2:8): $R_f = 0.20$; Light yellow solid; Yield = 85%; $^1\text{H NMR}$ (200 MHz, CDCl_3) 6.85 (d, $J = 8.9$ Hz, 2H), 6.78 (d, $J = 8.9$ Hz, 2H), 3.66 – 3.44 (m, 4H), 3.10 – 2.85 (m, 4H), 1.48 (s, 9H); LC-MS (ESI+): m/z 279.17 $[\text{M} + \text{H}]^+$.

(*R*)-*tert*-Butyl 4-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-*b*]oxazol-2-yl)methoxy)phenyl)piperazine-1-carboxylate **11: IIM/MCD-038**



To a mixture of epoxide compound **5** (1.08 g, 5 mmol) and phenol compound **10** (1.39 g, 5 mmol) in *N,N*-dimethylformamide (10

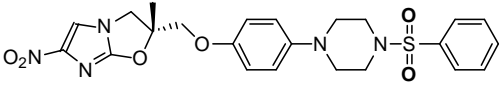
ml) was added 60% sodium hydride (0.36 g, 15 mmol) at 0 °C portionwise. After the mixture was stirred at 50 °C for 6 h under a nitrogen atmosphere, the reaction mixture was cooled in

an ice bath and carefully quenched with ethyl acetate (11.5 ml) and ice water (2.5 ml). The thus-obtained mixture was poured into water (150 ml) and extracted with ethyl acetate twice, washed with brine solution and dried under vacuo. This crude product was purified by silica gel column chromatography using a dichloromethane and ethyl acetate mixture as solvent. TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.55$; Light yellow solid; Yield: 32%; mp 211-213 °C ; ^1H NMR (500 MHz, CDCl_3) 7.56 (s, 1H), 6.88 (d, $J = 9.1$ Hz, 2H), 6.79 (d, $J = 9.1$ Hz, 2H), 4.49 (d, $J = 10.2$ Hz, 1H), 4.18 (d, $J = 10.1$ Hz, 1H), 4.05 – 4.01 (m, 2H), 3.59 – 3.55 (m, 4H), 3.03-3.0 (m, 4H), 1.77 (s, 3H), 1.48 (s, 9H); [α] $_D$ -8.52° (c 0.51, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{22}\text{H}_{29}\text{N}_5\text{O}_6$ [$\text{M} + \text{H}$] $^+$ 460.2196, found 460.2134; HPLC-purity 96.90%.

General procedure for the preparation of compounds 13(a-e):

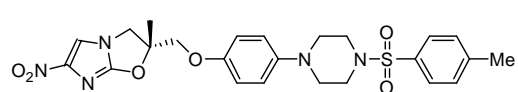
The Boc protected compound **11** (100 mg, 0.21 mmol) was dissolved in 20% TFA/DCM and the reaction mixture was stirred at room temperature for 2 h. Then the reaction mixture was evaporated under vacuo and the crude reaction mixture was dissolved in dichloromethane. The crude reaction mixture was added triethylamine (24.2 mg, 0.23 mmol), and a catalytic amount of 4- dimethylaminopyridine (DMAP). After stirring at room temperature for 15 min, a solution of substituted benzene sulphonyl chlorides **12** (0.21 mmol) in 5 ml of dichloromethane was added slowly in dropwise manner. The reaction mixture was stirred at room temperature under nitrogen atmosphere for 12 h. After complete conversion as indicated by TLC, the solvent was removed in vacuo, the residue was neutralized with saturated NaHCO_3 solution, and the aqueous layer was extracted with ethyl acetate, washed with water, and dried over anhydrous Na_2SO_4 . The solvent was evaporated in vacuo and the resultant crude compounds were purified by column chromatography.

(*R*)-2-Methyl-6-nitro-2-[[4-(4-phenylsulfonyl)piperazin-1-yl]phenoxy]methyl]-2,3-dihydroimidazo[2,1-*b*]oxazole 13a: IIIM/MCD-132

 TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.35$; Light yellow solid; Yield: 90%; mp 218-220 °C ; ^1H NMR (400 MHz, CDCl_3) 7.79 (d, $J = 7.3$ Hz, 2H), 7.62 (t, $J = 7.3$ Hz, 1H), 7.59 – 7.53 (m, 3H), 6.81 (d, $J = 9.1$ Hz, 2H), 6.75 (d, $J = 9.1$ Hz, 2H), 4.47 (d, $J = 10.2$ Hz, 1H), 4.16 (d, $J = 10.2$ Hz, 1H), 4.03 (d, $J = 4.1$ Hz, 1H), 4.01 (d, $J = 4.1$ Hz, 1H), 3.18 – 3.09 (m, 8H), 1.75 (s, 3H); ^{13}C NMR (126 MHz, Acetone- d_6) 156.96, 153.65, 147.67, 146.91, 136.61, 133.96, 130.14, 128.73, 119.40, 116.36, 115.02, 94.67, 73.31, 52.04, 50.72, 47.17, 22.69; [α] $_D$ -20° (c

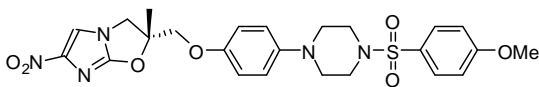
0.35, Acetone); HRMS (ESI-TOF) calcd for C₂₃H₂₅N₅O₆S [M + Na]⁺ 522.1424, found 522.1427; HPLC-purity 97.85%.

(R)-2-Methyl-6-nitro-2-[4-(4-tosylpiperazin-1-yl)phenoxyethyl]-2,3-dihydroimidazo[2,1-b]oxazole 13b: IIM/MCD-130



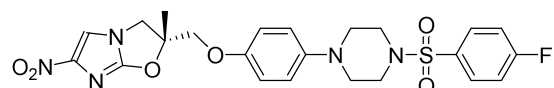
TLC (EtOAc:DCM 0.5:9.5): *R_f* = 0.40; Light yellow solid; Yield: 83%; mp 226-228 °C; ¹H NMR (400 MHz, CDCl₃) 7.67 (d, *J* = 7.5 Hz, 2H), 7.55 (s, 1H), 7.34 (d, *J* = 7.9 Hz, 2H), 6.78 (dd, *J* = 22.5, 8.2 Hz, 4H), 4.47 (d, *J* = 9.7 Hz, 1H), 4.16 (d, *J* = 10.0 Hz, 1H), 4.02 (d, *J* = 10.1 Hz, 2H), 3.13 (s, 8H), 2.44 (s, 3H), 1.75 (s, 3H); ¹³C NMR (101 MHz, Acetone-*d*₆) 156.96, 153.66, 147.76, 146.96, 144.72, 133.76, 130.59, 128.79, 119.39, 116.40, 114.92, 94.62, 73.36, 52.06, 50.73, 47.15, 22.69, 21.41; [α]_D -6.6° (*c* 0.75, Acetone); HRMS (ESI-TOF) calcd for C₂₄H₂₇N₅O₆S [M + Na]⁺ 536.1580, found 536.1575; HPLC-purity 95.92%.

(R)-2-Methyl-6-nitro-2-[[4-(4-(4-methoxyphenylsulfonyl)piperazin-1-yl)]phenoxyethyl]-2,3-dihydroimidazo[2,1-b]oxazole 13c: IIM/MCD-129



TLC (EtOAc:DCM 0.5:9.5): *R_f* = 0.35; Light yellow solid; Yield: 80%; mp 222-224 °C; ¹H NMR (400 MHz, CDCl₃) 7.72 (d, *J* = 8.9 Hz, 2H), 7.54 (s, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 6.81 (d, *J* = 9.1 Hz, 2H), 6.75 (d, *J* = 9.2 Hz, 2H), 4.47 (d, *J* = 10.2 Hz, 1H), 4.16 (d, *J* = 10.2 Hz, 1H), 4.04- 4.0 (m, 2H), 3.88 (s, 3H), 3.14 – 3.12 (m, 8H), 1.76 (s, 3H); ¹³C NMR (101 MHz, Acetone-*d*₆) 164.21, 156.96, 153.64, 146.97, 130.91, 128.19, 119.37, 116.39, 115.20, 114.94, 94.63, 73.34, 56.16, 52.04, 50.71, 47.16, 22.68; [α]_D -7.45° (*c* 0.42, Acetone); HRMS (ESI-TOF) calcd for C₂₄H₂₇N₅O₇S [M + Na]⁺ 552.1529, found 552.1519; HPLC-purity 96.42%.

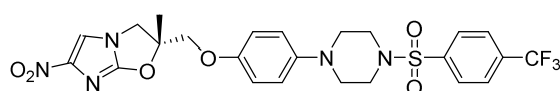
(R)-2-Methyl-6-nitro-2-[[4-(4-(4-fluorophenylsulfonyl)piperazin-1-yl)]phenoxyethyl]-2,3-dihydroimidazo[2,1-b]oxazole 13d: IIM/MCD-039/252



TLC (EtOAc:DCM 0.5:9.5): *R_f* = 0.45; Light yellow solid; Yield: 85%; mp 217-219 °C; ¹H NMR (400 MHz, CDCl₃) 7.74 (d, *J* = 8.9 Hz, 2H), 7.58 (s, 1H), 7.33 – 7.20 (m, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 4.52 (d, *J* = 10.3 Hz, 1H), 4.35 (d, *J* = 10.3 Hz, 1H), 4.17 (d, *J* = 10.3 Hz, 1H), 4.09 (d, *J* = 10.3 Hz, 1H), 3.92 – 3.90 (m, 2H), 2.34 – 2.31 (m, 4H), 2.04 – (m, 2H), 1.82 (s, 3H); ¹³C NMR (126 MHz, Acetone-*d*₆) 166.16 (d, *J* = 252.3 Hz), 165.65 (d, *J* = 2.6 Hz), 156.96, 153.67, 146.88, 132.95, 131.75 (d, *J* = 9.5 Hz),

119.42, 117.25 (d, $J = 22.8$ Hz), 116.35, 115.02, 94.66, 73.29, 52.03, 50.71, 47.16, 22.68; $[\]_D -13.42^\circ$ (c 0.35, Acetone); HRMS (ESI-TOF) calcd for $C_{23}H_{24}FN_5O_6S$ $[M + H]^+$ 518.1509, found 518.1514; HPLC-purity 93.21%.

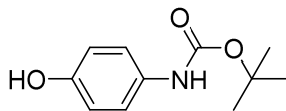
(R)-2-Methyl-6-nitro-2-[[4-(4-(4-trifluoromethylphenylsulfonyl)piperazin-1-yl)]phenoxy methyl]-2,3-dihydroimidazo[2,1-b]oxazole 13e: IIM/MCD-131



TLC (EtOAc:DCM 0.5:9.5): $R_f = 0.45$;
Light yellow solid; Yield: 82%; mp 243-
245 °C; 1H NMR (400 MHz, $CDCl_3$ + two

drops of Acetone- d_6) 7.93 (d, $J = 6.7$ Hz, 2H), 7.84 (d, $J = 6.9$ Hz, 2H), 7.57 (s, 1H), 6.80 (d, $J = 21.3$ Hz, 4H), 4.49 (s, 1H), 4.18 (s, 1H), 4.04 (s, 2H), 3.17 (d, $J = 19.5$ Hz, 8H), 1.77 (s, 3H). ^{13}C NMR (126 MHz, Acetone- d_6) 156.96, 153.73, 147.68, 146.85, 140.68, 134.53, 129.61, 127.38, 127.33, 119.49, 116.37, 115.02, 94.65, 73.32, 52.06, 50.79, 47.15, 22.70; $[\]_D -11.4^\circ$ (c 0.50, Acetone); HRMS (ESI-TOF) calcd for $C_{24}H_{24}F_3N_5O_6S$ $[M + Na]^+$ 590.1297, found 590.1283; HPLC-purity 97.35%.

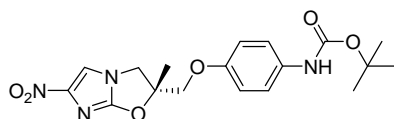
tert-Butyl (4-hydroxyphenyl)carbamate 15:



To a mixture of 4-amino phenol **14** (1.09 g, 10 mmol) in water (10 ml) was added $(Boc)_2O$ (2.4 g, 11 mmol) at room temperature. The reaction mixture was stirred at room temperature for 1h. The completion of the reaction is indicated by settling of white solid on

the bottom of the reaction vessel. The reaction mixture was filtered off and washes the solid obtained with water for several times and then the white solid was dried under vacuum. The crude product was purified by silica gel column chromatography using a dichloromethane and ethyl acetate mixture as solvent. TLC (EtOAc:Hexane 1:9): $R_f = 0.40$; white solid; Yield: 95%; 1H NMR (200 MHz, $CDCl_3$) 7.31 (d, $J = 8.56$ Hz, 2H), 7.78 (d, $J = 8.58$ Hz, 2H), 6.34 (s, 1H), 1.54 (s, 9H); LC-MS (ESI+): m/z 210.11 $[M + H]^+$.

tert-Butyl(R)-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl carbamate 16: IIM/MCD-049



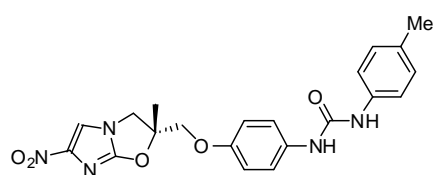
To a mixture of epoxide compound **5** (1.08 g, 5 mmol) and phenolic compound **15** (1.05 g, 5 mmol) in N,N -dimethylformamide (15 ml) was added 60% sodium hydride (0.36 g, 15 mmol) at 0 °C portionwise. After the reaction mixture was stirred at 50 °C for 6 h under a nitrogen atmosphere, the reaction mixture was cooled in an ice bath and

carefully quenched with ethyl acetate (11.5 ml) and ice water (2.5 ml). The thus-obtained mixture was poured into water (150 ml) and extracted with ethyl acetate twice, washed with brine solution and dried under vacuo. This crude product was purified by silica gel column chromatography using a dichloromethane and ethyl acetate mixture as solvent. TLC (EtOAc:DCM 1:9): $R_f = 0.40$; Light yellow solid; Yield: 35%; mp 233-235 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) 7.55 (s, 1H), 7.27 (d, $J = 6.7$ Hz, 2H), 6.78 (d, $J = 9.0$ Hz, 2H), 6.38 (s, 1H), 4.49 (d, $J = 10.2$ Hz, 1H), 4.19 (d, $J = 10.1$ Hz, 1H), 4.07 – 4.00 (m, 2H), 1.77 (s, 3H), 1.50 (s, 9H). $[\alpha]_D -10.4^\circ$ (c 0.52, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_5$ $[\text{M} + \text{H}]^+$ 391.16, found 391.1601; HPLC-purity 95.95%.

General procedure for the preparation of compounds 18(a-n):

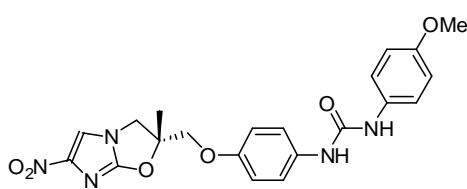
The compound **16** (100 mg, 0.25 mmol) was dissolved in 20% TFA/DCM and the reaction mixture was stirred at room temperature for 2 h. Then the reaction mixture was evaporated in vacuo and the crude reaction mixture was dissolved in dichloromethane. The reaction mixture was added triethyl amine (37.9 mg, 0.37 mmol) and stirred at room temperature for 5 minutes. Then the reaction mixture was added appropriate isocyanate or isothiocyanate **17** (0.27 mmol) and stirred at room temperature until one or both starting materials could not be detected by TLC. The product was then filtered off, washed, and the crude product was purified by column chromatography to give pure products **18(a-n)** in 60-80% yields.

(R)-1-(4-((2-Methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)-3-(p-tolyl)urea 18a: IIM/MCD-154



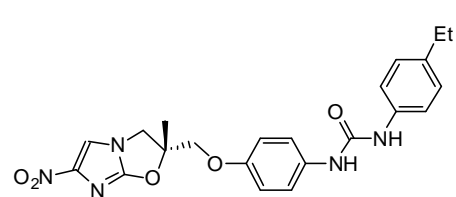
TLC (EtOAc:DCM 1:9): $R_f = 0.25$; Light yellow solid; Yield: 78%; mp 233-235 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 7.99 – 7.98 (m, 2H), 7.92 (s, 1H), 7.46 – 7.40 (m, 4H), 7.08 (d, $J = 8.2$ Hz, 2H), 6.87 (d, $J = 9.0$ Hz, 2H), 4.63 (d, $J = 10.8$ Hz, 1H), 4.36 – 4.29 (m, 3H), 2.27 (s, 3H), 1.82 (s, 3H); $^{13}\text{C NMR}$ (101 MHz, Acetone- d_6) 156.98, 154.58, 153.66, 138.49, 135.06, 131.96, 129.95, 121.08, 119.51, 115.93, 114.96, 94.62, 73.26, 52.08, 22.70, 20.69; $[\alpha]_D -10.4^\circ$ (c 0.50, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_5$ $[\text{M} + \text{Na}]^+$ 446.1441, found 446.1441; HPLC-purity 98.49%.

(R)-1-(4-Methoxyphenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)urea 18b: IIM/MCD-076



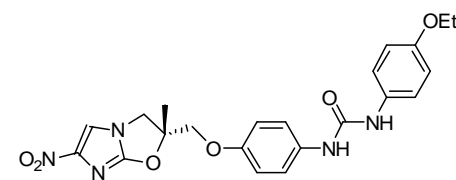
TLC (EtOAc:DCM 1:9): $R_f = 0.35$; Light yellow solid; Yield: 80%; mp 218-220 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 8.03 (s, 1H), 7.91 (s, 1H), 7.46 – 7.43 (m, 3H), 6.88 – 6.84 (m, 3H), 4.63 (d, $J = 10.7$ Hz, 1H), 4.36 – 4.28 (m, 3H), 3.76 (s, 3H), 1.82 (s, 3H); $[\alpha]_D -7.55^\circ$ (c 0.44, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_6$ $[\text{M} + \text{H}]^+$ 440.1570, found 440.1566; HPLC-purity 98.90%.

(R)-1-(4-Ethylphenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)urea 18c: IIM/MCD-156



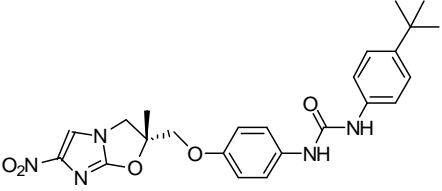
TLC (EtOAc:DCM 1:9): $R_f = 0.45$; Light yellow solid; Yield: 75%; mp 210-212 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 7.98 (d, $J = 5.9$ Hz, 2H), 7.92 (s, 1H), 7.46 – 7.42 (m, 4H), 7.12 (d, $J = 8.4$ Hz, 2H), 6.87 (d, $J = 9.0$ Hz, 2H), 4.63 (d, $J = 10.8$ Hz, 1H), 4.36 – 4.29 (m, 3H), 2.58 (q, $J = 7.6$ Hz, 2H), 1.82 (s, 3H), 1.19 (t, $J = 7.6$ Hz, 3H); $^{13}\text{C NMR}$ (101 MHz, Acetone- d_6) 156.99, 154.62, 153.65, 138.68, 135.04, 128.81, 121.14, 119.63, 115.96, 114.95, 94.63, 73.28, 52.09, 28.76, 22.71, 16.23; $[\alpha]_D -8.30^\circ$ (c 0.31, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{23}\text{H}_{23}\text{N}_5\text{O}_5$ $[\text{M} + \text{Na}]^+$ 460.1597, found 460.1602; HPLC-purity 97.99%.

(R)-1-(4-Ethoxyphenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)urea 18d: IIM/MCD-195



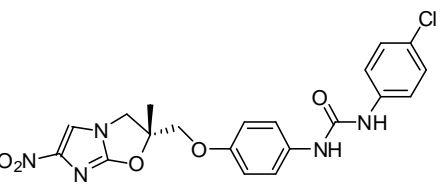
TLC (EtOAc:DCM 1:9): $R_f = 0.25$; Light yellow solid; Yield: 68%; mp 215-216 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 7.93 (s, 1H), 7.91 – 7.89 (m, 2H), 7.44 – 7.39 (m, 4H), 6.86 – 6.82 (m, 4H), 4.62 (d, $J = 10.7$ Hz, 1H), 4.34 – 4.27 (m, 3H), 3.99 (q, $J = 7.0$ Hz, 2H), 1.80 (s, 3H), 1.34 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, Acetone- d_6) 156.12, 154.55, 153.64, 134.28, 133.06, 120.42, 120.30, 120.18, 120.06, 115.03, 114.49, 114.16, 93.78, 72.37, 63.25, 51.20, 21.84, 14.33; $[\alpha]_D -8.41^\circ$ (c 0.49, Acetone); LC-MS (ESI+): m/z 454.2 $[\text{M} + \text{H}]^+$; HPLC-purity 95.95%.

(R)-1-(4-(tert-Butyl)phenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)urea 18e: IIM/MCD-155



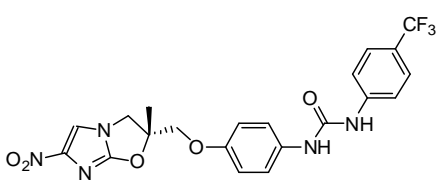
TLC (EtOAc:DCM 1:9): $R_f = 0.5$; Light yellow solid; Yield: 72%; mp 186-188 °C; ^1H NMR (400 MHz, Acetone- d_6) 8.04 (s, 1H), 8.00 (d, $J = 7.7$ Hz, 2H), 7.92 (s, 1H), 7.46 – 7.44 (m, 3H), 7.31 (d, $J = 8.7$ Hz, 2H), 6.88 (d, $J = 9.0$ Hz, 2H), 4.63 (d, $J = 10.8$ Hz, 1H), 4.37 – 4.29 (m, 3H), 1.82 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, Acetone- d_6) 157.00, 154.64, 153.68, 153.61, 145.50, 138.38, 135.02, 126.24, 121.17, 119.30, 115.97, 114.96, 94.64, 73.29, 52.10, 34.68, 31.74, 22.72; $[\alpha]_D -6.73^\circ$ (c 0.52, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{24}\text{H}_{27}\text{N}_5\text{O}_5$ $[\text{M} + \text{H}]^+$ 466.2090, found 466.2099; HPLC-purity 96.20%.

(R)-1-(4-Chlorophenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)urea 18f: IIM/MCD-192



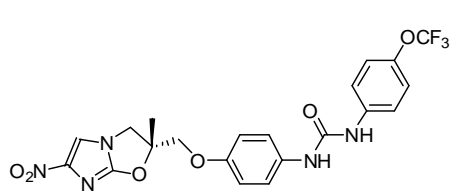
TLC (EtOAc:DCM 1:9): $R_f = 0.20$; Light yellow solid; Yield: 60%; mp 222-224 °C; ^1H NMR (400 MHz, Acetone- d_6) 8.24 (s, 1H), 8.06 (s, 1H), 7.91 (s, 1H), 7.56 (d, $J = 8.9$ Hz, 2H), 7.44 (d, $J = 9.0$ Hz, 2H), 7.29 (d, $J = 8.9$ Hz, 2H), 6.88 (d, $J = 9.0$ Hz, 2H), 4.63 (d, $J = 10.8$ Hz, 1H), 4.37 – 4.29 (m, 3H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, Acetone- d_6) 156.98, 154.80, 153.53, 140.01, 134.66, 129.42, 129.36, 127.02, 121.38, 121.33, 120.76, 116.00, 115.94, 115.01, 114.97, 100.89, 94.66, 73.26, 52.07, 22.71; $[\alpha]_D -8.34^\circ$ (c 0.53, Acetone); LC-MS (ESI+): m/z 444.1 $[\text{M} + \text{H}]^+$; HPLC-purity 98.32%.

(R)-1-(4-((2-Methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)-3-(4-(trifluoromethyl)phenyl)urea 18g: IIM/MCD-010



TLC (EtOAc:DCM 1:9): $R_f = 0.25$; Light yellow solid; Yield: 65%; mp 182-184 °C; ^1H NMR (400 MHz, Acetone- d_6) 8.65 (s, 1H), 8.30 (s, 1H), 7.90 (s, 1H), 7.75 (d, $J = 8.2$ Hz, 2H), 7.59 (d, $J = 8.2$ Hz, 2H), 7.46 (d, $J = 8.6$ Hz, 2H), 6.88 (d, $J = 8.7$ Hz, 2H), 4.62 (d, $J = 10.8$ Hz, 1H), 4.36 – 4.29 (m, 3H), 1.81 (s, 3H); $[\alpha]_D -8.69^\circ$ (c 0.45, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{18}\text{F}_3\text{N}_5\text{O}_5$ $[\text{M} + \text{Na}]^+$ 500.1158, found 500.1171; HPLC-purity 97.53%.

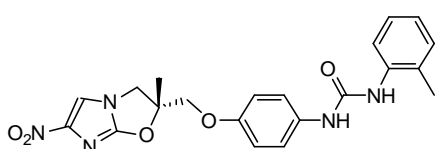
(R)-1-(4-((2-Methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)-3-(4-(trifluoromethoxy)phenyl)urea 18h: IIM/MCD-075



TLC (EtOAc:DCM 1:9): $R_f = 0.5$; Light yellow solid; Yield: 70%; mp 210-212 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 8.34 (s, 1H), 8.11 (s, 1H), 7.90 (s, 1H), 7.64 (d, $J = 9.1$ Hz, 2H), 7.44 (d, $J = 9.1$ Hz, 2H),

7.23 (d, $J = 8.4$ Hz, 2H), 6.87 (d, $J = 9.0$ Hz, 2H), 4.62 (d, $J = 10.8$ Hz, 1H), 4.36 – 4.28 (m, 3H), 1.80 (s, 3H); $[\alpha]_D -8.59^\circ$ (c 0.44, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{18}\text{F}_3\text{N}_5\text{O}_6$ $[\text{M} + \text{H}]^+$ 494.1287, found 494.1301; HPLC-purity 96.58%.

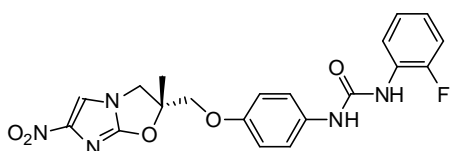
(R)-1-(4-((2-Methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)-3-(o-tolyl) urea 18i: IIM/MCD-157



TLC (EtOAc:DCM 1:9): $R_f = 0.30$; Light yellow solid; Yield: 79%; mp 220-222 °C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) 8.87 (s, 1H), 8.16 (s, 1H), 7.91 – 7.71 (m, 2H), 7.35 (d, $J = 8.4$ Hz, 2H), 7.17 – 7.11 (m, 2H), 6.93 (t, $J = 6.9$ Hz, 1H), 6.84 (d, $J = 8.4$ Hz, 2H), 4.38 (d, $J = 10.8$ Hz, 1H), 4.26 – 4.17 (m, 3H), 2.22 (s, 3H), 1.68 (s, 3H); $^{13}\text{C NMR}$

(126 MHz, Acetone- d_6) 155.17, 153.02, 152.01, 137.04, 133.49, 133.44, 129.43, 127.07, 125.50, 122.16, 120.81, 119.37, 114.35, 113.42, 93.04, 71.64, 50.47, 21.11, 16.49; $[\alpha]_D -8.77^\circ$ (c 0.43, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_5$ $[\text{M} + \text{Na}]^+$ 446.1441, found 446.1439; HPLC-purity 97.73%.

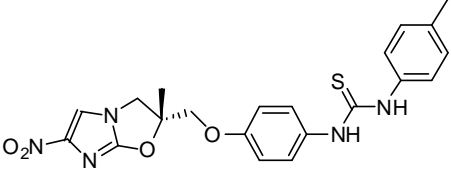
(R)-1-(2-Fluorophenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)urea 18j: IIM/MCD-194



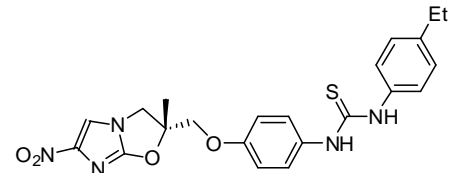
TLC (EtOAc:DCM 1:9): $R_f = 0.35$; Light yellow solid; Yield: 62%; mp 195-197 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 8.47 (s, 1H), 8.32 – 8.28 (m, 1H), 8.00 (s, 1H), 7.92 (s, 1H), 7.46 (d, $J = 8.8$ Hz,

2H), 7.16 – 7.12 (m, 2H), 7.02 – 6.97 (m, 1H), 6.89 (d, $J = 8.9$ Hz, 2H), 4.63 (d, $J = 10.7$ Hz, 1H), 4.36 – 4.29 (m, 3H), 1.81 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, Acetone- d_6) 156.99, 154.77, 153.24, 153.19 (d, $J = 240.7$ Hz), 147.64, 134.59, 129.02 (d, $J = 10.0$ Hz), 125.26 (d, $J = 3.4$ Hz), 123.15 (d, $J = 7.5$ Hz), 121.60, 121.08, 115.97, 115.48 (d, $J = 19.3$ Hz), 115.14, 94.71, 73.19, 52.07, 22.70; $[\alpha]_D -8.34^\circ$ (c 0.49, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{22}\text{H}_{19}\text{FN}_5\text{O}_5$ $[\text{M} + \text{Na}]^+$ 428.1361, found 428.1356; HPLC-purity 95.22%.

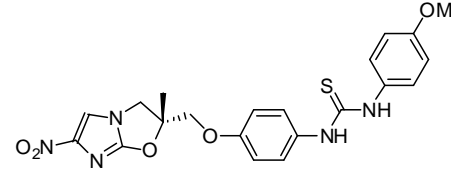
(R)-1-(4-((2-Methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)-3-(p-tolyl)thiourea 18k: IIM/MCD-0159/244


TLC (EtOAc:DCM 1:9): $R_f = 0.35$; Yellow solid;
Yield: 78%; mp 157-159 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 8.86 (s, 1H), 8.83 (s, 1H), 7.92 (s, 1H), 7.41 – 7.37 (m, 4H), 7.17 (d, $J = 8.1$ Hz, 2H), 6.92 (d, $J = 8.9$ Hz, 2H), 4.65 (d, $J = 10.8$ Hz, 1H), 4.42 – 4.34 (m, 3H), 2.31 (s, 3H), 1.83 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, Acetone- d_6) 181.77, 156.94, 156.92, 147.65, 137.48, 135.70, 133.82, 130.08, 127.67, 125.57, 115.62, 115.13, 94.63, 73.00, 52.08, 22.70, 20.96; $[\alpha]_D -24.8^\circ$ (c 0.75, Acetone); HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_4\text{S}$ $[\text{M} + \text{Na}]^+$ 462.1212, found 462.1218; HPLC-purity 91.94%.

(R)-1-(4-Ethylphenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)thiourea 18l: IIM/MCD-193

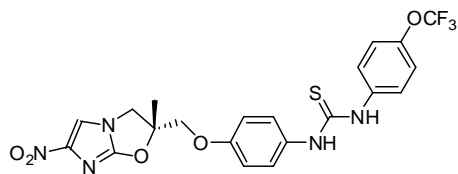

TLC (EtOAc:DCM 1:9): $R_f = 0.35$; Yellow solid;
Yield: 76%; mp 180-182 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 8.90 (s, 1H), 8.88 (s, 1H), 7.91 (s, 1H), 7.43 – 7.38 (m, 4H), 7.20 (d, $J = 8.3$ Hz, 2H), 6.92 (d, $J = 8.9$ Hz, 2H), 4.64 (d, $J = 10.8$ Hz, 1H), 4.41 – 4.33 (m, 3H), 2.63 (q, $J = 7.6$ Hz, 2H), 1.82 (s, 3H), 1.21 (t, $J = 7.6$ Hz, 3H); $^{13}\text{C NMR}$ (101 MHz, Acetone- d_6) 181.81, 156.96, 156.94, 147.70, 142.12, 137.71, 133.84, 128.88, 127.65, 125.53, 115.67, 115.03, 94.58, 73.03, 52.08, 28.89, 22.68, 16.02; $[\alpha]_D -23^\circ$ (c 0.46, Acetone); LC-MS (ESI+): m/z 454.2 $[\text{M} + \text{H}]^+$; HPLC-purity 96.52%.

(R)-1-(4-Methoxyphenyl)-3-(4-((2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)thiourea 18m: IIM/MCD-158


TLC (EtOAc:DCM 1:9): $R_f = 0.30$; Yellow solid;
Yield: 75%; mp 183-185 °C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6) 8.80 (s, 1H), 8.76 (s, 1H), 7.92 (s, 1H), 7.44 – 7.32 (m, 4H), 6.93 – 6.91 (m, 4H), 4.65 (d, $J = 10.8$ Hz, 1H), 4.41 – 4.33 (m, 3H), 3.81 (s, 3H), 1.83 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, Acetone- d_6) 180.25, 156.64, 155.04, 154.97, 132.04, 130.80, 129.62, 125.79, 125.76, 113.66, 113.13, 112.83, 92.66, 71.10, 53.80, 50.17, 20.78; $[\alpha]_D -25^\circ$ (c 0.48, Acetone);

HRMS (ESI-TOF) calcd for C₂₁H₂₁N₅O₅S [M + Na]⁺ 478.1161, found 478.1173; HPLC-purity 98.35%.

