Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis of new generation triazolyl and isoxazolyl containing 6-nitro-2,3-dihydroimidazooxazoles as anti-TB agents: I*n vitro*, Structure-activity relationship, pharmacokinetics and *in vivo* evaluation

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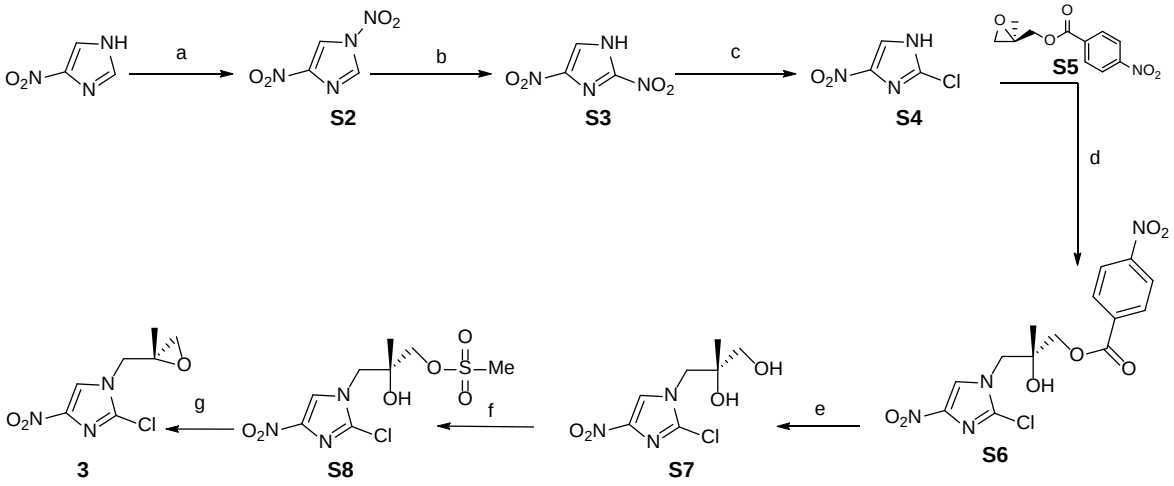
Synthesis of key intermediate 3:

Scheme S1:



Reagents and conditions: a) HNO_3, ACOH, AC_2O, 5 ^oC, 2 h, and then at rt, 12 h; b) chloro benzene, 120-125 ^oC, 50 h; c) con HCl, 90-95 ^oC, 12 h; d) Et_3N, AcOEt, 60-65 ^oC, 6 h; e) K_2CO_3, MeOH, rt, 2 h; f) MsCl, pyridine, <15 ^oC, 2 h; g) DBU, AcOEt, rt, 2 h.

1,4-Dinitroimidazole S2:

To a suspension of 4-nitroimidazole (4.0 g, 35.37 mmol) in glacial acetic acid (10 ml) cooled to 0-5 ^oC was added fuming nitric acid (d=1.52; 5.25 ml) drop wise with stirring, keeping the temperature at or below 5 ^oC over a period of 30 min. The mixture was cooled to 0 ^oC, acetic anhydride (19.5 ml) added drop wise, and stirred at 0 ^oC for 2 h and at room temperature over night. The solid gradually went into the solution, which was extracted with CH_2Cl_2 twice and combining the organic layers wash with saturated $NaHCO_3$ solution twice and combining organic layers wash with brine solution and dried over anhydrous $NaSO_4$ and filtered. The filtrate was concentrated under reduced pressure to give compound **S2** (3.85 g, 69%) as a light yellow solid. TLC (DCM:MeOH 9.5:0.5): R_f = 0.20; ^1H NMR (400 MHz, DMSO-d_6): δ 9.40 (s, 1H), 8.98 (s, 1H); LC-MS (ESI+): *m*/*z* 158.01.

2, 4-Dinitroimidazole S3:

A mixture of **S2** (3.85 g, 24.3 mmol) in chlorobenzene (40 ml) was heated with stirring at 120 – 125 ^{o}C for 50 h on an oil both, cooled, the solid was filtered and washed with cold chlorobenzene and hexane to yield **S3** (3.5 g, 90%) as a light yellow solid. TLC (DCM:MeOH 9.5:0.5): R_f = 0.30; ^{1}H NMR (200 MHz, DMSO-d_6): δ 8.48 (s, 1H); LC-MS (ESI+): *m*/*z* 158.01.

2-Chloro-4-nitroimidazole S4:

2, 4-Dinitroimidazole **S3** (3.5 g, 22.15 mmol) was added to 20 ml of 35 mass% of HCl. The reaction mixture was stirred for 7 hours at 95 ^{o}C. After completion of the reaction, 30 ml of water was added and the reaction mixture was cooled to 0 ^{o}C for crystallisation. The crystals were filtered and dried to obtain 2-chloro-4-nitroimidazole **S4** (3 g, 92%) as a white solid. TLC (DCM:MeOH 9.5:0.5): R_f = 0.30; ^{1}H NMR (200 MHz, DMSO-d_6): δ 8.44 (s, 1H); LC-MS (ESI+): *m*/*z* 146.98.

(*R*)-2-Chloro-1-[2-hydroxy-2-methyl-3-(4-nitrobenzoyloxy)]-propyl-4-nitroimidazole S6:

A solution of 2-chloro-4-nitro-1*H*-imidazole **S4** (12 g, 81.36 mmol), (*R*)-form epoxide **S5** (21.24 g, 89.48 mmol), and triethylamine (2.28 mL, 16.28 mmol) in ethyl acetate (40 ml) was heated at 60-65 °C for 6 h. The reaction mixture was allowed to cool to room temperature and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give **S6** (27.28 g, 87%) as colourless needles. TLC (EtOAc:hexane 4:6): R_f = 0.20; ^{1}H NMR (200 MHz, DMSO-d_6) δ 8.42 – 8.30 (m, 3H), 8.25 (d, *J* = 8.86 Hz, 2H), 5.61 (s, 1H), 4.32 –4.12 (m, 4H), 1.25 (s, 3H); LC-MS (ESI+): *m*/*z* 384.05.

(*R*)-2-Chloro-1-(2,3-dihydroxy-2-methyl)propyl-4-nitroimidazole S7:

To a solution of S**6** (13.6 g, 35.34 mmol) in methanol (136 mL) was added potassium carbonate (244 mg, 1.76 mmol). After the solution was stirred at room temperature for 2 h, 6 M hydrochloric acid (0.6 mL) and anhydrous sodium sulphate (3 g) were added at 0 °C, and the resulting mixture was stirred for 1 h. The insoluble materials were filtered off through celite, and the filtrate was concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give **S7** (8.18 g, 97%) as colorless needles. TLC (CH_2Cl_2:CH_3OH 9.5:0.5): R_f = 0.20; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28 (s, 1H), 5.07 (t, *J* = 5.6 Hz, 1H), 4.95 (s, 1H), 4.03 (s, 2H), 3.24 (d, *J* = 5.2 Hz, 2H), 1.01 (s, 3H); LC-MS (ESI+): *m*/*z* 235.04.

(*R*)-2-Chloro-1-(2-methyl-2,3-epoxypropyl)-4-nitroimidazole 3:

To a solution of **S7** (10 g, 42.44 mmol) in pyridine (20 ml) was added methanesulfonyl chloride (7.29 g, 63.66 mmol) at below 15 °C dropwise over 30 min. After the solution was stirred for 2 h, 6 M hydrochloric acid (63 ml) was added to the reaction mixture at below 30 °C. The resulting mixture was extracted with ethyl acetate twice, and the combined organic layer was washed with brine, dried over Sodium sulphate, and filtered. The filtrate was concentrated under reduced pressure to afford crude compound **S8.** To a solution of this crude **S8** in ethyl acetate (100 ml) was added 1,8-diazabicyclo[5.4.0]-7-undecene (7.10 g, 46.68 mmol), and the mixture was stirred at room temperature for 2 h. The reaction mixture was washed with brine, dried over sodium sulphate, and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give the (*R*)-form epoxide **3** (6.93 g, 75%) as colorless needles. TLC (EtOAc:hexane 4:6): R_f = 0.30; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.88 (s, 1H), 4.39 (d, *J* = 14.87 Hz, 1H), 4.00 (d, *J* = 14.88 Hz, 1H), 2.78 (d, *J* = 3.97 Hz, 1H), 2.63 (d, *J* = 3.92 Hz, 1H), 1.38 (s, 3H); LC-MS (ESI+): *m*/*z* 217.03.

General procedure for the preparation of *O*-Propargylated compounds 10:

To a solution of substituted phenols **9** (10 mmol) in ACN (20 mL) was added K_2CO_3 (20 mmol) and stirred for 5 minutes. Propargyl bromide **8** (15mmol) was added slowly to the reaction mixture at room temperature so that the temperature of the reaction should not be increased to above 30 ^oC. The mixture was stirred at room temperature for 12 h. Then the solvent was removed under reduced pressure and add water into the reaction mixture, extracted with EtOAc twice. The combined organic layers were washed with brine and dried over Na_2SO_4, and concentrated under *vaccuo* to afford compounds **10** in 90-95% as light yellow liquid. The residual crude product was used directly in the next reaction without purification.

General procedure for the preparation of azidophenols 12:

Amino phenols **11** (3.273 g, 30 mmol) was dissolved with 6 N HCl (30 mL) in an ice bath at 0-5 ^oC. $NaNO_2$ solution (3.105 g, 45 mmol in 75 ml of H_2O) was added drop wise. The reaction mixture was stirred for 30 min at 0-5 ^oC. Next, a solution of sodium azide (7.8 g, 120 mmol in 120 ml of H_2O) was added drop wise. After addition, the system was stirred for another hour. Next, the mixture was extracted with ethyl acetate and the combined organic extracts were washed with H_2O, dried over anhydrous Na_2SO_4, filtered, and concentrated in *vaccuo* to give **12** as yellow liquids. The residual crude product was used directly without purification.

General procedure for the preparation of triazolyl intermediate compounds 4a-m:

To a mixture of azido phenol **12** (10 mmol) and substituted phenoxymethylacetylenes **10a-i** (12mmol) in 1:1 ^{t}BuOH and water (10 mL) add $CuSO_4$ pentahydrate (1 mmol) and sodium ascorbate (2 mmol), The reaction mixture was stirred for 10 to 12 h at room temperature after completion of the reaction add 20 ml water and subsequently extracted with ethyl acetate twice. The combined organic extracts were washed with brine and dried over

anhydrous Na_2SO_4 filtered, and concentrated in *vaccuo*. The residual crude product was purified via silica gel column chromatography using a gradient mixture of hexane-ethyl acetate to obtain the pure triazole intermediate compounds **4a-m** in 85-90% yields.

4-{4-[(p-Tolyloxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4a): TLC (EtOAc:Hexane 2:8): R_f = 0.25; ^{1}H NMR (200 MHz, CD_3OD) δ 8.11 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 5.26 (s, 2H); LC-MS (ESI+): m\z 281.12.

4-{4-[(4-Ethylphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4b): TLC (EtOAc:Hexane 2:8): R_f = 0.28; ^{1}H NMR (200 MHz, CD_3OD) δ 8.34 (s, 1H), 7.52 (d, *J* = 8.9 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.87 – 6.83 (m, 4H), 5.09 (s, 2H), 2.48 (q, *J* = 7.5 Hz, 2H), 1.11 (t, *J* = 7.6 Hz, 3H); LC-MS (ESI+): m\z 295.15.

4-{4-[(4-*iso*-Propylphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4c): TLC (EtOAc: Hexane 2:8): R_f = 0.30; ^{1}H NMR (200 MHz, CD_3OD) δ 8.35 (s, 1H), 7.53 (d, *J* = 8.9 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 6.84 (d, *J* = 8.89 Hz, 2H), 5.09 (s, 2H), 2.82 – 2.68 (m, 2H), 1.14 (d, *J* = 6.93 Hz, 6H); LC-MS (ESI+): m\z 309.15.

4-{4-[(4-(*sec*-Butylphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4d): TLC (EtOAc: Hexane 2:8): R_f = 0.30; ^{1}H NMR (200 MHz, CD_3OD) δ 8.44 (s, 1H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 7.89 Hz, 2H), 6.97 – 6.93 (m, 4H), 5.19 (s, 2H), 2.59 – 2.50 (m, 1H), 1.57 – 1.51 (m, 2H), 1.18 (d, *J* = 6.87 Hz, 2H), 0.81 (t, *J* = 7.5 Hz, 3H); LC-MS (ESI+): m\z 323.16.

4-{4-[(4-Fluorophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4e): TLC (EtOAc:Hexane 2:8): R_f = 0.25; ^{1}H NMR (200 MHz, CD_3OD) δ 8.46 (s, 1H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.04 – 6.94 (m, 6H), 5.19 (s, 2H); LC-MS (ESI+): m\z 285.08.

4-{4-[(4-Trifluoromethylphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4f): TLC (EtOAc:Hexane 2:8): R_f = 0.32; ^{1}H NMR (400 MHz, CD_3OD): δ 8.40 (s, 1H), 7.80 (s, 1H),

7.52 (dd, *J* = 8.7, 6.4 Hz, 4H), 7.11 (d, *J* = 8.6 Hz, 2H), 6.85 (d, *J* = 8.9 Hz, 2H), 5.21 (s, 2H); LC-MS (ESI+): m\z 335.09.

4-{4-[(4-Trifluoromethoxyphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4g): TLC (EtOAc:Hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, CD_3OD) δ 8.38 (s, 1H), 7.52 (d, *J* = 9.0 Hz, 2H), 7.12 (d, *J* = 9.2 Hz, 2H), 7.02 (d, *J* = 9.2 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 2H), 5.15 (s, 2H); LC-MS (ESI+): m\z 351.08.

4-{4-[(2-Fluorophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4h): TLC (EtOAc:Hexane 2:8): R_f = 0.30; ^{1}H NMR (500 MHz, CD_3OD) δ 8.38 (s, 1H), 7.81 (s, 1H), 7.53 (d, *J* = 8.7 Hz, 2H), 7.16 (t, *J* = 8.4 Hz, 1H), 7.01 (dd, *J* = 12.4, 5.9 Hz, 2H), 6.85 (d, *J* = 9.8 Hz, 2H), 5.19 (s, 2H); LC-MS (ESI+): m\z 285.09.

4-{4-[(3-Clorophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4i): TLC (EtOAc:Hexane 2:8): R_f = 0.30; ^{1}H NMR (500 MHz, CD_3OD) δ 8.38 (s, 1H), 7.53 (d, *J* = 8.9 Hz, 2H), 7.18 (t, *J* = 8.2 Hz, 1H), 6.99 (t, *J* = 2.2 Hz, 1H), 6.91 – 6.86 (m, 2H), 6.85 (d, *J* = 8.9 Hz, 2H), 5.13 (s, 2H); LC-MS (ESI+): m\z 301.06.

3-{4-[(4-Trifluoromethoxyphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4j): TLC (EtOAc: Hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.91 (s, 1H), 7.38 (t, *J* = 8.3 Hz, 1H), 7.35 – 7.28 (m, 4H), 7.18 (d, *J* = 9.0 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 1H), 5.25 (s, 2H); LC-MS (ESI+): m\z 351.08.

3-{4-[(4-Fluorophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4k): TLC (EtOAc:Hexane 2:8): R_f = 0.30; ^{1}H NMR (500 MHz, CD_3OD): δ 8.30 (s, 1H), 7.41 – 7.35 (m, 3H), 7.06 – 7.01 (m, 4H), 6.95 (s, 1H), 5.25 (s, 2H); LC-MS (ESI+): m\z 285.08.

2-{4-[(4-Trifluoromethoxyphenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4l): TLC (EtOAc:Hexane 2:8): R_f = 0.35; ^{1}H NMR (200 MHz, Acetone-d_6) δ 8.63 (s, 1H), 7.89 (t, *J* = 8.3 Hz, 2H), 7.18 (t, *J* = 7.8 Hz, 3H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 9.0 Hz, 2H); LC-MS (ESI+): m\z 351.08.

2-{4-[(4-Fluorophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenol (4m): TLC (EtOAc:Hexane 2:8): R_f = 0.30; ^{1}H NMR (200 MHz, Acetone-d_6) δ 8.58 (s, 1H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.20 – 7.07 (m, 5H), 5.27 (s, 2H); LC-MS (ESI+): m\z 285.093.

General procedure for the preparation triazole intermediate compounds 5a-f:

Reaction of azido phenol **12** (10 mmol) and substitutedphenylacetylenes **13** (12mmol) under the same procedure as mentioned for the preparation of compounds **4 a-m**, followed by purification on silica gel column chromatography using a gradient mixture of hexane-ethyl acetate to obtain the pure triazole intermediate compounds **5a-f** in 85-90% yields.

4-[4-(4-Fluorophenyl)-1*H*-1,2,3-triazol-1-yl]phenol (5a): TLC (EtOAc:Hexane 2:8): R_f = 0.20; ^{1}H NMR (400 MHz, Acetone-d_6): δ 8.81 (s, 1H), 8.03 (dd, *J* = 6.1, 2.7 Hz, 2H), 7.75 (d, *J* = 9.1 Hz, 2H), 7.24 (t, *J* = 8.9 Hz, 2H), 7.05 (d, *J* = 9.1 Hz, 2H); LC-MS (ESI+): m\z 255.08.

4-[4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl]phenol (5b): TLC (EtOAc:Hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6): δ 8.70 (s, 1H), 7.90 (d, *J* = 8.9 Hz, 2H), 7.75 (d, *J* = 8.9 Hz, 2H), 7.04 (dd, *J* = 8.9, 5.9 Hz, 4H), 3.85 (s, 3H); LC-MS (ESI+): m\z 267.10.

4-[4-(4-Trifluoromethylphenyl)-1*H*-1,2,3-triazol-1-yl]phenol (5c): TLC (EtOAc:Hexane 2:8): R_f = 0.30; ^{1}H NMR (200 MHz, Acetone-d_6) δ 9.02 (s, 1H), 8.23 (d, *J* = 8.05Hz, 2H), 7.85 – 7.76 (m, 4H), 7.07 (d, *J* = 8.9 Hz, 2H); LC-MS (ESI+): m\z 305.08.

4-[4-(3-Trifluoromethylphenyl)-1*H*-1,2,3-triazol-1-yl]phenol (5d): TLC (EtOAc:hexane 2:8): R_f = 0.22;^{1}H NMR (400 MHz, CD_3OD) δ 8.80 (s, 1H), 8.13 (s, 1H), 8.06 (d, *J* = 2.3 Hz, 1H), 7.64 – 7.49 (m, 4H), 6.87 (d, *J* = 8.7 Hz, 2H); LC-MS (ESI+): m\z 305.07.

4-[4-(2-Trifluoromethylphenyl)-1*H*-1,2,3-triazol-1-yl]phenol (5e): TLC (EtOAc:Hexane 2:8): R_f = 0.20; ^{1}H NMR (200 MHz, Acetone-d_6): δ 8.24 (s, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.70 (d, *J* = 9.0 Hz, 2H), 7.69 – 7.65 (m, 1H), 7.50 (t, *J* = 8.2 Hz, 1H), 7.02 (d, *J* = 9.0 Hz, 2H); LC-MS (ESI+): m\z 305.08.

4-[4-(4-Trifluoromethoxyphenyl)-1*H*-1,2,3-triazol-1-yl]phenol (5f): TLC (EtOAc: Hexane 2:8): R_f = 0.30; ^{1}H NMR (200 MHz, Acetone-d_6) δ 8.95 (s, 1H), 8.09 (d, *J* = 8.3 Hz, 2H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 8.34 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 2H); LC-MS (ESI+): m\z 321.09.

4-Hydroxybenzaldehyde oxime 16:

To a suspension of 4-hydroxy benzaldehyde **15** (1.2 g, 10 mmol) in a 1:1:2 mixture of H_2O/EtOH/ ice (10 ml) was added hydroxylamine hydrochloride (0.695 g, 10 mmol), followed by NaOH solution (as a 50% solution in water) (1.0 g, 25 mmol) drop wise, while keeping the temperature below 30 °C. After being stirred at room temperature for 2 h, the solution was extracted with diethyl ether. The aqueous phase was acidified to P^H = 6 by adding 6N HCl while keeping the temperature below 30 ^{o}C and extracted with diethyl ether. The organic phase was dried over Na_2SO4, and the solvent was evaporated to give the oxime product **16** in 85% yield as yellow solid, which was used directly to the next reaction without purification.

(*Z*)-N,4-dihydroxybenzimidoyl chloride 17:

To a solution of oxime **16** (1.37 g, 10 mmol) in DMF (10 ml) was added *N*-chlorosuccinimide (0.24 g, 1.8 mmol) in one portion. The beginning of the reaction can be detected by a slight increase of the reaction temperature. The remaining NCS (1.09 g, 8.2 mmol) was added in small portions while keeping the temperature below 35 °C. The mixture was stirred at room temperature for 3 h, poured into water, and extracted with diethyl ether. The organic phase was washed with brine and dried over Na_2SO4, and the solvent was removed to give the imidoyl chloride **17** in 90% yields. The crude product was used in the next reaction directly.

General procedure for the preparation of isoxazolyl intermediate compounds 6a-l:

N-4-dihydroxybenzimidoyl chloride **17** (0.17 g, 1.0 mmol) and substituted phenoxymethyl acetylenes **14** (1.2 mmol) were dissolved in 6 ml of a 1:1 ^{t}BuOH/H_2O mixture. While the mixture was being stirred, sodium ascorbate (19.8 mg, 0.1mmol) was added, followed by copper (II) sulfate pentahydrate (2.7 mg, 0.05mmol). The reaction mixture was then treated with $KHCO_3$ (433 mg, 4.33 mmol,) and left stirring for 12 h at ambient temperature, after which time it was diluted with water and extract with ethyl acetate twice. Combined the organic layer wash with brine solution and dried over anhydrous $NaSO_4$ and filtered. The filtrate was concentrated under reduced pressure, the residue was purified by silica gel column chromatography using a gradient mixture of hexane-ethyl acetate to obtain the pure compounds **6a-l** as white solids in 80-85% yields.

4-{5-[(*p*-Tolyloxy)methyl]isoxazol-3-yl}phenol (6a): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.75 (d, *J* = 8.8 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.97 – 6.94 (m, 4H), 6.88 (s, 1H), 5.25 (s, 2H), 2.26 (s, 3H); LC-MS (ESI+): m\z 281.11.

4-{5-[(4-*iso*-Propylphenoxy)methyl]isoxazol-3-yl}phenol (6b): TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.75 (d, *J* = 8.7 Hz, 2H), 7.20 (d, *J* = 8.7 Hz, 2H), 7.00 – 6.94 (m, 4H), 6.90 (s, 1H), 5.26 (s, 2H), 2.90 – 2.78 (m, 1H), 1.21 (d, *J* = 6.9 Hz, 6H); LC-MS (ESI+): m\z 309.14.

4-{5-[(4-Trifluoromethylphenoxy)methyl]isoxazol-3-yl}phenol (6c): TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.88 – 7.82 (m, 4H), 7.12 (d, *J* = 8.4 Hz, 2H), 6.98 – 6.95 (m, 3H), 5.4 (s, 2H); LC-MS (ESI+): m\z 335.07.

4-{5-[(4-Methoxyphenoxy)methyl]isoxazol-3-yl}phenol (6d): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.75 (d, *J* = 8.7 Hz, 2H), 7.01 (d, *J* = 9.1 Hz, 2H), 6.95 (d, *J* = 8.7 Hz, 2H), 6.09 – 6.88 (m, 3H), 5.23 (s, 2H), 3.75 (s, 3H); LC-MS (ESI+): m\z 297.10.

4-{5-[(4-Trifluoromethoxyphenoxy)methyl]isoxazol-3-yl}phenol (6e):

TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.19 (d, *J* = 9.2 Hz, 2H), 6.97 - 6.95 (m, 3H), 5.35 (s, 2H); LC-MS (ESI+): m\z 351.07.

4-{5-[(4-Fluorophenoxy)methyl]isoxazol-3-yl}phenol (6f): TLC (EtOAc:hexane 2:8): R_f = 0.25; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.78 – 7.75 (m, 2H), 7.09 – 6.98 (m, 7H), 5.4 (s, 2H); LC-MS (ESI+): m\z 285.08.

4-{5-[(4-Bromophenoxy)methyl]isoxazol-3-yl}phenol (6g): TLC (EtOAc:hexane 2:8): R_f = 0.25; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.75 (d, *J* = 8.7 Hz, 2H), 7.48 (d, *J* = 9.0 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H), 6.99 – 6.91 (m, 3H), 5.32 (s, 2H); LC-MS (ESI+): m\z 345.00.

4-{5-[(3-Fluorophenoxy)methyl]isoxazol-3-yl}phenol (6h): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.36 (m, 1H), 6.99 – 6.87 (m, 5H), 6.81 – 6.74 (m, 1H), 5.35 (s, 2H); LC-MS (ESI+): m\z 285.08.

4-{5-[(2-Fluorophenoxy)methyl]isoxazol-3-yl}phenol (6i): TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.75 (d, *J* = 8.7 Hz, 2H), 7.33 – 7.29 (m, 1H), 7.21 – 7.12 (m, 2H), 7.05 – 6.99 (m, 1H), 6.98 – 6.92 (m, 3H), 5.38 (s, 2H); LC-MS (ESI+): m\z 285.07.

4-{5-[(*o*-Tolyloxy)methyl]isoxazol-3-yl}phenol (6j): TLC (EtOAc:hexane 2:8): R_f = 0.25; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.17 (m, 2H), 7.09 (d, *J* = 8.2 Hz, 1H), 6.95 (d, *J* = 8.7 Hz, 2H), 6.93 – 6.87 (m, 2H), 5.31 (s, 1H), 2.23 (s, 3H); LC-MS (ESI+): m\z 281.10.

4-{5-[(3-Chlorophenoxy)methyl]isoxazol-3-yl}phenol (6k): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, CD_3OD) δ 7.57 (d, *J* = 8.8 Hz, 2H), 7.18 (t, *J* = 8.2 Hz, 1H), 6.99 (t, *J* = 2.2 Hz, 1H), 6.93 – 6.86 (m, 2H), 6.77 (d, *J* = 8.8 Hz, 2H), 6.73 (s, 1H), 5.14 (s, 2H); LC-MS (ESI+): m\z 301.05.

4-{5-[(4-*iso*-Propyl-3-methylphenoxy)methyl]isoxazol-3-yl}phenol (6l): TLC (EtOAc:hexane 2:8): R_f = 0.37; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.75 (d, *J* = 8.8 Hz, 2H), 7.18 (d, *J* = 8.2 Hz, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.89 (s, 1H), 6.85 (s, 1H), 5.24 (s, 2H), 3.20 – 3.00 (m, 1H), 2.31 (s, 3H), 1.18 (d, *J* = 6.9 Hz, 6H); LC-MS (ESI+): m\z 323.15.

General procedure for the preparation of isoxazolyl intermediate compounds 7a-j:

Reaction of N-4-dihydroxybenzimidoyl chloride **17**(0.17 g, 1.0 mmol) and substitutedphenylacetylene **18** (12mmol) under the same procedure as mentioned for the preparation of compounds **6 a-l**, followed by purification on silica gel column chromatography using a gradient mixture of hexane-ethyl acetate to obtain the pure isoxazole intermediate compounds **7a-j** as a white solids in 85-90% yields.

4-(5-Phenylisoxazol-3-yl)phenol (7a): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.92 – 7.98 (m, 2H), 7.78 (d, *J* = 8.6 Hz, 2H), 7.50 – 7.55 (m, 3H), 7.15 (s, 1H), 6.92 (d, *J* = 8.6 Hz, 2H); LC-MS (ESI+): m\z 237.08.

4-[5-(*p*-Tolyl)isoxazol-3-yl]phenol (7b): TLC (EtOAc:hexane 2:8): R_f = 0.32; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.85 **–** 7.81 (m, 4H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.18 (s, 1H), 6.98 (d, *J* = 8.6 Hz, 2H), 2.38 (s, 3H); LC-MS (ESI+): m\z 251.09.

4-[5-(4-Fluorophenyl)isoxazol-3-yl]phenol (7c): TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.97-8.05 (m, 2H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.25-7.31 (m, 3H), 6.92 (d, *J* = 8.5 Hz, 2H); LC-MS (ESI+): m\z 255.06.

4-[5-(4-Methoxyphenyl)isoxazol-3-yl]phenol (7d): TLC (EtOAc:hexane 2:8): R_f = 0.20; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.74-7.81 (m, 4H), 6.95 – 7.11 (m, 5H), 3.92 (s, 3H); LC-MS (ESI+): m\z 267.08.

4-[5-(4-Trifluoromethylphenyl)isoxazol-3-yl]phenol (7e): TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (200 MHz, CD_3OD) δ 8.11 (d, *J* = 7.6Hz, 2H), 7.88-7.92 (m, 4H), 7.52 (s, 1H), 7.02 (d, *J* = 8.5 Hz, 2H); LC-MS (ESI+): m\z 305.06.

4-[5-(4-Trifluoromethoxyphenyl)isoxazol-3-yl]phenol (7f): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.07 (d, *J* = 7.3 Hz, 2H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.37 (s, 1H), 6.99 (d, *J* = 8.3 Hz, 2H); LC-MS (ESI+): m\z 321.06.

4-[5-(3-Trifluoromethylphenyl)isoxazol-3-yl]phenol (7g): TLC (EtOAc:hexane 2:8): R_f = 0.35; ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.22 (m, 1H), 7.89 – 7.79 (m, 5H), 7.51 (s, 1H), 6.99 (d, *J* = 8.7 Hz, 2H); LC-MS (ESI+): m\z 305.08.

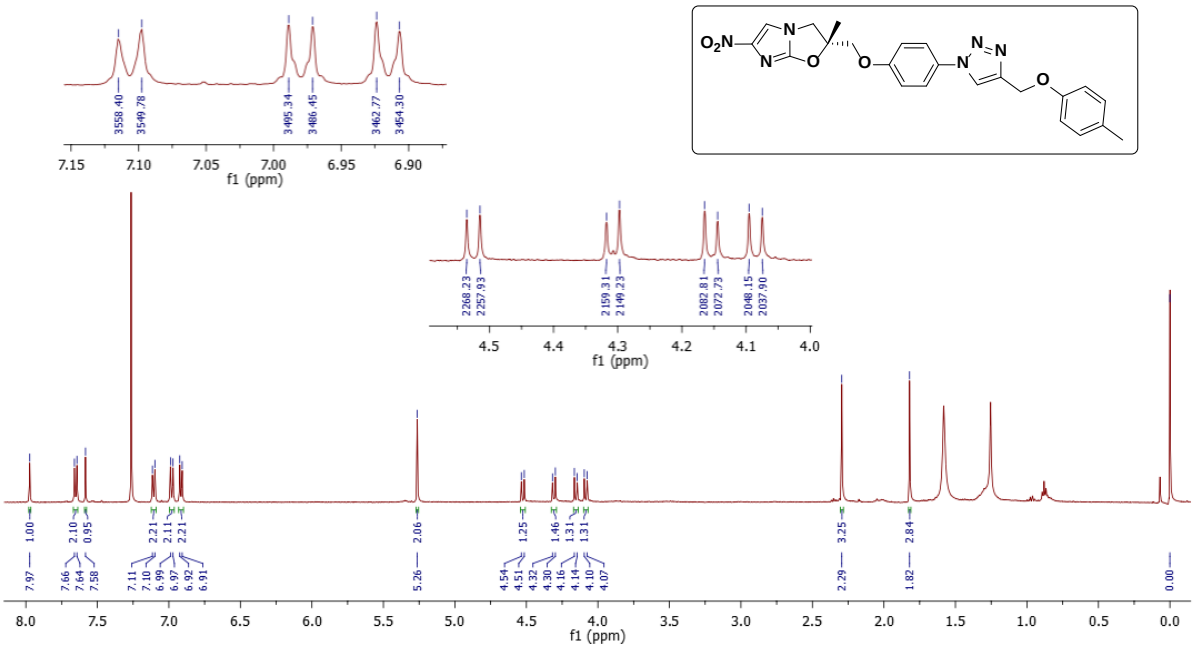
4-[5-(2-Trifluoromethylphenyl)isoxazol-3-yl]phenol (7h): TLC (EtOAc:hexane 2:8): R_f = 0.30; ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.98 (d, *J* = 7.8 Hz, 1H), 7.93 – 7.78 (m, 5H), 7.11 (s, 1H), 6.99 (d, *J* = 8.5 Hz, 2H); LC-MS (ESI+): m\z 305.08.

4-[5-(2-Fluorophenyl)isoxazol-3-yl]phenol (7i): TLC (EtOAc:hexane 2:8): R_f = 0.25; ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.03 – 8.01 (m, 1H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.44 – 7.35 (m, 2H), 7.20 – 7.18 (m, 1H), 6.99 (d, *J* = 8.5 Hz, 2H); LC-MS (ESI+): m\z 255.08.

4-[5-(2,4-Difluorophenyl)isoxazol-3-yl]phenol (7j): TLC (EtOAc:hexane 2:8): R_f = 0.40; ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.07 – 8.03 (m, 1H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.33 –7.26 (m, 2H), 7.17 (s, 1H), 6.98 (d, *J* = 8.8 Hz, 2H); LC-MS (ESI+): m\z 273.07.

^{1}H NMR, ^{13}C NMR, DEPT and HRMS of triazolyl and isoxazolyl based NHIO compounds 1 & 2:

^{1}H NMR (500 MHz, $CDCl_3$) of compound **1a (IIIM/MCD-023):**

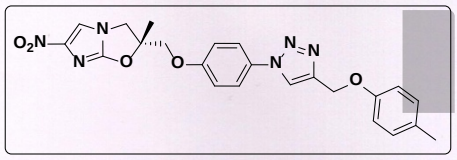


HRMS (ESI-TOF) of compound **1a (IIIM/MCD-023)**:

Qualitative Compound Report

Data File	23.d	**Sample Name**	23
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:16:25
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)

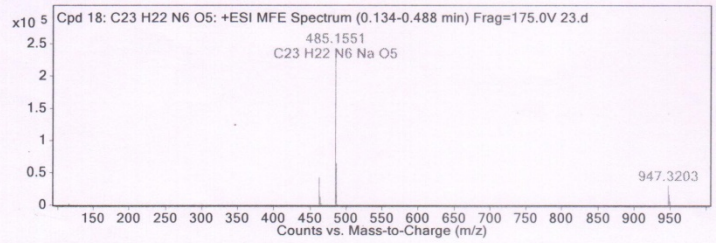


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C23 H22 N6 O5	0.188	462.1658	C23 H22 N6 O5	C23 H22 N6 O5	-1.39	C23 H22 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C23 H22 N6 O5	485.1551	0.188	Find by Molecular Feature	462.1658

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
463.1721	1	42349.98	C23 H23 N6 O5	(M+H)+
464.175	1	12992.68	C23 H23 N6 O5	(M+H)+
465.177	1	2368.35	C23 H23 N6 O5	(M+H)+
485.1551	1	231872.69	C23 H22 N6 Na O5	(M+Na)+
486.1576	1	64527.79	C23 H22 N6 Na O5	(M+Na)+
487.1602	1	9918.08	C23 H22 N6 Na O5	(M+Na)+
488.1622	1	1392.22	C23 H22 N6 Na O5	(M+Na)+
947.3203	1	30861.52		(2M+Na)+
948.3232	1	16080.84		(2M+Na)+
949.3265	1	5420.24		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	463.1721	463.1724	0.79	100	100	73.01	75.31
2	464.175	464.1753	0.6	30.68	27.52	22.4	20.73
3	465.177	465.1779	1.84	5.59	4.68	4.08	3.52
4	466.1848	466.1803	-9.5	0.7	0.59	0.51	0.45

--- End Of Report ---

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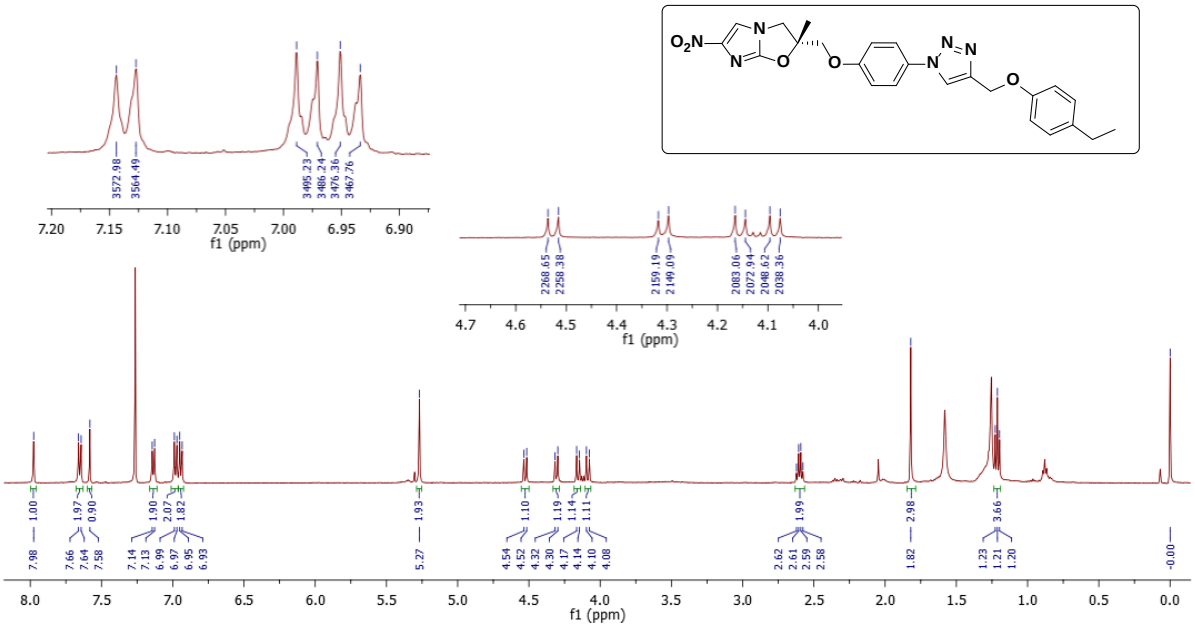
^{1}H NMR (500 MHz, $CDCl_3$) of compound **1b (IIIM/MCD-024):**

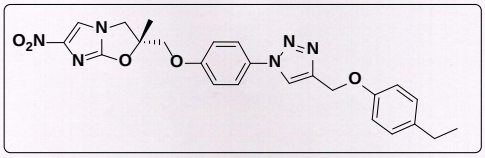


HRMS (ESI-TOF) of compound **1b** (**IIIM/MCD-024)**:

Qualitative Compound Report

Data File	24.d	**Sample Name**	24
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	26-04-2013 PM 1:38:06
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)	

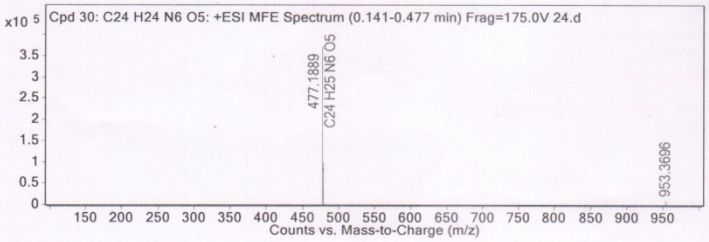


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C24 H24 N6 O5	0.188	476.1816	C24 H24 N6 O5	C24 H24 N6 O5	-1.54	C24 H24 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C24 H24 N6 O5	477.1889	0.188	Find by Molecular Feature	476.1816

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
477.1889	1	372797.22	C24 H25 N6 O5	(M+H)+
478.1914	1	98501.73	C24 H25 N6 O5	(M+H)+
479.1937	1	16648	C24 H25 N6 O5	(M+H)+
480.1952	1	2668.85	C24 H25 N6 O5	(M+H)+
953.3696	1	11159.06		(2M+H)+
954.372	1	6366.11		(2M+H)+
955.3732	1	1962.74		(2M+H)+
956.3781	1	422.6		(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	477.1889	477.1881	-1.78	100	100	75.99	74.49
2	478.1914	478.191	-0.92	26.42	28.63	20.08	21.32
3	479.1937	479.1936	-0.2	4.47	4.98	3.39	3.71
4	480.1952	480.1961	1.81	0.72	0.64	0.54	0.48