(R)-1-(4-((2-Methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazol-2-yl)methoxy)phenyl)-3-(4-(trifluoromethoxy)phenyl)thiourea 18n: IIM/MCD-160



TLC (EtOAc:DCM 1:9): R_f = 0.45; Yellow solid; Yield: 60%; mp 122-124 °C; ¹H NMR (400 MHz, CDCl₃) 7.83 (s, 1H), 7.78 (s, 1H), 7.47 (d, J = 8.7 Hz, 2H), 7.32 – 7.19 (m, 4H), 6.85 (d, J = 8.6 Hz, 2H), 4.49 (d, J = 10.2 Hz, 1H), 4.25 (d, J = 10.4 Hz, 1H), 4.09 – 4.06 (m, 2H), 1.78 (s, 3H); ¹³C NMR (126 MHz, Acetone-*d*₆) 181.91, 157.13, 156.94, 139.70, 133.40, 127.69, 126.63, 127.60, 121.98, 115.82, 115.06, 94.60, 73.02, 52.07, 22.66; [α]_D -21° (c 0.40, Acetone); HRMS (ESI-TOF) calcd for C₂₁H₁₈F₃N₅O₅S [M + Na]⁺ 532.0879, found 532.0897; HPLC-purity 94.85%.

2. Biological protocols for the determination of *in vitro* activities:

2.1. *In vitro* activity of compounds against *M. tuberculosis* H₃₇Rv and two clinical isolates (*M. tuberculosis* MDR & *M. tuberculosis* Rif^R)

MIC determination

MIC was determined by broth dilution method against *M. tuberculosis* H₃₇Rv (ATCC 27294; American Type Culture Collection, Manassas, VA, USA), *M. tuberculosis* MDR (resistant to isoniazid and rifampicin) and one of laboratory generated mutant *M. tuberculosis* Rif^R 1 (resistant to rifampicin) using micro-broth dilution method. The bacterial strains were grown for 10 to 15 days in Middlebrook 7H9 broth (Difco Laboratories, Detroit, Mich.) supplemented with 0.5% (v/v) glycerol, 0.25% (v/v) Tween 80 (Himedia, Mumbai India), and 10% ADC (albumin dextrose catalase, Becton Dickinson, Sparks, MD) under shaking conditions at 37 °C in 5% CO₂ to facilitate exponential-phase growth of the organism. Bacterial suspension was prepared by suspending *M. tuberculosis* growth in normal saline containing 0.5% tween 80 and turbidity was adjusted to 1 McFarland (McF) standard which is equivalent to 1.0 x 10⁷ CFU/ml. The 2-fold serial dilutions of compounds were prepared in Middle brook 7H9 (Difco laboratories) for *M. tuberculosis* in 100 μl per well in 96-well U bottom microtitre plates (Tarson, Mumbai, India). The above-mentioned bacterial suspension was further diluted 1:10 in the growth media and 100 μl volume of this diluted inoculum was

added to each well of the plate resulting in the final inoculum of 1.0×10^6 CFU/ml in the well and the final concentrations of compounds ranged from 0.015 to 32 $\mu\text{g/ml}$. The plates were incubated at 37 °C for seven days in 5% CO_2 . For evaluation of results (Resaurin Microtitre Assay) REMA method was used. After incubation, 15 μl of 0.04% resazurin and 12.5 μl of 20% tween 80 was added in each well of plate including media and growth controls. After 48 h incubation, plates were read visually and the minimum concentration of the compound showing no change of colour was recorded as MIC.

2.2. *In vitro* activity against Non-Replicating MTB:

Streptomycin starved *M. tuberculosis* 18b (ss18b) in non replicating phase (NRP) of growth was grown according to method described earlier² using 7H9 media. In brief streptomycin of normal strain of 18b was removed by phosphate buffer saline (pH 7.4) wash three times and then grown in STR free 7H9 media for a period of two weeks/14-16 days until mid log so that optical density of culture become nearly constant. A total of 0.2 O.D was used as inoculum for setting up MIC. Other conditions were same as used for MIC determination and evaluation by REMA method.

2.3. Evaluation of cytotoxicity in HepG2 cells:

Cytotoxicity of the compounds was evaluated using the MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide] assay.³ Human HepG2 cell line was maintained in the *Dulbecco's Modified Eagle's medium* (Gibco Life Technology, NY). Cells were plated at a density of 10,000 cell /well in 96 microwell flat bottom plate and incubated for 24 h (37°C; 5% CO_2). Cells monolayer was exposed to the single concentration of 40 $\mu\text{g/ml}$ of the tested compounds and incubated for 24 h (37°C; 5% CO_2). MTT dye was added at concentration of 2.5mg/ml dissolved in phosphate buffer saline (PBS) and cell viability was determined by measuring the absorbance of the reduced formazan at 570 nm in a plate reader. The percent cytotoxicity achieved by the compounds was calculated according to standard methods using tamoxifen as a negative control and healthy cells as positive control. Cytotoxicity is reported as CC_{50} , the concentration that causes a 50% reduction in cell viability.

3. Solubility determination method (96-well plate based assay):

The compound was dissolved in methanol to get a stock solution of 2000 $\mu\text{g/ml}$. The stock solution was introduced into 96-well plates and allowed to evaporate at room temperature to ensure that the compound (1, 2, 4, 8, 16, 25, 40, 80, 160, and 300 μg) is in solid form in the beginning of the experiment. Thereafter, 200 μl of dissolution medium

(water, PBS, SGF, and SIF) was added to the wells, and plates were shaken horizontally at 300 rpm (Eppendorf Thermoblock Adapter, North America) for 4 h at room temperature ($25\pm 1^\circ\text{C}$). The plates were covered with aluminum foil and were kept overnight at room temperature for equilibration. Later, the plates were centrifuged at 3000 rpm for 15 min (Jouan centrifuge BR4i). Supernatant (50 μl) was withdrawn into UV 96-well plates (Corning 96 well clearflat bottom UV-transparent microplate) for analyses with microplate reader (Molecular Devices, USA) at corresponding λ_{max} of the sample or the samples were also analysed by HPLC. The analysis was performed in triplicate for each compound. The solubility curve of concentration ($\mu\text{g}/\text{ml}$) vs absorbance was plotted to find out saturation point and the corresponding concentration was noted.^{4,5}

4. Metabolic stability assessed by Rat Liver Microsomes:

Pooled rat liver microsomes (20 mg/ml) were prepared from rat liver homogenate with the aim of isolating endoplasmic reticulum which are responsible for drug metabolism. 100 mM phosphate buffer saline was prepared and the pH was maintained at 7.4. 0.5 mM of the test compound was prepared in DMSO (final DMSO concentration should not be more than 0.4%). The incubation mixture contained 100mM phosphate buffer (pH 7.4), NADP, glucose-6-phosphate, glucose-6-phosphate dehydrogenase, $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ and 0.5mg/ml microsomal protein in a final incubation volume of 300 μl . the reaction was performed in triplicates in a water bath maintained at 37°C for 30 minutes. The reaction was quenched using methanol and centrifuged at 14000 rpm for 10 min. The supernatant was collected and analysed by LC-MS/MS.^{6,7}

5. *In vivo* oral Pharmacokinetic studies of compound 6d and IIM/MCD-019 in Swiss mice:

Compounds were administered orally to female Balb/c mice (5 mice in each group) at a dose of 5 mg/kg as a suspension in 0.5% CMC and Tween 80. Samples derived from plasma at different time points 0.16 h, 0.5 h, 1 h, 2 h, 4 h, 6 h, 8 h and 24 h, which were then analyzed by LC-MS/MS to generate the required pharmacokinetic parameters.

Table 1: Plasma concentrations (ng/ml) of compound **6d** and **IIIM/MCD-019** in mice

Compound ^a	Concentration (ng/ml) ^b							
	0.16 h	0.5 h	1 h	2 h	4 h	6 h	8 h	24 h
6d	612.26 ±118.92	642.68 ±105.78	226.49 ±63.10	157.37 ±68.04	79.52 ±62.09	ND	ND	ND
IIIM/MCD-019	183.03 ±105.62	364.3 ±142.53	491.57 ±242.33	544.85 ±153.81	451.55 ±70.29	318.43 ±67.11	298.92 ±77.88	226.74 ±118.41

^a p.o. at 5 mg/kg, ^b each value represents mean ± SD (n=5)

6. *In vivo* efficacy determination of the lead compound **6d**:

Quick *in vivo* model was used to determine the comparative efficacy of lead molecules among selected potent molecules. Brief experiment was run for one week using Balb/c mice and dosing was done for five days. Infection of actively growing culture suspension of *M. tuberculosis* H₃₇Rv with final density of 1.0 McF was given through nasal route. A total of four groups of Balb/c mice having six animals in each group with average body weight of 20-22 g were used. Animal were kept for acclimatization under BSL-3 conditions for two days following infection. Animal cages were labeled with drug control (Rifampicin 20 mg/kg), placebo, **6d** (25 mg/kg) and **IIIM/MCD-019** (100 mg/kg). Culture of *M. tuberculosis* was given small sonication thrashes to break clumps. 20µl of this uniform suspension was given by intranasal instillation. Dosing announced 48 h post-infection and continued for five days. Two days post dosing all animal were sacrificed to dissect left lung for enumeration of bacilli load. To determine bacilli load, left lung was homogenized in 1 ml of phosphate buffer saline (pH 7.4) supplemented with 0.05% tween 80. Serial tenfold dilutions were spotted on 7H10 agar supplemented with 10% OADC plates. Results were determined as Log CFU/ml.

6.1. Dose preparation and administration

For preparing the dose compound or drug was dissolved in minimum amount of DMSO and then mixed in alcohol so as to make final volume upto 5% ethanol and 95% PEG 400 (v/v) mixed. Compounds were dissolved to make final concentration of 25 mg/kg for **6d** and 100 mg/kg for **IIIM/MCD-019** while Rifampicin was prepared at a concentration of 20 mg/kg. A total of 200 µl volume of respective dose was administered orally (oral gavage) in a biosafety cabinet to each group. Same volume of mixture i.e. 5% ethanol and 95% PEG 400

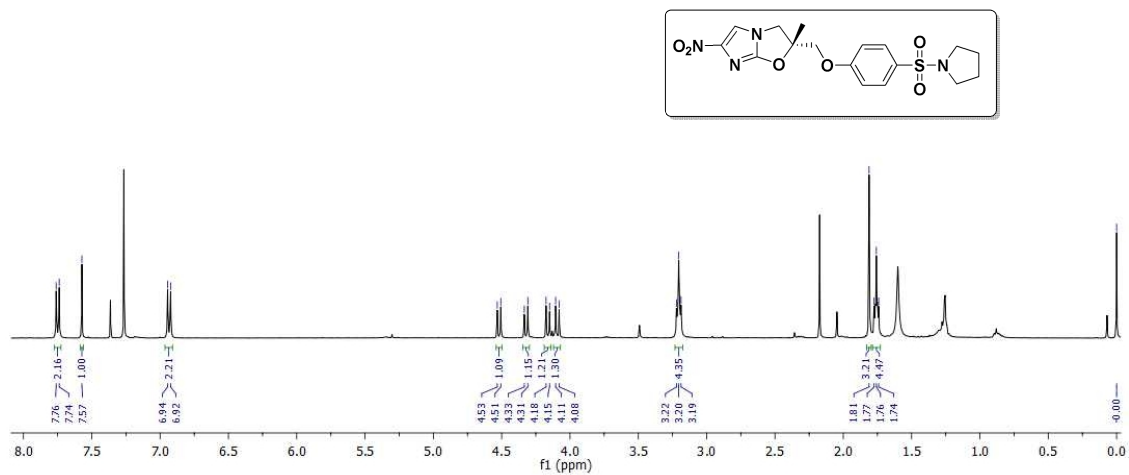
(v/v) was given to placebo group. A group of mice was kept without dosing which served as control.

7. References:

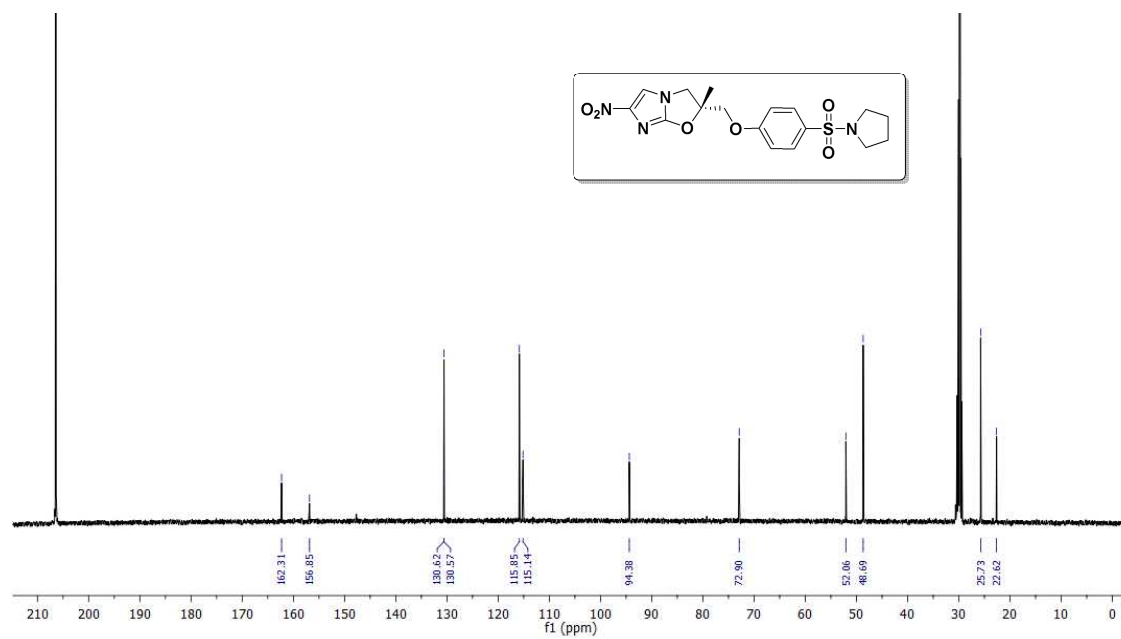
1. Sharma, S.; Kumar, M.; Sharma, S.; Nargotra, A.; Koul, S.; Khan, I. A. Piperine as an inhibitor of Rv1258c, a putative multidrug efflux pump of *Mycobacterium tuberculosis*. *J Antimicrob Chemother.* **2010**, *65*, 1694.
2. a) Sala, C.; Dhar, N.; Hartkoorn, R.C.; Zhang, M.; Ha, Y.H.; Schneider, P.; Cole, S.T. Simple model for testing drugs against nonreplicating *Mycobacterium tuberculosis*. *Antimicrob. Agents Chemother.* **2010**, *54*, 4150.
3. Zhang, M.; Sala, C.; Hartkoorn, R.C.; Dhar, N.; Losana.A.F.; and Cole, S.T. Streptomycin starved *Mycobacterium tuberculosis* 18b, a drug discovery tool for latent tuberculosis. *Antimicrob. Agents Chemother.* **2012**, *56*, 4150.
4. Dorsey, W. C.; Tchounwou, P. B.; Sutton, D. Mitogenic and cytotoxic effects of pentachlorophenol to AML 12 mouse hepatocytes. *Int J Environ Res Public Health.* **2004**, *1*, 100.
5. Roy, D.; Ducher, F.; Laumain, A.; Legendre, J. Y. Determination of the aqueous solubility of drugs using a convenient 96-well platebased assay. *Drug Dev. Ind. Pharm.* **2001**, *27*, 107-109.
6. Heikkila, T.; Karjalainen, M.; Ojala, K.; Partola, K.; Lammert, F.; Augustijns, P.; Urtti, A.; Yliperttula, M.; Peltonen, L.; Hirvonen, J. Equilibrium drug solubility measurements in 96-well plates reveal similar drug solubilities in phosphate buffer pH 6.8 and human intestinal fluid. *Int. J. Pharm.* **2011**, *405*, 132-136.
7. Seglen, P. O. Preparation of isolated rat liver cells. *Methods Cell. Biol.* **1976**, *13*, 29-83.
8. LeCluyse, E. L., Bullock, P. L., Parkinson, A., and Hochman, J. H. Cultured rat hepatocytes, in *Models for Assessing Drug Absorption and Metabolism.* **1996** (Borchardt, R. T., et al., eds.), Plenum, New York, pp. 121–159.

8. Spectras (^1H NMR, ^{13}C NMR, DEPT and HRMS) of sulphonyl and uridy/thiouridyl based NHIO compounds:

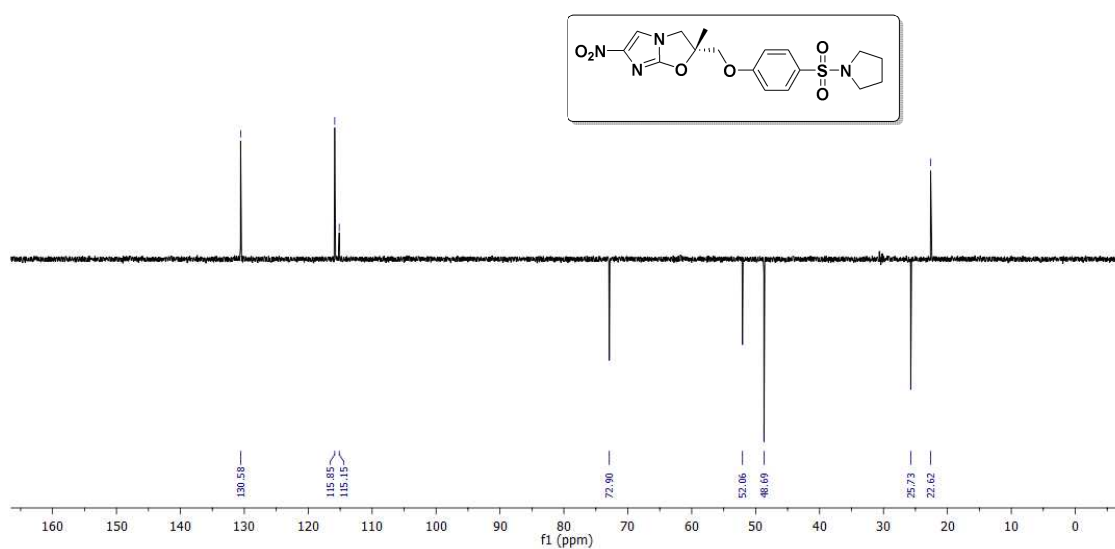
^1H NMR (400 MHz, CDCl_3 + two drops of Acetone- d_6) of compound **6a**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **6a**:



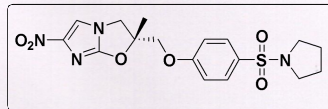
DEPT (126 MHz, Acetone- d_6) of compound **6a**:



HRMS of compound **6a**:

Qualitative Compound Report

Data File	33.d	Sample Name	33
Sample Type	Sample	Position	Vial 4
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	26-04-2013 PM 1:47:17
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			



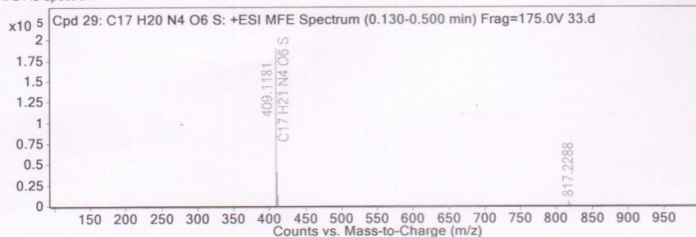
Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C17 H20 N4 O6 S	0.187	408.1108	C17 H20 N4 O6 S	C17 H20 N4 O6 S	-1.11	C17 H20 N4 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 29: C17 H20 N4 O6 S	409.1181	0.187	Find by Molecular Feature	408.1108

MFE MS Spectrum



MS Spectrum Peak List

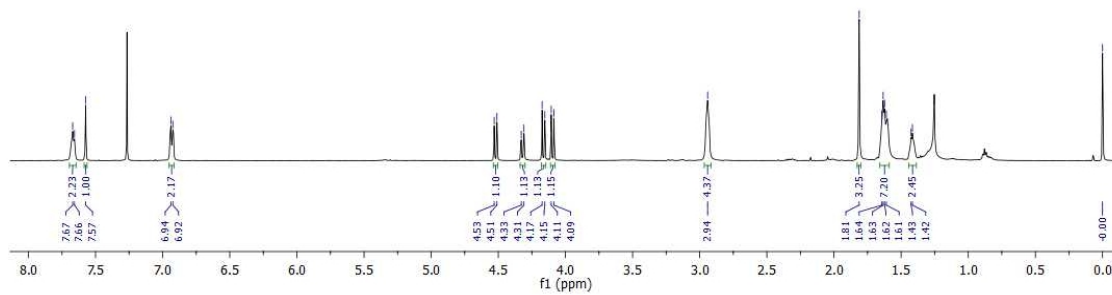
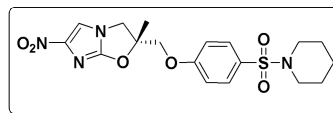
m/z	z	Abund	Formula	Ion
409.1181	1	189415.42	C17 H21 N4 O6 S	(M+H)+
410.1207	1	40705.55	C17 H21 N4 O6 S	(M+H)+
411.1187	1	12864.01	C17 H21 N4 O6 S	(M+H)+
412.1194	1	2580.01	C17 H21 N4 O6 S	(M+H)+
413.1211	1	561.34	C17 H21 N4 O6 S	(M+H)+
817.2288	1	5628.19		(2M+H)+
818.2314	1	2224		(2M+H)+
819.2348	1	1092.44		(2M+H)+

Predicted Isotope Match Table

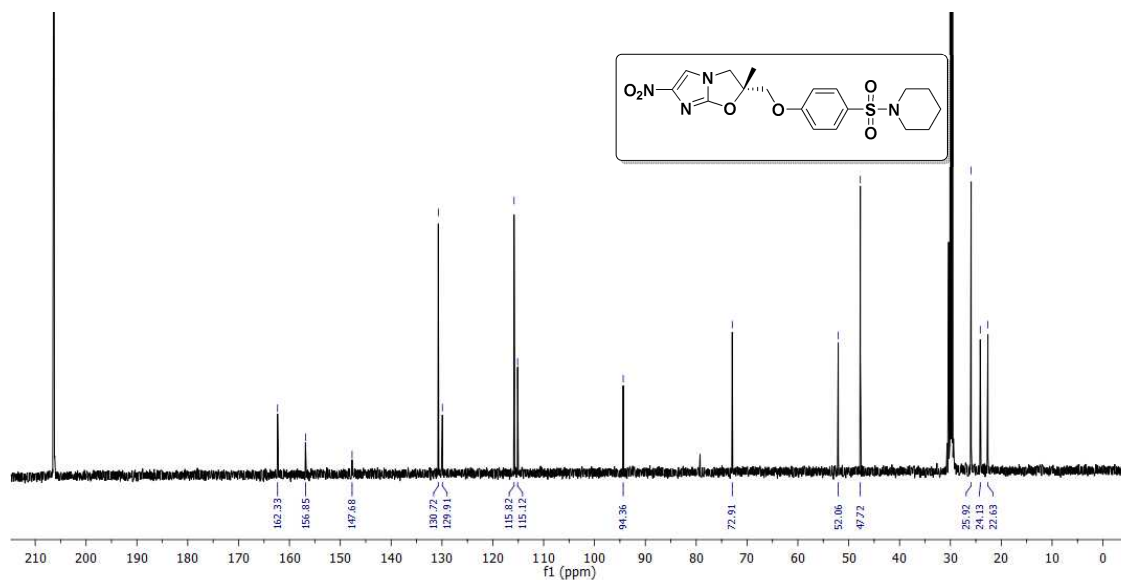
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	409.1181	409.1176	-1.07	100	100	76.96	76.67
2	410.1207	410.1204	-0.63	21.49	21.11	16.54	16.18
3	411.1187	411.1174	-3.12	6.79	7.83	5.23	6
4	412.1194	412.119	-1	1.36	1.3	1.05	1
5	413.1211	413.1201	-2.48	0.3	0.19	0.23	0.15

--- End Of Report ---

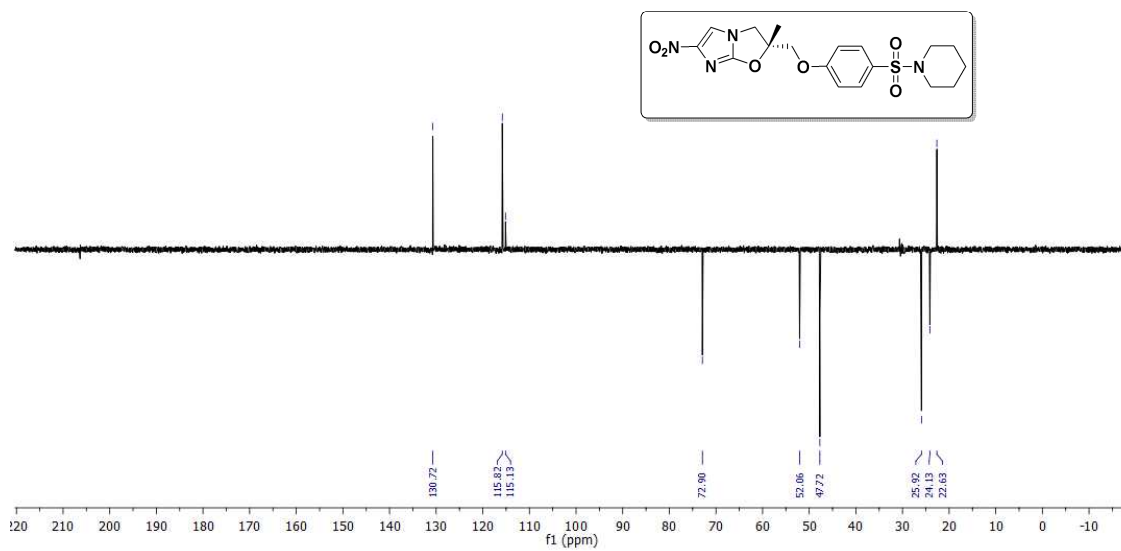
^1H NMR (500 MHz, CDCl_3) of compound **6b**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **6b**:



DEPT (126 MHz, Acetone- d_6) of compound **6b**:

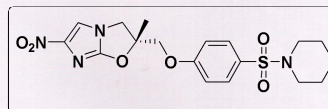


HRMS of compound **6b**:

Qualitative Compound Report

Data File	34.d	Sample Name	34
Sample Type	Sample	Position	Vial 6
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	26-04-2013 PM 2:03:34
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

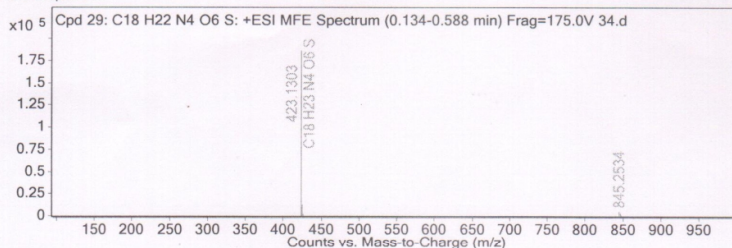


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C18 H22 N4 O6 S	0.187	422.123	C18 H22 N4 O6 S	C18 H22 N4 O6 S	7.22	C18 H22 N4 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 29: C18 H22 N4 O6 S	423.1303	0.187	Find by Molecular Feature	422.123

MFE MS Spectrum



MS Spectrum Peak List

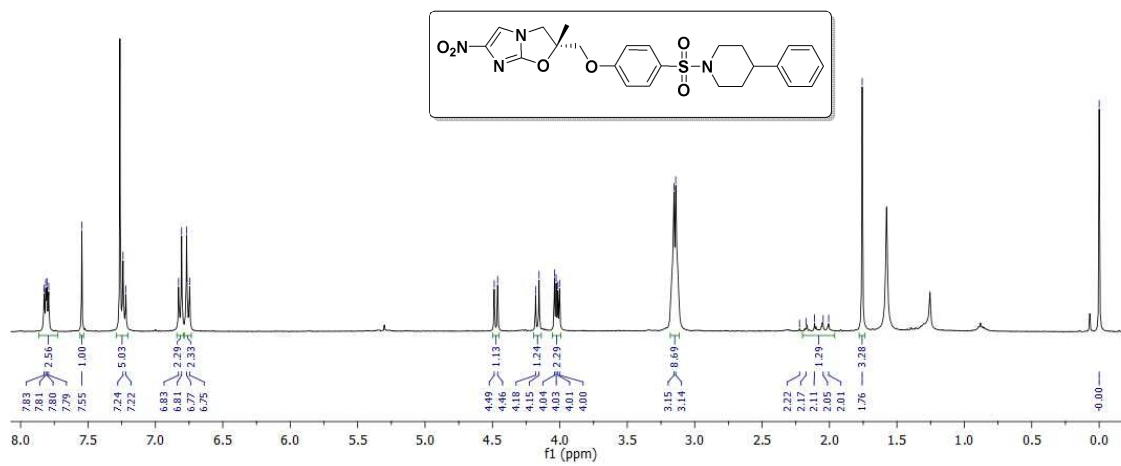
m/z	z	Abund	Formula	Ion
423.1303	1	186501.16	C18 H23 N4 O6 S	(M+H)+
424.1327	1	42984.6	C18 H23 N4 O6 S	(M+H)+
425.1306	1	13006.8	C18 H23 N4 O6 S	(M+H)+
426.1324	1	2556.17	C18 H23 N4 O6 S	(M+H)+
427.1345	1	416.77	C18 H23 N4 O6 S	(M+H)+
845.2534	1	4909.81		(2M+H)+
846.2522	1	2642.01		(2M+H)+
847.2579	1	1104.59		(2M+H)+

Predicted Isotope Match Table

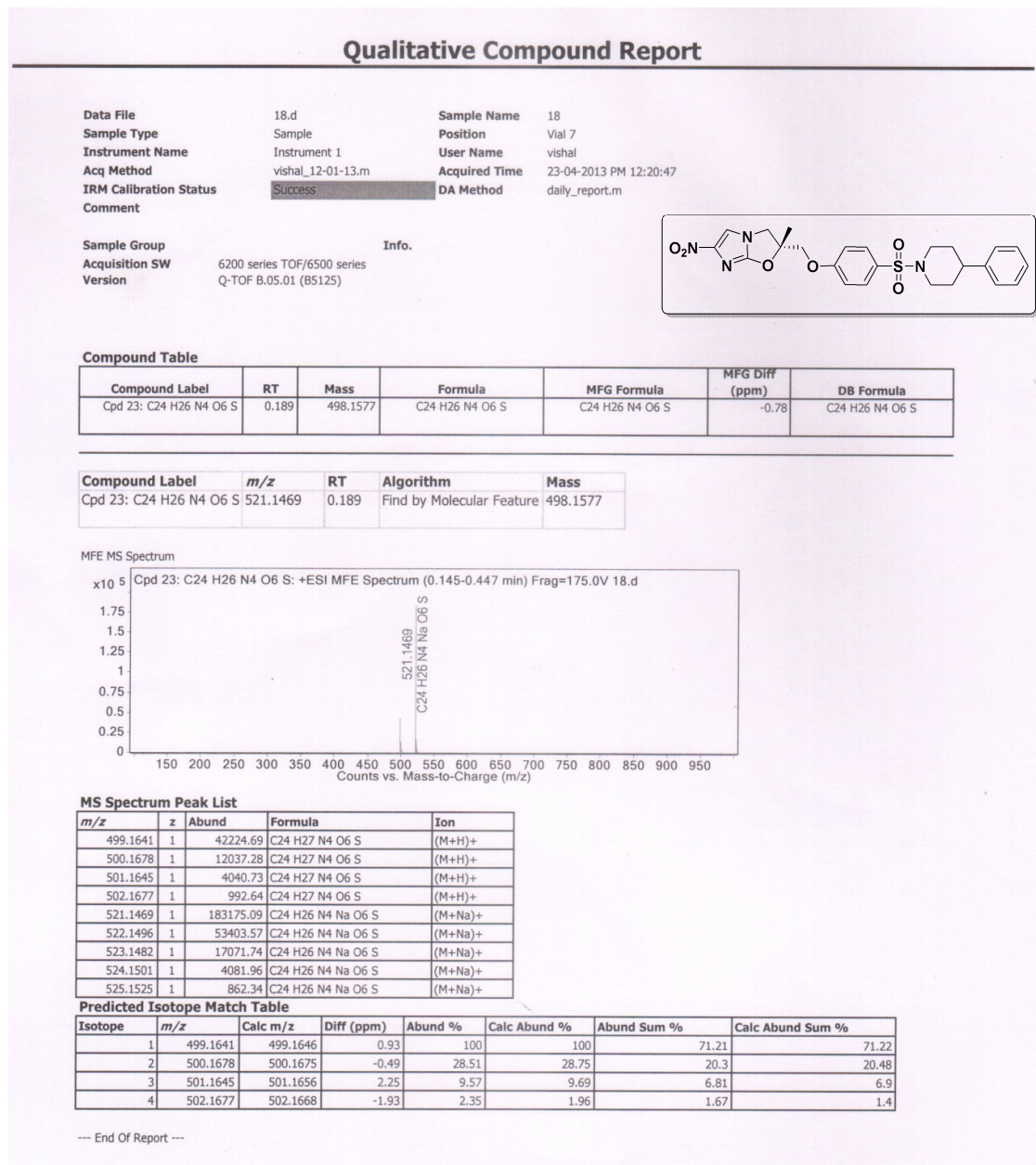
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	423.1303	423.1333	7.11	100	100	75.98	75.83
2	424.1327	424.1361	8	23.05	22.21	17.51	16.84
3	425.1306	425.1333	6.3	6.97	8.06	5.3	6.11
4	426.1324	426.1348	5.5	1.37	1.39	1.04	1.05
5	427.1345	427.1359	3.4	0.22	0.21	0.17	0.16