--- End Of Report ---

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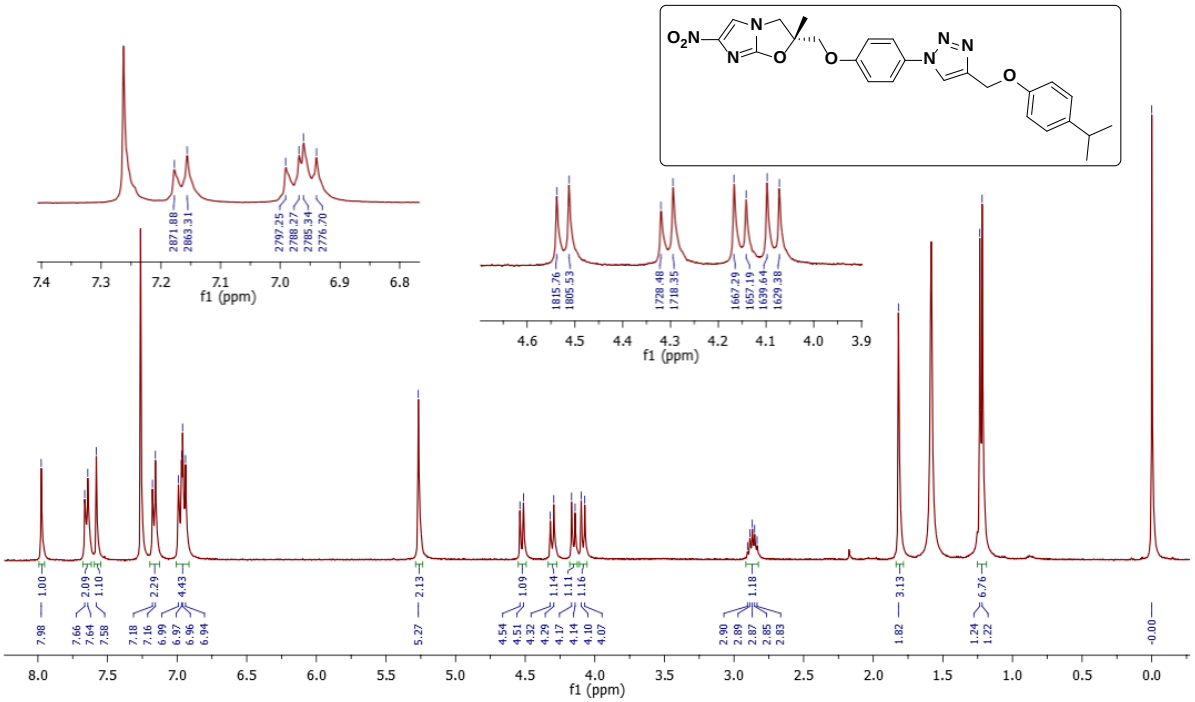
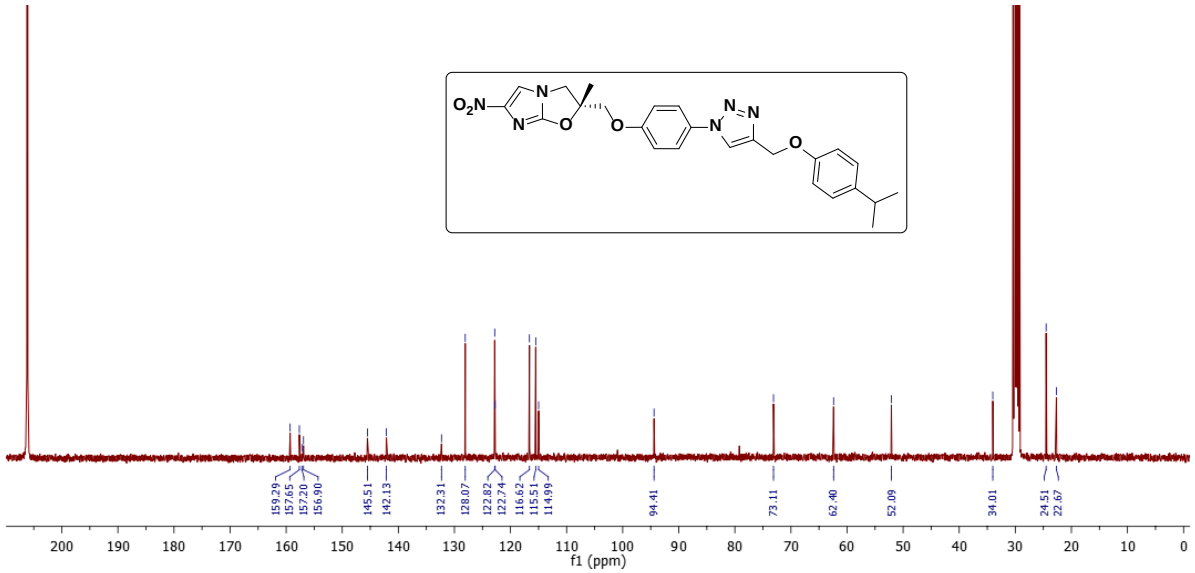
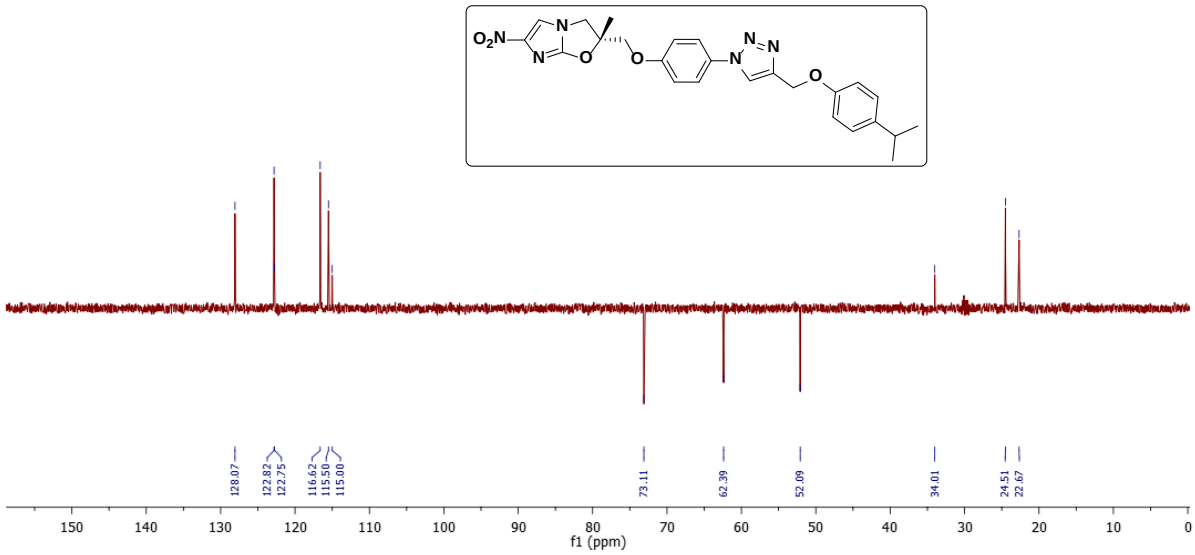
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1c** (**IIIM/MCD-026):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **1c** (**IIIM/MCD-026):**



DEPT (101 MHz, Acetone-d_6) of compound **1c (IIIM/MCD-026):**

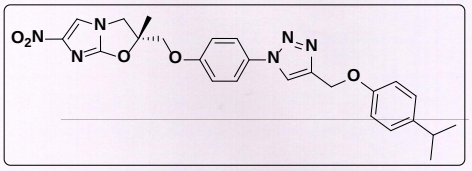


HRMS (ESI-TOF) of compound **1c (IIIM/MCD-026):**

Qualitative Compound Report

Data File	26.d	**Sample Name**	26
Sample Type	Sample	**Position**	Vial 7
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:21:02
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)		

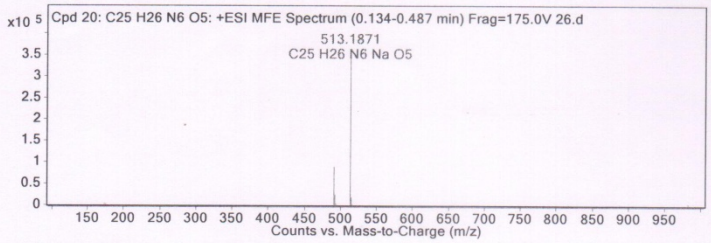


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 20: C25 H26 N6 O5	0.19	490.1977	C25 H26 N6 O5	C25 H26 N6 O5	-2.49	C25 H26 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 20: C25 H26 N6 O5	513.1871	0.19	Find by Molecular Feature	490.1977

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
491.2042	1	88769.41	C25 H27 N6 O5	(M+H)+
492.2071	1	25399.91	C25 H27 N6 O5	(M+H)+
493.208	1	4073.94	C25 H27 N6 O5	(M+H)+
513.1871	1	348285.06	C25 H26 N6 Na O5	(M+Na)+
514.1895	1	97278.2	C25 H26 N6 Na O5	(M+Na)+
515.1913	1	17739.9	C25 H26 N6 Na O5	(M+Na)+
516.1939	1	2318.02	C25 H26 N6 Na O5	(M+Na)+
981.4001	1	3518.02		(2M+H)+
982.4022	1	2416.43		(2M+H)+
983.4032	1	869.25		(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	491.2042	491.2037	-0.84	100	100	74.61	73.68
2	492.2071	492.2067	-0.88	28.61	29.73	21.35	21.91
3	493.208	493.2093	2.52	4.59	5.3	3.42	3.9
4	494.2119	494.2118	-0.23	0.83	0.7	0.62	0.52

--- End Of Report ---

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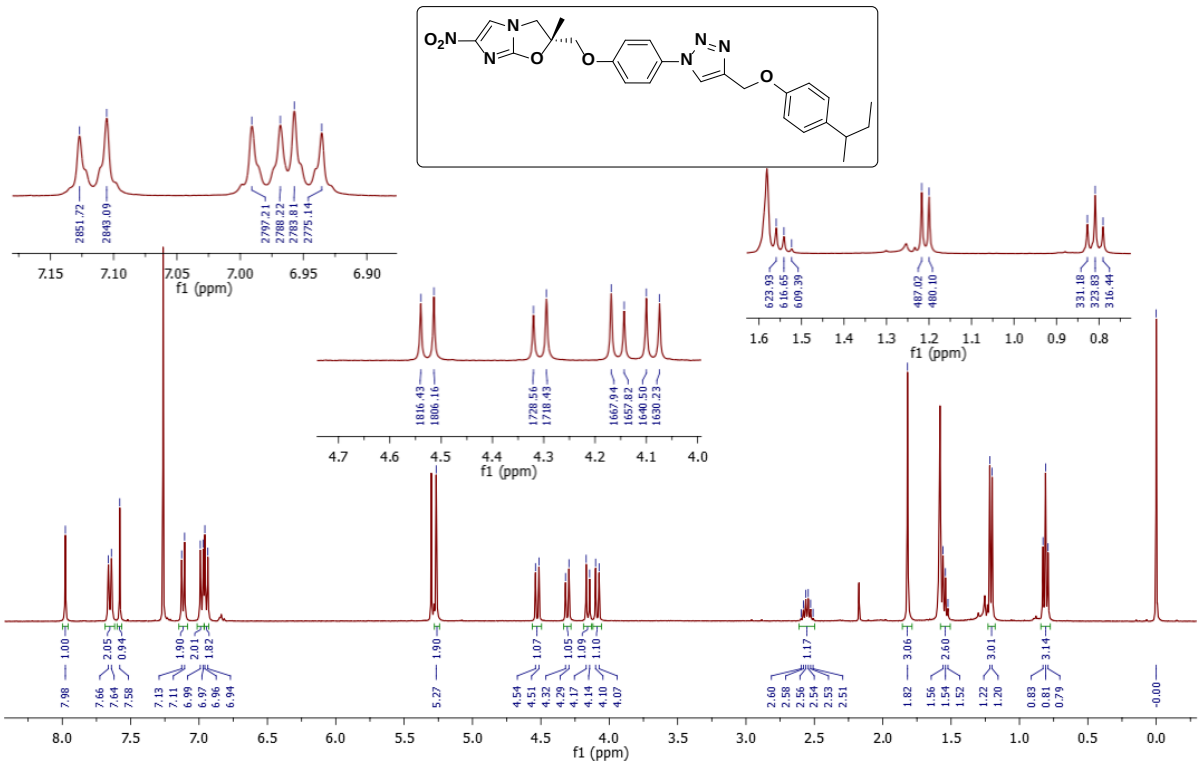
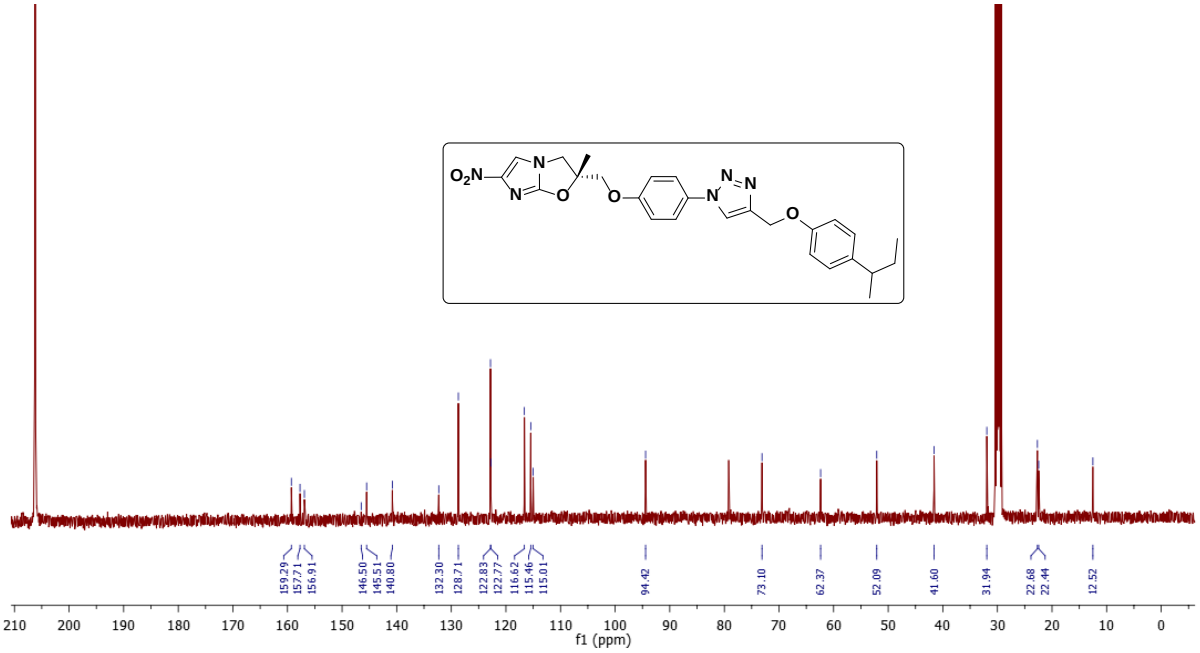
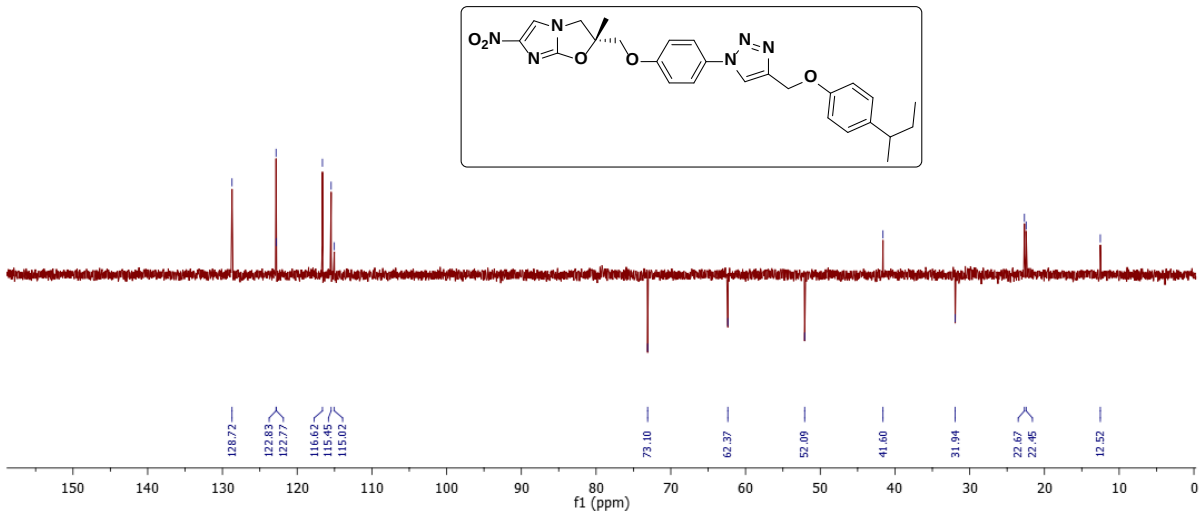
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1d** (**IIIM/MCD-027):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **1d** (**IIIM/MCD-027**)**:**



DEPT (101 MHz, Acetone-d_6) of compound **1d** (**IIIM/MCD-027**)**:**

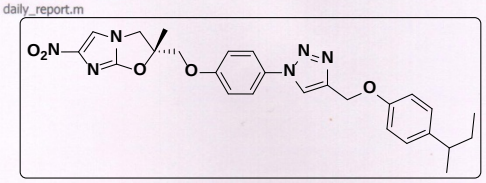


HRMS (ESI-TOF) of compound **1d** (**IIIM/MCD-027)**:

Qualitative Compound Report

Data File	27.d	**Sample Name**	27
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:11:51
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)

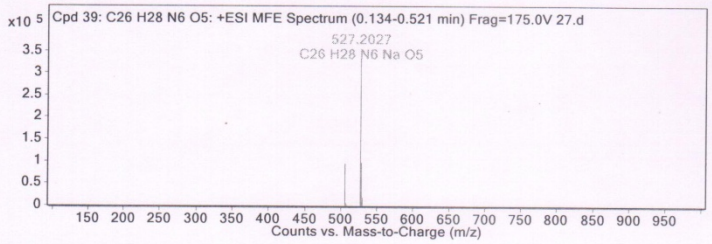


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 39: C26 H28 N6 O5	0.194	504.2132	C26 H28 N6 O5	C26 H28 N6 O5	-2.16	C26 H28 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 39: C26 H28 N6 O5	527.2027	0.194	Find by Molecular Feature	504.2132

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
505.2198	1	95963.11	C26 H29 N6 O5	(M+H)+
506.2222	1	30354.89	C26 H29 N6 O5	(M+H)+
507.2243	1	6577.15	C26 H29 N6 O5	(M+H)+
508.223	1	1132.3	C26 H29 N6 O5	(M+H)+
527.2027	1	339465.75	C26 H28 N6 Na O5	(M+Na)+
528.2048	1	98090.96	C26 H28 N6 Na O5	(M+Na)+
529.2072	1	18354.73	C26 H28 N6 Na O5	(M+Na)+
530.2096	1	2898.29	C26 H28 N6 Na O5	(M+Na)+
531.2096	1	353.2	C26 H28 N6 Na O5	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	505.2198	505.2194	-0.9	100	100	71.6	72.88
2	506.2222	506.2223	0.25	31.63	30.84	22.65	22.47
3	507.2243	507.225	1.23	6.85	5.63	4.91	4.1
4	508.223	508.2275	8.94	1.18	0.76	0.84	0.55

--- End Of Report ---

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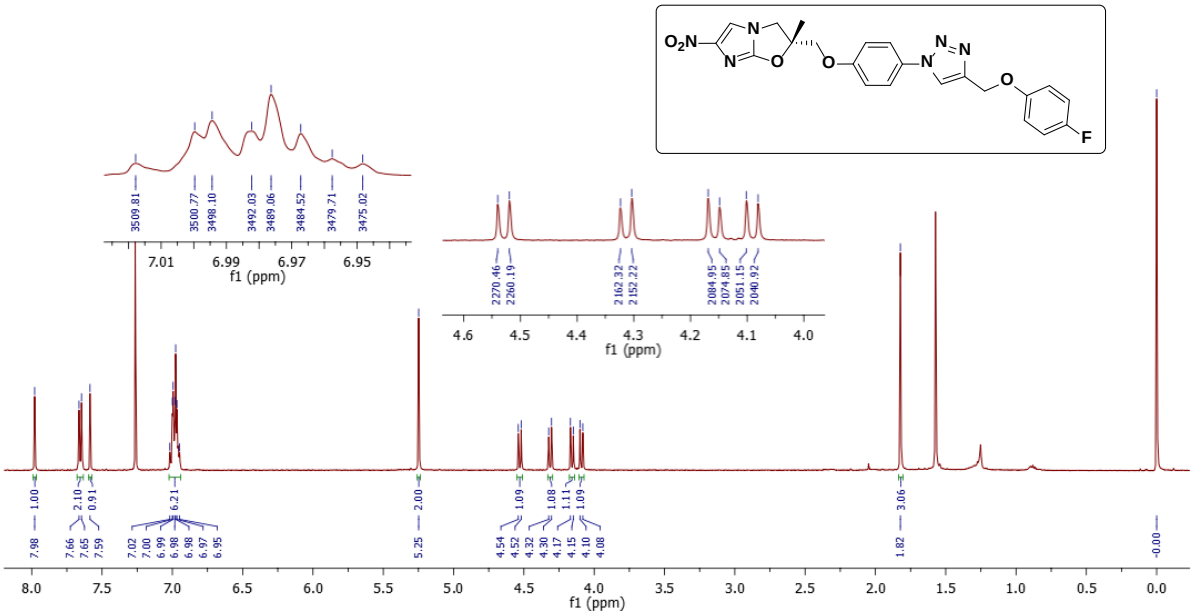
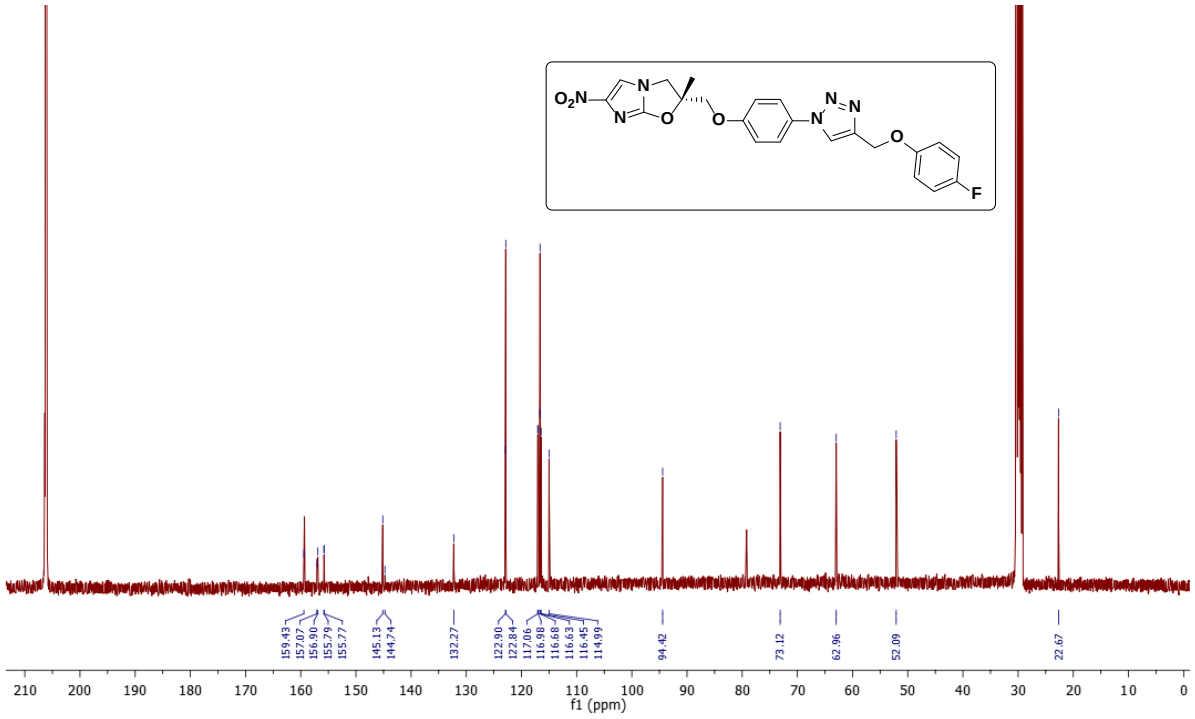
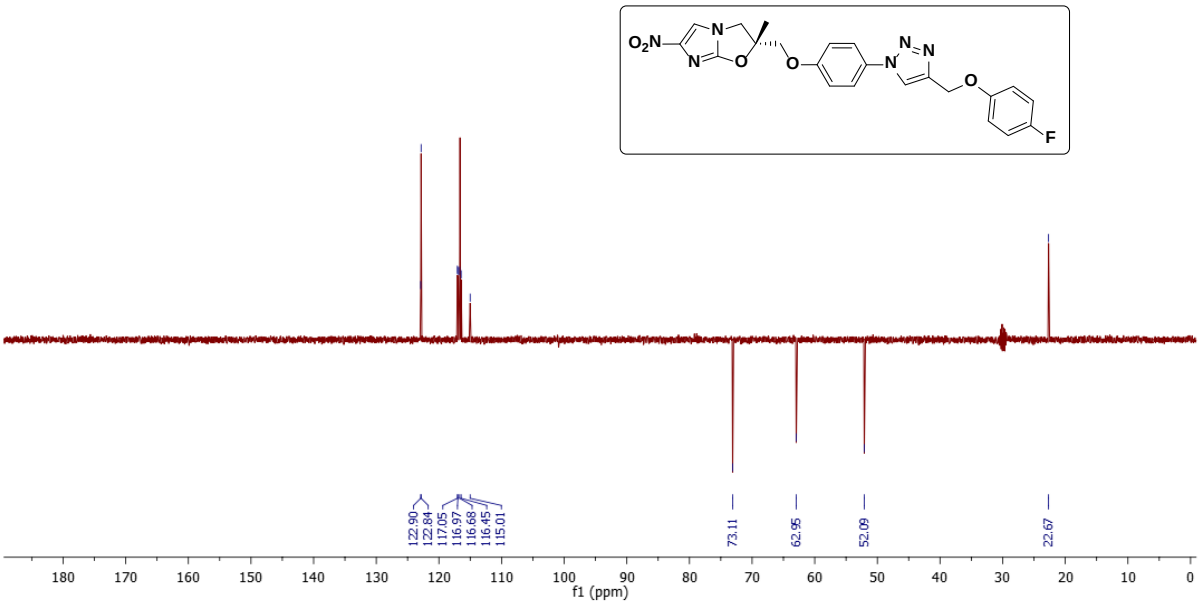
^{1}H NMR (500 MHz, $CDCl_3$) of compound **1e** (**IIIM/MCD-028):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **1e** (**IIIM/MCD-028):**



DEPT (101 MHz, Acetone-d_6) of compound **1e** (**IIIM/MCD-028):**

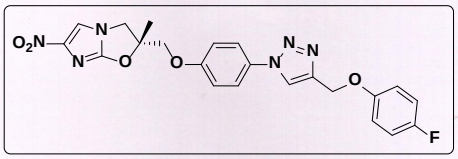


HRMS (ESI-TOF) of compound **1e** (**IIIM/MCD-028)**:

Qualitative Compound Report

Data File	28.d	**Sample Name**	28
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 2:07:11
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)

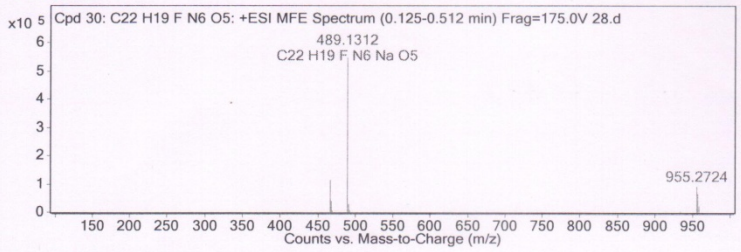


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C22 H19 F N6 O5	0.19	466.142	C22 H19 F N6 O5	C22 H19 F N6 O5	-4.14	C22 H19 F N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C22 H19 F N6 O5	489.1312	0.19	Find by Molecular Feature	466.142

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
467.1479	1	115388.3	C22 H20 F N6 O5	(M+H)+
468.1518	1	39308.95	C22 H20 F N6 O5	(M+H)+
469.1553	1	7389.04	C22 H20 F N6 O5	(M+H)+
489.1312	1	548353.44	C22 H19 F N6 Na O5	(M+Na)+
490.1343	1	178834.5	C22 H19 F N6 Na O5	(M+Na)+
491.1367	1	30611.18	C22 H19 F N6 Na O5	(M+Na)+
955.2724	1	93464.19		(2M+Na)+
956.2753	1	66257.42		(2M+Na)+
957.2781	1	23515.46		(2M+Na)+
958.2803	1	5978.36		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	467.1479	467.1474	-1.03	100	100	70.66	76.14
2	468.1518	468.1502	-3.31	34.07	26.41	24.07	20.11
3	469.1553	469.1527	-5.44	6.4	4.38	4.53	3.34
4	470.1569	470.1552	-3.6	1.04	0.54	0.74	0.41

--- End Of Report ---

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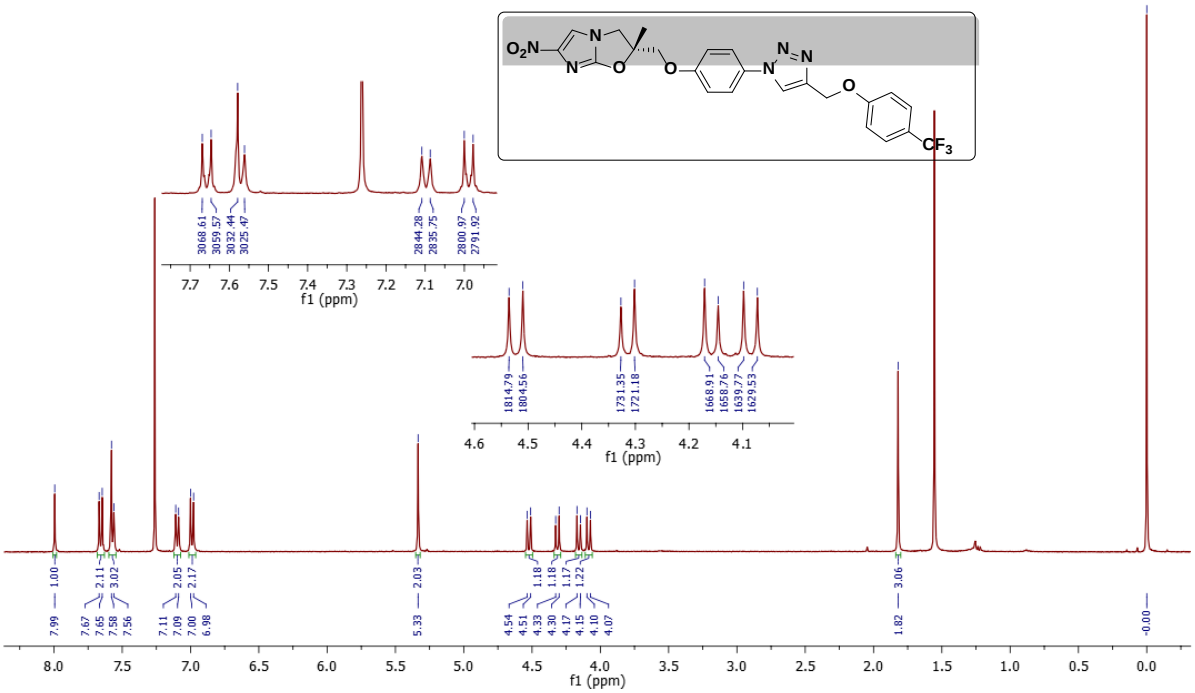
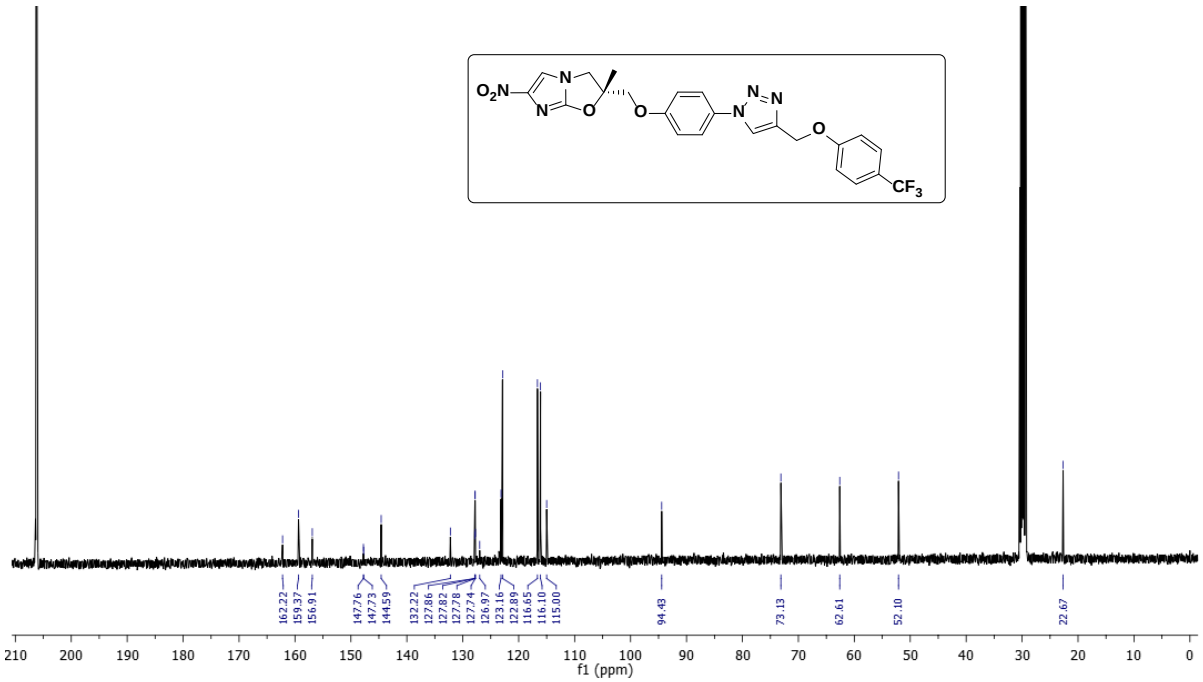
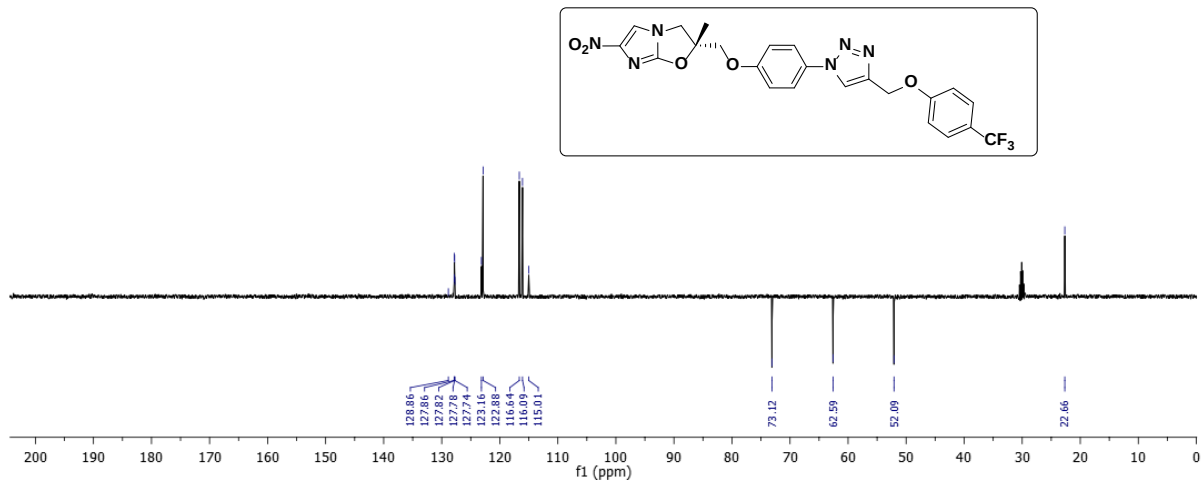
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1f** (**IIIM/MCD-025):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **1f** (**IIIM/MCD-025):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **1f** (**IIIM/MCD-025):**

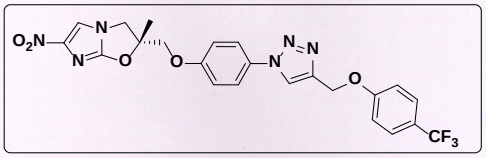


HRMS (ESI-TOF) of compound **1f (IIIM/MCD-025)**:

Qualitative Compound Report

Data File	25.d	**Sample Name**	25
Sample Type	Sample	**Position**	Vial 9
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:38:00
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)

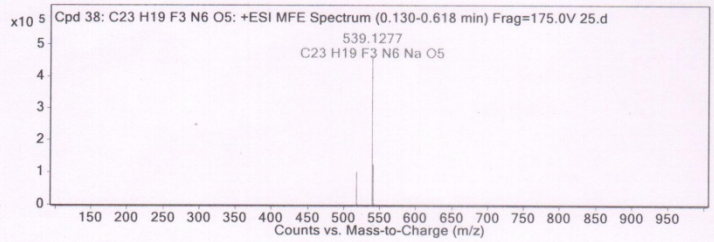


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 38: C23 H19 F3 N6 O5	0.189	516.1383	C23 H19 F3 N6 O5	C23 H19 F3 N6 O5	-2.68	C23 H19 F3 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 38: C23 H19 F3 N6 O5	539.1277	0.189	Find by Molecular Feature	516.1383

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
517.1444	1	103022.23	C23 H20 F3 N6 O5	(M+H)+
518.1473	1	26483.53	C23 H20 F3 N6 O5	(M+H)+
519.1496	1	3956.01	C23 H20 F3 N6 O5	(M+H)+
520.1521	1	929.27	C23 H20 F3 N6 O5	(M+H)+
539.1277	1	466341.94	C23 H19 F3 N6 Na O5	(M+Na)+
540.1298	1	124198.54	C23 H19 F3 N6 Na O5	(M+Na)+
541.1315	1	18573.32	C23 H19 F3 N6 Na O5	(M+Na)+
542.1345	1	2460.49	C23 H19 F3 N6 Na O5	(M+Na)+
543.1446	1	310.04	C23 H19 F3 N6 Na O5	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	517.1444	517.1442	-0.44	100	100	76.66	75.33
2	518.1473	518.1471	-0.56	25.71	27.49	19.71	20.71
3	519.1496	519.1496	-0.04	3.84	4.67	2.94	3.52
4	520.1521	520.1521	0.01	0.9	0.59	0.69	0.45