--- End Of Report ---

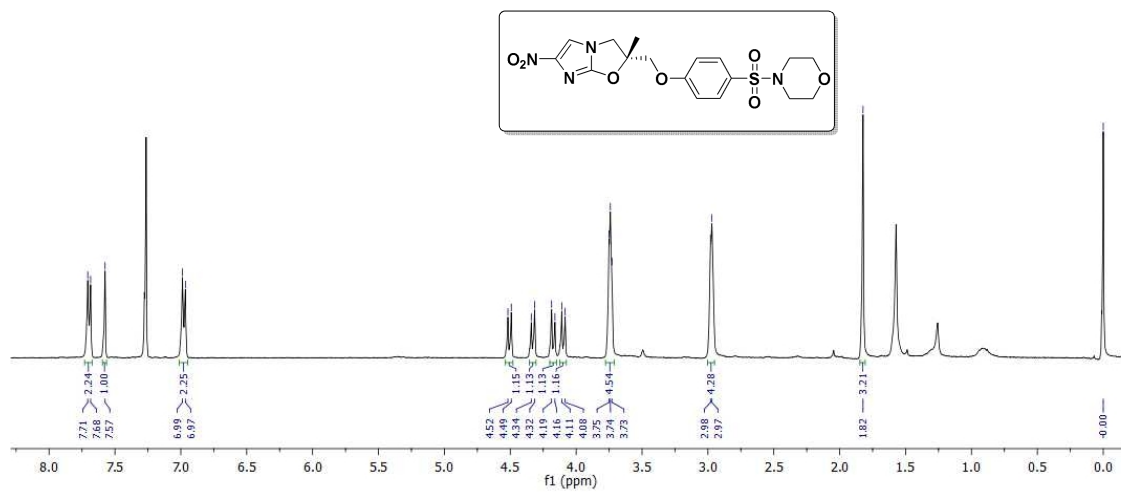
^1H NMR (400 MHz, CDCl_3) of compound **6c**:



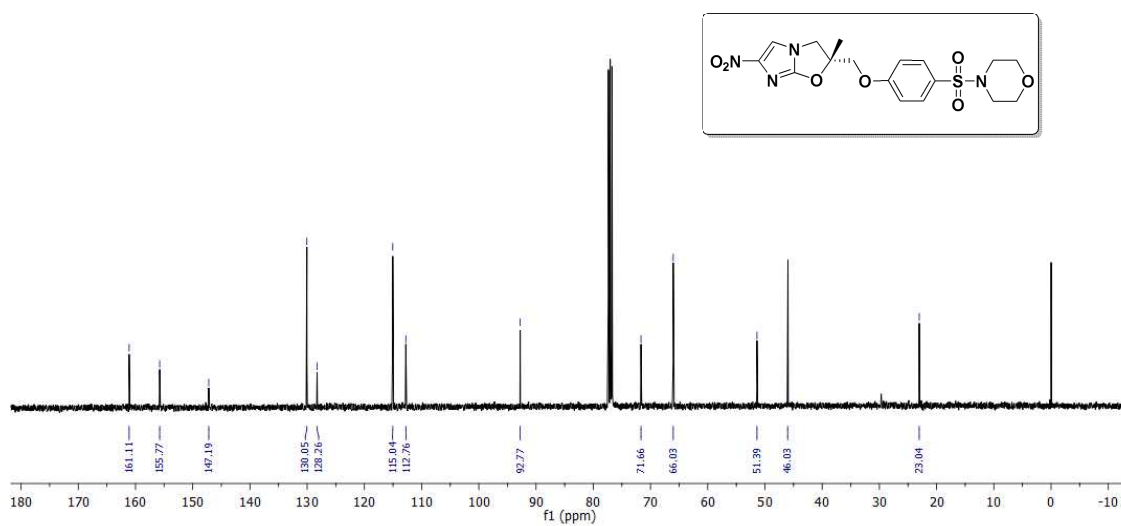
HRMS of compound 6c:



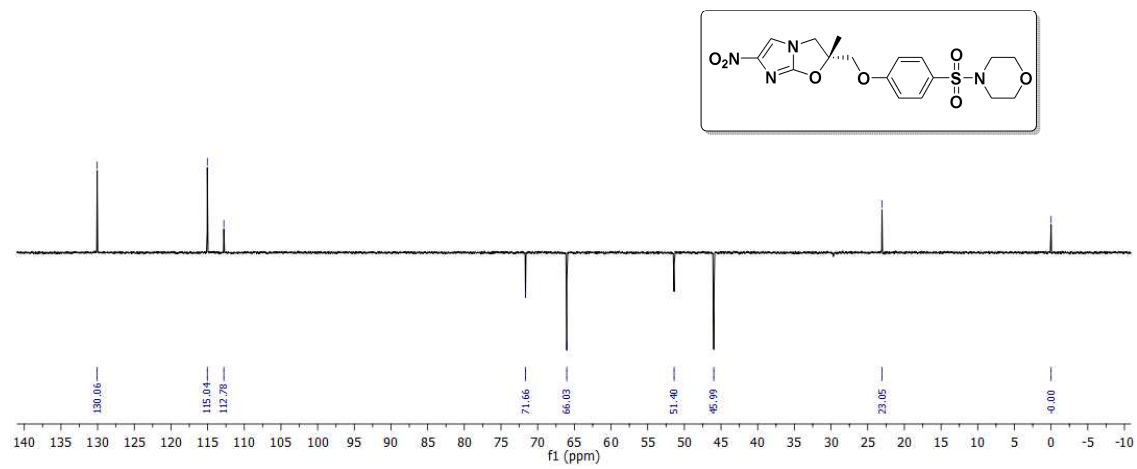
^1H NMR (400 MHz, CDCl_3) of compound **6d**:



^{13}C NMR (101 MHz, CDCl_3) of compound **6d**:



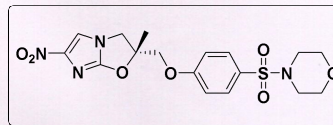
DEPT (101 MHz, CDCl₃) of compound **6d**:



HRMS of compound **6d**:

Qualitative Compound Report

Data File	17.d	Sample Name	17
Sample Type	Sample	Position	Vial 4
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	23-04-2013 PM 12:02:23
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			



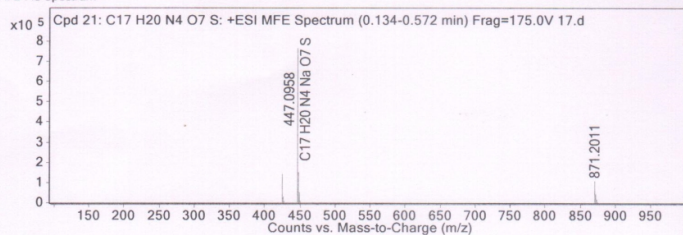
Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C17 H20 N4 O7 S	0.188	424.1063	C17 H20 N4 O7 S	C17 H20 N4 O7 S	-2.52	C17 H20 N4 O7 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 21: C17 H20 N4 O7 S	447.0958	0.188	Find by Molecular Feature	424.1063

MFE MS Spectrum



MS Spectrum Peak List

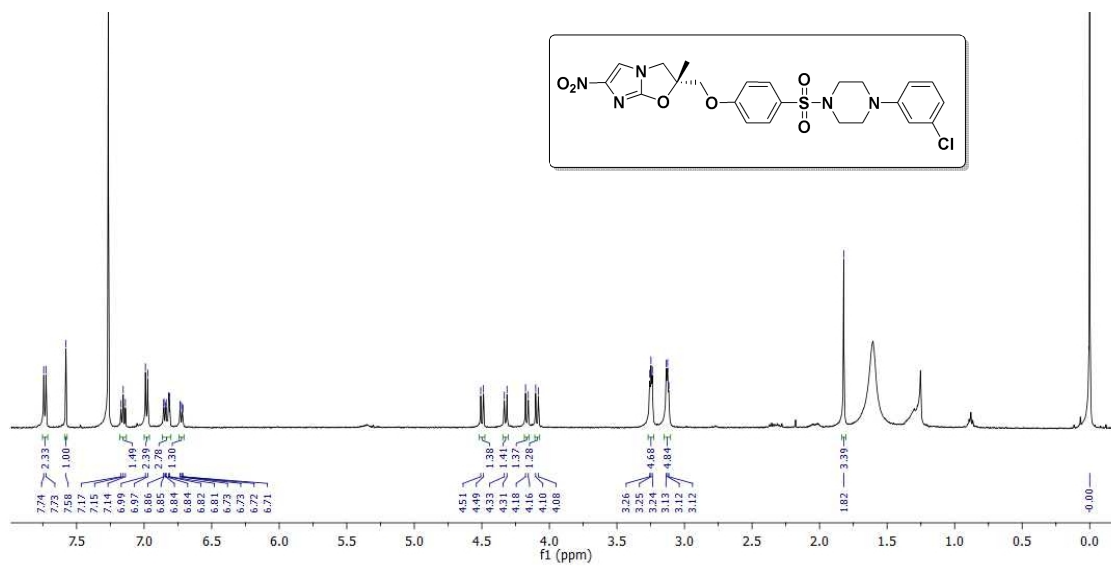
m/z	z	Abund	Formula	Ion
425.1126	1	144300.92	C17 H21 N4 O7 S	(M+H)+
426.1151	1	28460.53	C17 H21 N4 O7 S	(M+H)+
427.1129	1	9165.86	C17 H21 N4 O7 S	(M+H)+
447.0958	1	763722.19	C17 H20 N4 Na O7 S	(M+Na)+
448.0975	1	151583.17	C17 H20 N4 Na O7 S	(M+Na)+
449.095	1	52981.03	C17 H20 N4 Na O7 S	(M+Na)+
450.0966	1	7336.96	C17 H20 N4 Na O7 S	(M+Na)+
871.2011	1	106743.52		(2M+Na)+
872.2028	1	42656.6		(2M+Na)+
873.2017	1	18329.96		(2M+Na)+

Predicted Isotope Match Table

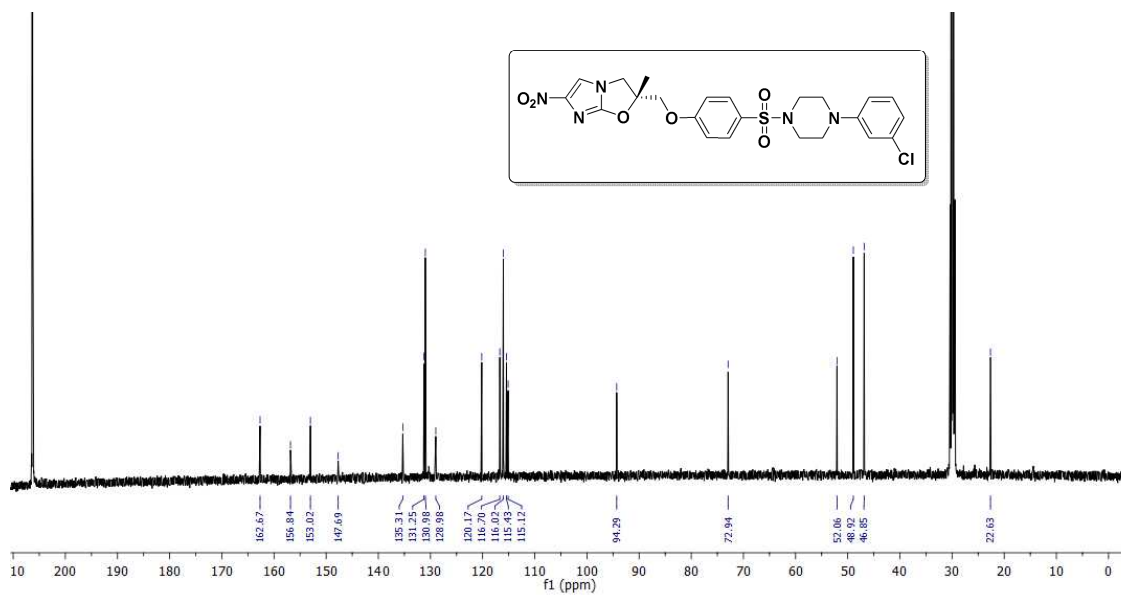
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	425.1126	425.1125	-0.22	100	100	78.56	76.61
2	426.1151	426.1154	0.57	19.72	21.15	15.49	16.2
3	427.1129	427.1125	-1.01	6.35	8.04	4.99	6.16
4	428.1138	428.1141	0.66	1.22	1.35	0.96	1.03

--- End Of Report ---

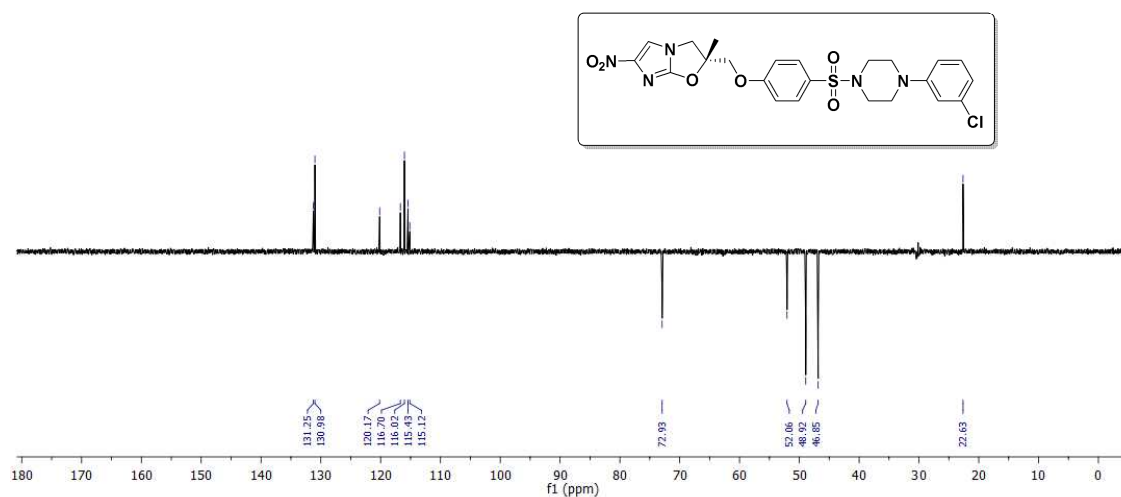
^1H NMR (500 MHz, CDCl_3) of compound **6e**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **6e**:



DEPT (126 MHz, Acetone- d_6) of compound **6e**:

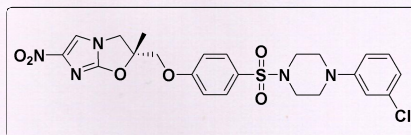


HRMS of compound 6e:

Qualitative Compound Report

Data File 36.d **Sample Name** 36
Sample Type Sample **Position** Vial 8
Instrument Name Instrument 1 **User Name** vishal
Acq Method vishal_12-01-13.m **Acquired Time** 23-04-2013 PM 12:25:19
IRM Calibration Status Success **DA Method** daily_report.m
Comment

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

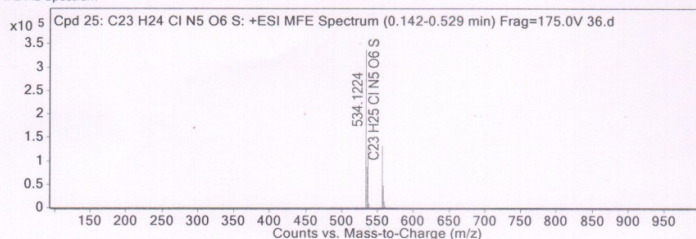


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 25: C23 H24 Cl N5 O6 S	0.189	533.1149	C23 H24 Cl N5 O6 S	C23 H24 Cl N5 O6 S	-2.56	C23 H24 Cl N5 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 25: C23 H24 Cl N5 O6 S	534.1224	0.189	Find by Molecular Feature	533.1149

MFE MS Spectrum



MS Spectrum Peak List

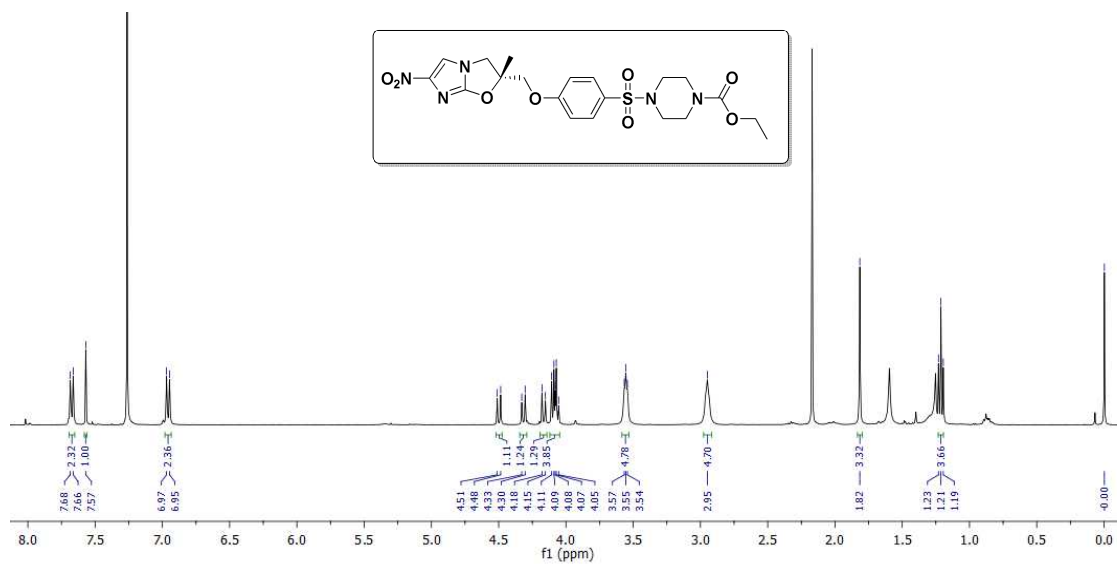
m/z	z	Abund	Formula	Ion
534.1224	1	337289.19	C23 H25 Cl N5 O6 S	(M+H)+
535.1249	1	87723.89	C23 H25 Cl N5 O6 S	(M+H)+
536.12	1	134114.31	C23 H25 Cl N5 O6 S	(M+H)+
537.1219	1	32344.32	C23 H25 Cl N5 O6 S	(M+H)+
538.1205	1	9408.5	C23 H25 Cl N5 O6 S	(M+H)+
556.104	1	130812.28	C23 H24 Cl N5 Na O6 S	(M+Na)+
557.1061	1	36808.99	C23 H24 Cl N5 Na O6 S	(M+Na)+
558.1017	1	47855.59	C23 H24 Cl N5 Na O6 S	(M+Na)+
559.1052	1	12717.17	C23 H24 Cl N5 Na O6 S	(M+Na)+
560.1047	1	4286.65	C23 H24 Cl N5 Na O6 S	(M+Na)+

Predicted Isotope Match Table

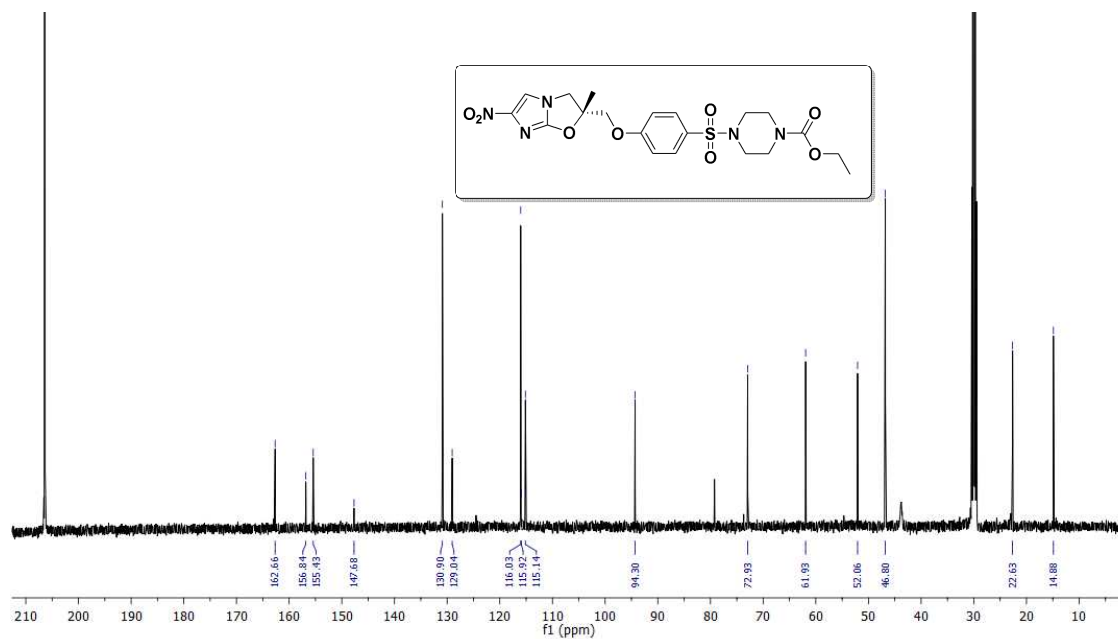
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	534.1224	534.1209	-2.9	100	100	55.89	54.22
2	535.1249	535.1237	-2.13	26.01	28.01	14.54	15.19
3	536.12	536.1188	-2.33	39.76	41.48	22.22	22.49
4	537.1219	537.1211	-1.35	9.59	10.85	5.36	5.88
5	538.1205	538.1192	-2.43	2.79	3.33	1.56	1.81
6	539.1187	539.1202	2.78	0.64	0.64	0.36	0.35
7	540.121	540.1214	0.76	0.14	0.1	0.08	0.05

--- End Of Report ---

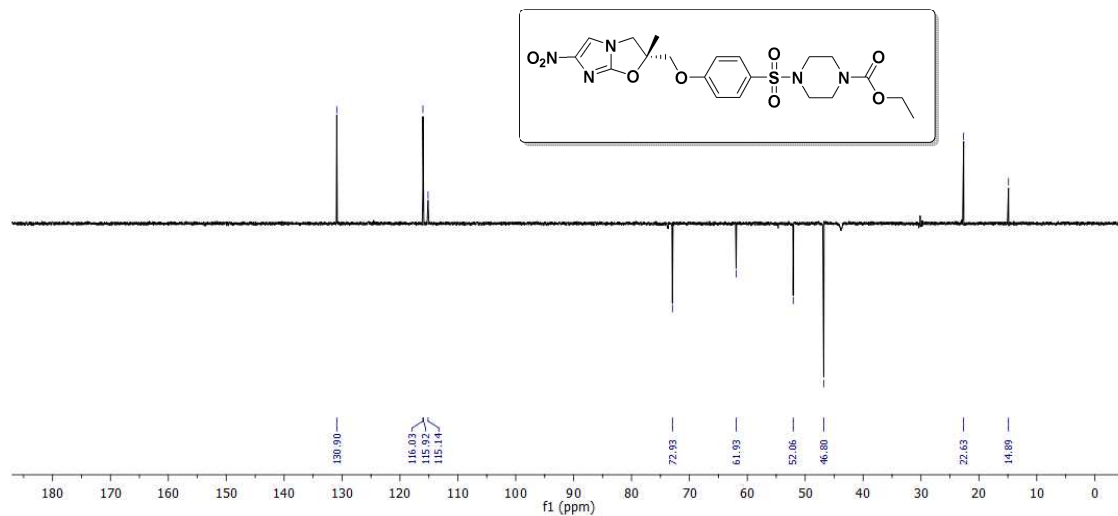
^1H NMR (400 MHz, CDCl_3 + two drops of Acetone- d_6) of compound **6f**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **6f**:



DEPT (126 MHz, Acetone- d_6) of compound **6f**:

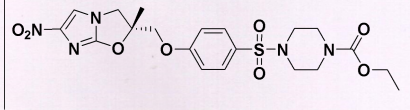


HRMS of compound 6f:

Qualitative Compound Report

Data File	37.d	Sample Name	37
Sample Type	Sample	Position	Vial 11
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	23-04-2013 PM 12:43:51
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

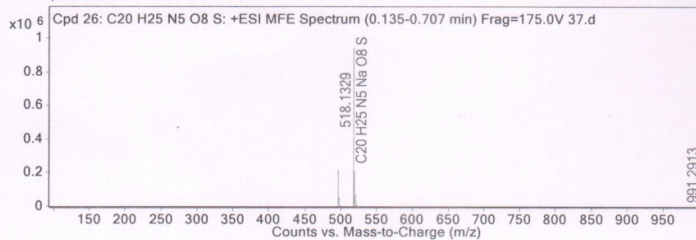


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 26: C20 H25 N5 O8 S	0.188	495.1436	C20 H25 N5 O8 S	C20 H25 N5 O8 S	-2.43	C20 H25 N5 O8 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 26: C20 H25 N5 O8 S	518.1329	0.188	Find by Molecular Feature	495.1436

MFE MS Spectrum



MS Spectrum Peak List

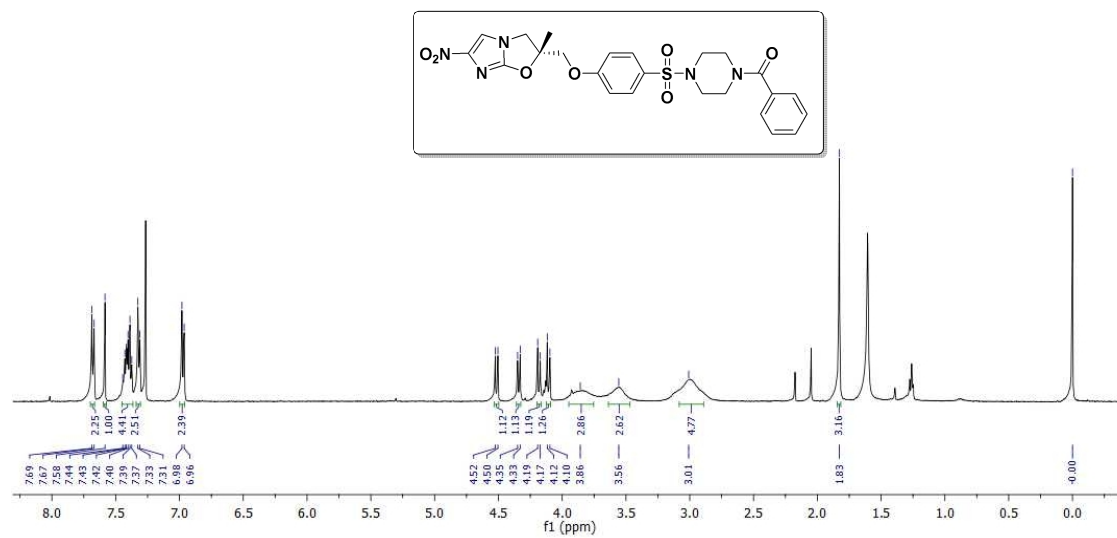
m/z	z	Abund	Formula	Ion
496.1501	1	219960.8	C20 H26 N5 O8 S	(M+H)+
497.1524	1	54242.38	C20 H26 N5 O8 S	(M+H)+
498.1507	1	18768.63	C20 H26 N5 O8 S	(M+H)+
499.1519	1	3979.86	C20 H26 N5 O8 S	(M+H)+
518.1329	1	942935.19	C20 H25 N5 Na O8 S	(M+Na)+
519.1352	1	209418.05	C20 H25 N5 Na O8 S	(M+Na)+
520.133	1	67265.67	C20 H25 N5 Na O8 S	(M+Na)+
521.1342	1	12925.16	C20 H25 N5 Na O8 S	(M+Na)+
522.1358	1	2344.13	C20 H25 N5 Na O8 S	(M+Na)+
991.2913	1	5505.8		(2M+H)+

Predicted Isotope Match Table

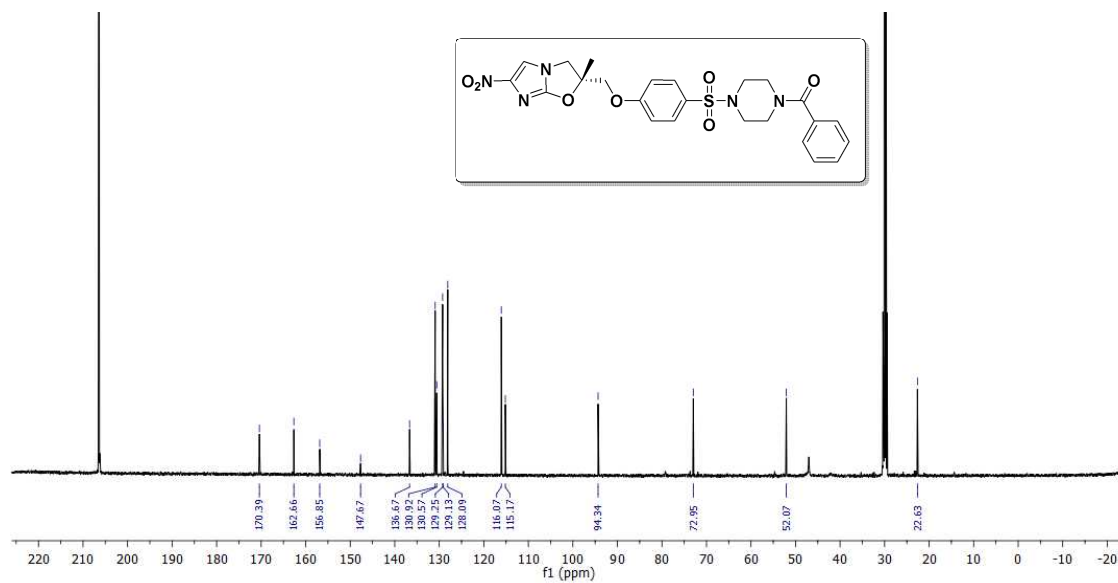
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	496.1501	496.1497	-0.95	100	100	73.86	73.57
2	497.1524	497.1525	0.18	24.66	24.85	18.21	18.28
3	498.1507	498.1502	-0.98	8.53	9.08	6.3	6.68
4	499.1519	499.1516	-0.51	1.81	1.71	1.34	1.26
5	500.1488	500.1527	7.88	0.39	0.28	0.29	0.21

--- End Of Report ---

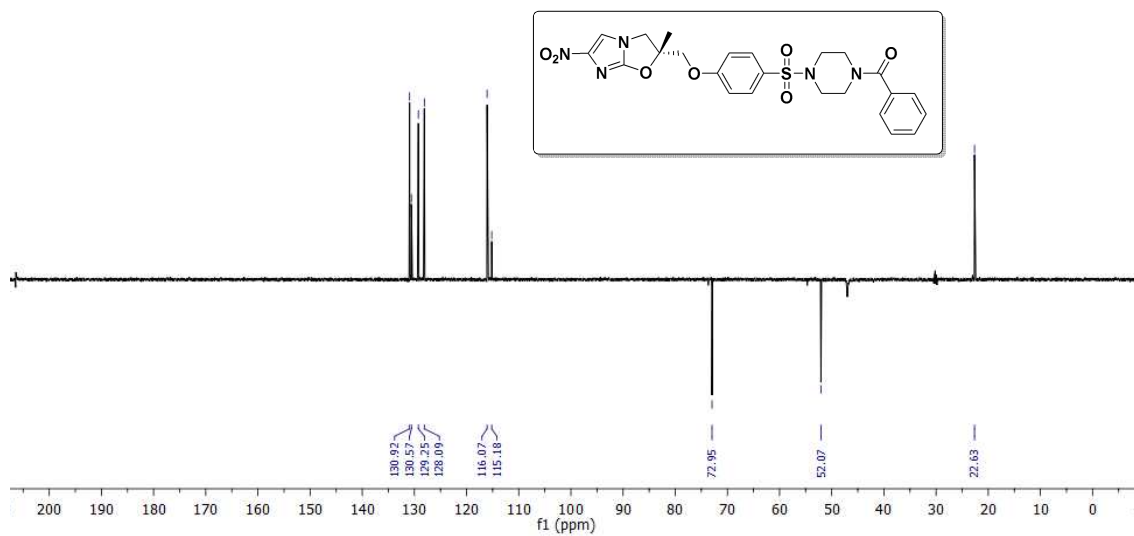
^1H NMR (500 MHz, CDCl_3) of compound **6g**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **6g**:



DEPT NMR (126 MHz, Acetone- d_6) of compound **6g**:

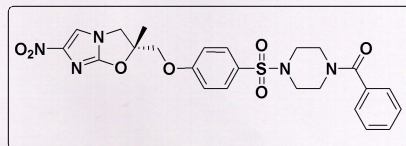


HRMS of compound 6g:

Qualitative Compound Report

Data File 35.d **Sample Name** 35
Sample Type Sample **Position** Vial 10
Instrument Name Instrument 1 **User Name** vishal
Acq Method vishal_12-01-13.m **Acquired Time** 26-04-2013 PM 2:27:17
IRM Calibration Status Success **DA Method** daily_report.m
Comment

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

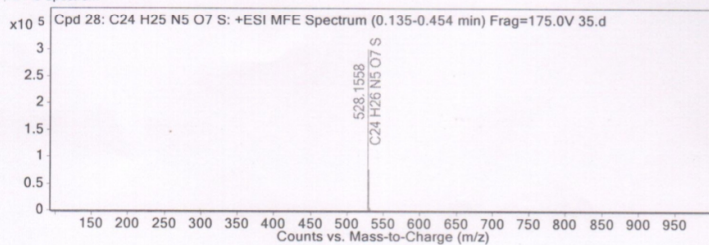


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C24 H25 N5 O7 S	0.188	527.1483	C24 H25 N5 O7 S	C24 H25 N5 O7 S	-1.65	C24 H25 N5 O7 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 28: C24 H25 N5 O7 S	528.1558	0.188	Find by Molecular Feature	527.1483

MFE MS Spectrum



MS Spectrum Peak List

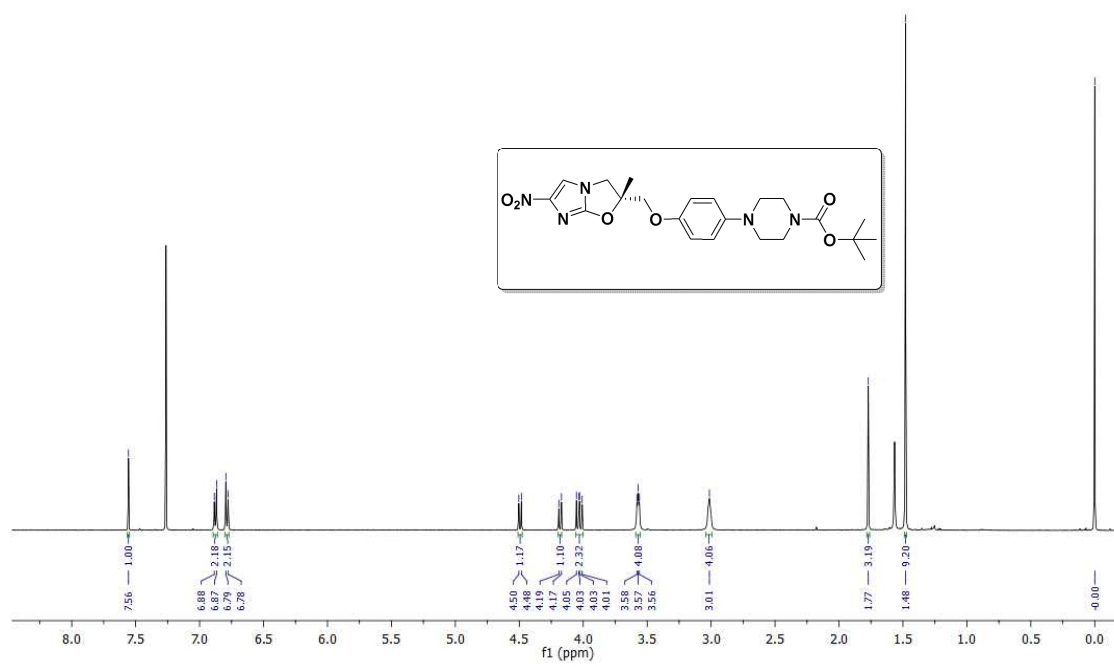
m/z	z	Abund	Formula	Ion
528.1558	1	299787	C24 H26 N5 O7 S	(M+H)+
529.1582	1	76985.31	C24 H26 N5 O7 S	(M+H)+
530.1561	1	26161.64	C24 H26 N5 O7 S	(M+H)+
531.1568	1	5723.65	C24 H26 N5 O7 S	(M+H)+
532.1563	1	1188.38	C24 H26 N5 O7 S	(M+H)+
533.1602	1	288.71	C24 H26 N5 O7 S	(M+H)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	528.1558	528.1547	-1.96	100	100	73.09	70.62
2	529.1582	529.1576	-1.09	25.68	29.14	18.77	20.58
3	530.1561	530.1558	-0.44	8.73	10.01	6.38	7.07
4	531.1568	531.157	0.42	1.91	2.06	1.4	1.45
5	532.1563	532.1583	3.61	0.4	0.34	0.29	0.24
6	533.1602	533.1599	-0.47	0.1	0.05	0.07	0.03

--- End Of Report ---

^1H NMR (500 MHz, CDCl_3) of compound **11**:

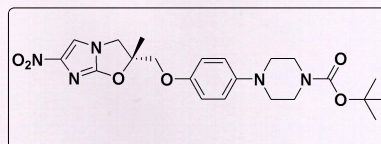


HRMS of compound 11:

Qualitative Compound Report

Data File 38.d **Sample Name** 38
Sample Type Sample **Position** Vial 3
Instrument Name Instrument 1 **User Name** vishal
Acq Method vishal_12-01-13.m **Acquired Time** 23-04-2013 AM 11:57:48
IRM Calibration Status Success **DA Method** daily_report.m
Comment

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

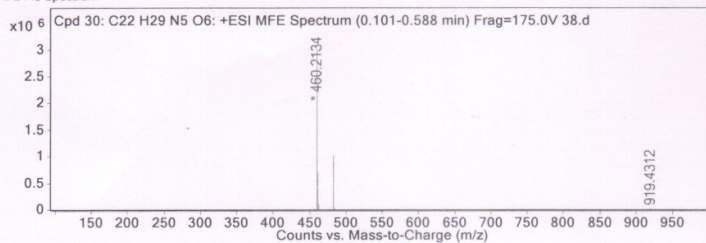


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C22 H29 N5 O6	0.188	459.2076	C22 H29 N5 O6	C22 H29 N5 O6	9.03	C22 H29 N5 O6

Compound Label	m/z	RT	Algorithm	Mass
Cpd 30: C22 H29 N5 O6	460.2134	0.188	Find by Molecular Feature	459.2076

MFE MS Spectrum



MS Spectrum Peak List

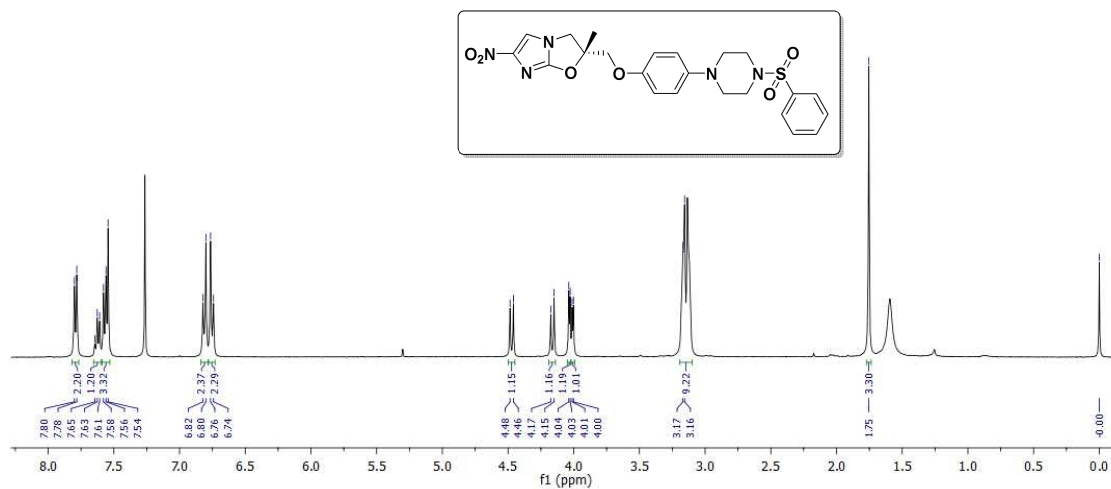
m/z	z	Abund	Formula	Ion
460.2134	1	3002174		(M+H)+
461.2181	1	701989.38		(M+H)+
462.2196	1	110083.15		(M+H)+
463.2217	1	14467.03		(M+H)+
482.1969	1	1019884.44	C22 H29 N5 Na O6	(M+Na)+
483.1997	1	239956.47	C22 H29 N5 Na O6	(M+Na)+
484.2012	1	38049.29	C22 H29 N5 Na O6	(M+Na)+
485.2038	1	6027.41	C22 H29 N5 Na O6	(M+Na)+
919.4312	1	11932.95		(2M+H)+
920.4322	1	5934.29		(2M+H)+

Predicted Isotope Match Table

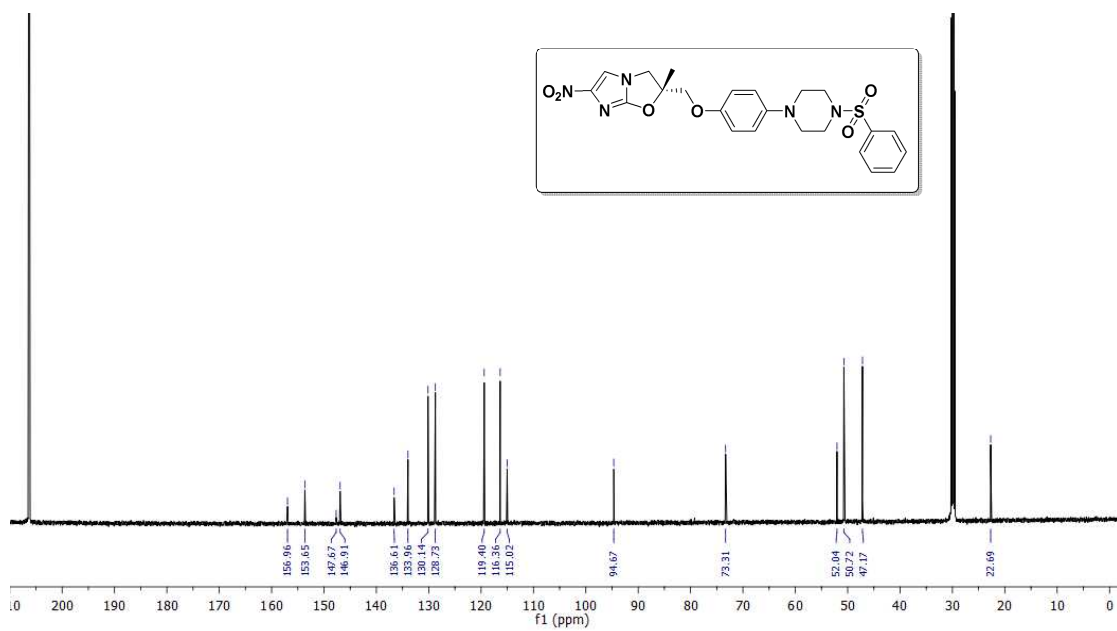
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	482.1969	482.201	8.45	100	100	78.17	76.13
2	483.1997	483.204	8.77	23.53	26.18	18.39	19.93
3	484.2012	484.2065	10.86	3.73	4.53	2.92	3.45
4	485.2038	485.2089	10.58	0.59	0.59	0.46	0.45
5	486.2053	486.2114	12.42	0.08	0.06	0.06	0.05

--- End Of Report ---

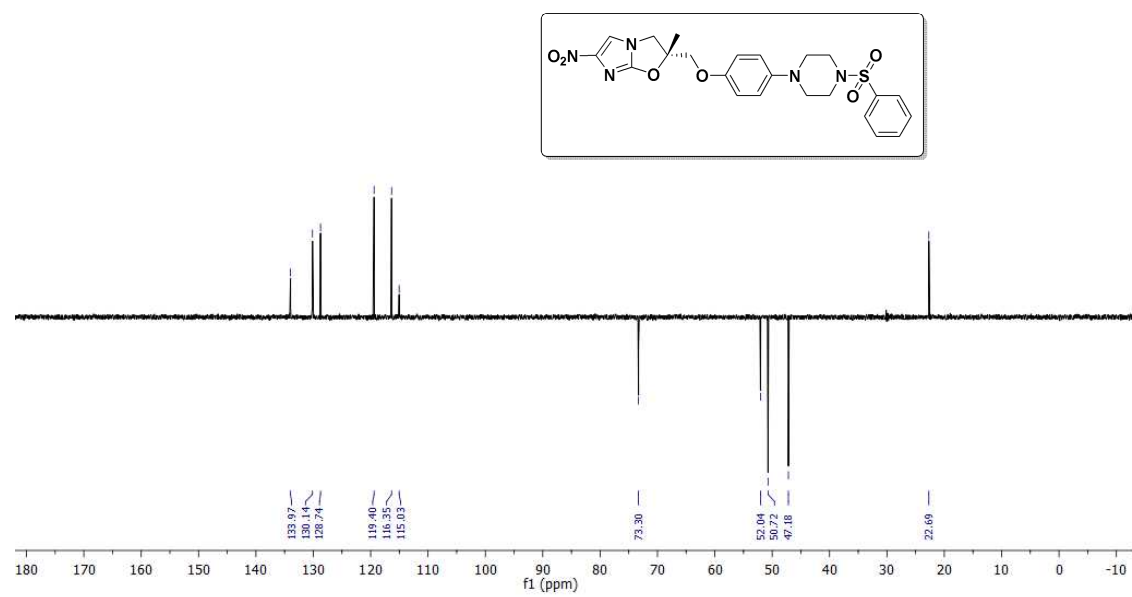
^1H NMR (400 MHz, CDCl_3) of compound **13a**:



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



DEPT NMR (126 MHz, Acetone- d_6) of compound **13a**:

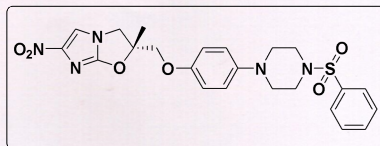


HRMS of compound **13a**:

Qualitative Compound Report

Data File: 132.d Sample Name: 132
 Sample Type: Sample Position: Vial 28
 Instrument Name: Instrument 1 User Name:
 Acq Method: vishal_12-01-13.m Acquired Time: 05-03-2013 PM 3:24:24
 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)

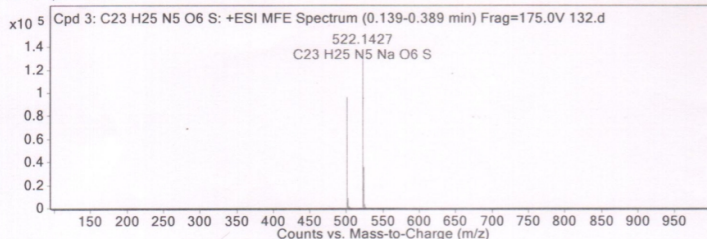


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C23 H25 N5 O6 S	0.19	499.1533	C23 H25 N5 O6 S	C23 H25 N5 O6 S	-1.57	C23 H25 N5 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C23 H25 N5 O6 S	522.1427	0.19	Find by Molecular Feature	499.1533

MFE MS Spectrum



MS Spectrum Peak List

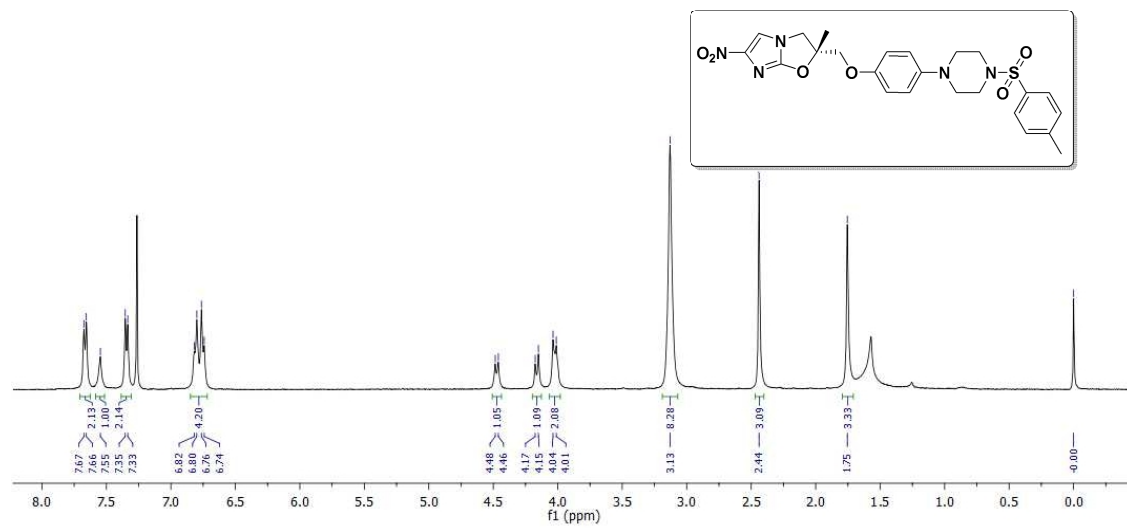
m/z	z	Abund	Formula	Ion
500.1606	1	95973.61	C23 H26 N5 O6 S	(M+H)+
501.1627	1	26608.09	C23 H26 N5 O6 S	(M+H)+
502.1616	1	8355.98	C23 H26 N5 O6 S	(M+H)+
503.1607	1	1819.11	C23 H26 N5 O6 S	(M+H)+
522.1427	1	131673.11	C23 H25 N5 Na O6 S	(M+Na)+
523.1449	1	35452.16	C23 H25 N5 Na O6 S	(M+Na)+
524.1438	1	11939.44	C23 H25 N5 Na O6 S	(M+Na)+
525.1448	1	2933.57	C23 H25 N5 Na O6 S	(M+Na)+
526.1442	1	554.8	C23 H25 N5 Na O6 S	(M+Na)+
999.3129	1	7780.4		(2M+H)+

Predicted Isotope Match Table

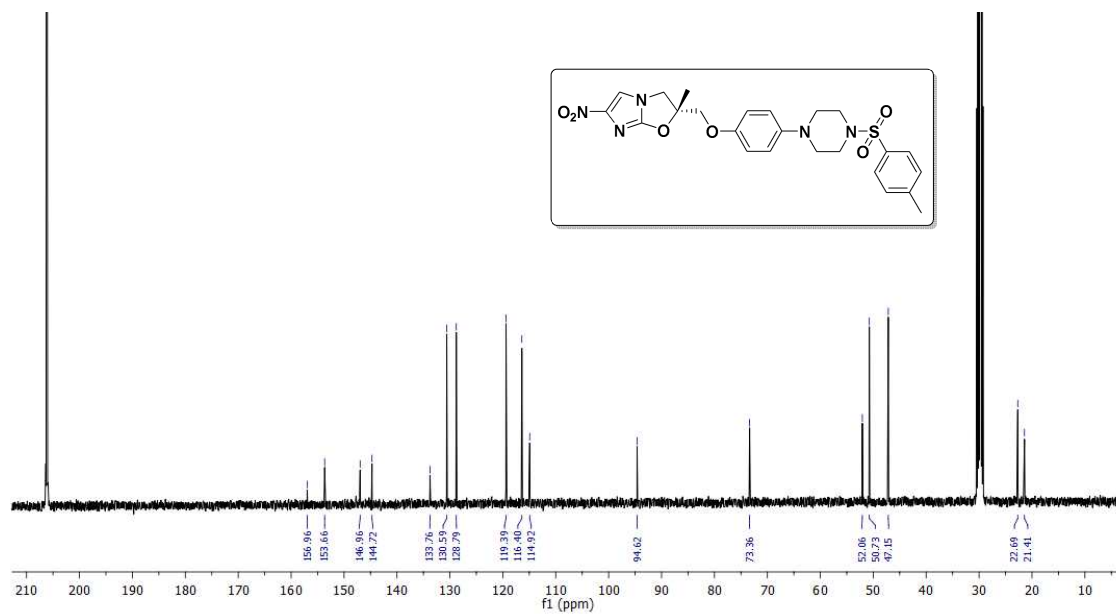
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	500.1606	500.1598	-1.48	100	100	72.05	71.58
2	501.1627	501.1627	-0.03	27.72	28.02	19.97	20.06
3	502.1616	502.1607	-1.77	8.71	9.49	6.27	6.79
4	503.1607	503.1618	2.3	1.9	1.89	1.37	1.35
5	504.1635	504.1631	-0.74	0.47	0.3	0.34	0.21

--- End Of Report ---

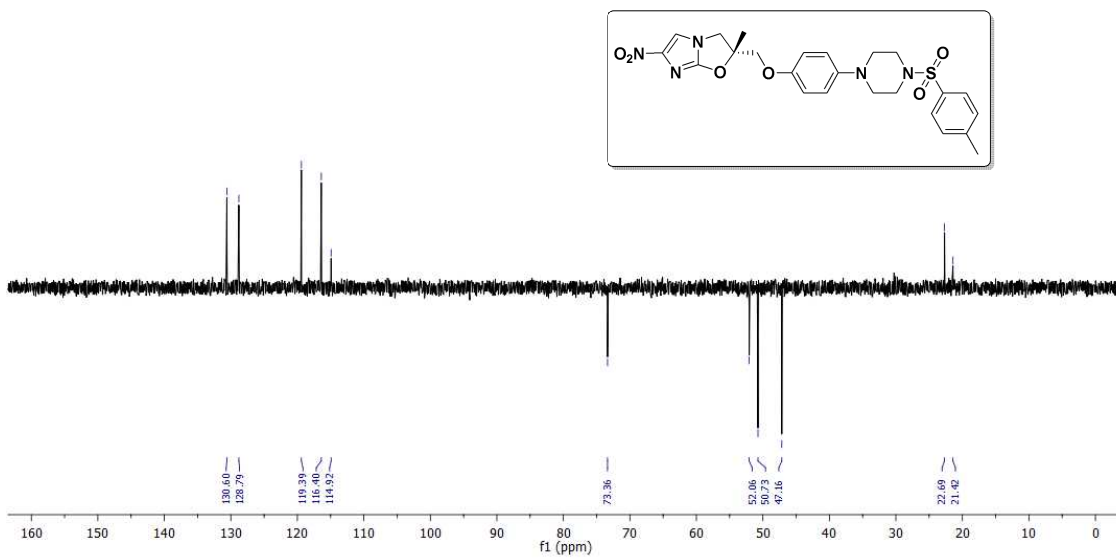
^1H NMR (400 MHz, CDCl_3) of compound **13b**:



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



DEPT (101 MHz, Acetone- d_6) of compound **13b**:

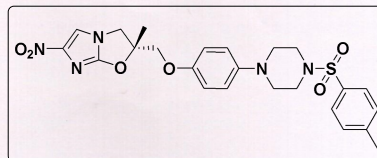


HRMS of compound 13b:

Qualitative Compound Report

Data File 130.d **Sample Name** 130
Sample Type Sample **Position** Vial 29
Instrument Name Instrument 1 **User Name**
Acq Method vishal_12-01-13.m **Acquired Time** 04-03-2013 PM 2:54:21
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)

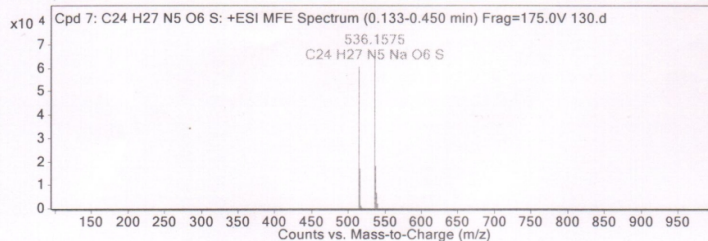


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C24 H27 N5 O6 S	0.189	513.1682	C24 H27 N5 O6 S	C24 H27 N5 O6 S	0.06	C24 H27 N5 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 7: C24 H27 N5 O6 S	536.1575	0.189	Find by Molecular Feature	513.1682

MFE MS Spectrum



MS Spectrum Peak List

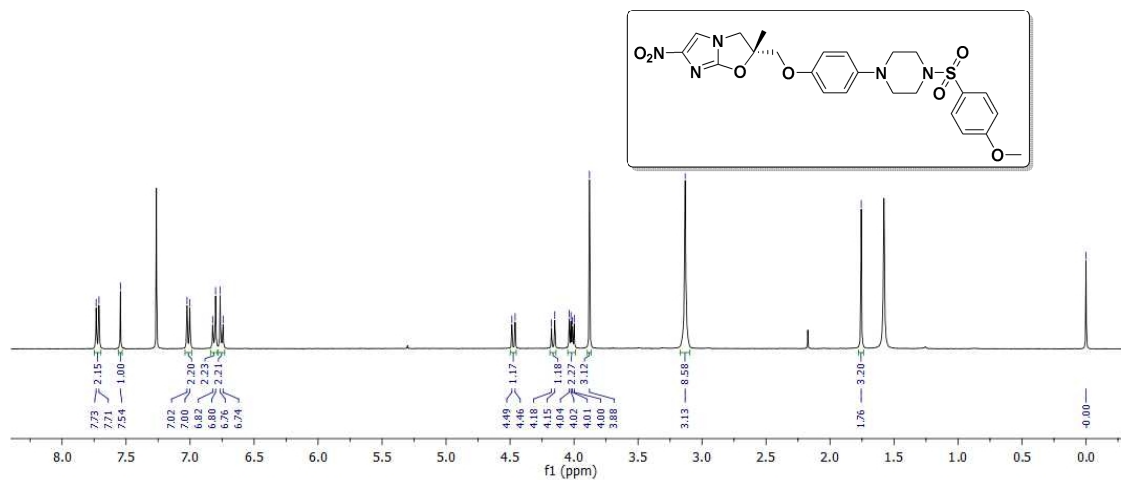
m/z	z	Abund	Formula	Ion
514.1756	1	60715.67	C24 H28 N5 O6 S	(M+H)+
515.1774	1	17094.04	C24 H28 N5 O6 S	(M+H)+
516.1768	1	5631.22	C24 H28 N5 O6 S	(M+H)+
517.177	1	1253.21	C24 H28 N5 O6 S	(M+H)+
518.1843	1	303.74	C24 H28 N5 O6 S	(M+H)+
536.1575	1	65085.88	C24 H27 N5 Na O6 S	(M+Na)+
537.1599	1	18342.49	C24 H27 N5 Na O6 S	(M+Na)+
538.1583	1	6474.68	C24 H27 N5 Na O6 S	(M+Na)+
539.161	1	1824.41	C24 H27 N5 Na O6 S	(M+Na)+
540.1525	1	461.27	C24 H27 N5 Na O6 S	(M+Na)+

Predicted Isotope Match Table

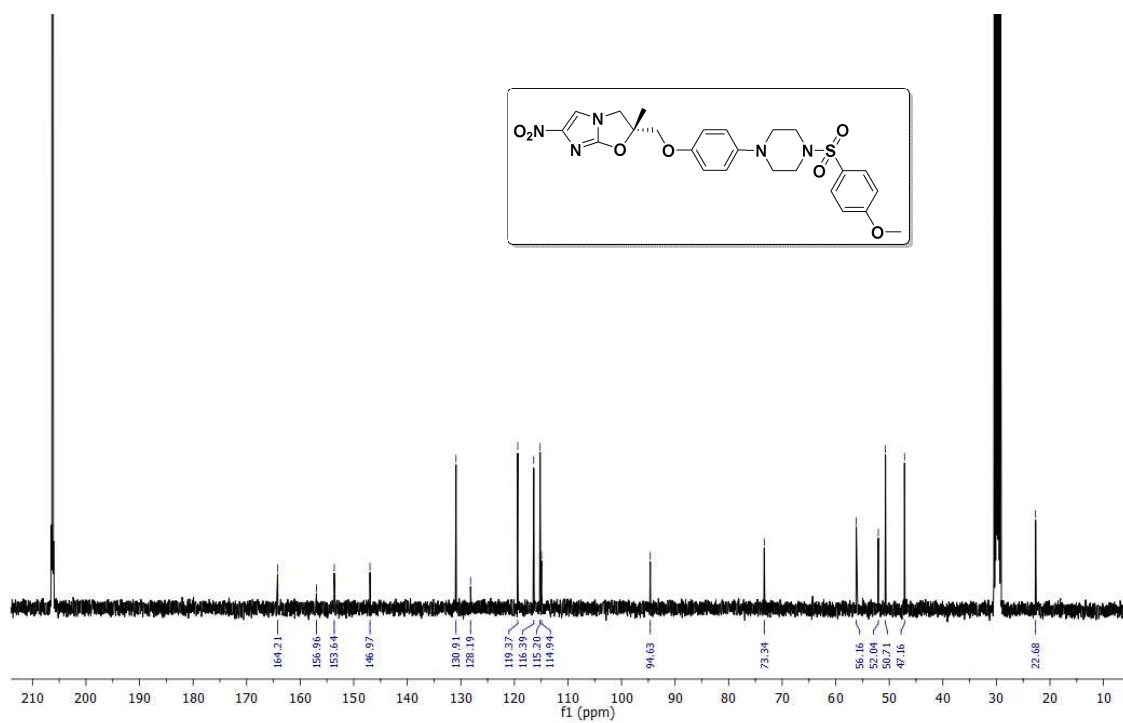
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	514.1756	514.1755	-0.16	100	100	71.43	70.8
2	515.1774	515.1784	1.88	28.15	29.12	20.11	20.62
3	516.1768	516.1765	-0.54	9.27	9.8	6.63	6.94
4	517.177	517.1776	1.16	2.06	2	1.47	1.41
5	518.1843	518.1789	-10.51	0.5	0.32	0.36	0.23

--- End Of Report ---

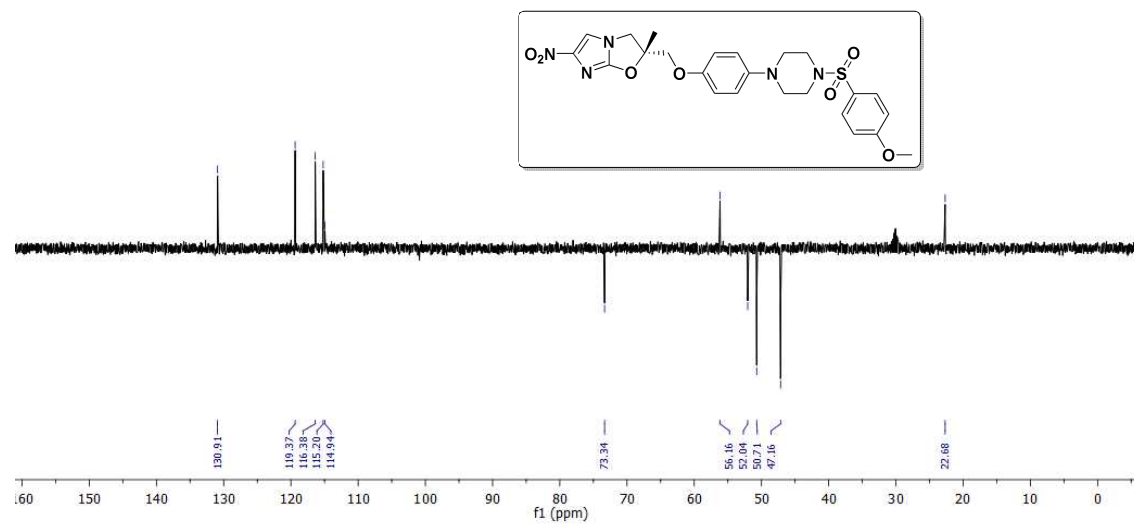
^1H NMR (400 MHz, CDCl_3) of compound **13c**:



^{13}C NMR (101 MHz, $\text{Acetone-}d_6$) of compound **13c**:



DEPT (101 MHz, Acetone- d_6) of compound **13c**:



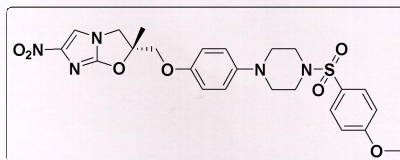
HRMS of compound 13c:

Qualitative Compound Report

Data File: 129.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: vishal_12-01-13.m
 IRM Calibration Status: Success
 Comment:

Sample Name: 129
 Position: Vial 28
 User Name:
 Acquired Time: 04-03-2013 PM 2:52:50
 DA Method: SamplePurity-Default.m

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

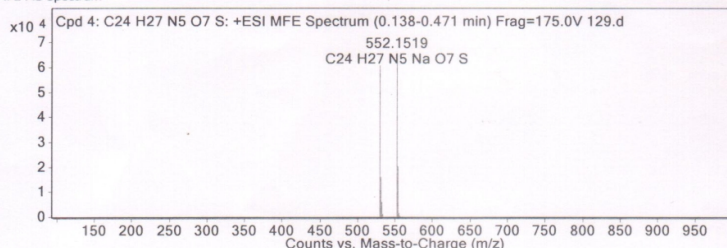


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C24 H27 N5 O7 S	0.193	529.1625	C24 H27 N5 O7 S	C24 H27 N5 O7 S	1.11	C24 H27 N5 O7 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 4: C24 H27 N5 O7 S	552.1519	0.193	Find by Molecular Feature	529.1625

MFE MS Spectrum



MS Spectrum Peak List

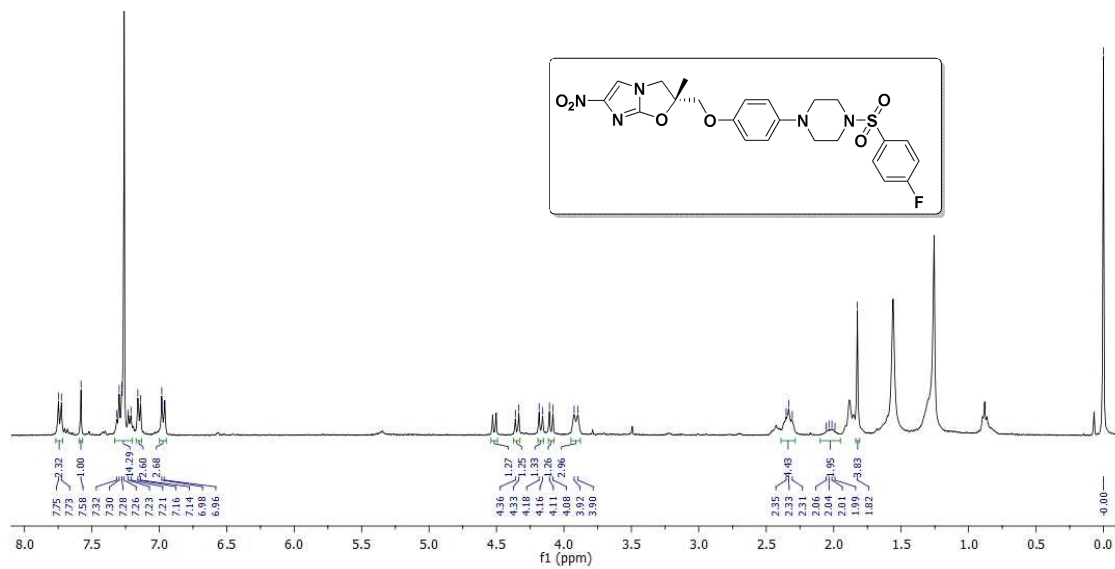
m/z	z	Abund	Formula	Ion
530.17	1	60821.04	C24 H28 N5 O7 S	(M+H)+
531.1725	1	16136.43	C24 H28 N5 O7 S	(M+H)+
532.1713	1	6062.18	C24 H28 N5 O7 S	(M+H)+
533.1722	1	1298.96	C24 H28 N5 O7 S	(M+H)+
534.1701	1	314.62	C24 H28 N5 O7 S	(M+H)+
552.1519	1	62713.42	C24 H27 N5 Na O7 S	(M+Na)+
553.1543	1	20132.32	C24 H27 N5 Na O7 S	(M+Na)+
554.153	1	6592.82	C24 H27 N5 Na O7 S	(M+Na)+
555.1548	1	1416.09	C24 H27 N5 Na O7 S	(M+Na)+
556.1532	1	303.69	C24 H27 N5 Na O7 S	(M+Na)+

Predicted Isotope Match Table

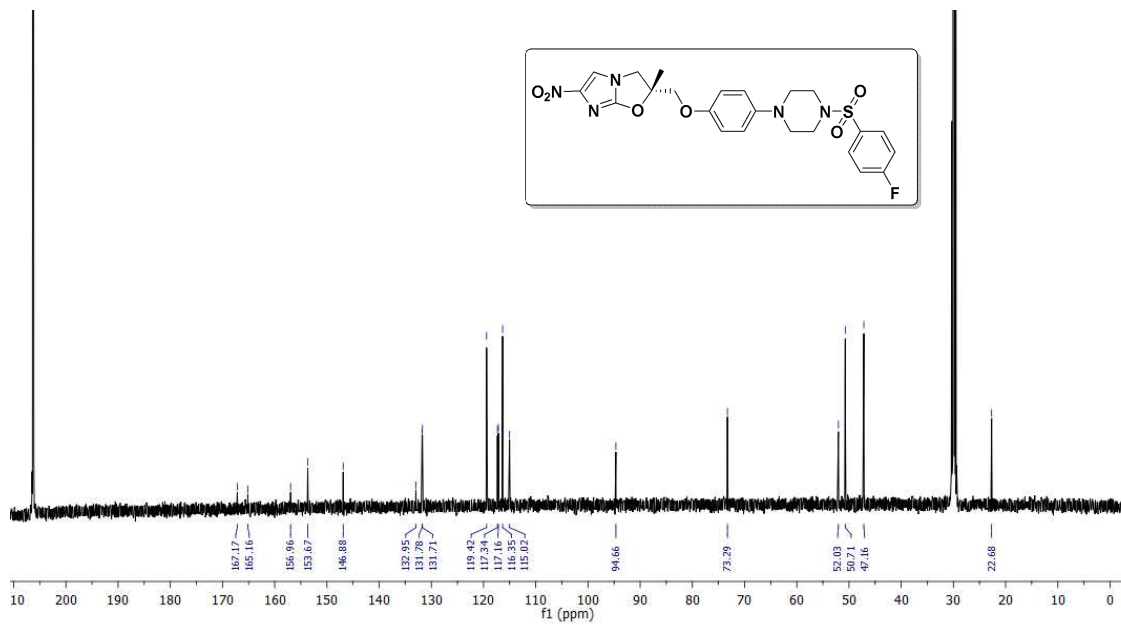
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	530.17	530.1704	0.7	100	100	71.86	70.63
2	531.1725	531.1733	1.46	26.53	29.16	19.07	20.6
3	532.1713	532.1715	0.44	9.97	10.02	7.16	7.08
4	533.1722	533.1727	0.85	2.14	2.06	1.53	1.45
5	534.1701	534.1739	7.21	0.52	0.34	0.37	0.24

--- End Of Report ---

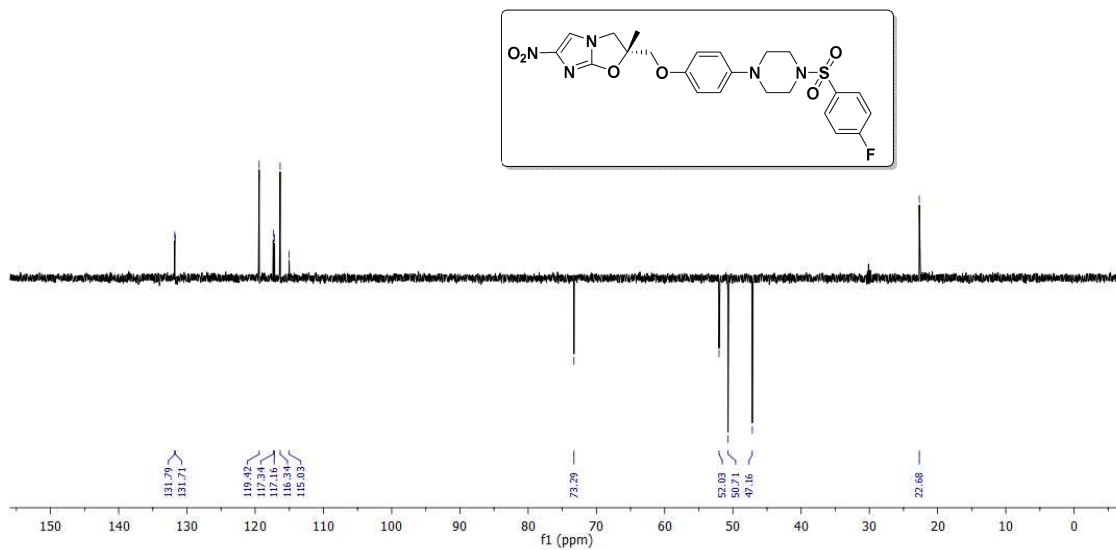
¹H NMR (400 MHz, CDCl₃) of compound **13d**:



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



DEPT (126 MHz, Acetone- d_6) of compound **13d**:

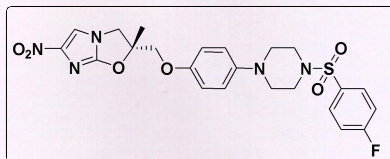


HRMS of compound 13d:

Qualitative Compound Report

Data File 39.d **Sample Name** 39
Sample Type Sample **Position** Vial 10
Instrument Name Instrument 1 **User Name** vishal
Acq Method vishal_12-01-13.m **Acquired Time** 23-04-2013 PM 12:34:28
IRM Calibration Status Success **DA Method** daily_report.m
Comment

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

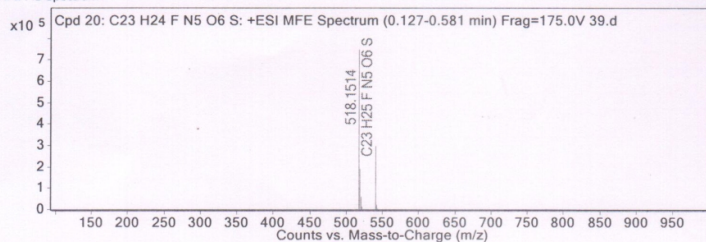


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 20: C23 H24 F N5 O6 S	0.189	517.1439	C23 H24 F N5 O6 S	C23 H24 F N5 O6 S	-1.56	C23 H24 F N5 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 20: C23 H24 F N5 O6 S	518.1514	0.189	Find by Molecular Feature	517.1439

MFE MS Spectrum



MS Spectrum Peak List

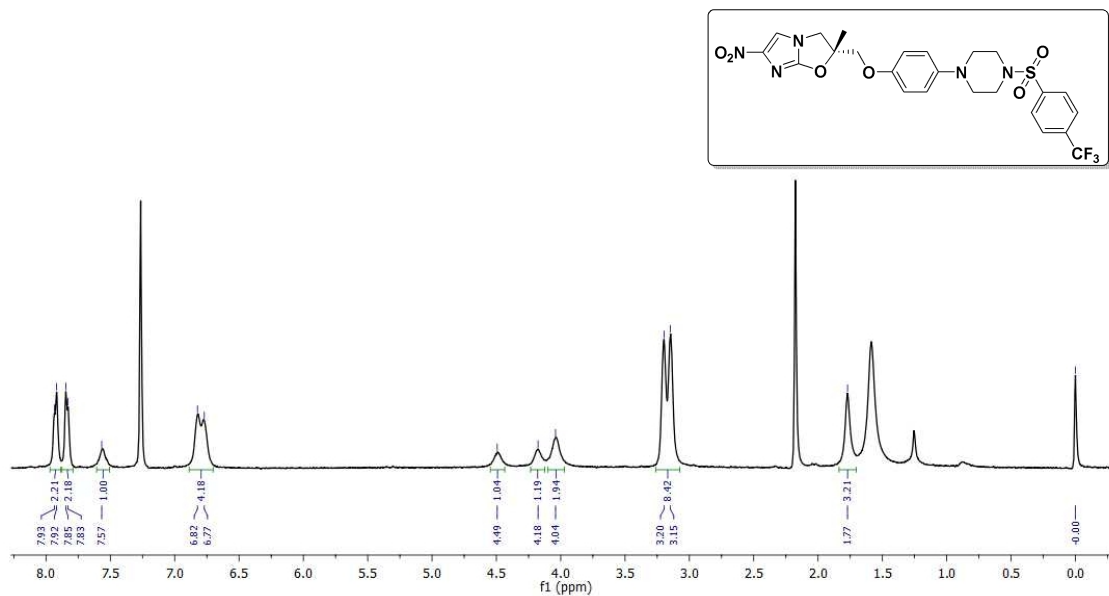
m/z	z	Abund	Formula	Ion
518.1514	1	747523.13	C23 H25 F N5 O6 S	(M+H)+
519.1535	1	192352.86	C23 H25 F N5 O6 S	(M+H)+
520.1517	1	58434.13	C23 H25 F N5 O6 S	(M+H)+
521.1527	1	11963.62	C23 H25 F N5 O6 S	(M+H)+
522.1535	1	2321.01	C23 H25 F N5 O6 S	(M+H)+
540.1329	1	296718.03	C23 H24 F N5 Na O6 S	(M+Na)+
541.1351	1	77581.06	C23 H24 F N5 Na O6 S	(M+Na)+
542.1337	1	21806.8	C23 H24 F N5 Na O6 S	(M+Na)+
543.1338	1	4367.32	C23 H24 F N5 Na O6 S	(M+Na)+
544.1365	1	1012.07	C23 H24 F N5 Na O6 S	(M+Na)+

Predicted Isotope Match Table

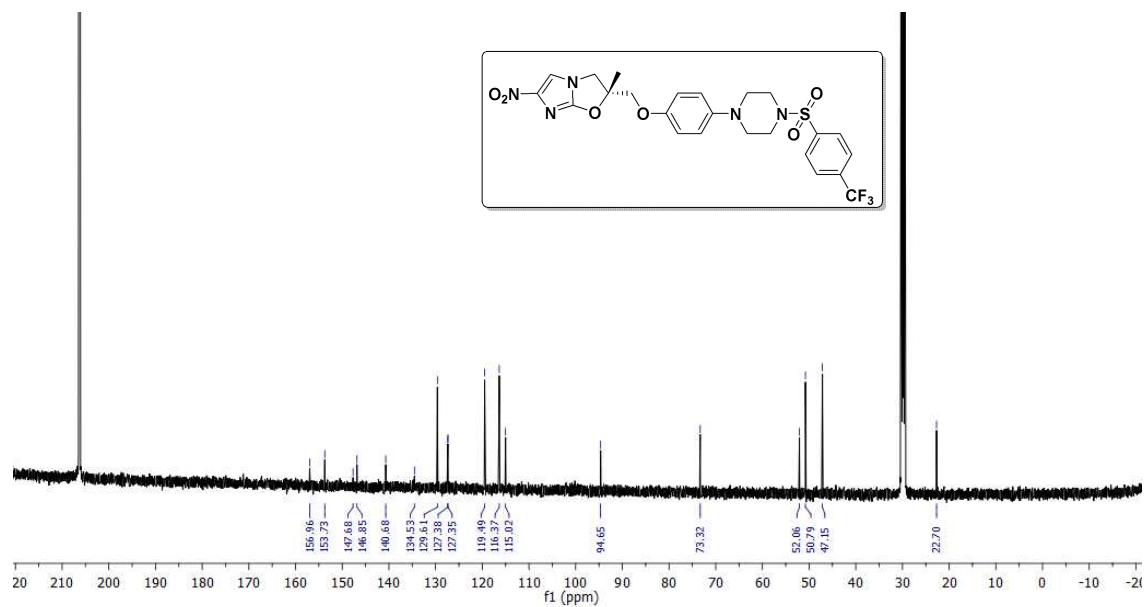
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	518.1514	518.1504	-1.91	100	100	73.8	71.57
2	519.1535	519.1533	-0.46	25.73	28.01	18.99	20.05
3	520.1517	520.1513	-0.86	7.82	9.49	5.77	6.79
4	521.1527	521.1524	-0.62	1.6	1.89	1.18	1.35
5	522.1535	522.1537	0.24	0.31	0.3	0.23	0.21
6	523.1615	523.1553	-11.88	0.03	0.04	0.03	0.03

--- End Of Report ---

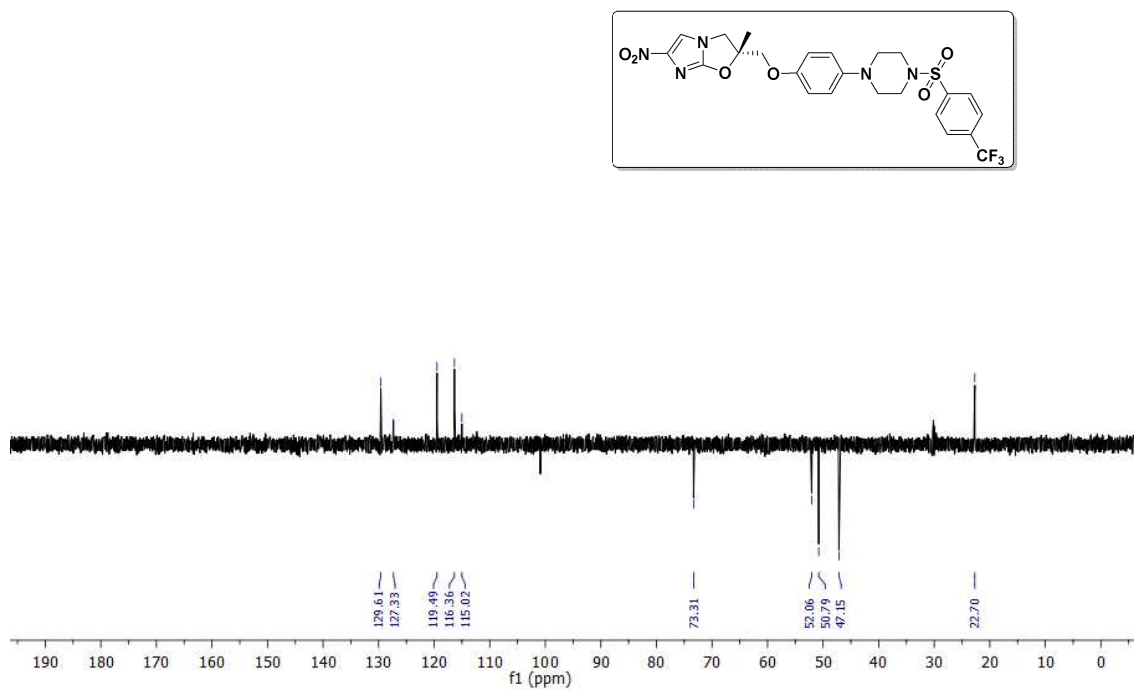
^1H NMR (400 MHz, CDCl_3 + two drops of Acetone- d_6) of compound **13e**:



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



DEPT (126 MHz, Acetone- d_6) of compound **13e**:

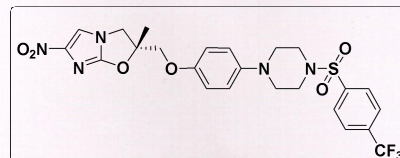


HRMS of compound **13e**:

Qualitative Compound Report

Data File	131.d	Sample Name	131
Sample Type	Sample	Position	Vial 30
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_12-01-13.m	Acquired Time	05-03-2013 PM 3:33:31
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)

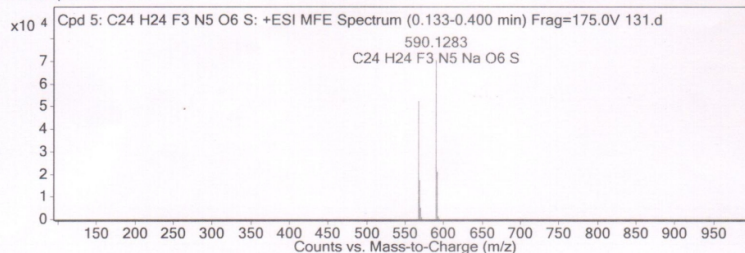


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C24 H24 F3 N5 O6 S	0.191	567.139	C24 H24 F3 N5 O6 S	C24 H24 F3 N5 O6 S	1.74	C24 H24 F3 N5 O6 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 5: C24 H24 F3 N5 O6 S	590.1283	0.191	Find by Molecular Feature	567.139

MFE MS Spectrum



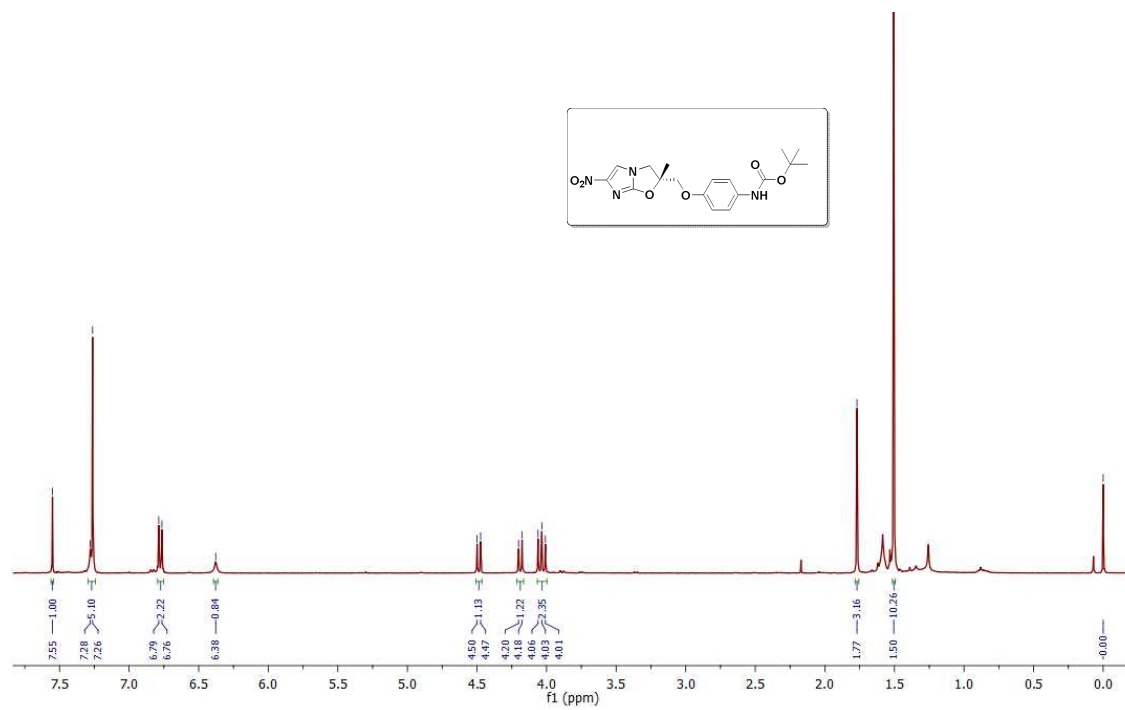
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
568.1467	1	52409.59	C24 H25 F3 N5 O6 S	(M+H)+
569.1478	1	17337.64	C24 H25 F3 N5 O6 S	(M+H)+
570.147	1	5142.97	C24 H25 F3 N5 O6 S	(M+H)+
571.1492	1	966.04	C24 H25 F3 N5 O6 S	(M+H)+
590.1283	1	70586.38	C24 H24 F3 N5 Na O6 S	(M+Na)+
591.1307	1	21044.2	C24 H24 F3 N5 Na O6 S	(M+Na)+
592.1288	1	7011.18	C24 H24 F3 N5 Na O6 S	(M+Na)+
593.1298	1	1421.15	C24 H24 F3 N5 Na O6 S	(M+Na)+
594.1295	1	392.26	C24 H24 F3 N5 Na O6 S	(M+Na)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	568.1467	568.1472	0.97	100	100	69.09	70.99
2	569.1478	569.1501	3.97	33.08	29.09	22.86	20.65
3	570.147	570.1482	2.24	9.81	9.79	6.78	6.95
4	571.1492	571.1493	0.2	1.84	1.99	1.27	1.41

^1H NMR (400 MHz, CDCl_3) of compound **16**:

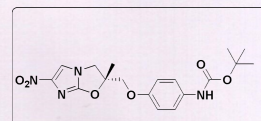


HRMS of compound 16:

Qualitative Compound Report

Data File	49.d	* Sample Name	49
Sample Type	Sample	Position	Vial 9
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	23-04-2013 PM 12:29:51
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

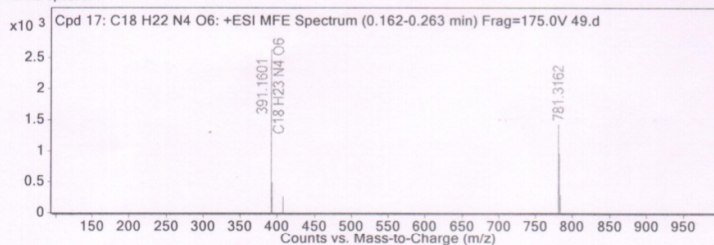


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 17: C18 H22 N4 O6	0.186	390.1522	C18 H22 N4 O6	C18 H22 N4 O6	4.35	C18 H22 N4 O6

Compound Label	m/z	RT	Algorithm	Mass
Cpd 17: C18 H22 N4 O6	391.1601	0.186	Find by Molecular Feature	390.1522

MFE MS Spectrum



MS Spectrum Peak List

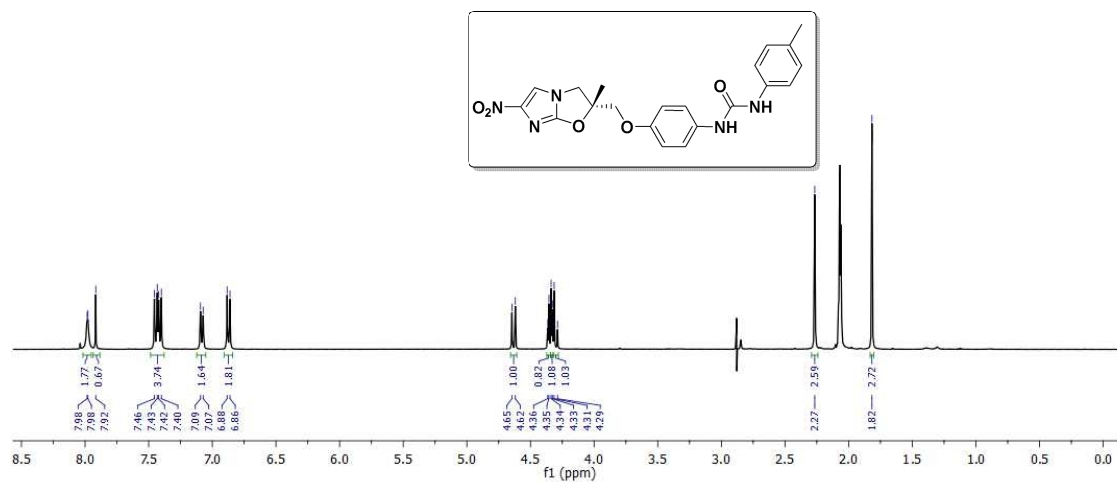
m/z	z	Abund	Formula	Ion
391.1601	1	2645.8	C18 H23 N4 O6	(M+H)+
392.1606	1	643.4	C18 H23 N4 O6	(M+H)+
393.1644	1	492.58	C18 H23 N4 O6	(M+H)+
408.1895	1	264.91	C18 H26 N5 O6	(M+NH4)+
781.3162	1	1422.69		(2M+H)+
782.3162	1	966.88		(2M+H)+
783.312	1	299.26		(2M+H)+

Predicted Isotope Match Table

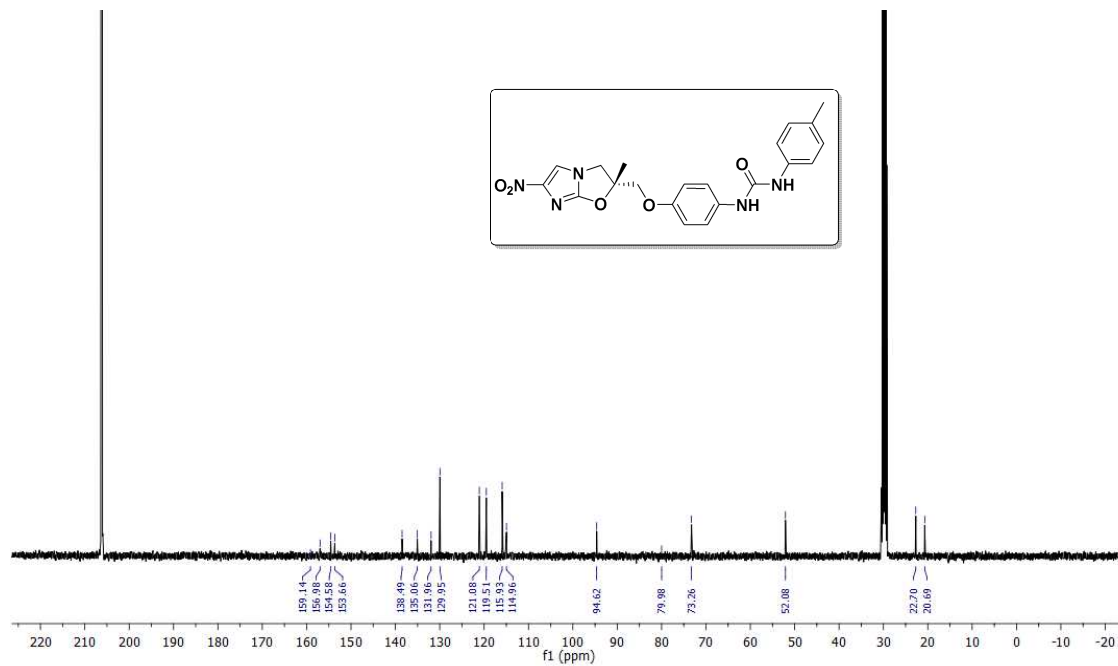
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	391.1601	391.1612	2.96	100	100	69.96	80.1
2	392.1606	392.1642	9.05	24.32	21.42	17.01	17.16
3	393.1644	393.1665	5.52	18.62	3.42	13.03	2.74

--- End Of Report ---

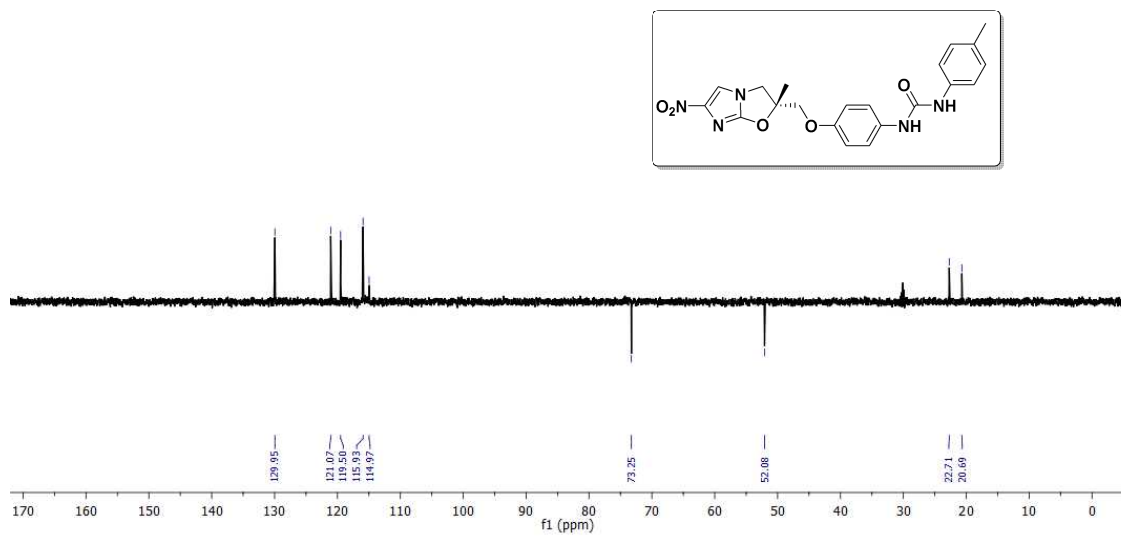
^1H NMR (400 MHz, Acetone- d_6) of compound **18a**:



^{13}C NMR (101 MHz, Acetone- d_6) of compound **18a** :



DEPT (101 MHz, Acetone- d_6) of compound **18a**:

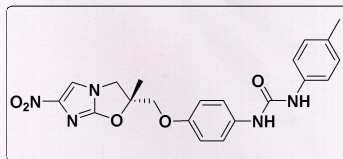


HRMS of compound **18a**:

Qualitative Compound Report

Data File	154.d	Sample Name	154
Sample Type	Sample	Position	Vial 10
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	25-04-2013 PM 2:24:03
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

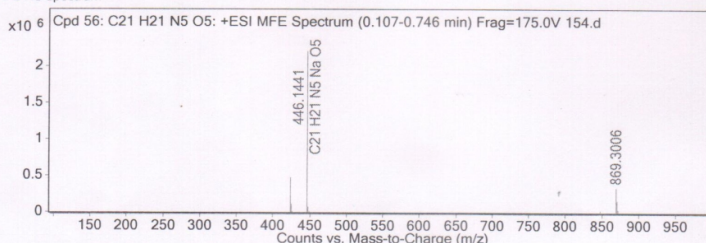


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 56: C21 H21 N5 O5	0.196	423.155	C21 H21 N5 O5	C21 H21 N5 O5	-1.74	C21 H21 N5 O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 56: C21 H21 N5 O5	446.1441	0.196	Find by Molecular Feature	423.155