--- End Of Report ---

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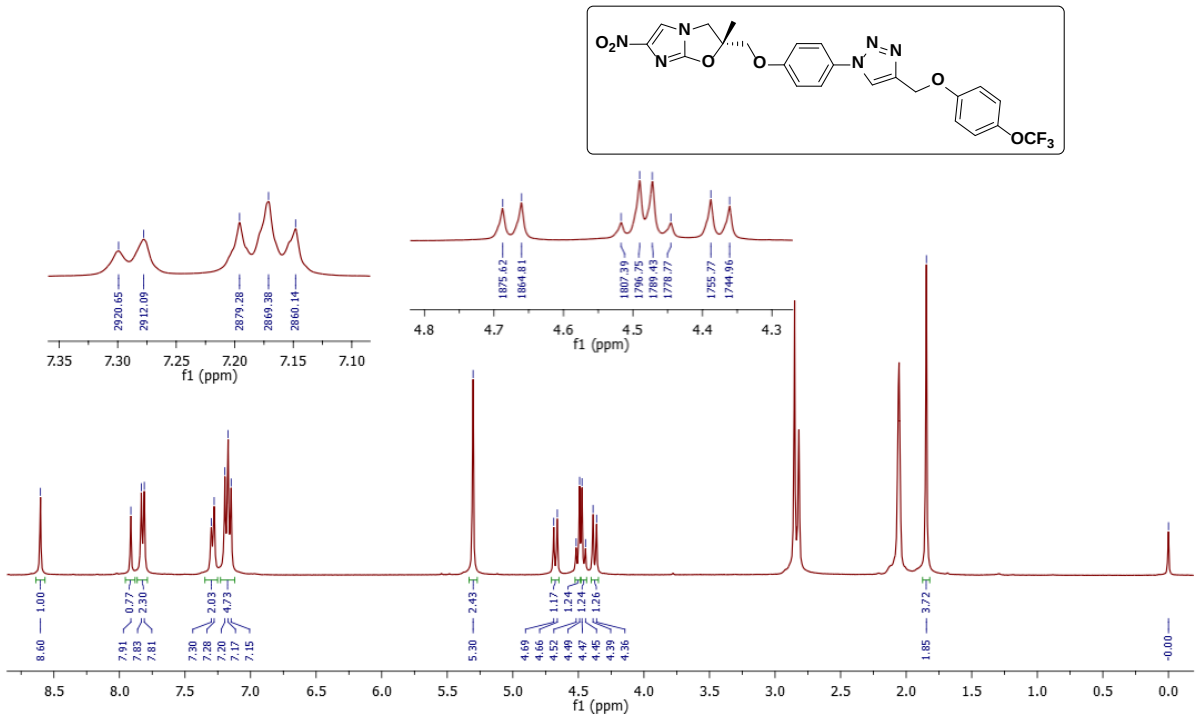
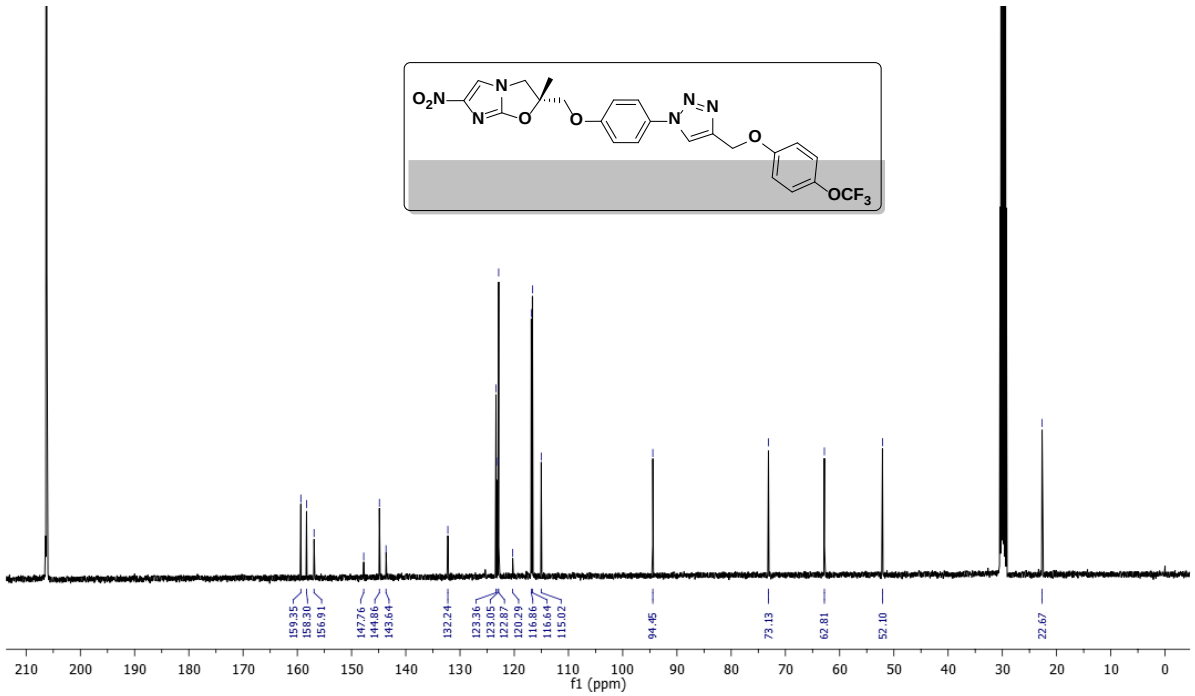
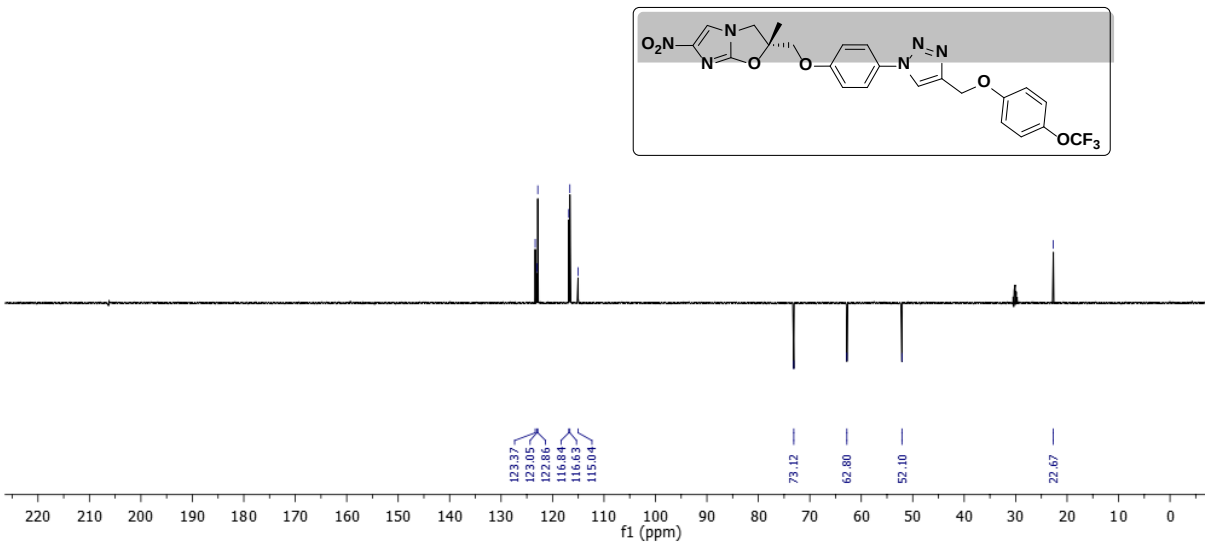
^{1}H NMR (400 MHz, Acetone-d_6) of compound **1g** (**IIIM/MCD-019):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **1g** (**IIIM/MCD-019):**



DEPT (101 MHz, Acetone-d_6) of compound **1g** (**IIIM/MCD-019):**

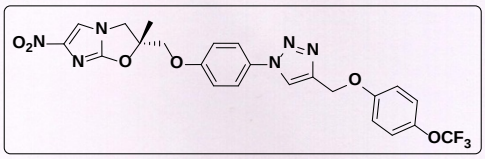


HRMS (ESI-TOF) of compound **1g** (**IIIM/MCD-019)**:

Qualitative Compound Report

Data File	19.d	**Sample Name**	19
Sample Type	Sample	**Position**	Vial 13
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:56:18
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)

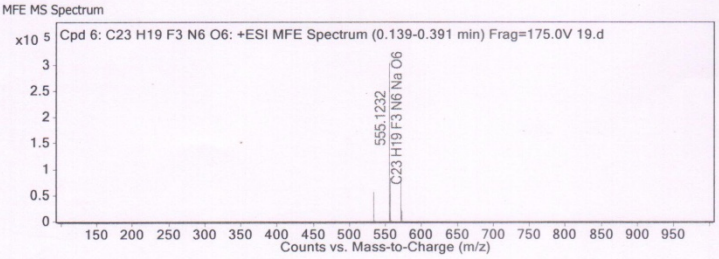


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C23 H19 F3 N6 O6	0.189	532.1337	C23 H19 F3 N6 O6	C23 H19 F3 N6 O6	-3.55	C23 H19 F3 N6 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C23 H19 F3 N6 O6	555.1232	0.189	Find by Molecular Feature	532.1337

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
533.1401	1	56520.39	C23 H20 F3 N6 O6	(M+H)+
534.1425	1	15064.11	C23 H20 F3 N6 O6	(M+H)+
535.1459	1	2376.52	C23 H20 F3 N6 O6	(M+H)+
555.1232	1	302473.06	C23 H19 F3 N6 Na O6	(M+Na)+
556.1251	1	81562.34	C23 H19 F3 N6 Na O6	(M+Na)+
557.1268	1	13193.54	C23 H19 F3 N6 Na O6	(M+Na)+
571.096	1	75946.52	C23 H19 F3 K N6 O6	(M+K)+
572.0991	1	20405.25	C23 H19 F3 K N6 O6	(M+K)+
573.0972	1	9116.58	C23 H19 F3 K N6 O6	(M+K)+
574.0991	1	2169.57	C23 H19 F3 K N6 O6	(M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	533.1401	533.1391	-1.91	100	100	76.42	75.52
2	534.1425	534.142	-0.96	26.65	27.53	20.37	20.79
3	535.1459	535.1445	-2.66	4.2	4.88	3.21	3.69

--- End Of Report ---

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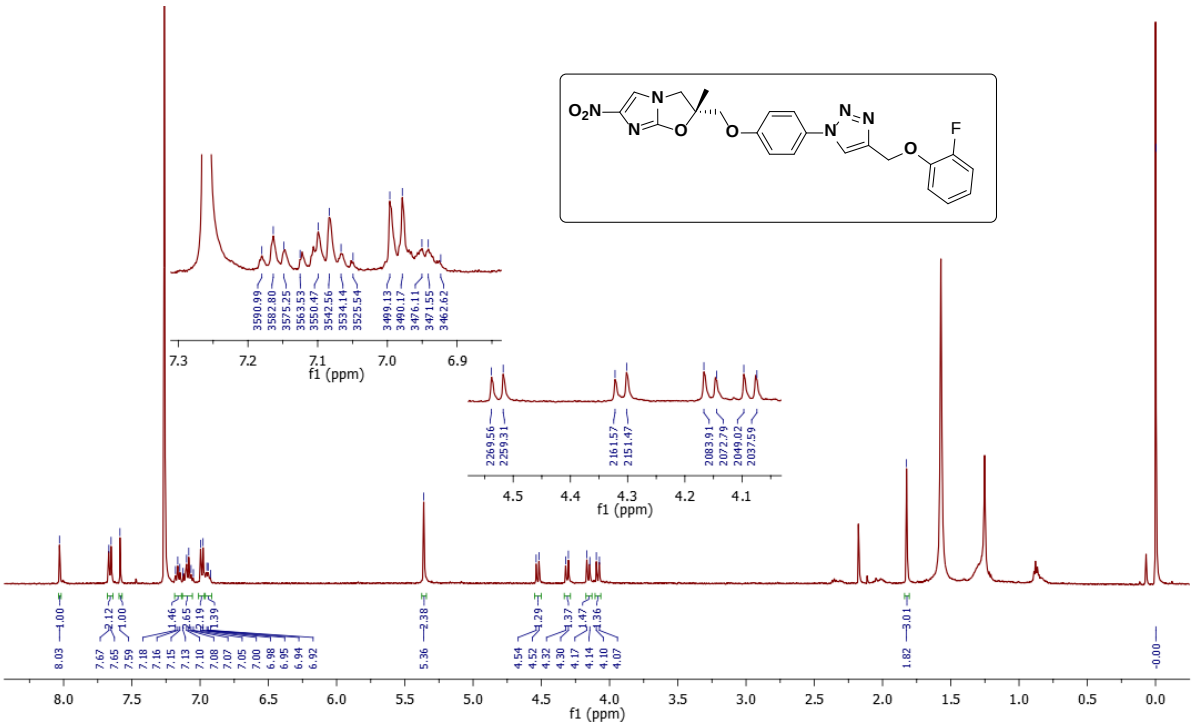
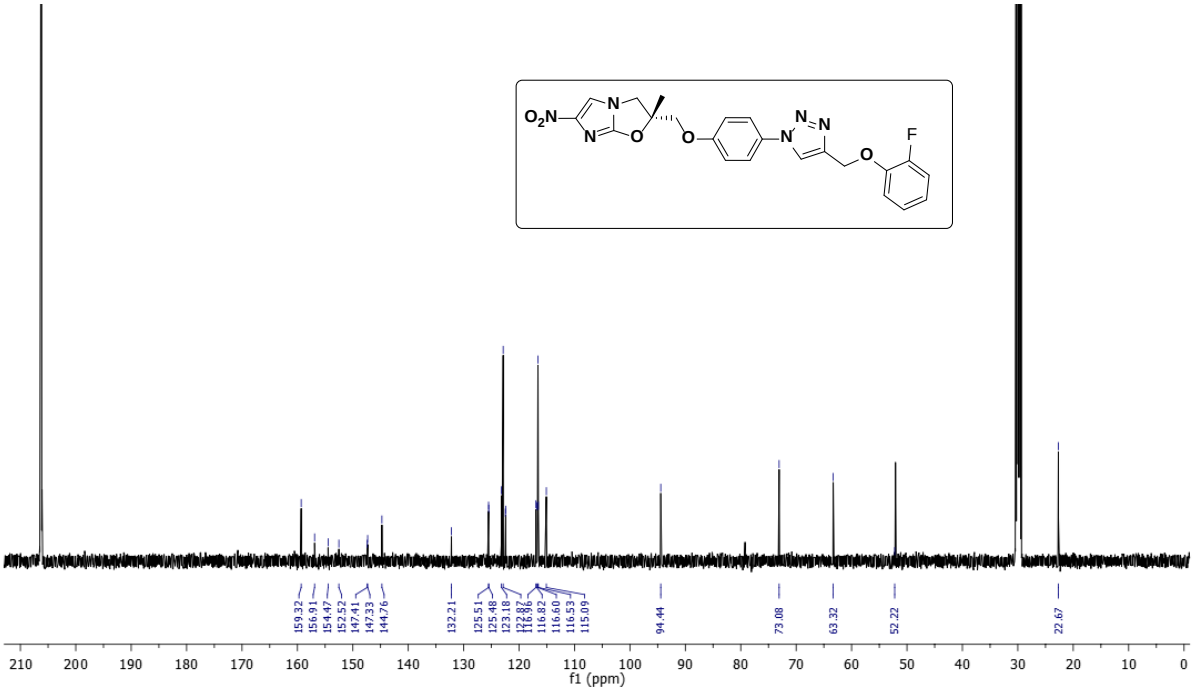
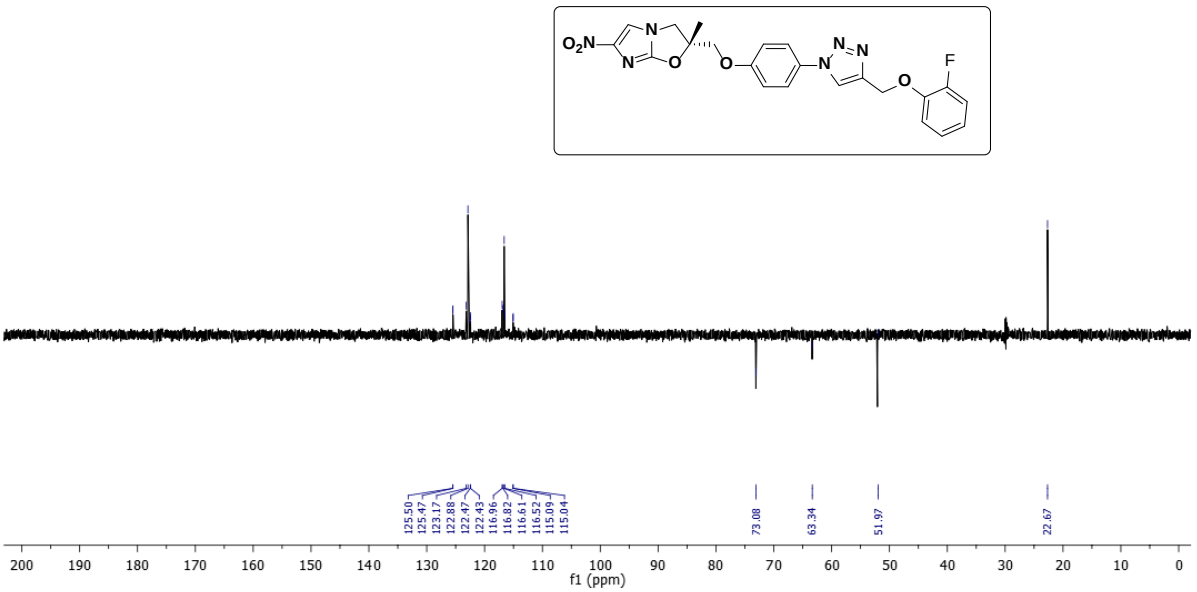
^{1}H NMR (500 MHz, $CDCl_3$) of compound **1h** (**IIIM/MCD-031):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **1h** (**IIIM/MCD-031):**



DEPT (126 MHz, Acetone-d_6) of compound **1h** (**IIIM/MCD-031):**

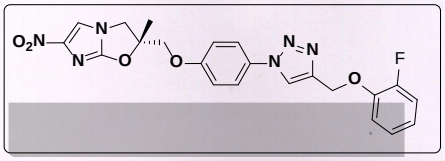


HRMS (ESI-TOF) of compound **1h** (**IIIM/MCD-031)**:

Qualitative Compound Report

Data File	31.d	**Sample Name**	31
Sample Type	Sample	**Position**	Vial 4
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:07:16
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)

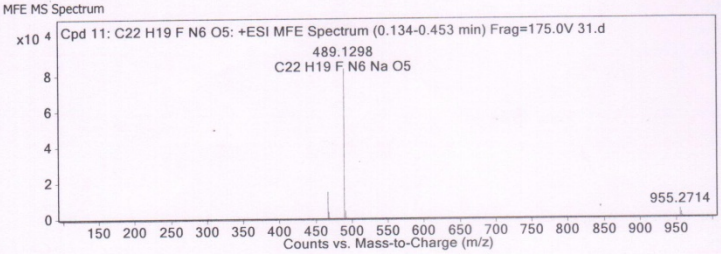


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C22 H19 F N6 O5	0.187	466.1405	C22 H19 F N6 O5	C22 H19 F N6 O5	-0.87	C22 H19 F N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C22 H19 F N6 O5	489.1298	0.187	Find by Molecular Feature	466.1405