MFE MS Spectrum



MS Spectrum Peak List

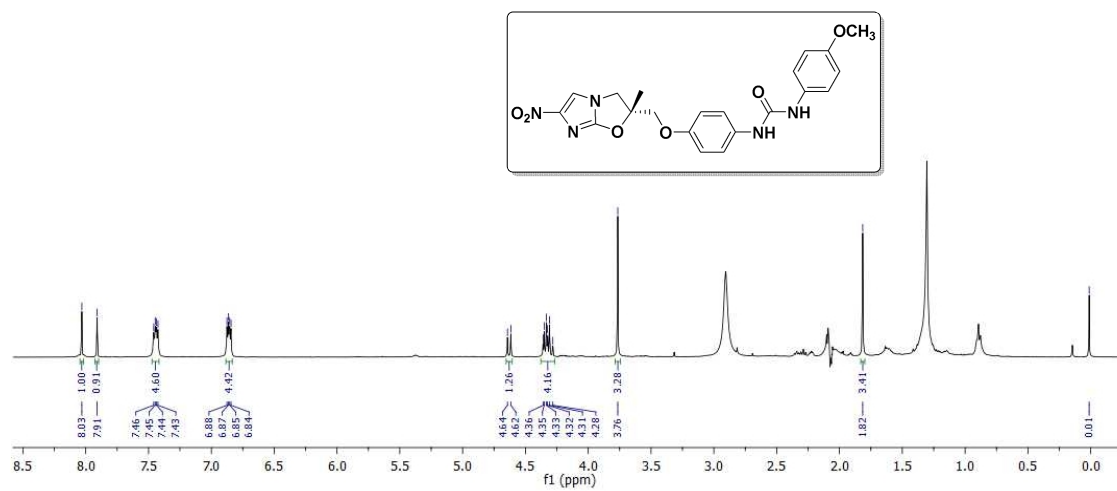
m/z	z	Abund	Formula	Ion
424.1625	1	481020.06	C21 H22 N5 O5	(M+H)+
425.1651	1	116235.84	C21 H22 N5 O5	(M+H)+
426.1671	1	18291.17	C21 H22 N5 O5	(M+H)+
446.1441	1	2215807.75	C21 H21 N5 Na O5	(M+Na)+
447.1476	1	501260.72	C21 H21 N5 Na O5	(M+Na)+
448.1494	1	70581.26	C21 H21 N5 Na O5	(M+Na)+
847.3158	1	23094.38		(2M+H)+
869.3006	1	340590.78		(2M+Na)+
870.3025	1	160836.86		(2M+Na)+
871.3041	1	41154.98		(2M+Na)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	424.1625	424.1615	-2.26	100	100	77.64	77.2
2	425.1651	425.1645	-1.48	24.16	24.98	18.76	19.29
3	426.1671	426.167	-0.39	3.8	4.02	2.95	3.1
4	427.169	427.1694	0.95	0.77	0.49	0.6	0.37
5	428.1696	428.1719	5.37	0.06	0.05	0.05	0.04

--- End Of Report ---

^1H NMR (400 MHz, Acetone- d_6) of compound **18b**:

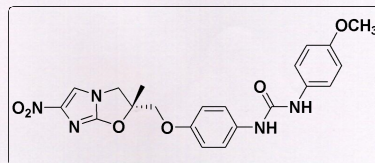


HRMS of compound **18b**:

Qualitative Compound Report

Data File 76.d Sample Name 76
 Sample Type Sample Position Vial 3
 Instrument Name Instrument 1 User Name vishal
 Acq Method vishal_12-01-13.m Acquired Time 26-04-2013 PM 1:42:40
 IRM Calibration Status Success DA Method daily_report.m
 Comment

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

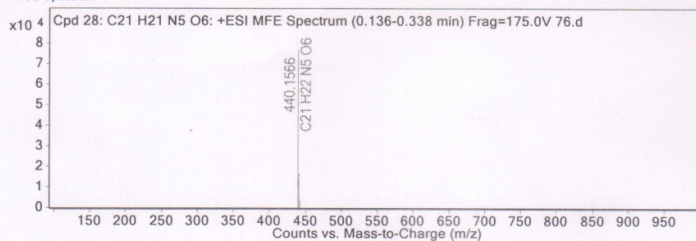


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C21 H21 N5 O6	0.188	439.1493	C21 H21 N5 O6	C21 H21 N5 O6	-0.24	C21 H21 N5 O6

Compound Label	m/z	RT	Algorithm	Mass
Cpd 28: C21 H21 N5 O6	440.1566	0.188	Find by Molecular Feature	439.1493

MFE MS Spectrum



MS Spectrum Peak List

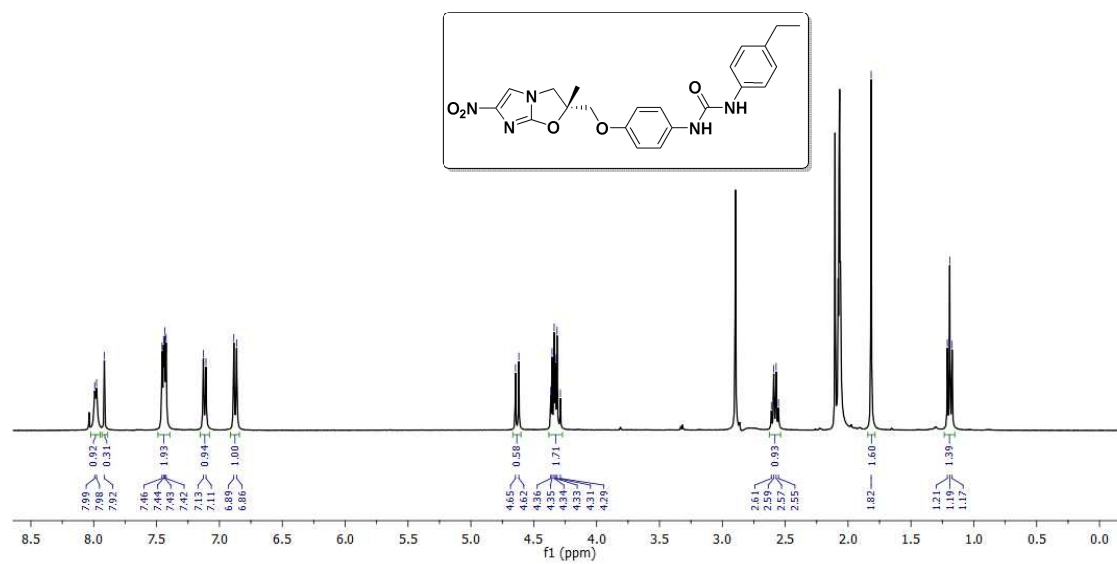
m/z	z	Abund	Formula	Ion
440.1566	1	76818.89	C21 H22 N5 O6	(M+H)+
441.1593	1	16960.28	C21 H22 N5 O6	(M+H)+
442.162	1	3512.6	C21 H22 N5 O6	(M+H)+
443.1663	1	806.32	C21 H22 N5 O6	(M+H)+

Predicted Isotope Match Table

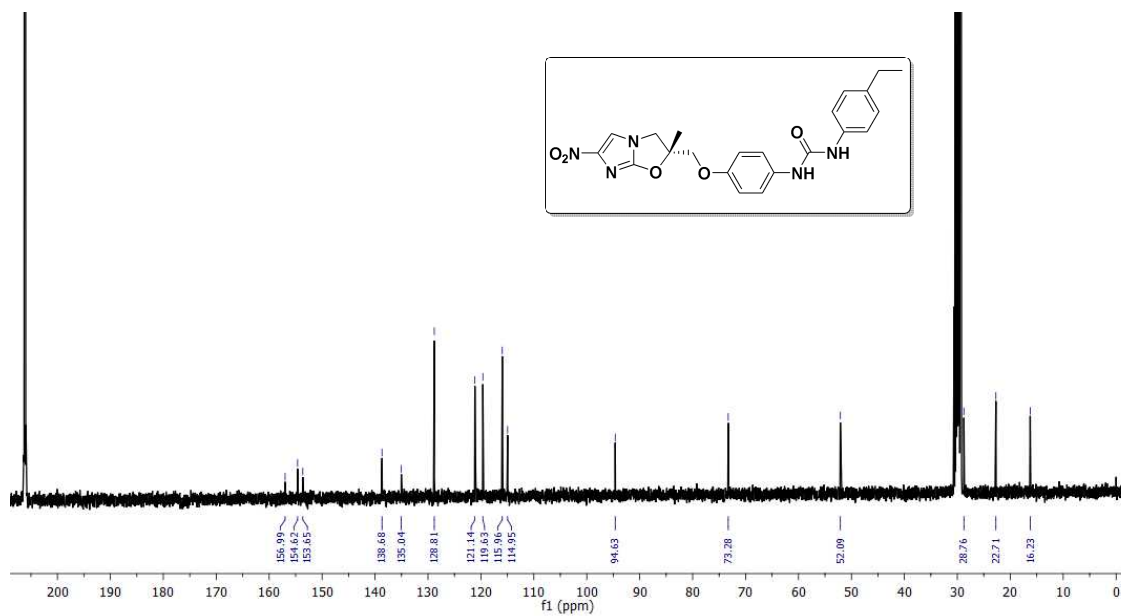
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	440.1566	440.1565	-0.27	100	100	78.31	77.04
2	441.1593	441.1594	-0.16	22.08	25.02	17.29	19.28
3	442.162	442.1618	-0.43	4.57	4.24	3.58	3.26
4	443.1663	443.1643	-4.59	1.05	0.54	0.82	0.41

--- End Of Report ---

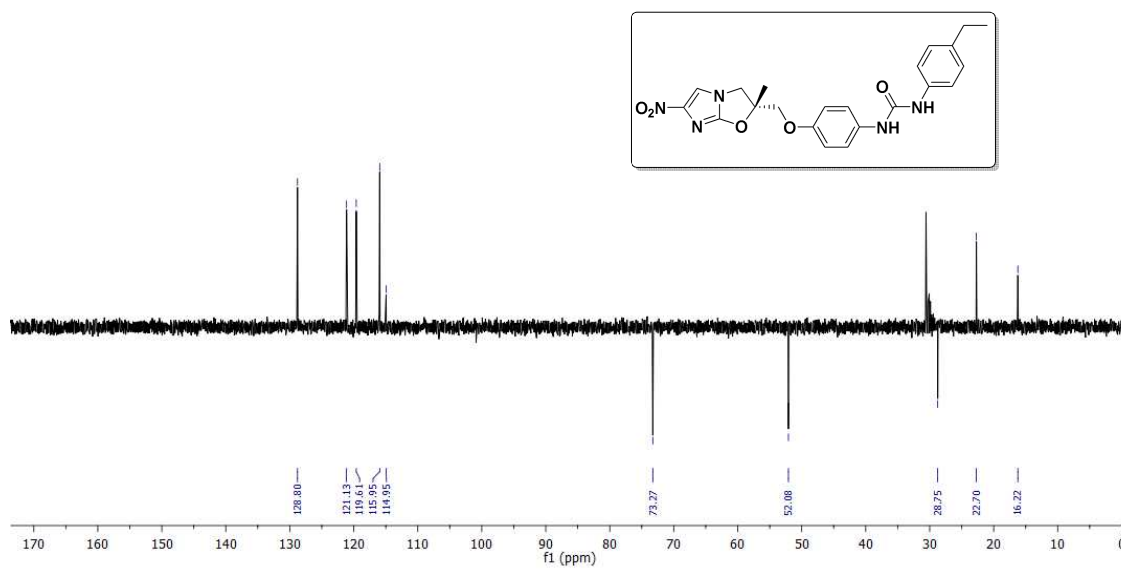
^1H NMR (400 MHz, Acetone- d_6) of compound **18c**:



^{13}C NMR (101 MHz, Acetone- d_6) of compound **18c**:



DEPT (101 MHz, Acetone- d_6) of compound **18c**:

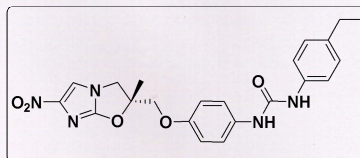


HRMS of compound **18c**:

Qualitative Compound Report

Data File	156.d	Sample Name	156
Sample Type	Sample	Position	Vial 8
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	25-04-2013 PM 2:12:57
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

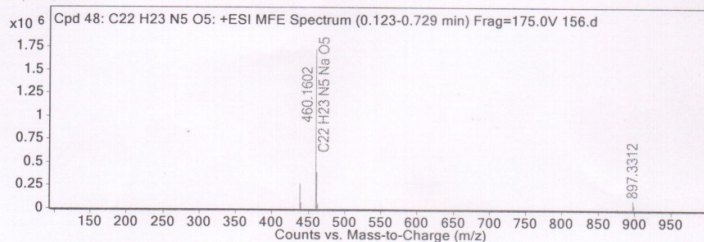


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 48: C22 H23 N5 O5	0.194	437.1711	C22 H23 N5 O5	C22 H23 N5 O5	-2.6	C22 H23 N5 O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 48: C22 H23 N5 O5	460.1602	0.194	Find by Molecular Feature	437.1711

MFE MS Spectrum



MS Spectrum Peak List

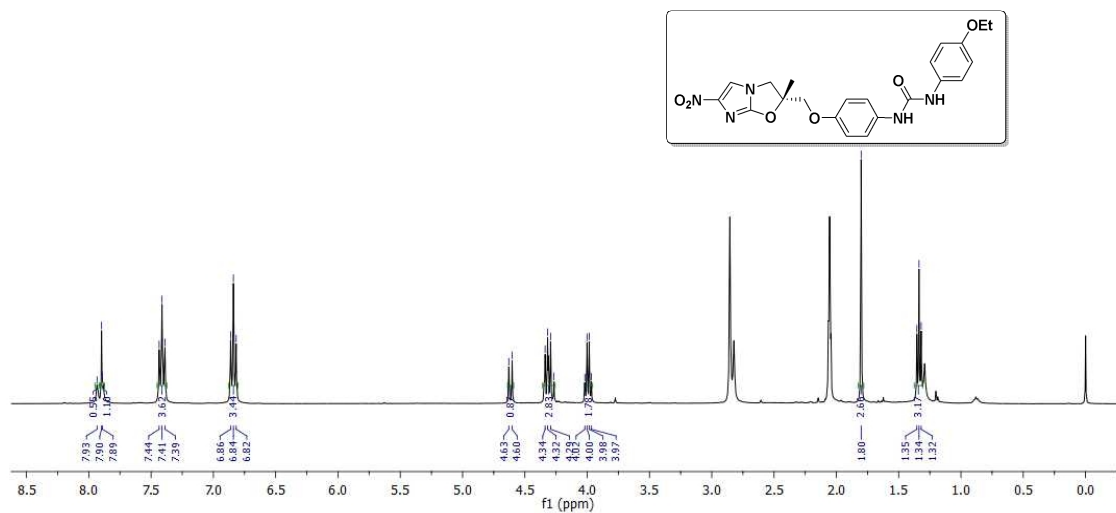
m/z	z	Abund	Formula	Ion
438.1781	1	276302.25	C22 H24 N5 O5	(M+H)+
439.1807	1	70332.48	C22 H24 N5 O5	(M+H)+
440.1832	1	10671.2	C22 H24 N5 O5	(M+H)+
460.1602	1	1729835.5	C22 H23 N5 Na O5	(M+Na)+
461.1635	1	403361.31	C22 H23 N5 Na O5	(M+Na)+
462.1653	1	61601.47	C22 H23 N5 Na O5	(M+Na)+
463.1678	1	8330.23	C22 H23 N5 Na O5	(M+Na)+
897.3312	1	97882.28		(2M+Na)+
898.3339	1	44786.88		(2M+Na)+
899.3355	1	13765.58		(2M+Na)+

Predicted Isotope Match Table

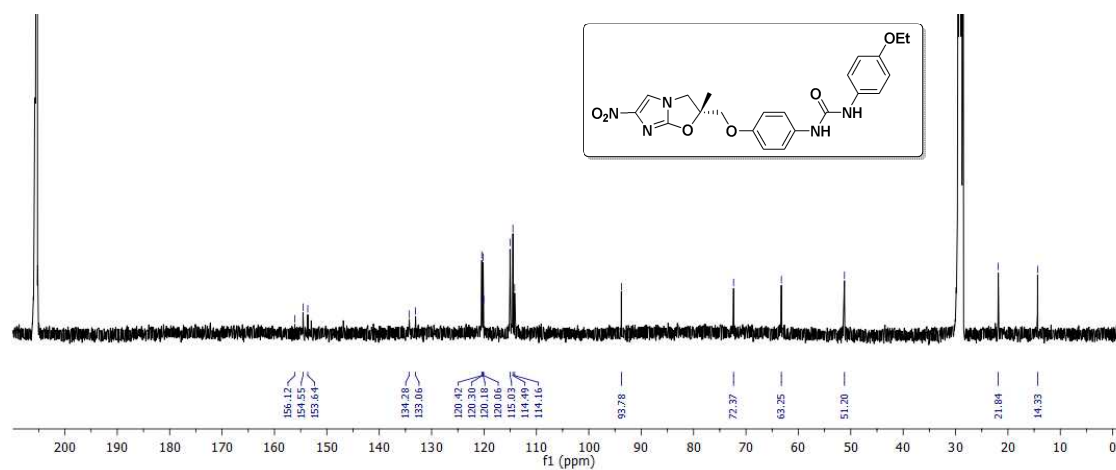
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	438.1781	438.1772	-2.17	100	100	77.02	76.38
2	439.1807	439.1801	-1.35	25.45	26.09	19.61	19.93
3	440.1832	440.1827	-1.16	3.86	4.3	2.97	3.28
4	441.1873	441.1852	-4.9	0.52	0.53	0.4	0.4

--- End Of Report ---

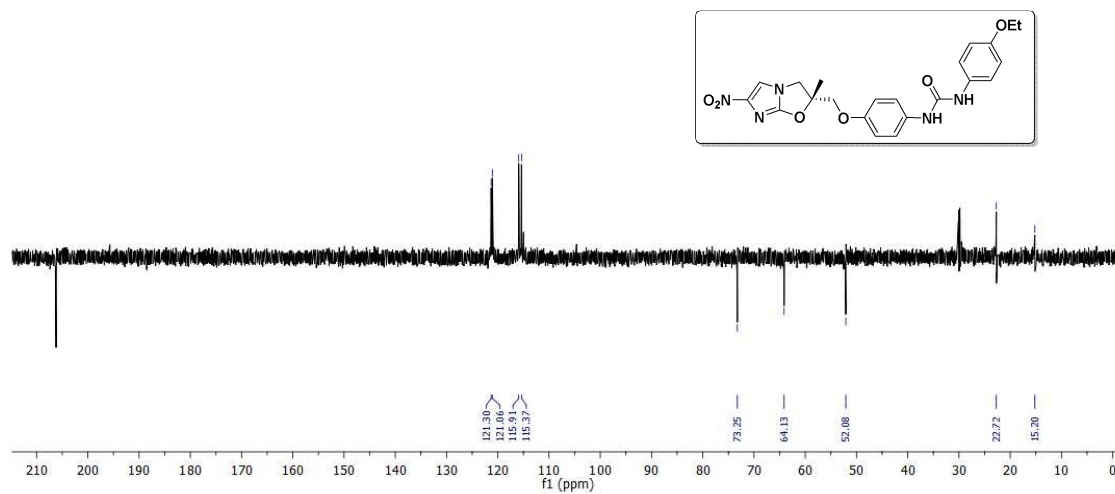
^1H NMR (400 MHz, Acetone- d_6) of compound **18d**:



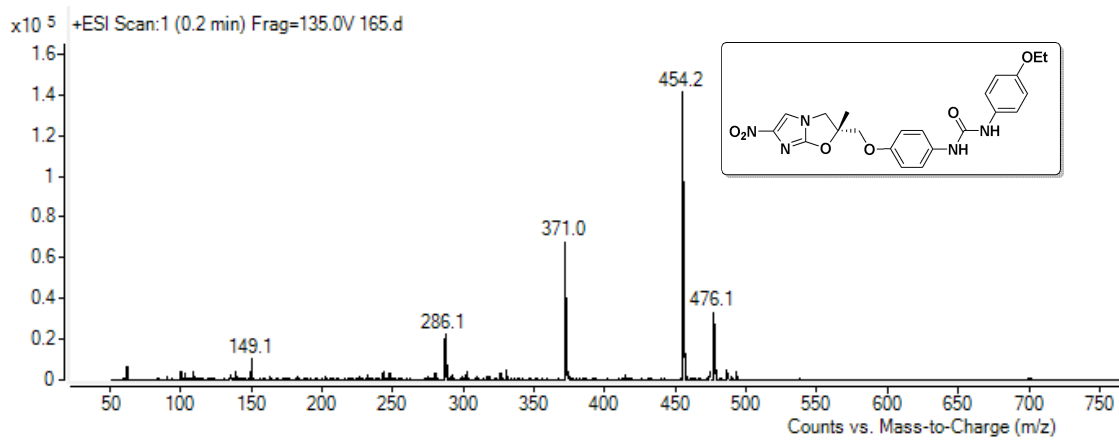
^{13}C NMR (126 MHz, Acetone- d_6) of compound **18d**:



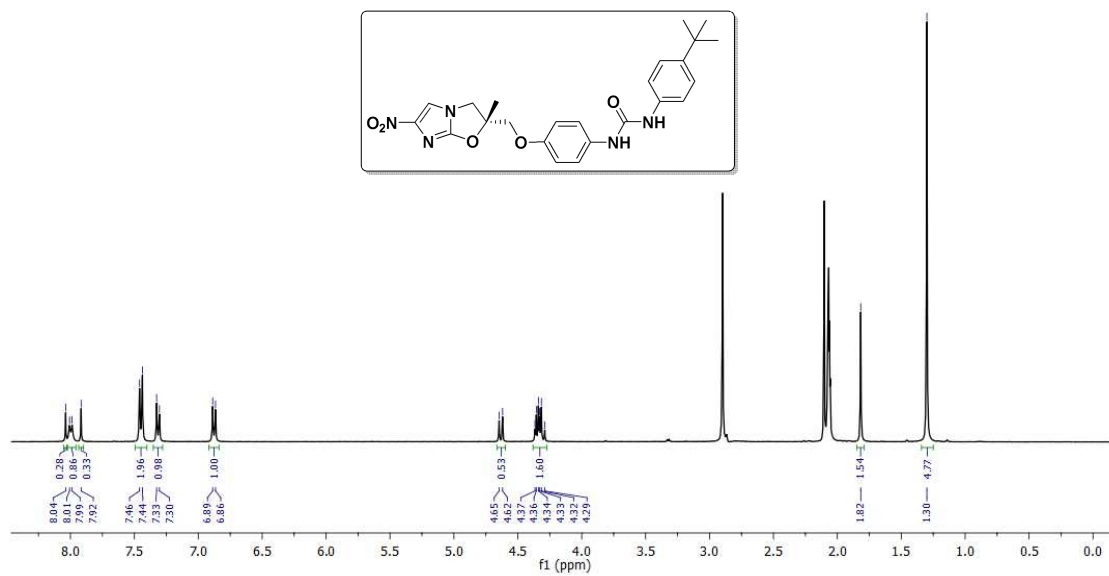
DEPT (101 MHz, Acetone- d_6) of compound **18d**:



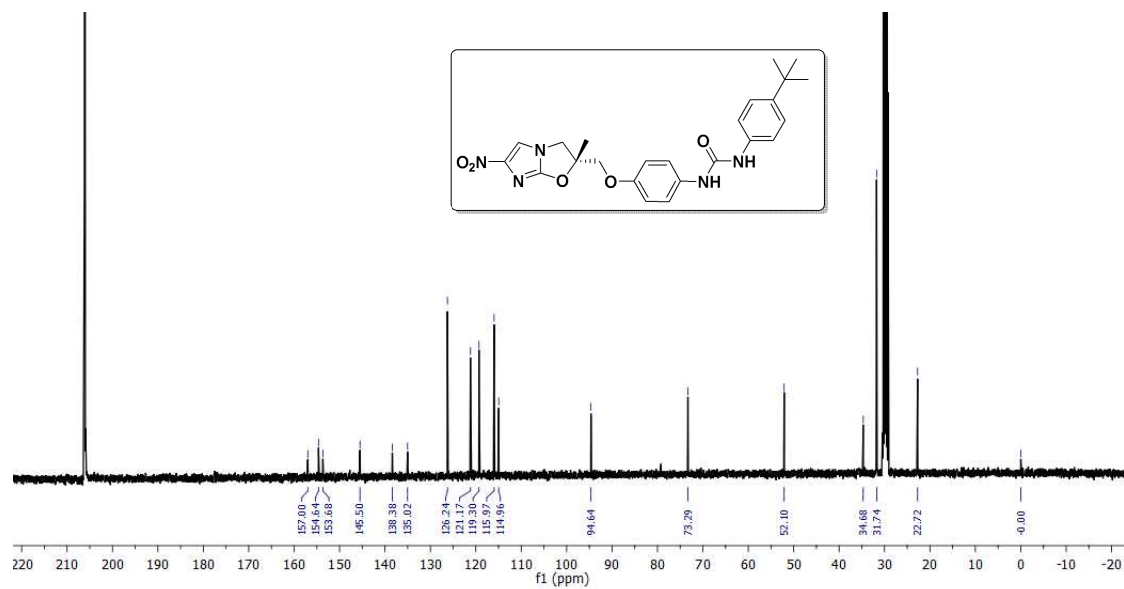
LC-MS of compound **18d**:



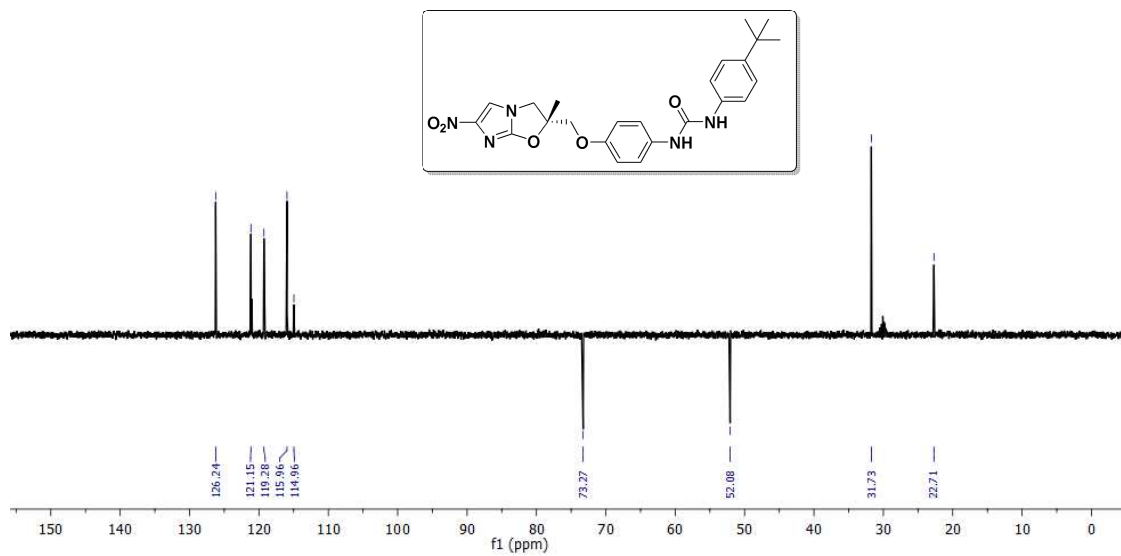
^1H NMR (400 MHz, Acetone- d_6) of compound **18e**:



^{13}C NMR (101 MHz, Acetone- d_6) of compound **18e**:



DEPT (101 MHz, Acetone- d_6) of compound **18e**:

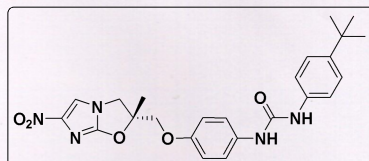


HRMS of compound **18e**:

Qualitative Compound Report

Data File	155.d	Sample Name	155
Sample Type	Sample	Position	Vial 2
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	25-04-2013 PM 1:33:54
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

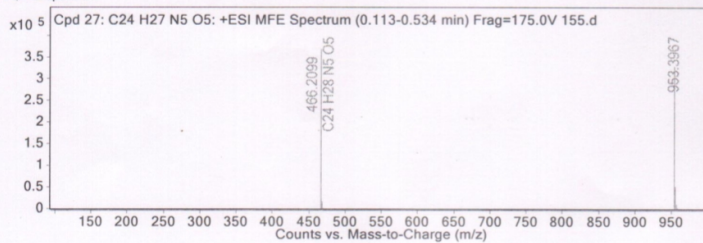


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 27: C24 H27 N5 O5	0.195	465.2025	C24 H27 N5 O5	C24 H27 N5 O5	-2.81	C24 H27 N5 O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 27: C24 H27 N5 O5	466.2099	0.195	Find by Molecular Feature	465.2025

MFE MS Spectrum



MS Spectrum Peak List

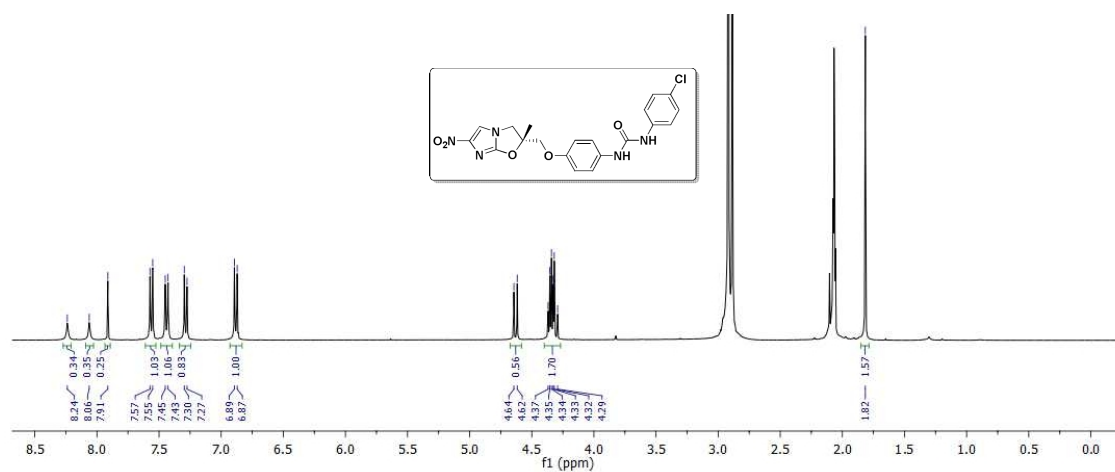
m/z	z	Abund	Formula	Ion
466.2099	1	369189.31	C24 H28 N5 O5	(M+H)+
467.2126	1	97556.08	C24 H28 N5 O5	(M+H)+
468.2152	1	15774.59	C24 H28 N5 O5	(M+H)+
469.2174	1	2409.28	C24 H28 N5 O5	(M+H)+
470.2223	1	633.19	C24 H28 N5 O5	(M+H)+
953.3967	1	329411.44		(2M+Na)+
954.399	1	172062.36		(2M+Na)+
955.4005	1	52302.04		(2M+Na)+
956.4025	1	11259.03		(2M+Na)+
957.4058	1	2029.35		(2M+Na)+

Predicted Isotope Match Table

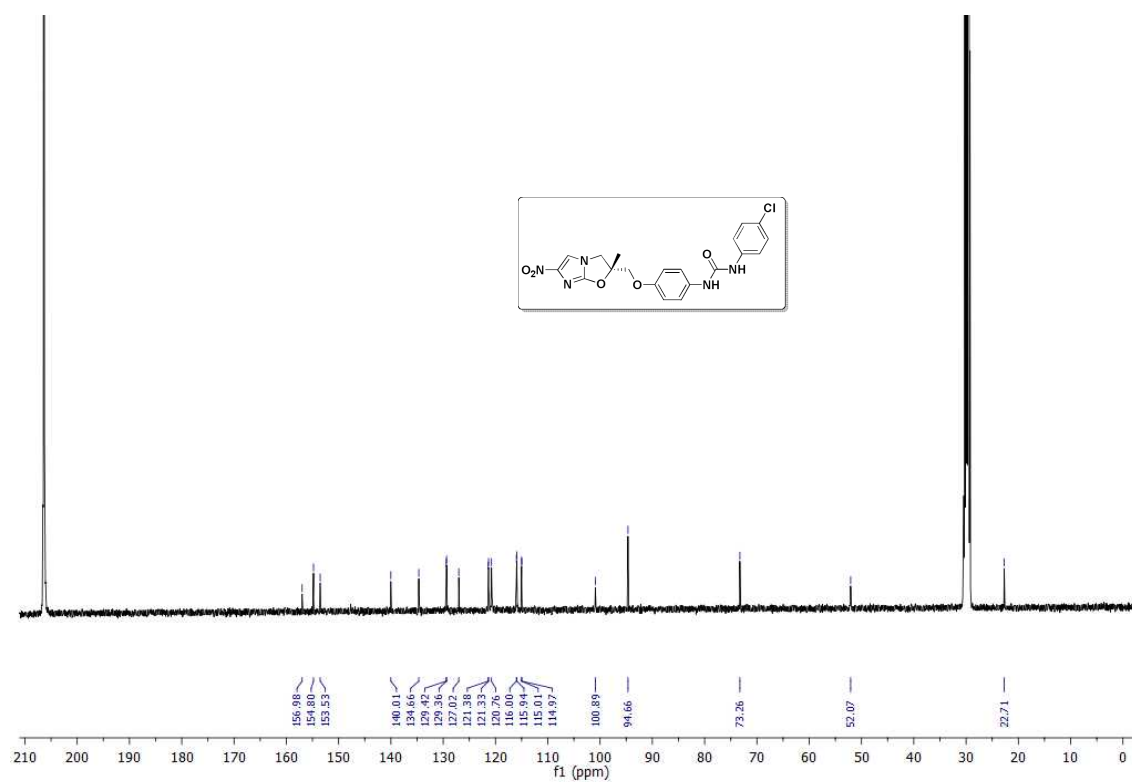
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	466.2099	466.2085	-2.94	100	100	76.03	74.7
2	467.2126	467.2115	-2.35	26.42	28.3	20.09	21.14
3	468.2152	468.2141	-2.26	4.27	4.89	3.25	3.65
4	469.2174	469.2166	-1.72	0.65	0.63	0.5	0.47
5	470.2223	470.2191	-6.84	0.17	0.07	0.13	0.05

--- End Of Report ---

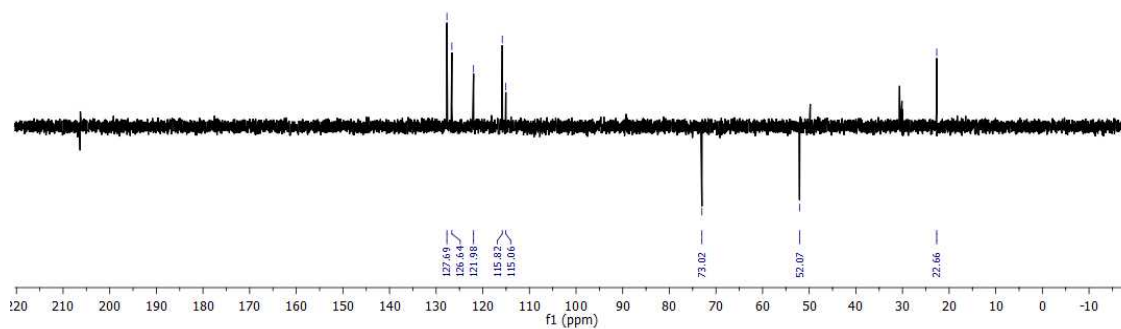
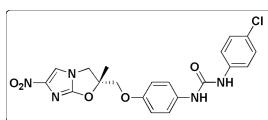
^1H NMR (400 MHz, Acetone- d_6) of compound **18f**:



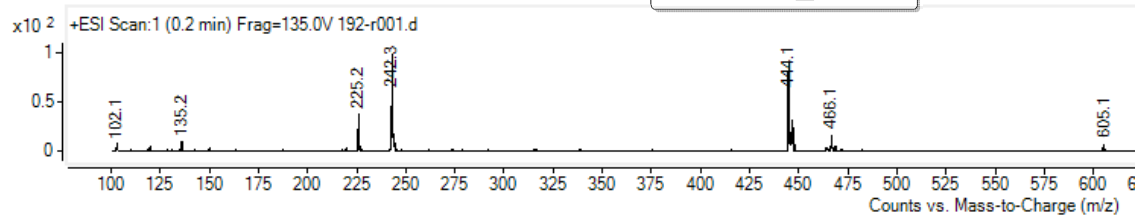
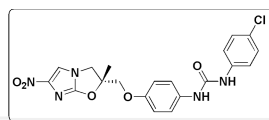
^{13}C NMR (101 MHz, Acetone- d_6) of compound **18f**:



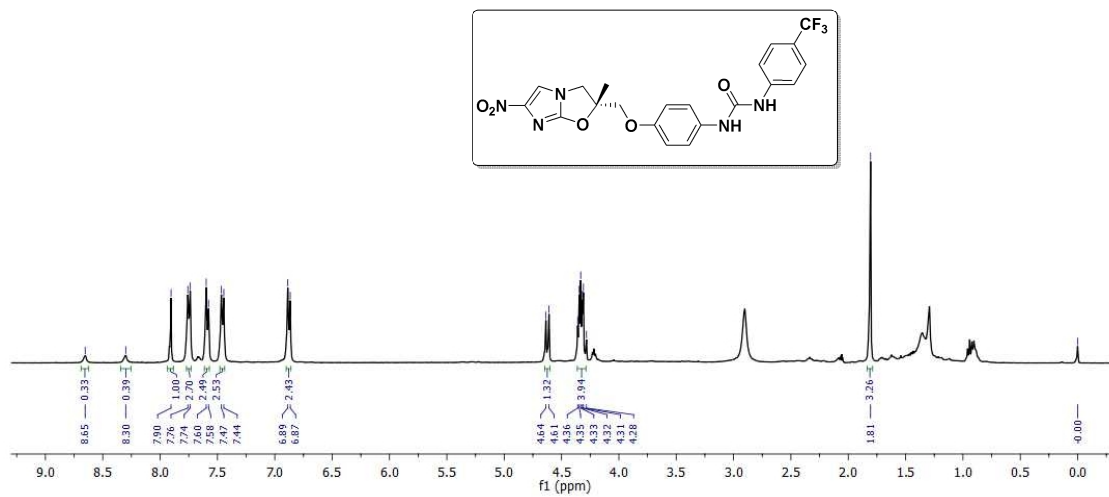
DEPT (101 MHz, Acetone- d_6) of compound **18f**:



LC-MS of compound **18f**:



^1H NMR (400 MHz, Acetone- d_6) of compound **18g**:

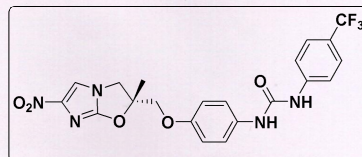


HRMS of compound **18g**:

Qualitative Compound Report

Data File	10.d	Sample Name	10
Sample Type	Sample	Position	Vial 2
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	23-04-2013 AM 11:53:16
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

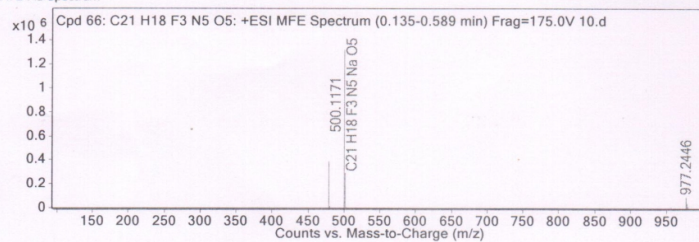


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 66: C21 H18 F3 N5 O5	0.194	477.1278	C21 H18 F3 N5 O5	C21 H18 F3 N5 O5	-3.85	C21 H18 F3 N5 O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 66: C21 H18 F3 N5 O5	500.1171	0.194	Find by Molecular Feature	477.1278

MFE MS Spectrum



MS Spectrum Peak List

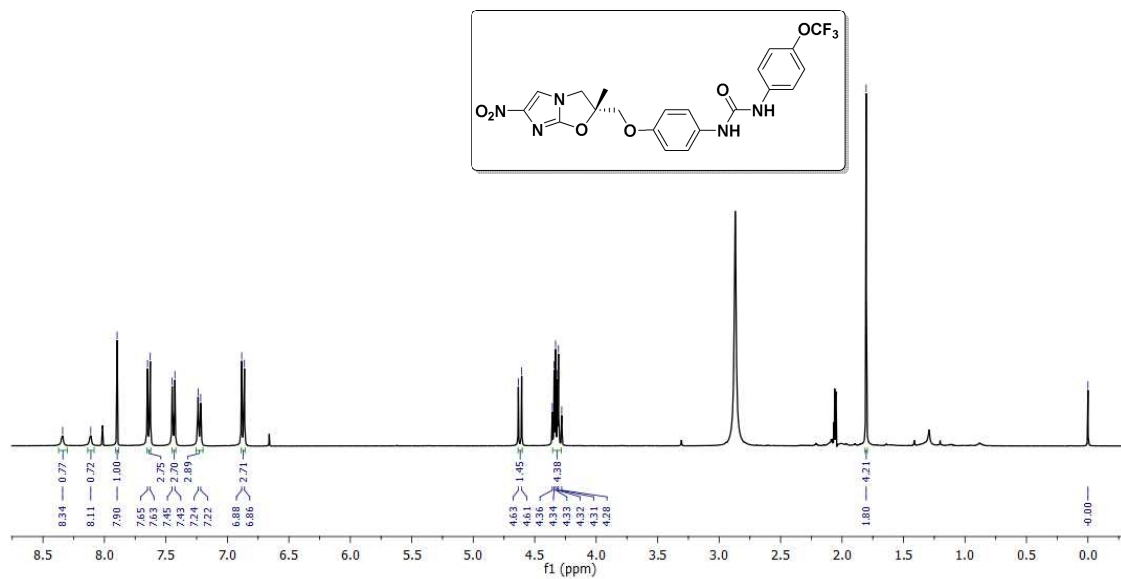
m/z	z	Abund	Formula	Ion
478.1351	1	391020.72	C21 H19 F3 N5 O5	(M+H)+
479.1377	1	89762.49	C21 H19 F3 N5 O5	(M+H)+
480.1399	1	16418.73	C21 H19 F3 N5 O5	(M+H)+
500.1171	1	1318063.88	C21 H18 F3 N5 Na O5	(M+Na)+
501.12	1	292724.84	C21 H18 F3 N5 Na O5	(M+Na)+
502.1218	1	45504.16	C21 H18 F3 N5 Na O5	(M+Na)+
955.2603	1	10123.84		(2M+H)+
977.2446	1	87354.54		(2M+Na)+
978.2472	1	40698.2		(2M+Na)+
979.2481	1	11685.93		(2M+Na)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	478.1351	478.1333	-3.88	100	100	78.25	77.25
2	479.1377	479.1362	-3.2	22.96	24.95	17.96	19.27
3	480.1399	480.1387	-2.48	4.2	4.01	3.29	3.1
4	481.1418	481.1412	-1.36	0.64	0.48	0.5	0.37

--- End Of Report ---

^1H NMR (400 MHz, Acetone- d_6) of compound **18h**:

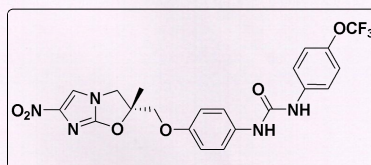


HRMS of compound 18h:

Qualitative Compound Report

Data File 75.d **Sample Name** 75
Sample Type Sample **Position** Vial 12
Instrument Name Instrument 1 **User Name** vishal
Acq Method vishal_12-01-13.m **Acquired Time** 23-04-2013 PM 12:48:21
IRM Calibration Status Success **DA Method** daily_report.m
Comment

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

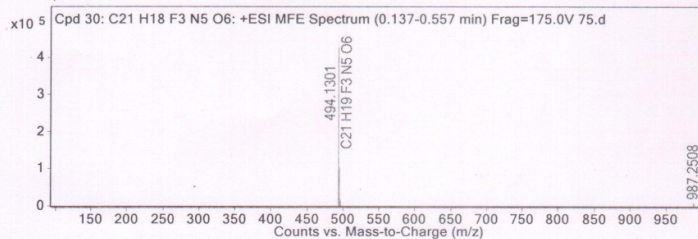


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C21 H18 F3 N5 O6	0.19	493.1226	C21 H18 F3 N5 O6	C21 H18 F3 N5 O6	-3.43	C21 H18 F3 N5 O6

Compound Label	m/z	RT	Algorithm	Mass
Cpd 30: C21 H18 F3 N5 O6	494.1301	0.19	Find by Molecular Feature	493.1226

MFE MS Spectrum



MS Spectrum Peak List

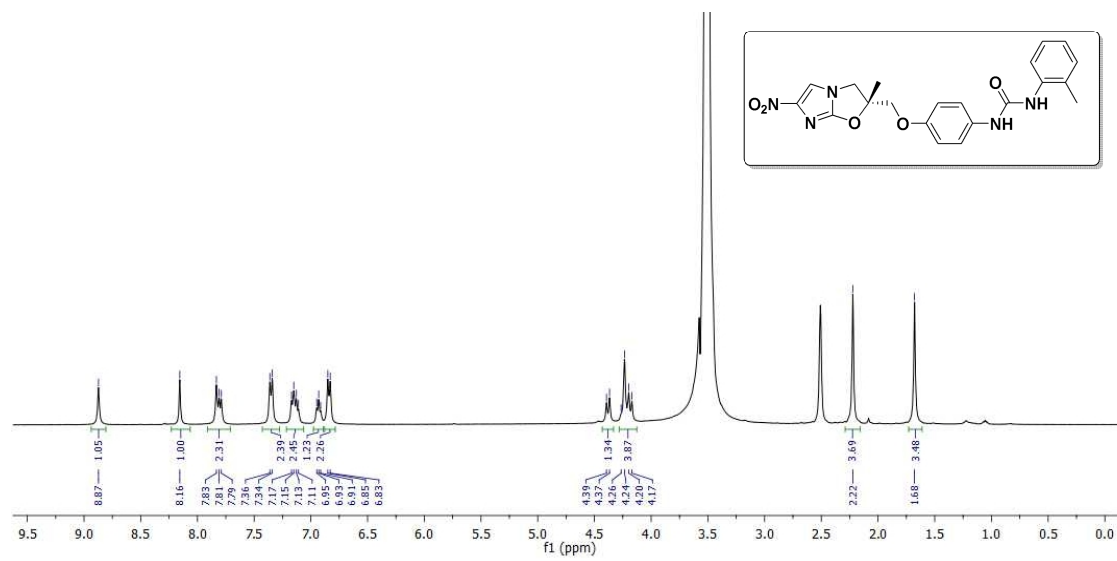
m/z	z	Abund	Formula	Ion
494.1301	1	425507.5	C21 H19 F3 N5 O6	(M+H)+
495.1321	1	102443.92	C21 H19 F3 N5 O6	(M+H)+
496.1346	1	17593.5	C21 H19 F3 N5 O6	(M+H)+
497.1371	1	2305.29	C21 H19 F3 N5 O6	(M+H)+
498.1403	1	513.64	C21 H19 F3 N5 O6	(M+H)+
987.2508	1	9960.06		(2M+H)+
988.254	1	5149.56		(2M+H)+
989.2548	1	1316.09		(2M+H)+
990.2558	1	507.89		(2M+H)+

Predicted Isotope Match Table

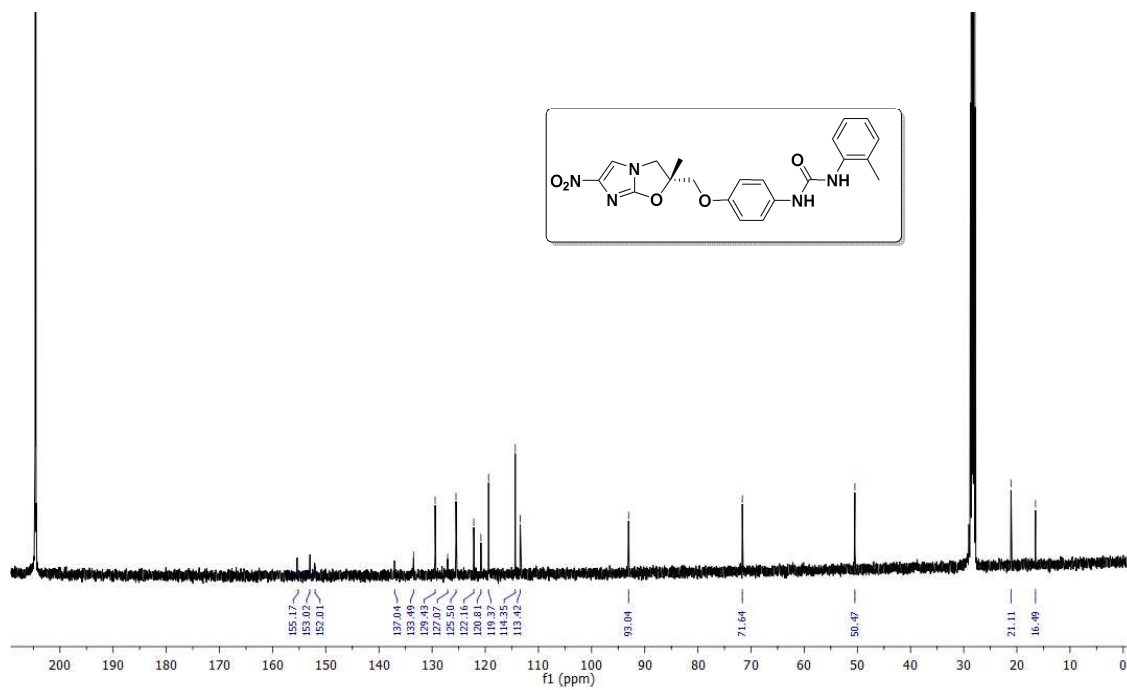
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	494.1301	494.1282	-3.84	100	100	77.6	77.04
2	495.1321	495.1311	-1.93	24.08	24.99	18.68	19.25
3	496.1346	496.1336	-2.04	4.13	4.23	3.21	3.26
4	497.1371	497.136	-2.16	0.54	0.54	0.42	0.41
5	498.1403	498.1384	-3.71	0.12	0.06	0.09	0.04

--- End Of Report ---

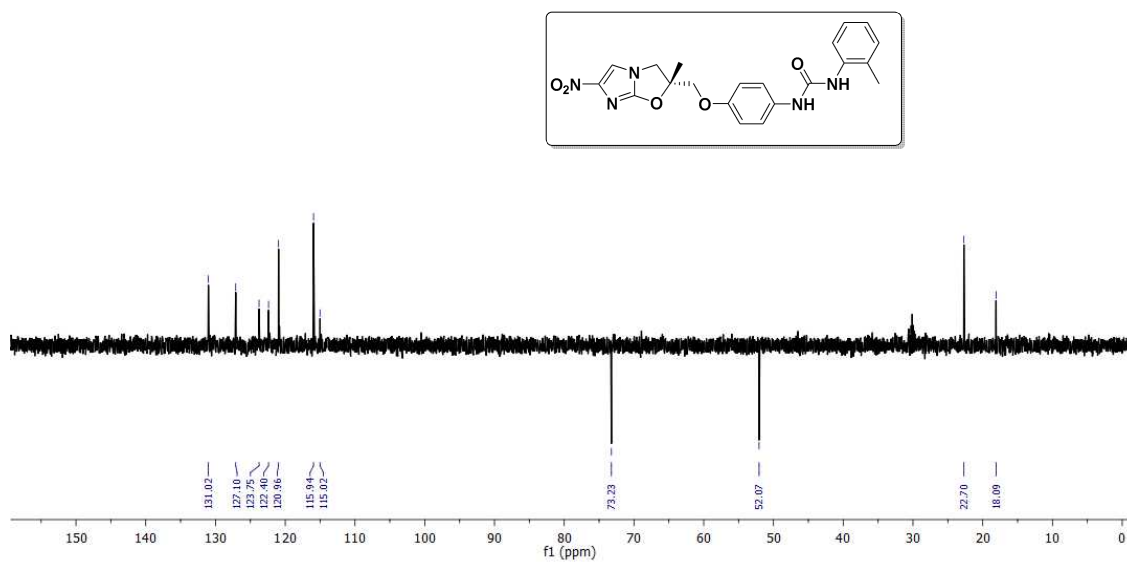
^1H NMR (400 MHz, DMSO- d_6) **18i**:



^{13}C (126 MHz, Acetone- d_6) of compound **18i**:



DEPT (126 MHz, Acetone- d_6) of compound **18i**:

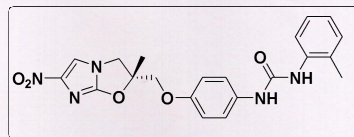


HRMS of compound **18i**:

Qualitative Compound Report

Data File	157.d	Sample Name	157
Sample Type	Sample	Position	Vial 11
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	25-04-2013 PM 2:29:34
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

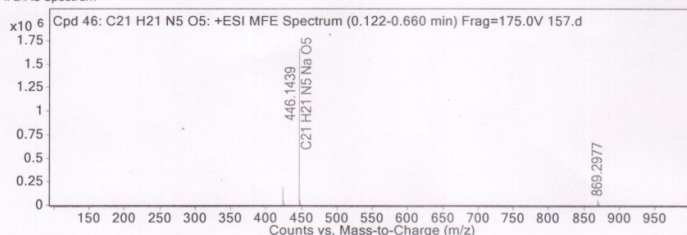


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 46: C21 H21 N5 O5	0.191	423.1547	C21 H21 N5 O5	C21 H21 N5 O5	-1.09	C21 H21 N5 O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 46: C21 H21 N5 O5	446.1439	0.191	Find by Molecular Feature	423.1547

MFE MS Spectrum



MS Spectrum Peak List

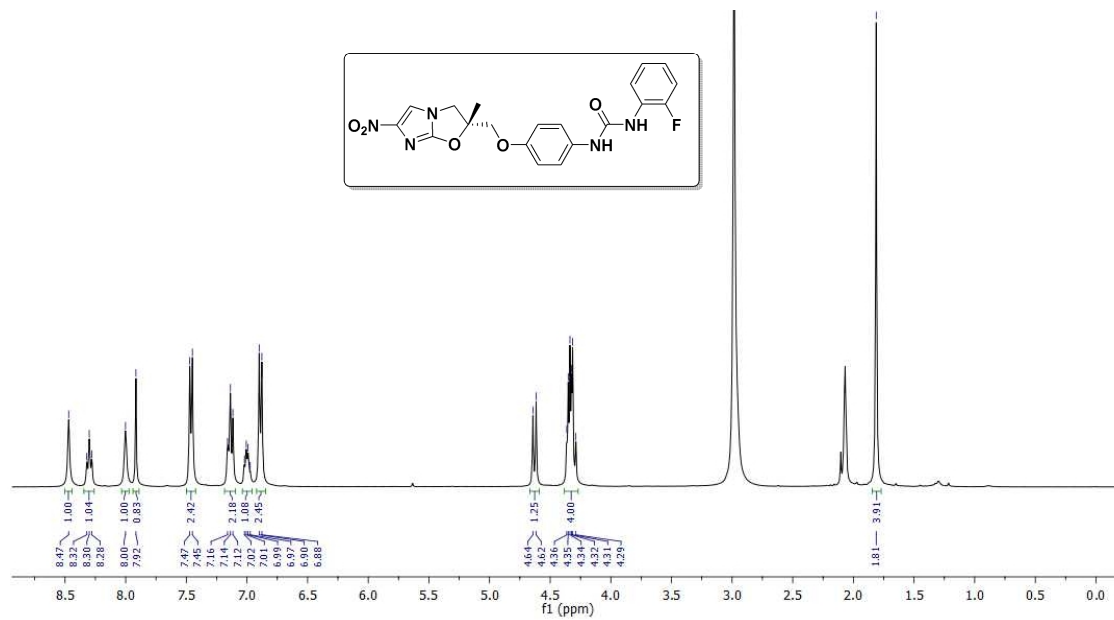
m/z	z	Abund	Formula	Ion
424.1615	1	190094.02	C21 H22 N5 O5	(M+H)+
425.1644	1	45985.77	C21 H22 N5 O5	(M+H)+
426.1668	1	7359.09	C21 H22 N5 O5	(M+H)+
446.1439	1	1654300	C21 H21 N5 Na O5	(M+Na)+
447.1471	1	365540.19	C21 H21 N5 Na O5	(M+Na)+
448.1488	1	54503.18	C21 H21 N5 Na O5	(M+Na)+
449.1512	1	6121.76	C21 H21 N5 Na O5	(M+Na)+
869.2977	1	60737.33		(2M+Na)+
870.3005	1	29825.42		(2M+Na)+
871.3036	1	7960.52		(2M+Na)+

Predicted Isotope Match Table

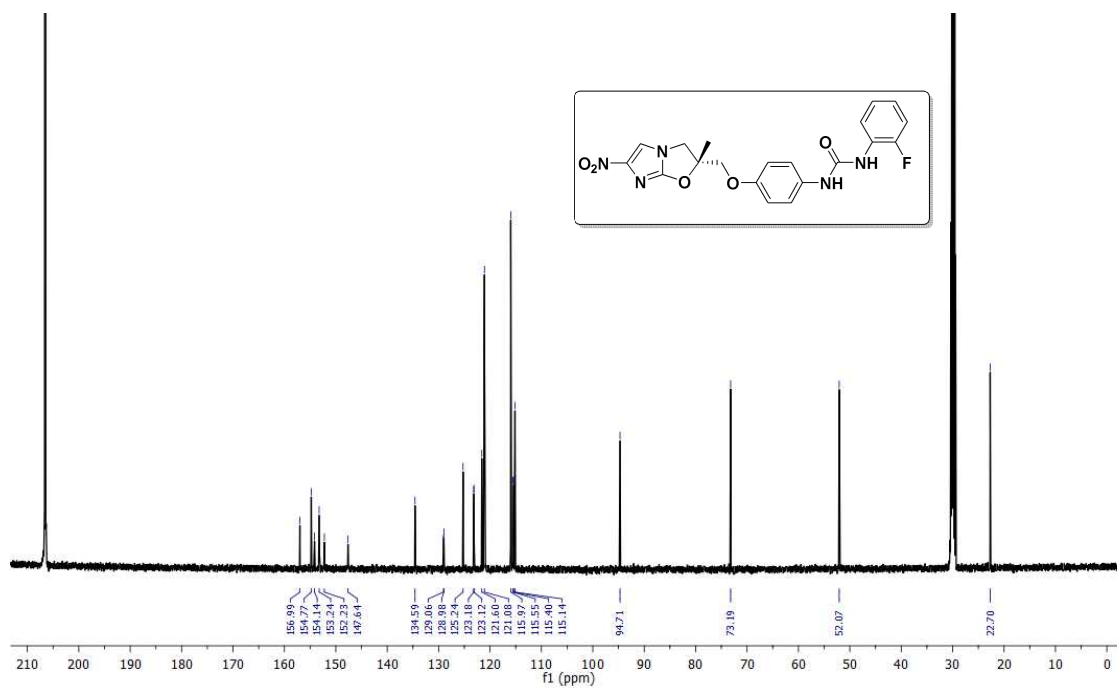
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	424.1615	424.1615	0.01	100	100	77.68	77.23
2	425.1644	425.1645	0.18	24.19	24.98	18.79	19.29
3	426.1668	426.167	0.38	3.87	4.02	3.01	3.11
4	427.167	427.1694	5.67	0.66	0.49	0.52	0.37

--- End Of Report ---

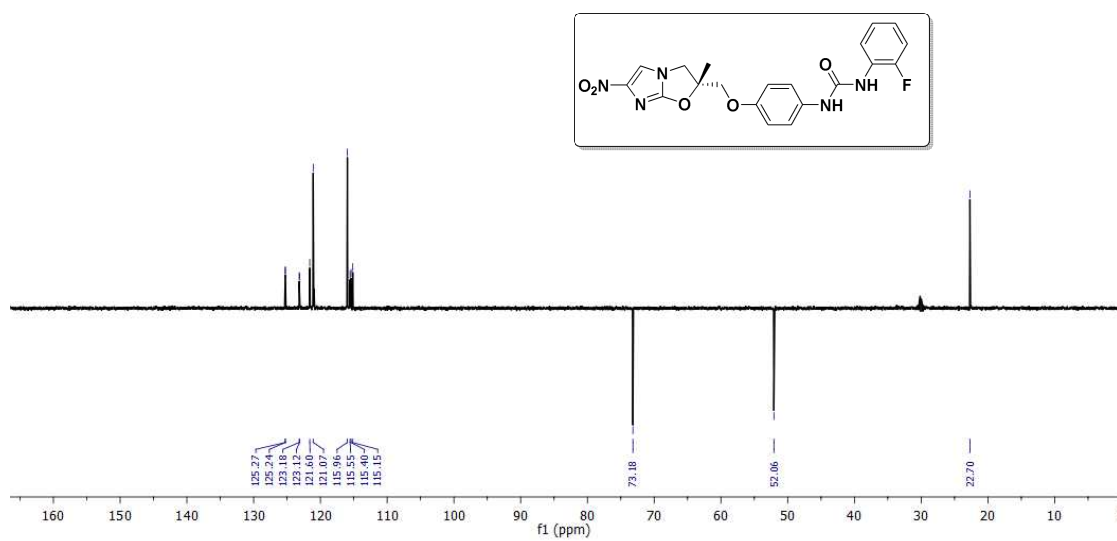
^1H NMR (400 MHz, Acetone- d_6) of compound **18j**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **18j**:



DEPT (126 MHz, Acetone- d_6) of compound **18j**:



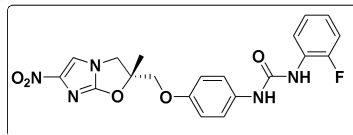
HRMS of compound 18j:

Qualitative Compound Report

Data File: 194.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: new method.m
 IRM Calibration Status: Success
 Comment:

Sample Name: 194
 Position: Vial 6
 User Name:
 Acquired Time: 13-10-2014 PM 4:31:53
 DA Method: daily_report.m

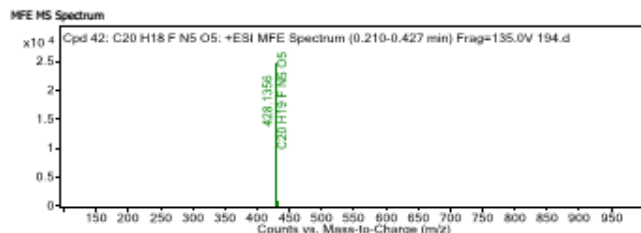
Sample Group: Info.
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF 8.05.01 (85125)



Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 42: C20 H18 F N5 O5	0.272	427.1283	C20 H18 F N5 O5	C20 H18 F N5 O5	2.14	C20 H18 F N5 O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 42: C20 H18 F N5 O5	428.1356	0.272	Find by Molecular Feature	427.1283



MS Spectrum Peak List

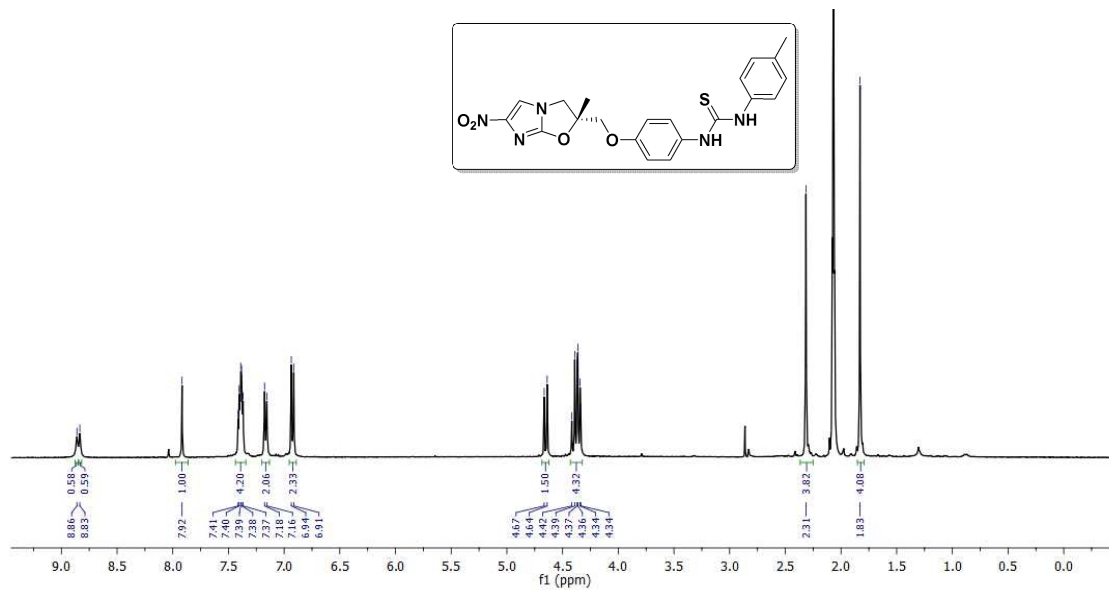
m/z	z	Abund	Formula	Ion
428.1356	1	24661.77	C20 H19 F N5 O5	(M+H) ⁺
429.1386	1	5598.37	C20 H19 F N5 O5	(M+H) ⁺
430.1382	1	1064.69	C20 H19 F N5 O5	(M+H) ⁺