MFE MS Spectrum



MS Spectrum Peak List

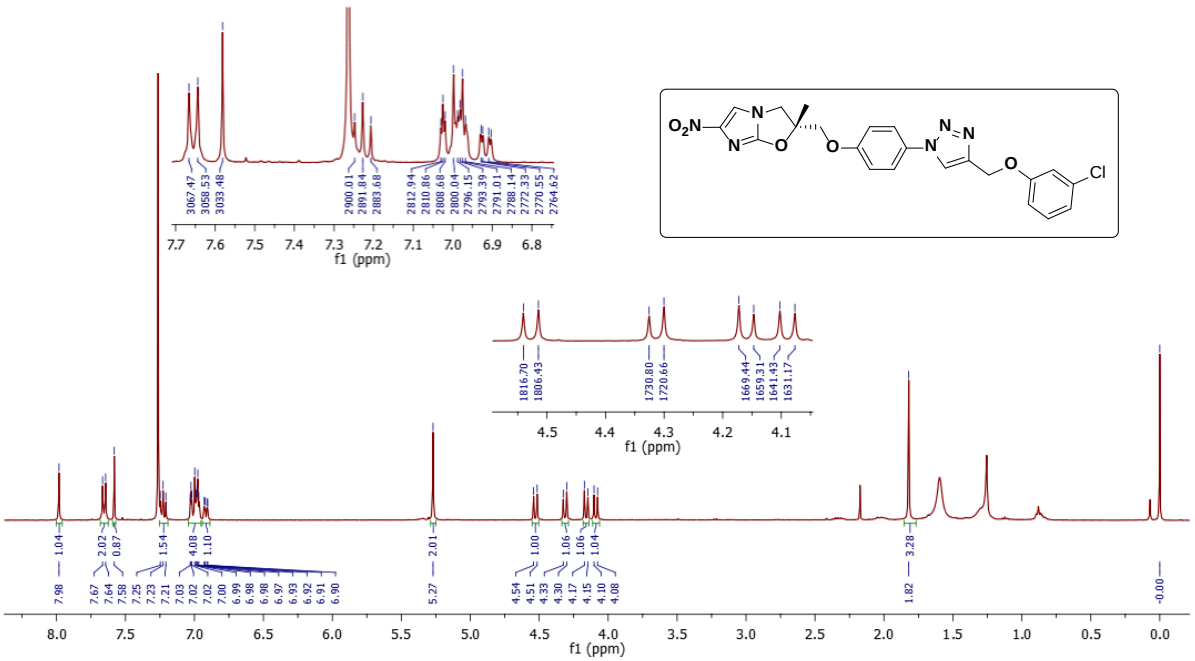
m/z	z	Abund	Formula	Ion
467.1469	1	14419.83	C22 H20 F N6 O5	(M+H)+
468.1506	1	3541.57	C22 H20 F N6 O5	(M+H)+
469.1558	1	680.4	C22 H20 F N6 O5	(M+H)+
489.1298	1	83419.87	C22 H19 F N6 Na O5	(M+Na)+
490.1325	1	19893.75	C22 H19 F N6 Na O5	(M+Na)+
491.1342	1	3916.56	C22 H19 F N6 Na O5	(M+Na)+
492.1348	1	584.65	C22 H19 F N6 Na O5	(M+Na)+
955.2714	1	4372.3		(2M+Na)+
956.2728	1	2736.44		(2M+Na)+
957.2742	1	682.4		(2M+Na)+

Predicted Isotope Match Table

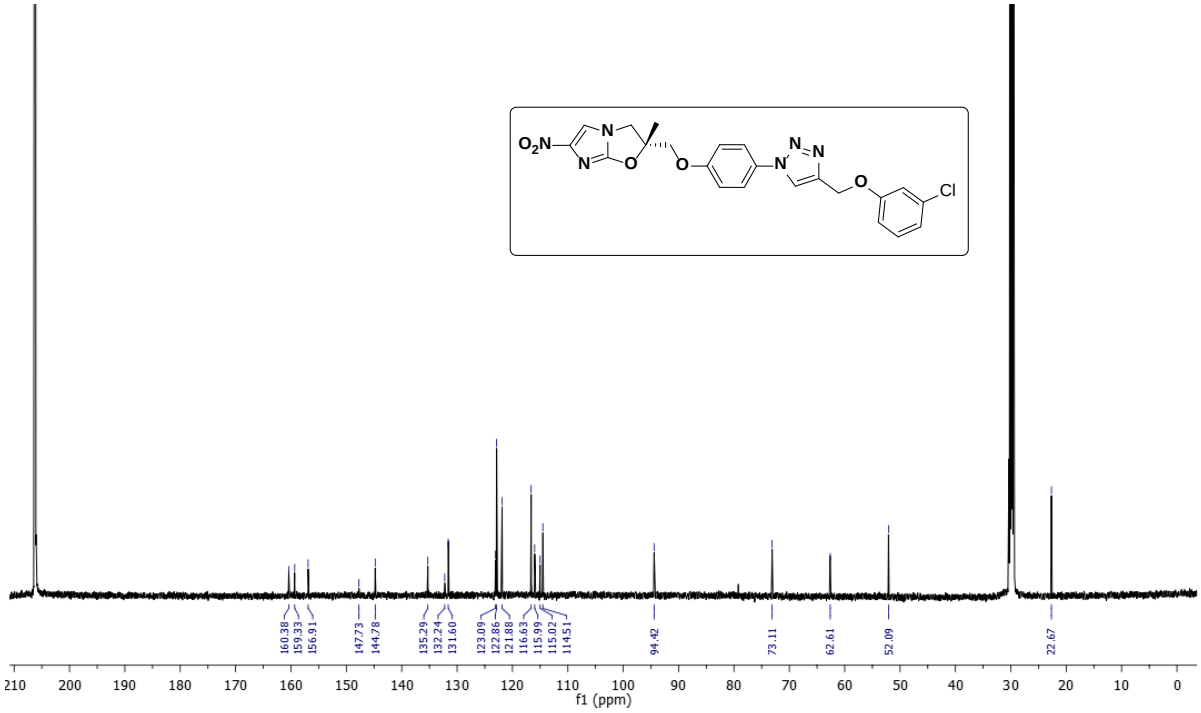
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	467.1469	467.1474	0.98	100	100	77.35	76.46
2	468.1506	468.1502	-0.72	24.56	26.41	19	20.19
3	469.1558	469.1527	-6.45	4.72	4.38	3.65	3.35

--- End Of Report ---

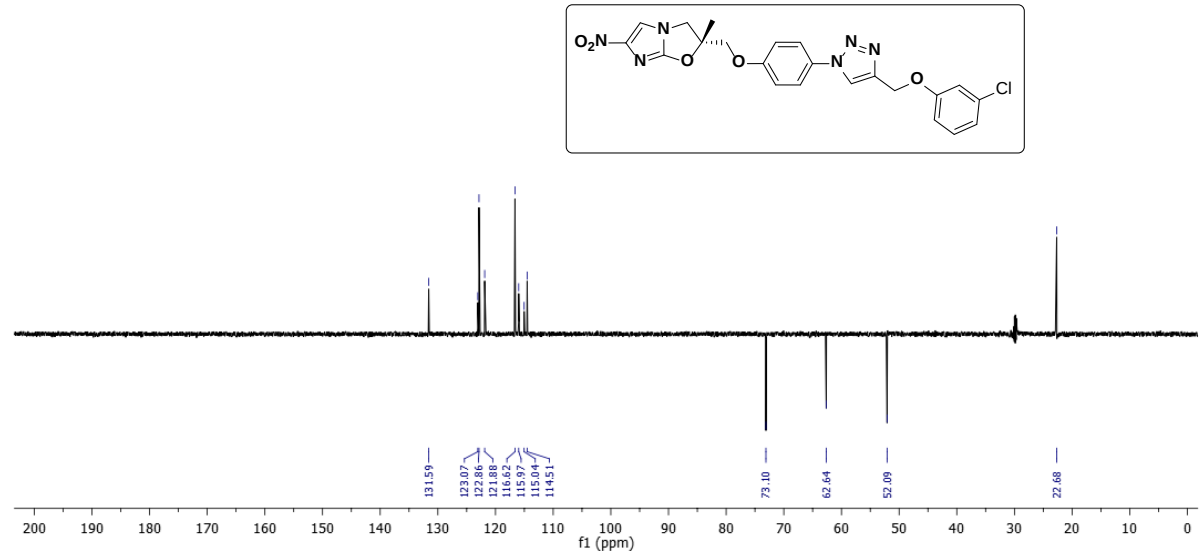
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1i (IIIM/MCD-030):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **1i** (**IIIM/MCD-030):**



DEPT (126 MHz, Acetone-d_6) of compound **1i** (**IIIM/MCD-030):**

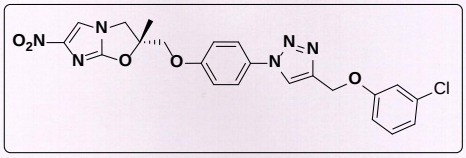


HRMS (ESI-TOF) of compound **1i** (**IIIM/MCD-030)**:

Qualitative Compound Report

Data File	30.d	**Sample Name**	30
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:44:12
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)

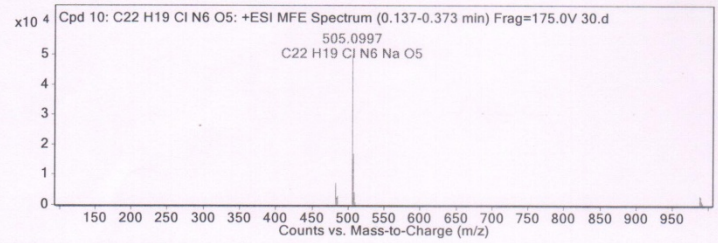


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C22 H19 Cl N6 O5	0.188	482.1107	C22 H19 Cl N6 O5	C22 H19 Cl N6 O5	-0.23	C22 H19 Cl N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C22 H19 Cl N6 O5	505.0997	0.188	Find by Molecular Feature	482.1107

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
483.118	1	7217.02	C22 H20 Cl N6 O5	(M+H)+
484.1202	1	2467.89	C22 H20 Cl N6 O5	(M+H)+
485.1156	1	3131.2	C22 H20 Cl N6 O5	(M+H)+
505.0997	1	49952.33	C22 H19 Cl N6 Na O5	(M+Na)+
506.1024	1	12780.01	C22 H19 Cl N6 Na O5	(M+Na)+
507.0981	1	16888.85	C22 H19 Cl N6 Na O5	(M+Na)+
508.1019	1	4314	C22 H19 Cl N6 Na O5	(M+Na)+
987.2115	1	2955.65		(2M+Na)+
988.2116	1	1664.04		(2M+Na)+
989.2084	1	2764.53		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	483.118	483.1178	-0.39	100	100	52.43	58.21
2	484.1202	484.1207	0.96	34.2	26.41	17.93	15.37
3	485.1156	485.1159	0.51	43.39	36.38	22.75	21.18
4	486.1173	486.1182	1.78	13.16	8.99	6.9	5.24

--- End Of Report ---

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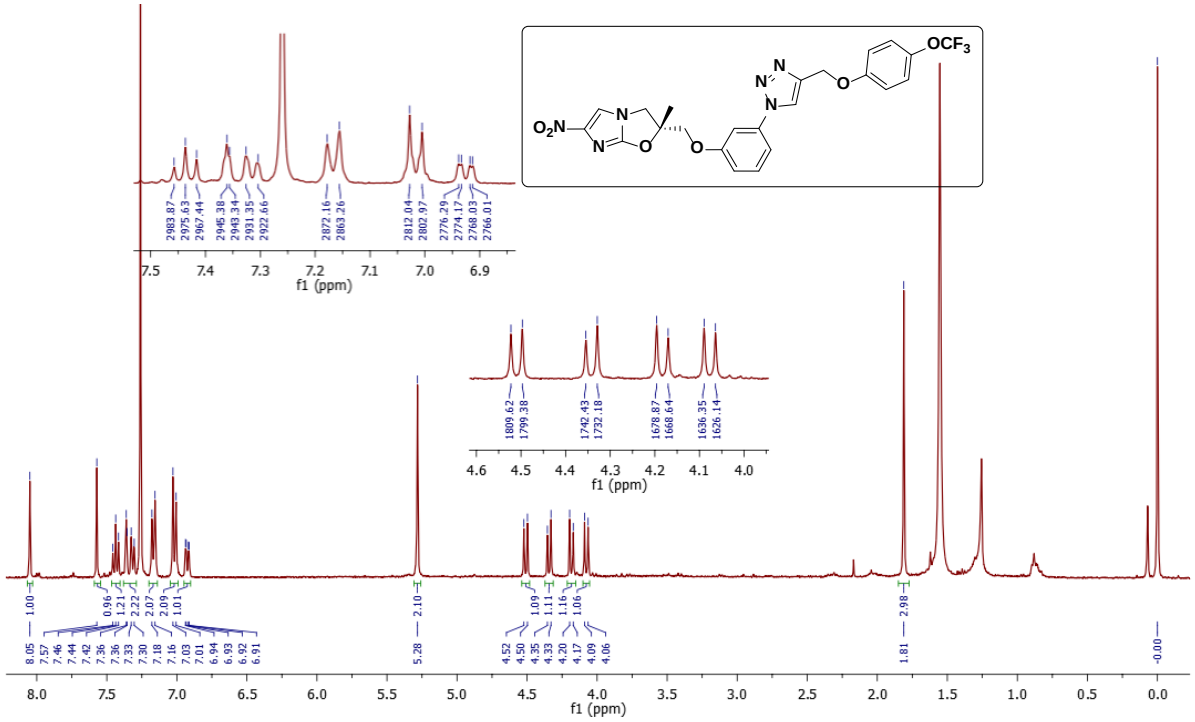
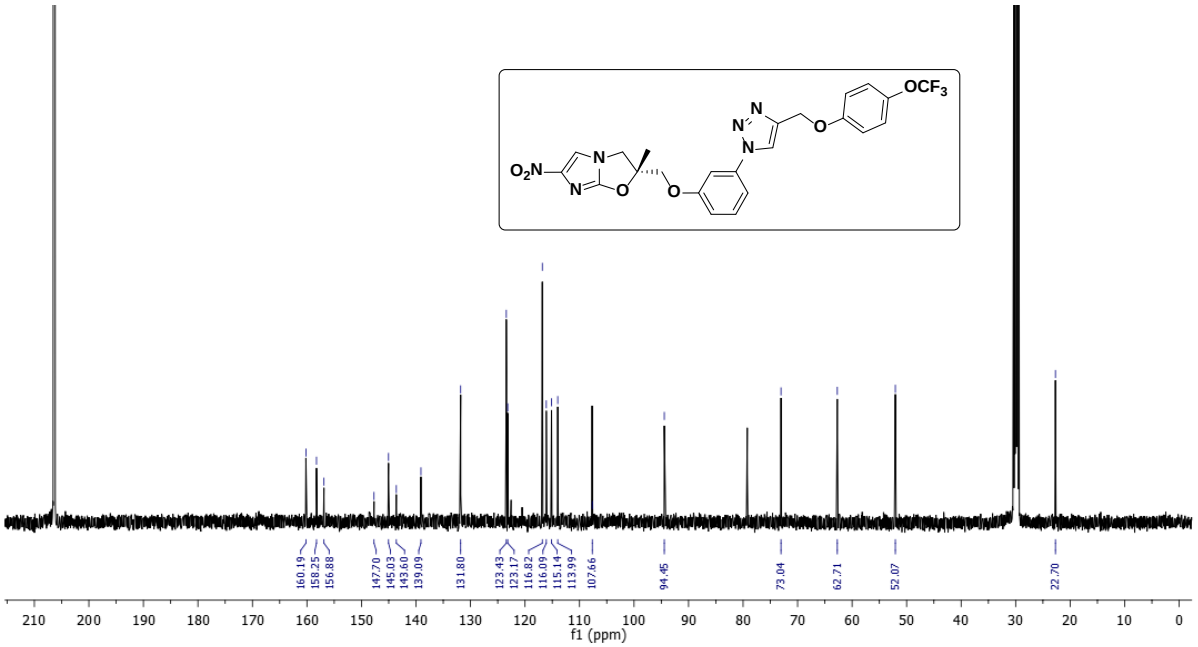
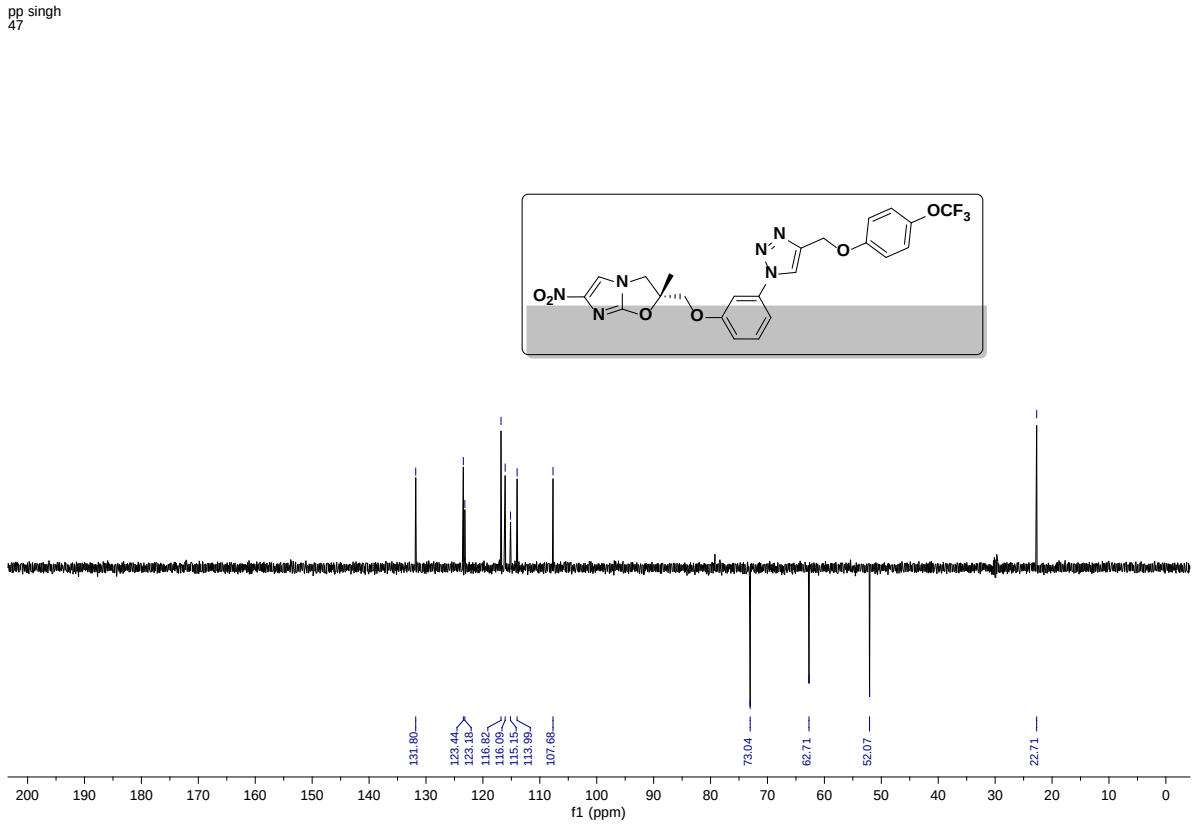
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1j (IIIM/MCD-047):**



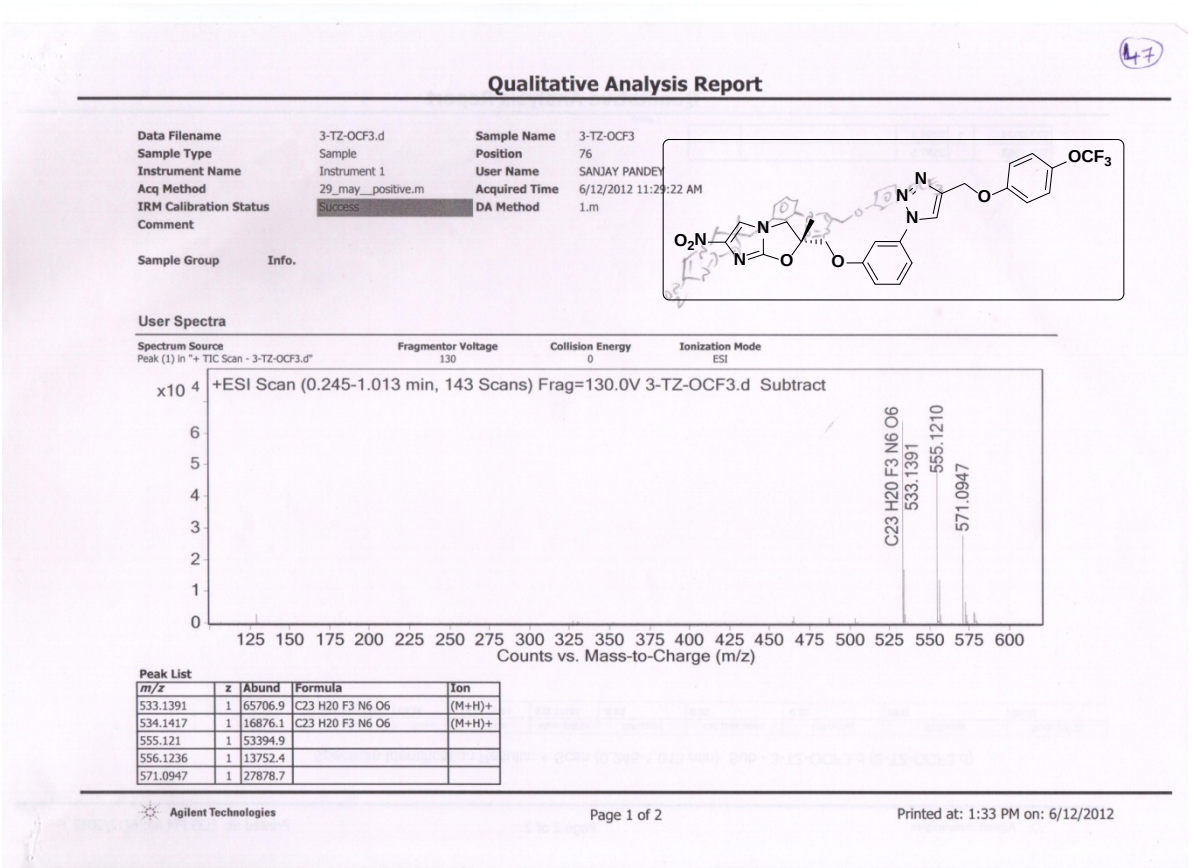
^{13}C NMR (126 MHz, Acetone-d_6) of compound **1j (IIIM/MCD-047):**



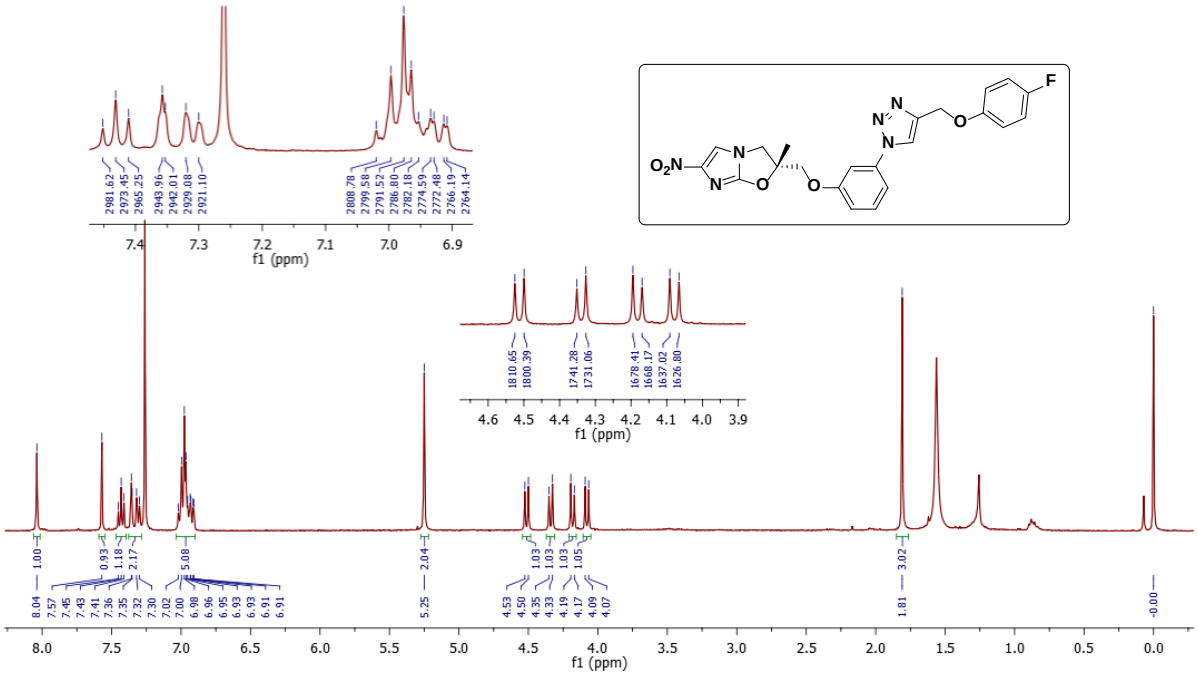
DEPT (126 MHz, Acetone-d_6) of compound **1j** (**IIIM/MCD-047):**



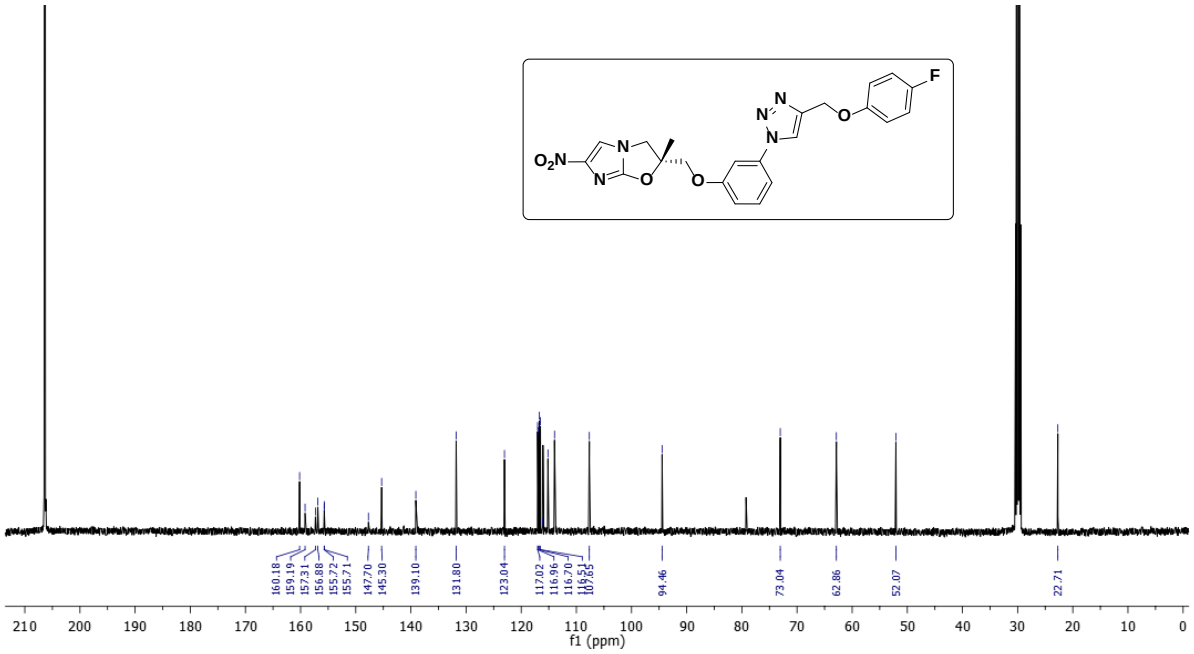
HRMS (ESI-TOF) of compound **1j** (**IIIM/MCD-047)**:



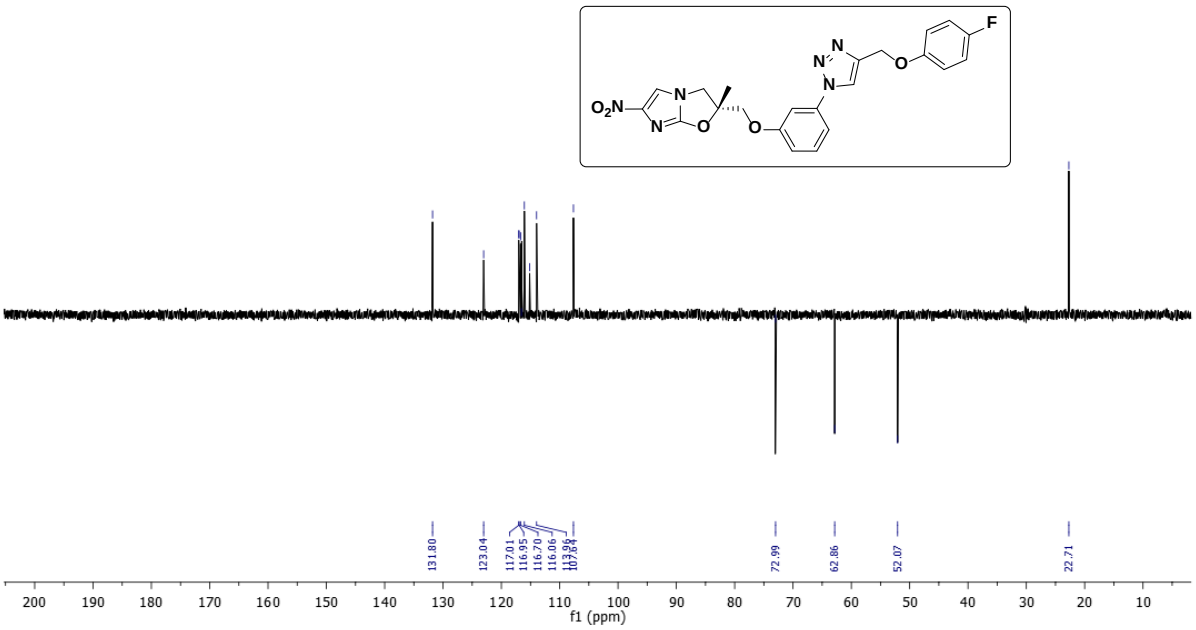
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1k** (**IIIM/MCD-048):**



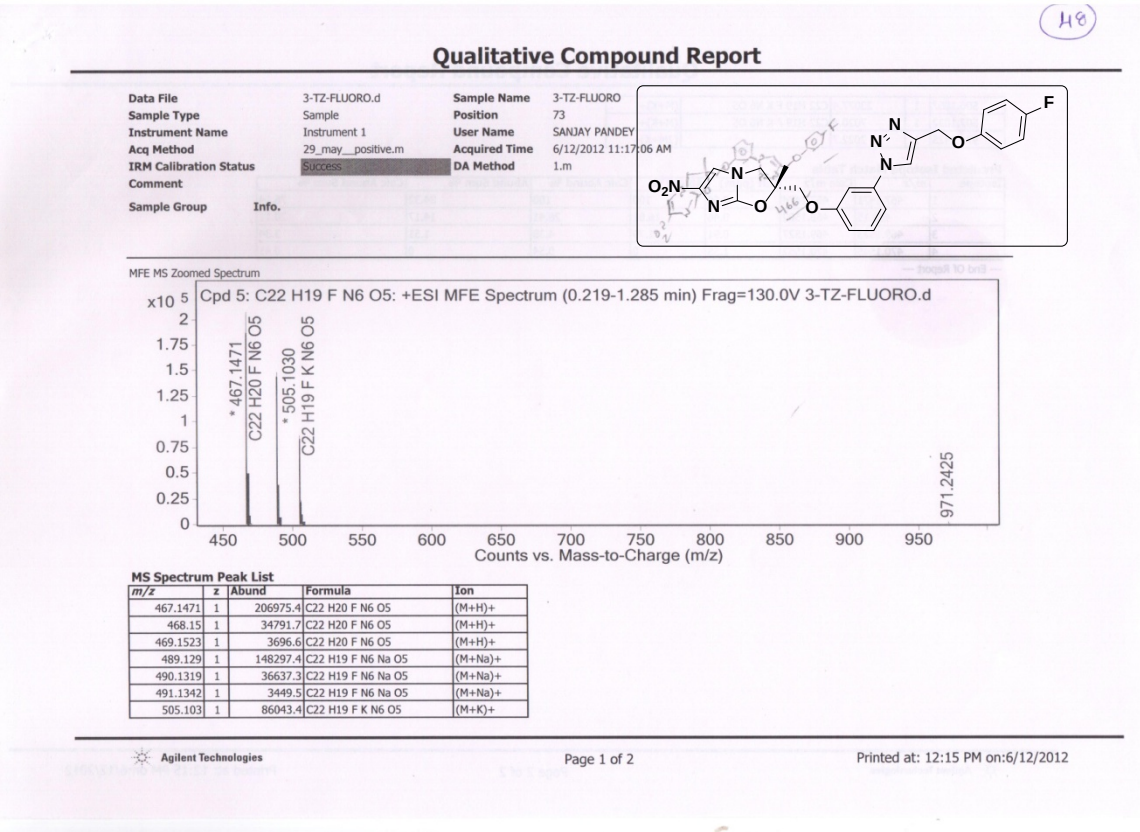
^{13}C NMR (126 MHz, Acetone-d_6) of compound **1k** (**IIIM/MCD-048):**



DEPT (126 MHz, Acetone-d_6) of compound **1k** (**IIIM/MCD-048):**



HRMS (ESI-TOF) of compound **1k** (**IIIM/MCD-048)**:



Qualitative Compound Report

Data File	3-TZ-FLUORO.d	**Sample Name**	3-TZ-FLUORO
Sample Type	Sample	**Position**	73
Instrument Name	Instrument 1	**User Name**	SANJAY PANDEY
Acq Method	29_may__positive.m	**Acquired Time**	6/12/2012 11:17:06 AM
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group	**Info.**		

MFE MS Zoomed Spectrum

Cpd 5: C22 H19 F N6 O5: +ESI MFE Spectrum (0.219-1.285 min) Frag=130.0V 3-TZ-FLUORO.d

x10 5 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0

* 467.1471 C22 H20 F N6 O5

* 505.1030 C22 H19 F K N6 O5

971.2425

450 500 550 600 650 700 750 800 850 900 950

Counts vs. Mass-to-Charge (m/z)

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
467.1471	1	206975.4	C22 H20 F N6 O5	(M+H)+
468.15	1	34791.7	C22 H20 F N6 O5	(M+H)+
469.1523	1	3696.6	C22 H20 F N6 O5	(M+H)+
489.129	1	148297.4	C22 H19 F N6 Na O5	(M+Na)+
490.1319	1	36637.3	C22 H19 F N6 Na O5	(M+Na)+
491.1342	1	3449.5	C22 H19 F N6 Na O5	(M+Na)+
505.103	1	86043.4	C22 H19 F K N6 O5	(M+K)+

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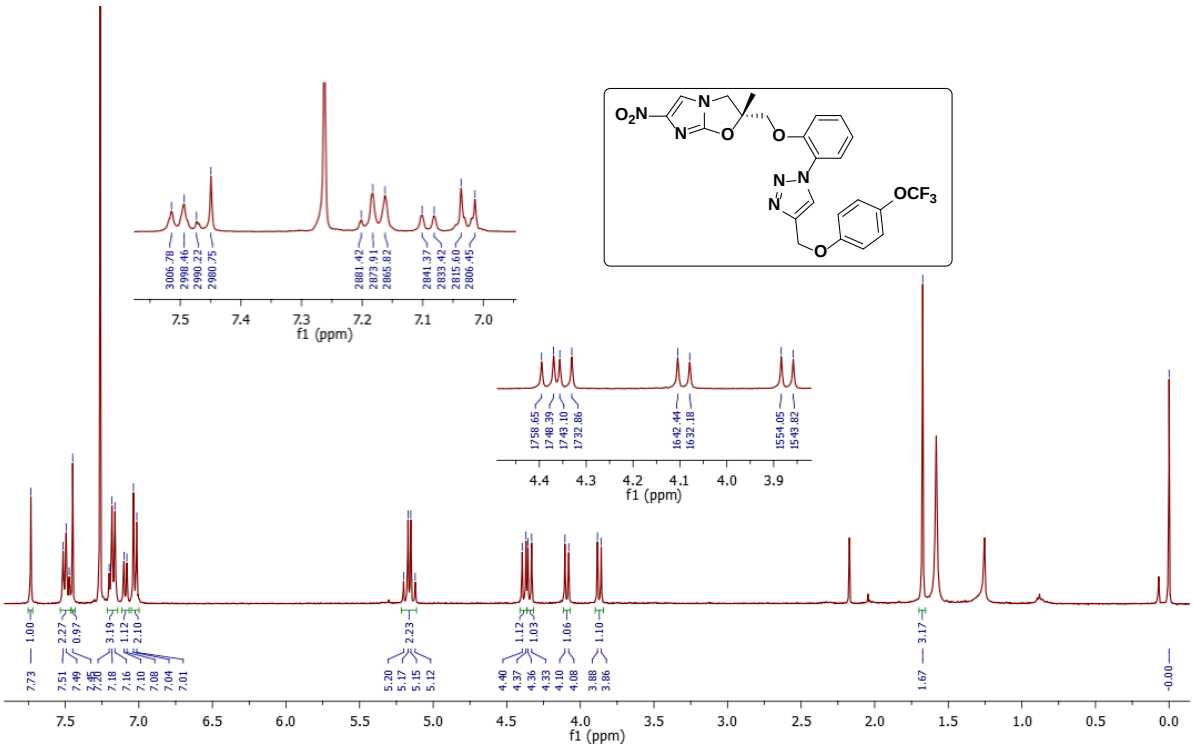
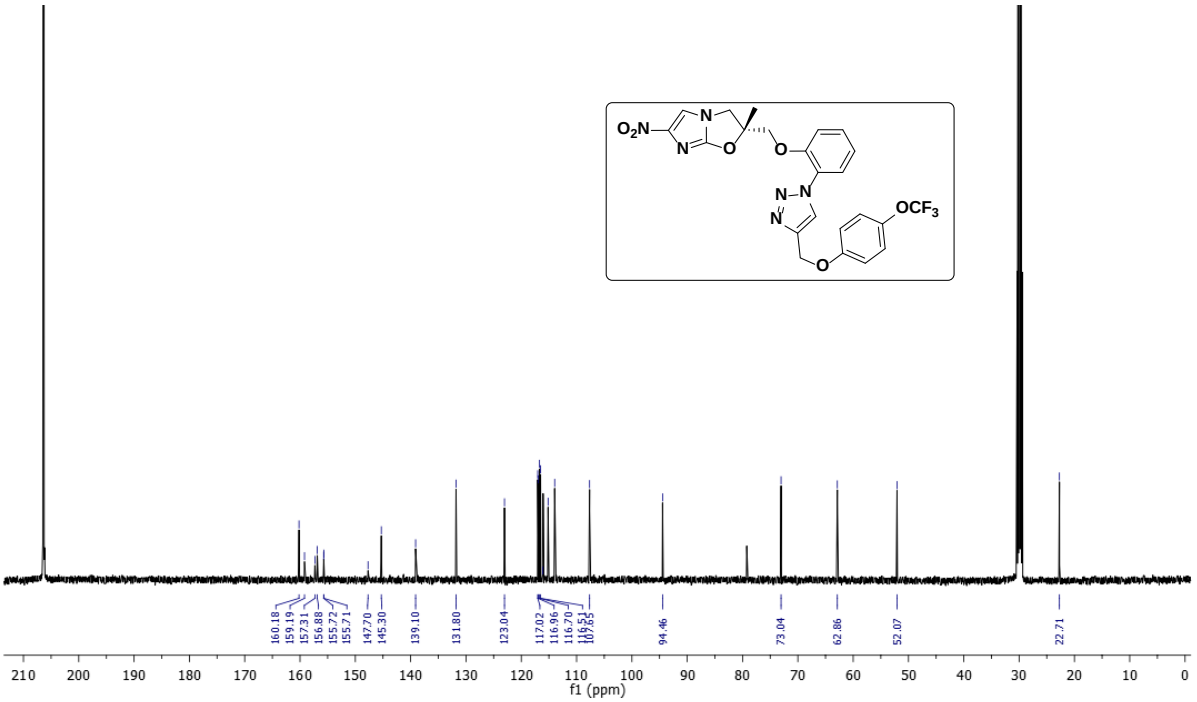
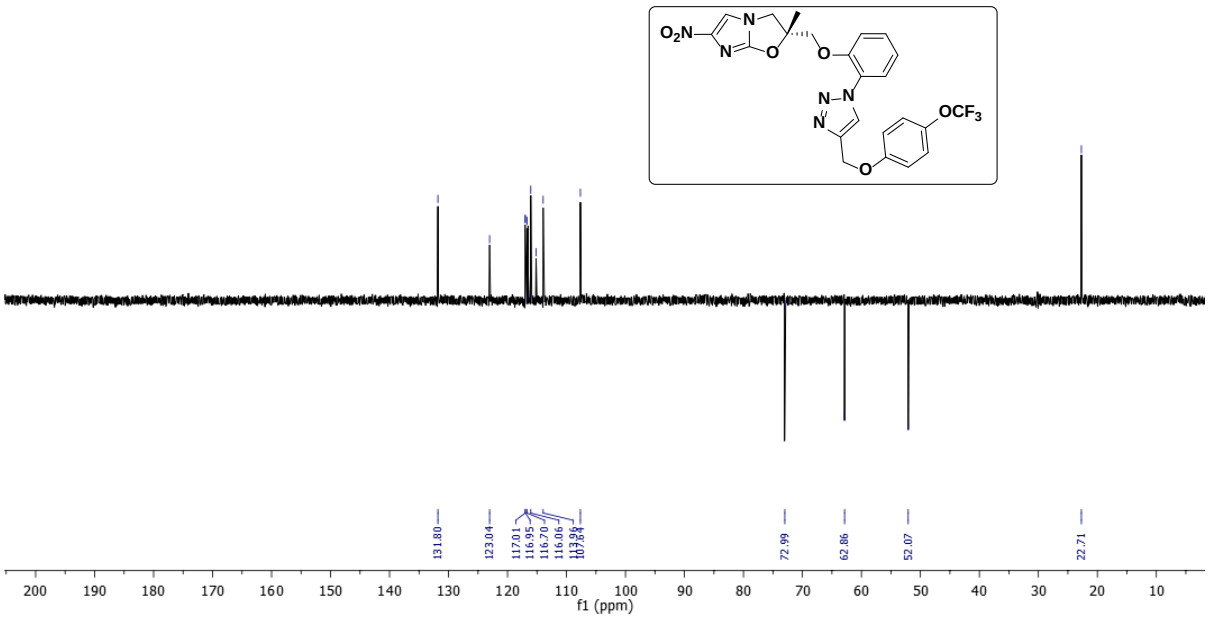
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1l** (**IIIM/MCD-052):**