Predicted Isotope Match Table

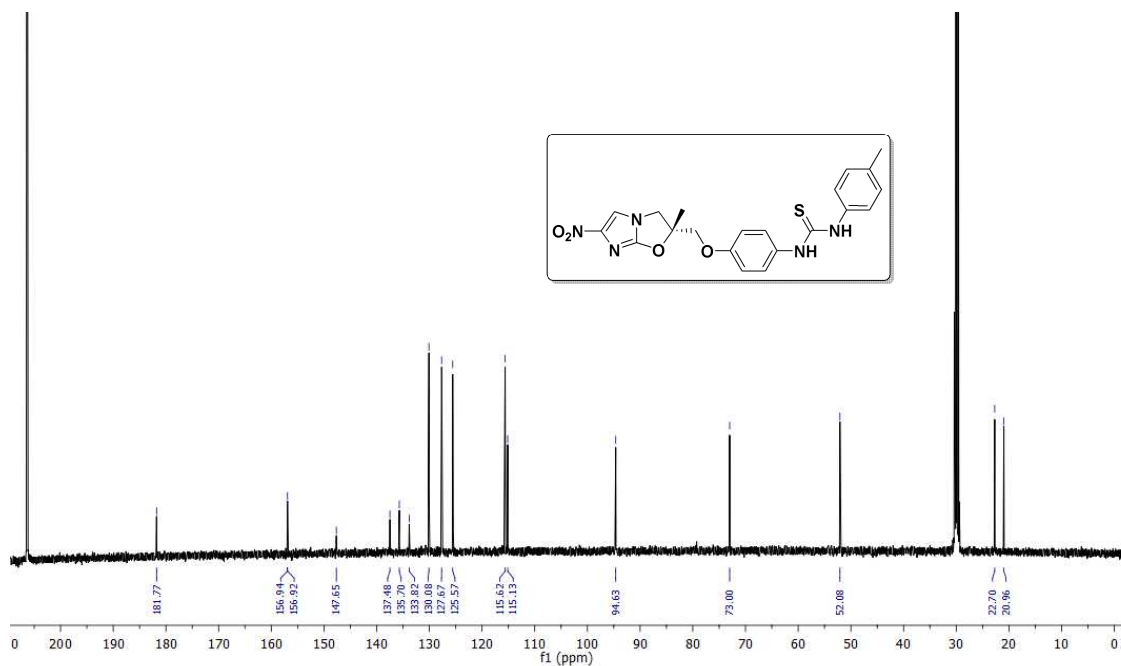
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	428.1356	428.1365	1.93	100	100	78.73	78.36
2	429.1386	429.1394	1.86	22.7	23.87	17.87	18.7
3	430.1382	430.1418	8.43	4.32	3.76	3.4	2.94

--- End Of Report ---

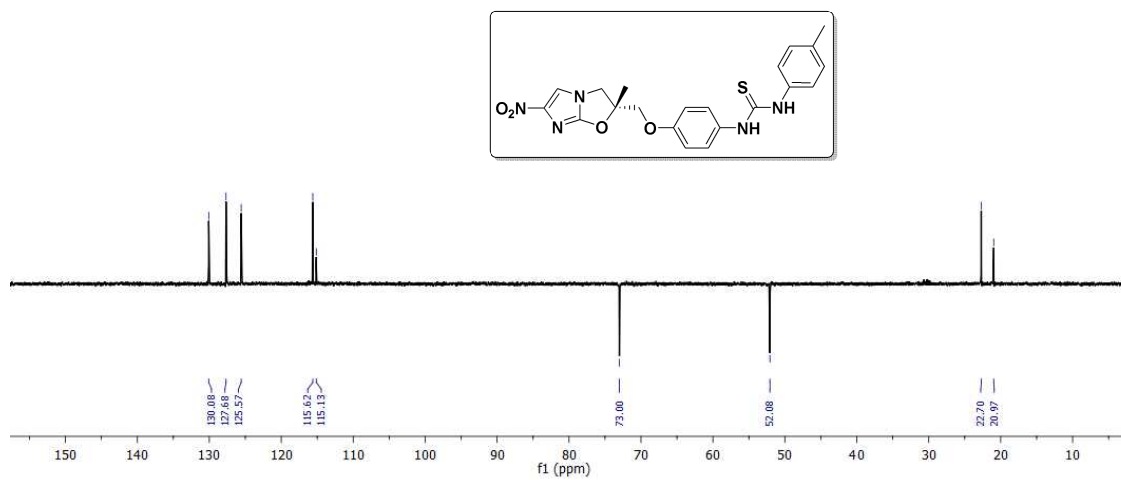
^1H NMR (400 MHz, Acetone- d_6) of compound **18k**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **18k**:



DEPT (126 MHz, Acetone- d_6) of compound **18k**:

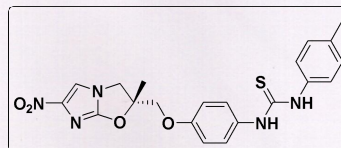


HRMS of compound **18k**:

Qualitative Compound Report

Data File	159.d	Sample Name	159
Sample Type	Sample	Position	Vial 5
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	25-04-2013 PM 1:50:31
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

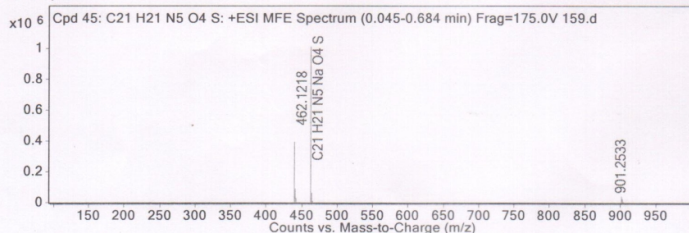


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 45: C21 H21 N5 O4 S	0.192	439.1325	C21 H21 N5 O4 S	C21 H21 N5 O4 S	-2.42	C21 H21 N5 O4 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 45: C21 H21 N5 O4 S	462.1218	0.192	Find by Molecular Feature	439.1325

MFE MS Spectrum



MS Spectrum Peak List

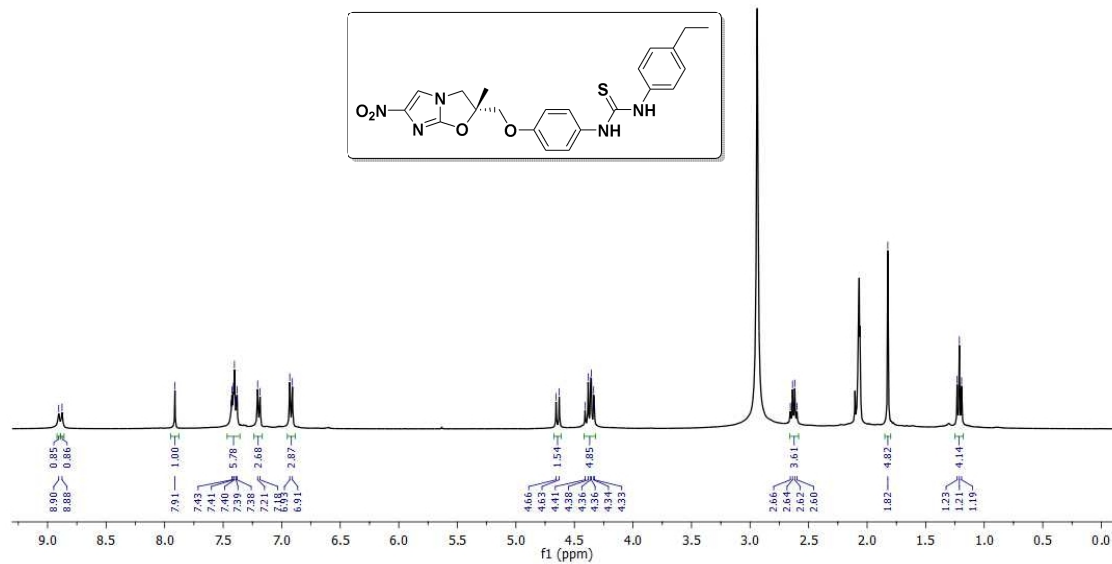
m/z	z	Abund	Formula	Ion
440.1397	1	392716.75	C21 H22 N5 O4 S	(M+H)+
441.1419	1	92456.56	C21 H22 N5 O4 S	(M+H)+
442.1396	1	29126.16	C21 H22 N5 O4 S	(M+H)+
462.1218	1	1009893.38	C21 H21 N5 Na O4 S	(M+Na)+
463.1242	1	237781.36	C21 H21 N5 Na O4 S	(M+Na)+
464.1218	1	65488.94	C21 H21 N5 Na O4 S	(M+Na)+
465.1225	1	12407.11	C21 H21 N5 Na O4 S	(M+Na)+
901.2533	1	39404.55		(2M+Na)+
902.256	1	20450.59		(2M+Na)+
903.2542	1	9607.17		(2M+Na)+

Predicted Isotope Match Table

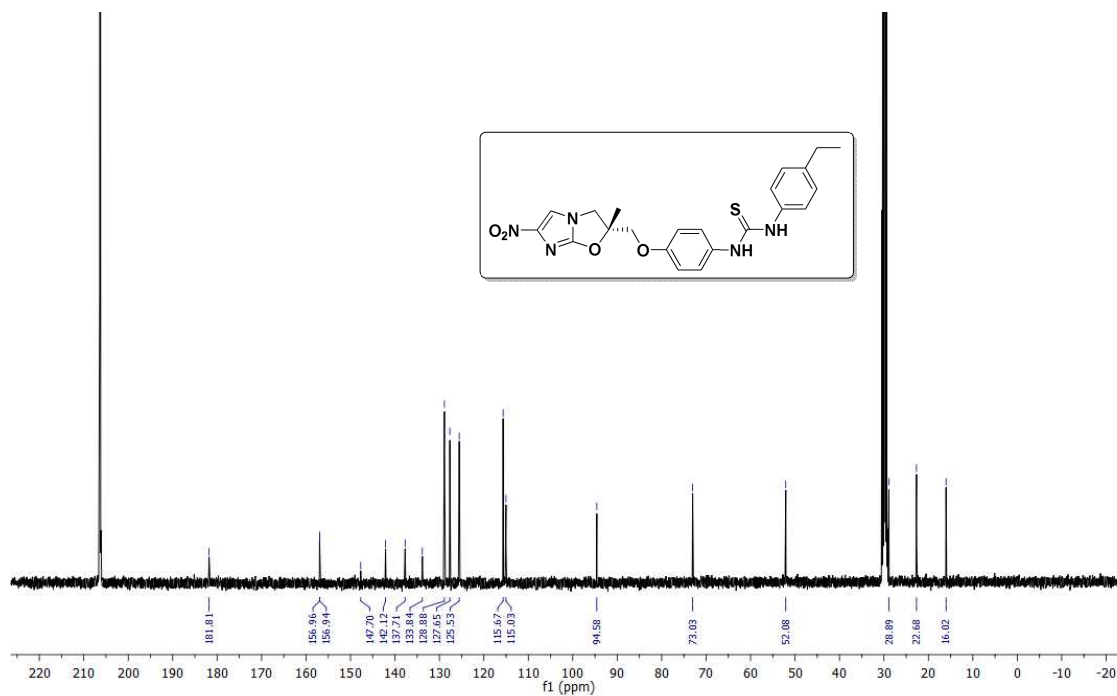
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	440.1397	440.1387	-2.31	100	100	75.54	73.64
2	441.1419	441.1415	-0.92	23.54	25.73	17.78	18.95
3	442.1396	442.139	-1.31	7.42	8.48	5.6	6.24
4	443.1397	443.1401	0.88	1.42	1.58	1.07	1.16

--- End Of Report ---

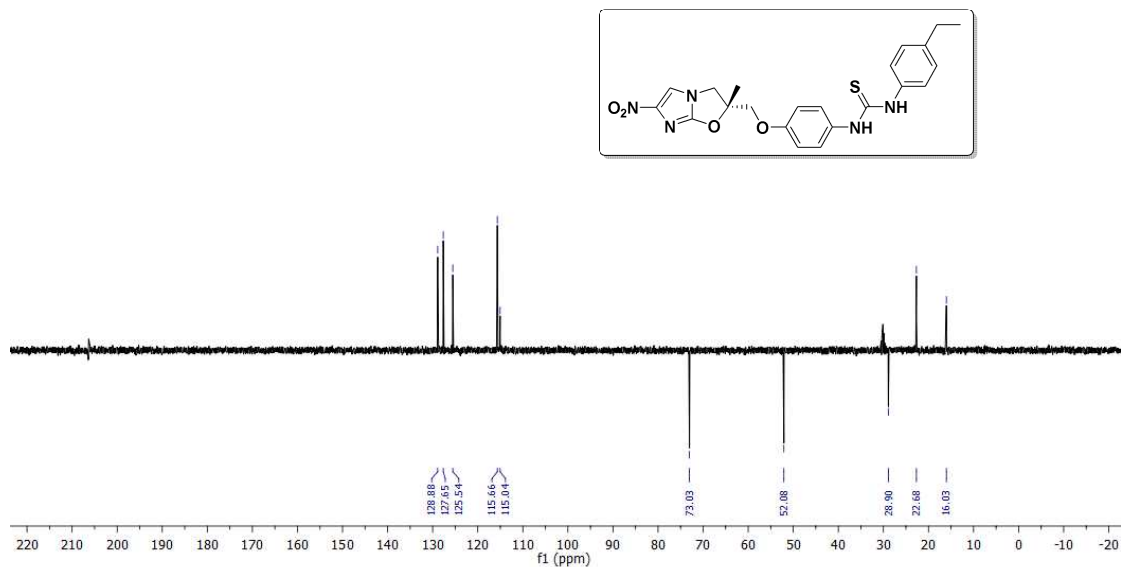
^1H NMR (400 MHz, Acetone- d_6) of compound **18l**:



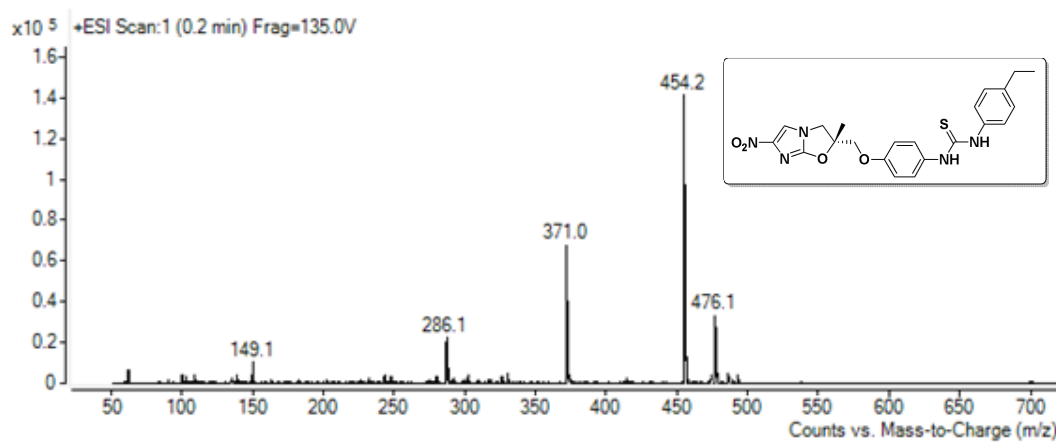
^{13}C NMR (101 MHz, Acetone- d_6) of compound **18l**:



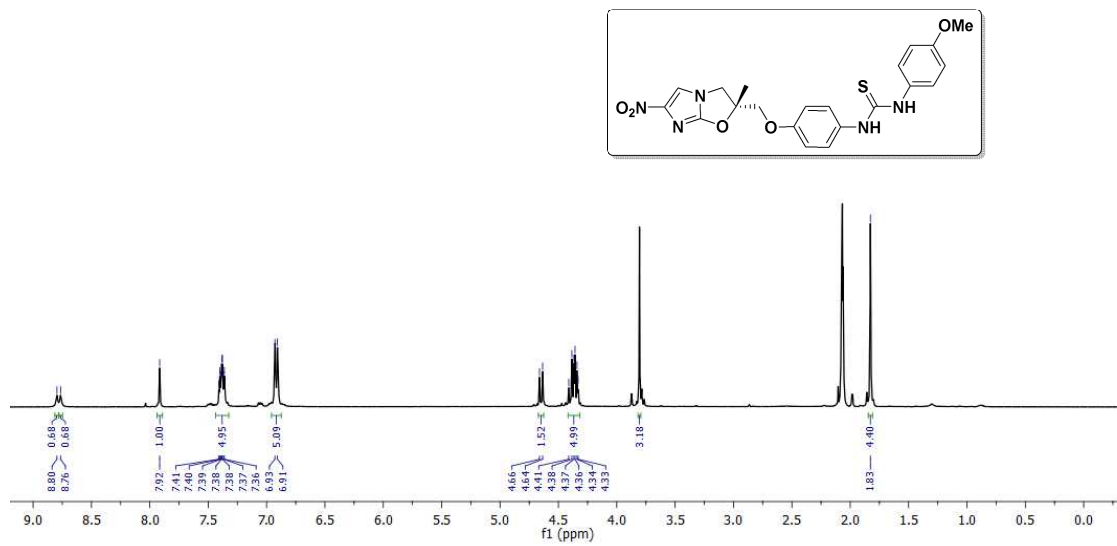
DEPT (101 MHz, Acetone- d_6) of compound **18l**:



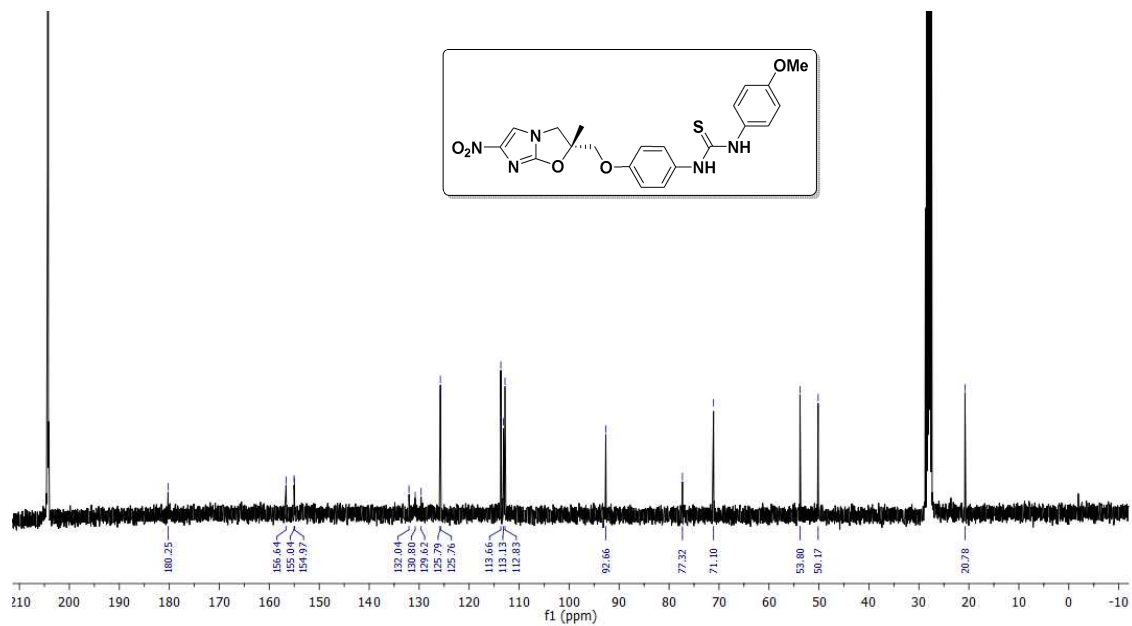
LC-MS of compound **18l**:



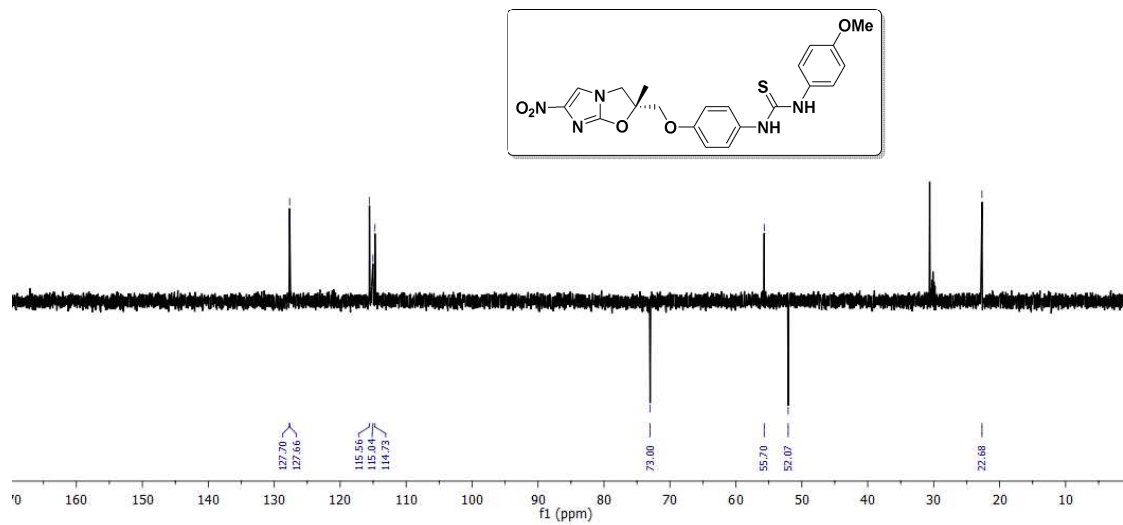
^1H NMR (400 MHz, Acetone- d_6) of compound **18m**:



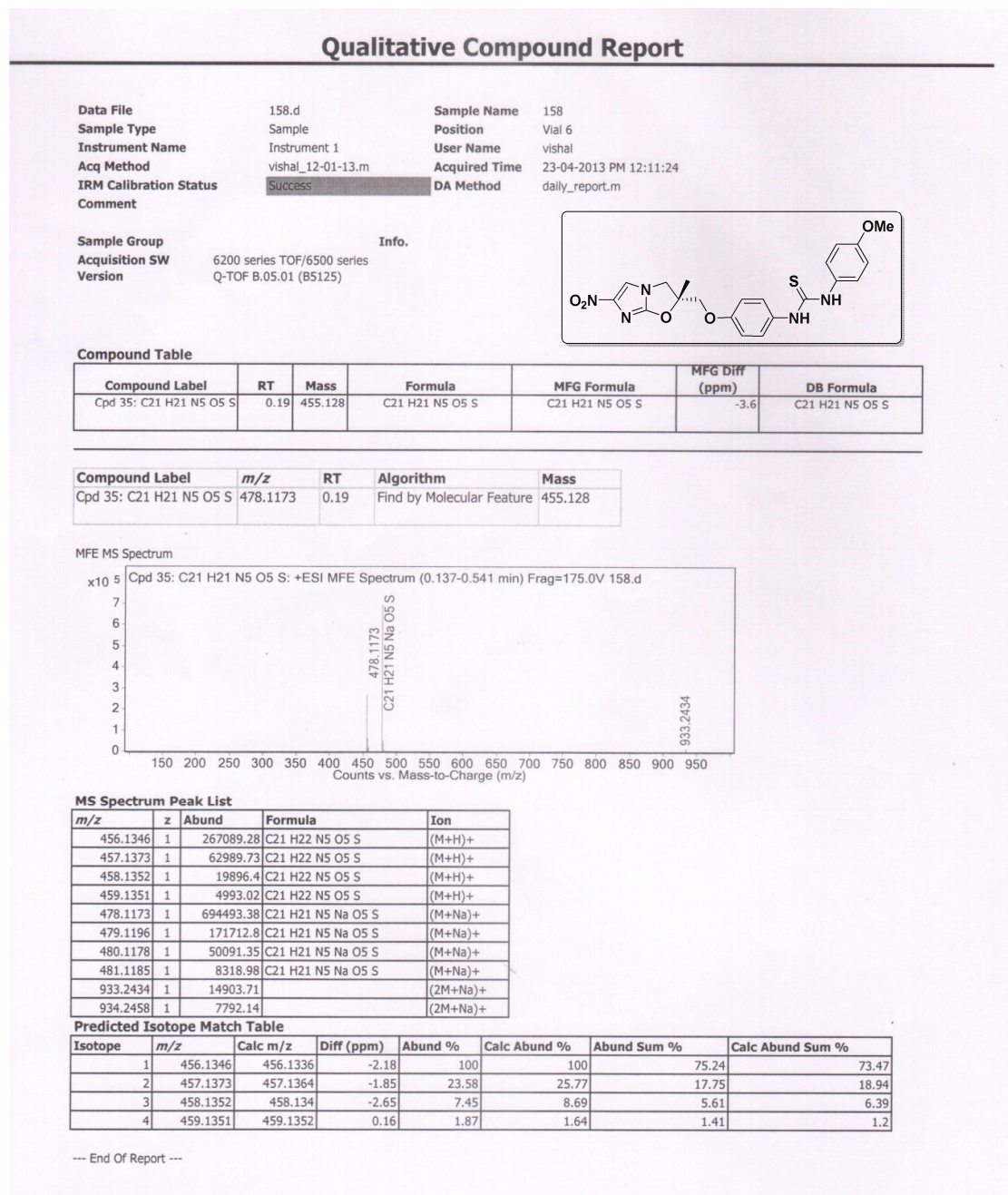
^{13}C NMR (126 MHz, Acetone- d_6) of compound **18m**:



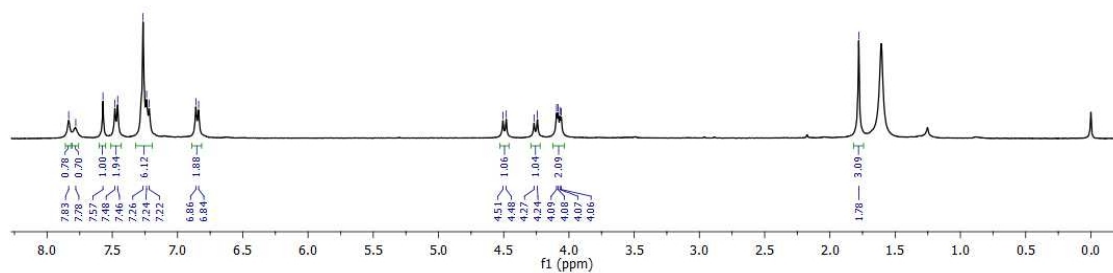
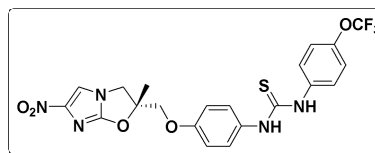
DEPT (126 MHz, Acetone- d_6) of compound **18m**:



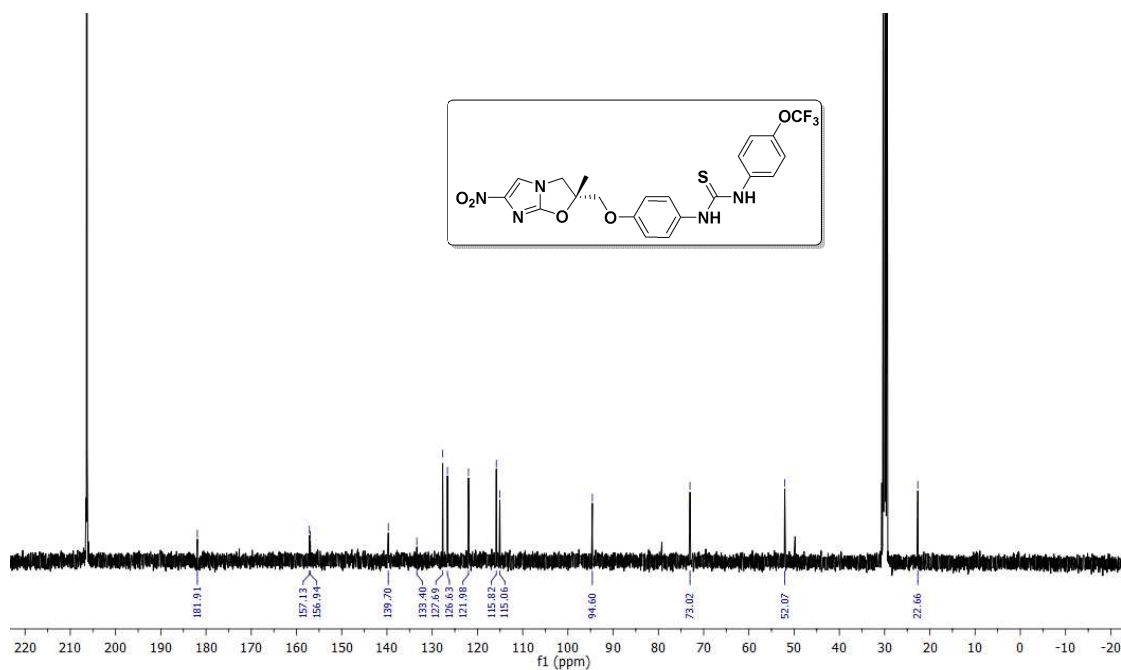
HRMS of compound **18m**:



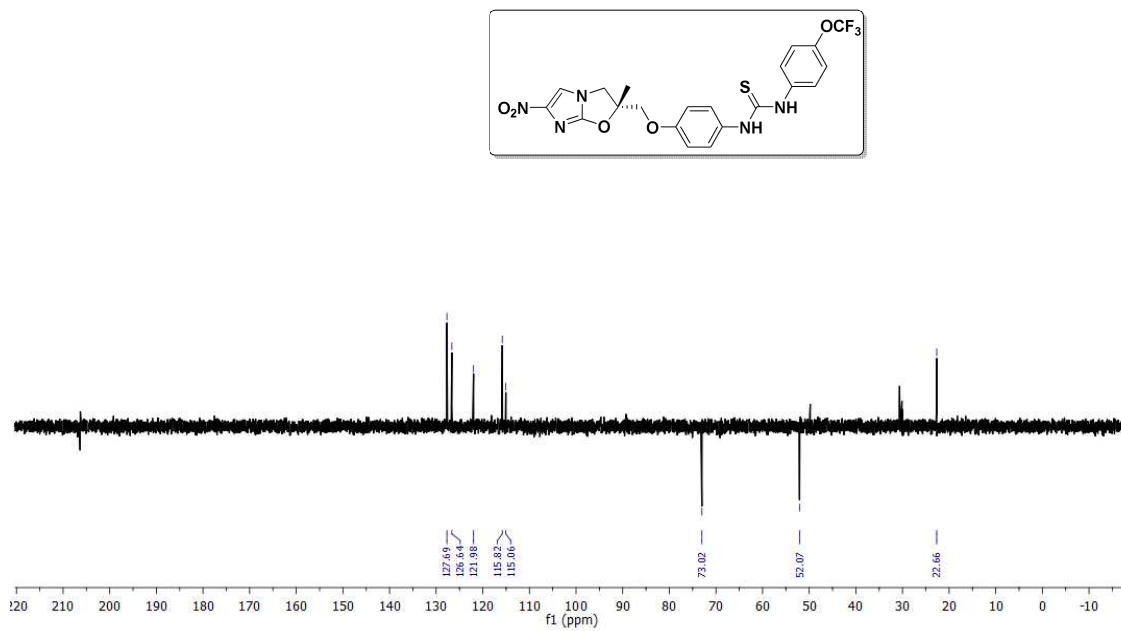
^1H NMR (400 MHz, CDCl_3) of compound **18n**:



^{13}C NMR (126 MHz, Acetone- d_6) of compound **18n**:



DEPT (126 MHz, Acetone- d_6) of compound **18n**:

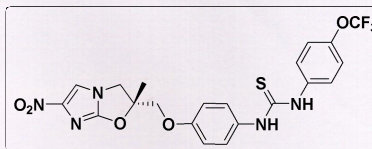


HRMS of compound **18n**:

Qualitative Compound Report

Data File	160.d	Sample Name	160
Sample Type	Sample	Position	Vial 4
Instrument Name	Instrument 1	User Name	vishal
Acq Method	vishal_12-01-13.m	Acquired Time	25-04-2013 PM 1:45:01
IRM Calibration Status	Success	DA Method	daily_report.m
Comment			

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

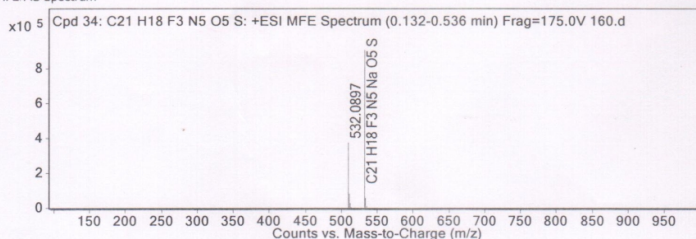


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 34: C21 H18 F3 N5 O5 S	0.189	509.1003	C21 H18 F3 N5 O5 S	C21 H18 F3 N5 O5 S	-4.46	C21 H18 F3 N5 O5 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 34: C21 H18 F3 N5 O5 S	532.0897	0.189	Find by Molecular Feature	509.1003

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
510.1072	1	372018.91	C21 H19 F3 N5 O5 S	(M+H)+
511.1093	1	82208.01	C21 H19 F3 N5 O5 S	(M+H)+
512.1063	1	26629.29	C21 H19 F3 N5 O5 S	(M+H)+
513.1074	1	5909.52	C21 H19 F3 N5 O5 S	(M+H)+
532.0897	1	906346.94	C21 H18 F3 N5 Na O5 S	(M+Na)+
533.092	1	213711	C21 H18 F3 N5 Na O5 S	(M+Na)+
534.0894	1	58201.91	C21 H18 F3 N5 Na O5 S	(M+Na)+
535.0898	1	12644.91	C21 H18 F3 N5 Na O5 S	(M+Na)+
536.0905	1	1676.35	C21 H18 F3 N5 Na O5 S	(M+Na)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	510.1072	510.1054	-3.59	100	100	76.43	73.5
2	511.1093	511.1082	-2.3	22.1	25.74	16.89	18.92
3	512.1063	512.1057	-1	7.16	8.68	5.47	6.38
4	513.1074	513.1069	-0.96	1.59	1.63	1.21	1.2

--- End Of Report ---