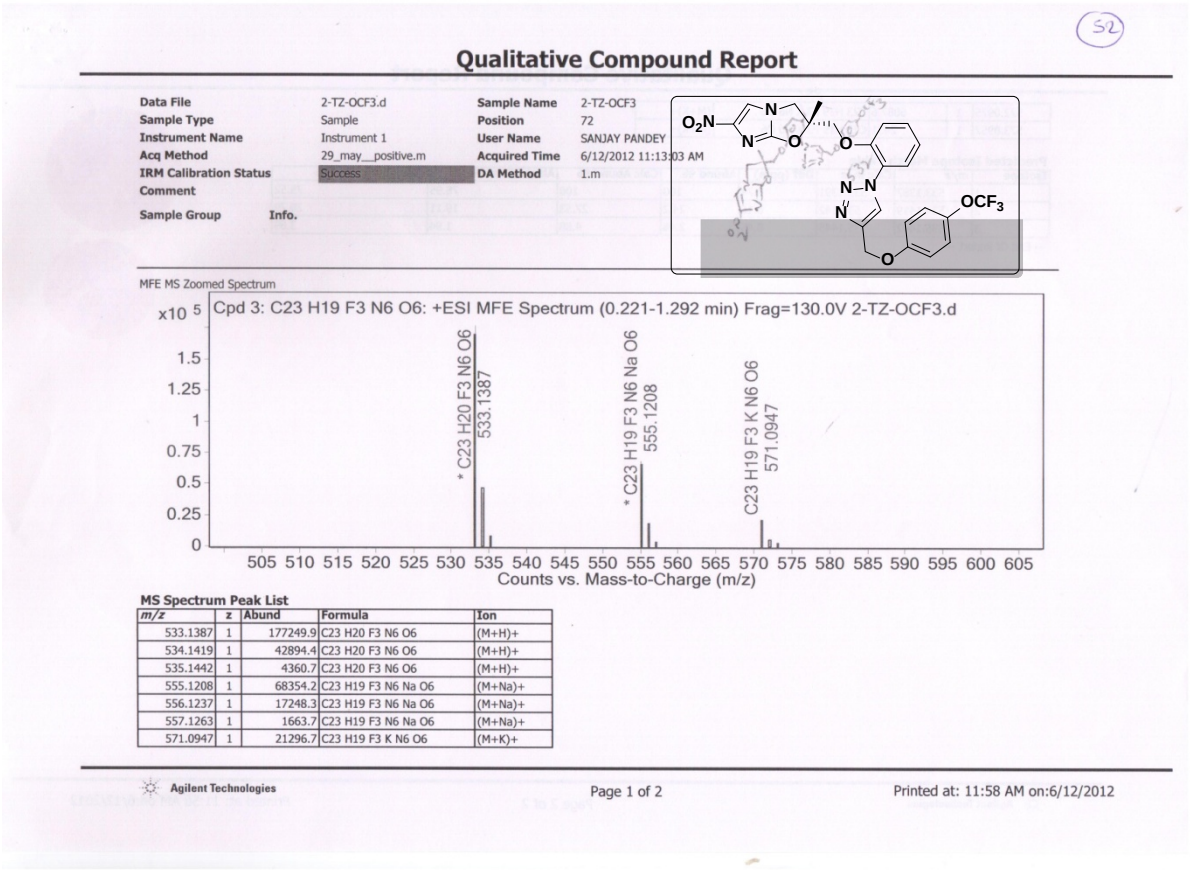
^{13}C NMR (101 MHz, $CDCl_3$) of compound **1l** (**IIIM/MCD-052):**



DEPT (101 MHz, $CDCl_3$) of compound **1l** (**IIIM/MCD-052):**



HRMS (ESI-TOF) of compound **1l** (**IIIM/MCD-052)**:



Qualitative Compound Report

Data File	2-TZ-OCF3.d	Sample Name	2-TZ-OCF3
Sample Type	Sample	Position	72
Instrument Name	Instrument 1	User Name	SANJAY PANDEY
Acq Method	29_may__positive.m	Acquired Time	6/12/2012 11:13:03 AM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group	Info.		

MFE MS Zoomed Spectrum

Cpd 3: C23 H19 F3 N6 O6: +ESI MFE Spectrum (0.221-1.292 min) Frag=130.0V 2-TZ-OCF3.d

x10 5

* C23 H20 F3 N6 O6 533.1387

* C23 H19 F3 N6 Na O6 555.1208

C23 H19 F3 K N6 O6 571.0947

Counts vs. Mass-to-Charge (m/z)

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
533.1387	1	177249.9	C23 H20 F3 N6 O6	(M+H)+
534.1419	1	42894.4	C23 H20 F3 N6 O6	(M+H)+
535.1442	1	4360.7	C23 H20 F3 N6 O6	(M+H)+
555.1208	1	68354.2	C23 H19 F3 N6 Na O6	(M+Na)+
556.1237	1	17248.3	C23 H19 F3 N6 Na O6	(M+Na)+
557.1263	1	1663.7	C23 H19 F3 N6 Na O6	(M+Na)+
571.0947	1	21296.7	C23 H19 F3 K N6 O6	(M+K)+

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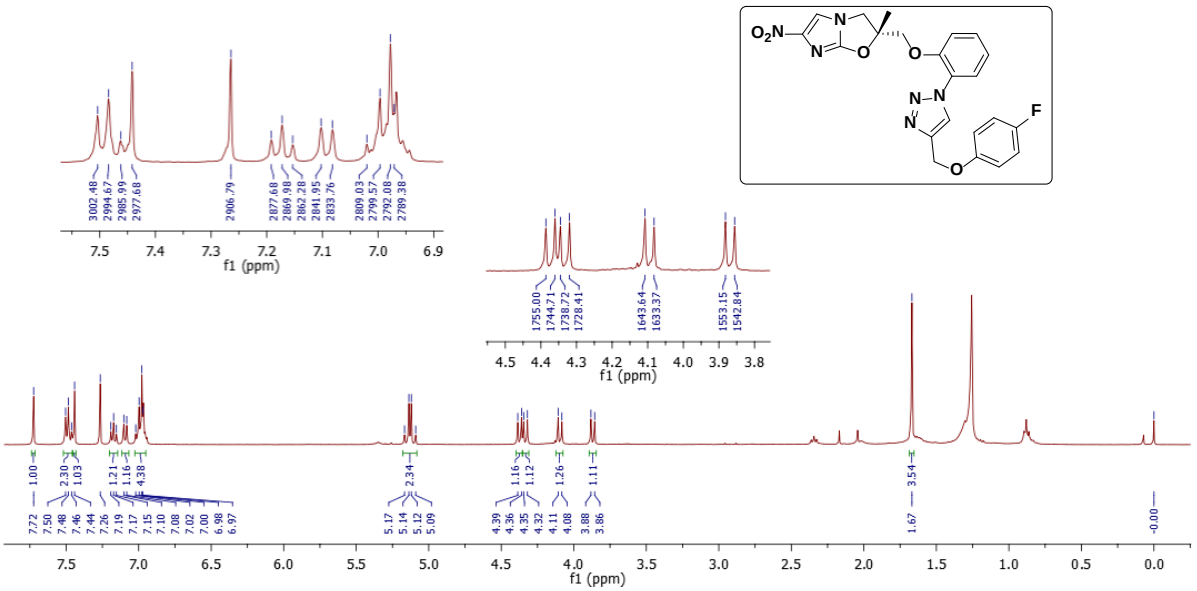
Printed at: 11:58 AM on:6/12/2012

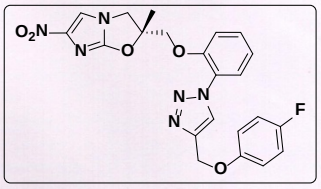
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1m** (**IIIM/MCD-063):**



HRMS (ESI-TOF) of compound **1m (IIIM/MCD-063)**:

Qualitative Compound Report

Data File	63.d	**Sample Name**	63
Sample Type	Sample	**Position**	Vial 24
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	26-07-2012 PM 09:44:19
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

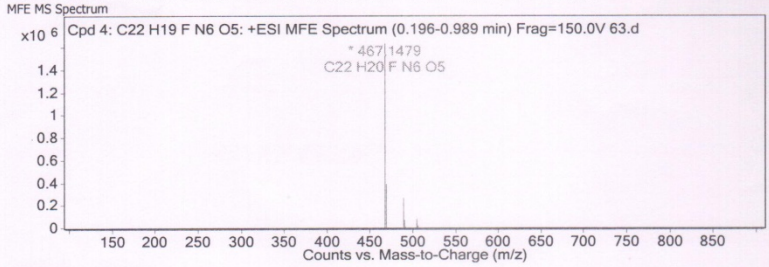


Compound Table

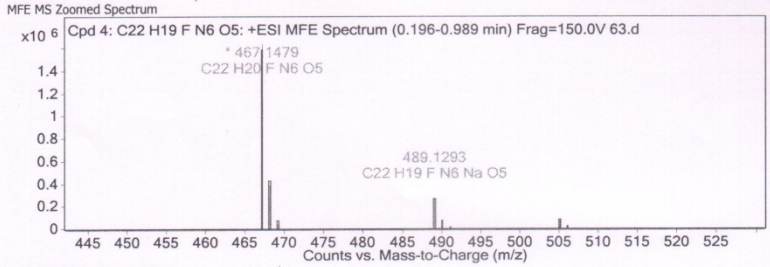
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C22 H19 F N6 O5	0.303	466.1406	C22 H19 F N6 O5	C22 H19 F N6 O5	-1.06	C22 H19 F N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C22 H19 F N6 O5	467.1479	0.303	Find by Molecular Feature	466.1406

MFE MS Spectrum



MFE MS Zoomed Spectrum

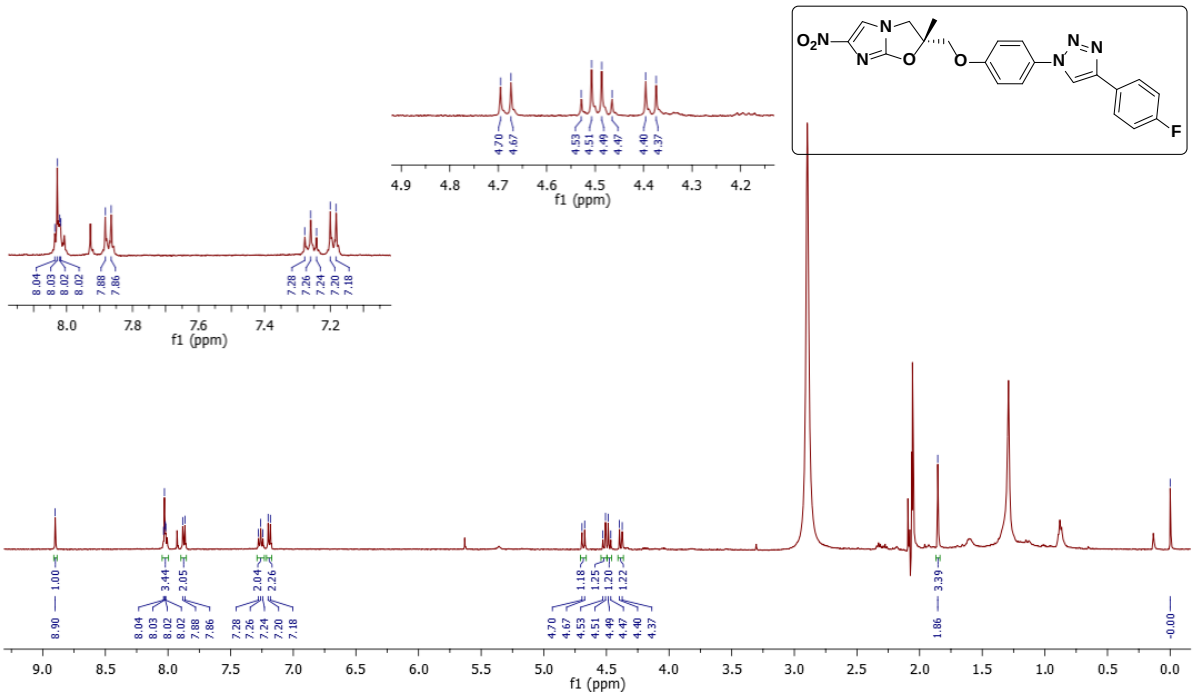


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
467.1479	1	1634766.8	C22 H20 F N6 O5	(M+H)+
468.1507	1	389274.9	C22 H20 F N6 O5	(M+H)+
469.1525	1	43992.1	C22 H20 F N6 O5	(M+H)+
489.1293	1	262385.6	C22 H19 F N6 Na O5	(M+Na)+
490.1318	1	70958.1	C22 H19 F N6 Na O5	(M+Na)+
491.1341	1	12631.2	C22 H19 F N6 Na O5	(M+Na)+
505.1034	1	75771	C22 H19 F K N6 O5	(M+K)+
506.106	1	18624.4	C22 H19 F K N6 O5	(M+K)+

--- End Of Report ---

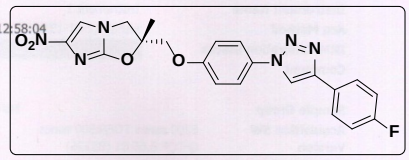
^{1}H NMR (500 MHz, Acetone-d_6) of compound **1n** (**IIIM/MCD-065):**



HRMS (ESI-TOF) of compound **1n** (**IIIM/MCD-065)**:

Qualitative Compound Report

Data File	65.d	**Sample Name**	65
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 12:58:04
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



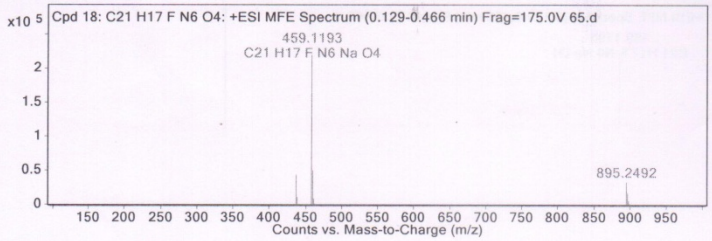
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C21 H17 F N6 O4	0.189	436.1301	C21 H17 F N6 O4	C21 H17 F N6 O4	-1.22	C21 H17 F N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C21 H17 F N6 O4	459.1193	0.189	Find by Molecular Feature	436.1301

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
437.1369	1	43860.13	C21 H18 F N6 O4	(M+H)+
438.1395	1	10522.2	C21 H18 F N6 O4	(M+H)+
439.1418	1	1938.93	C21 H18 F N6 O4	(M+H)+
459.1193	1	219992.16	C21 H17 F N6 Na O4	(M+Na)+
460.122	1	49384.63	C21 H17 F N6 Na O4	(M+Na)+
461.1247	1	7977.61	C21 H17 F N6 Na O4	(M+Na)+
462.1247	1	1143.44	C21 H17 F N6 Na O4	(M+Na)+
895.2492	1	33434.67		(2M+Na)+
896.2513	1	16655.05		(2M+Na)+
897.2543	1	4730.77		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	437.1369	437.1368	-0.29	100	100	77.87	77.43
2	438.1395	438.1396	0.26	23.99	25.26	18.68	19.56
3	439.1418	439.1422	0.88	4.42	3.89	3.44	3.01

--- End Of Report ---

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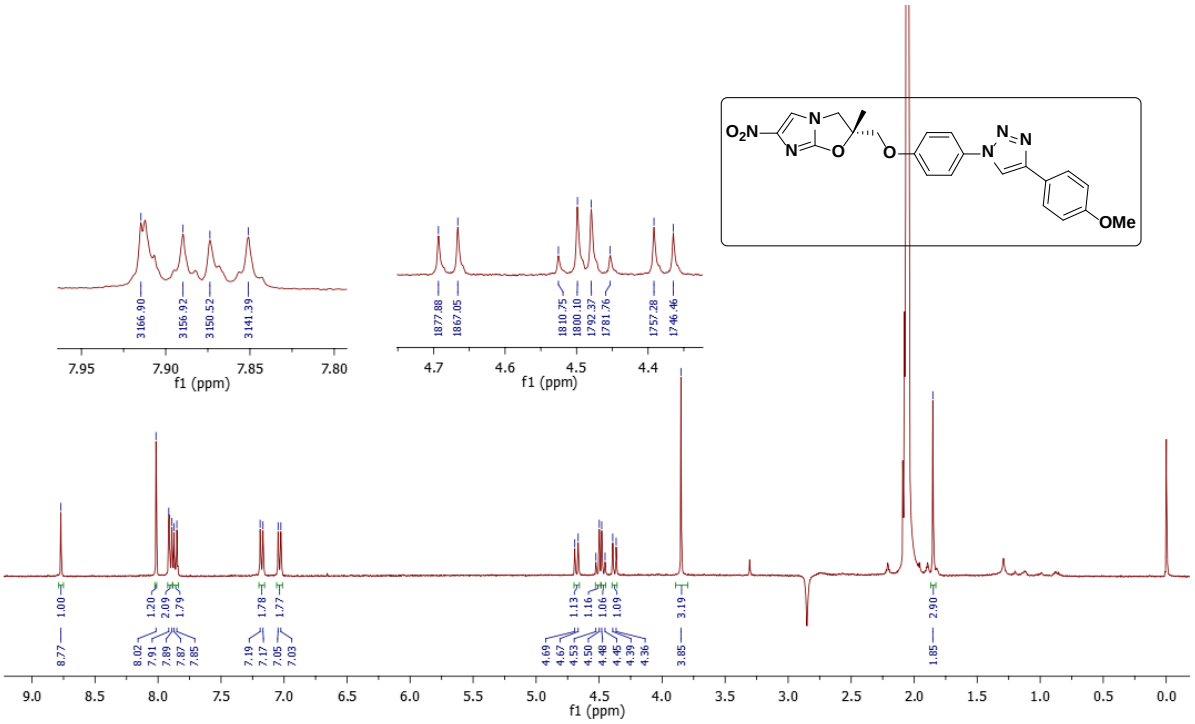
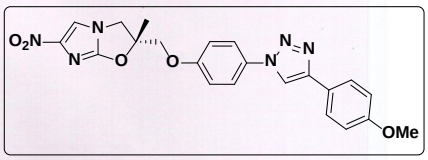
^{1}H NMR (400 MHz, Acetone-d_6) of compound **1o** (**IIIM/MCD-066):**



HRMS (ESI-TOF) of compound **1o** (**IIIM/MCD-066)**:

Qualitative Compound Report

Data File	66.d	**Sample Name**	66
Sample Type	Sample	**Position**	Vial 26
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	27-07-2012 PM 01:01:55
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

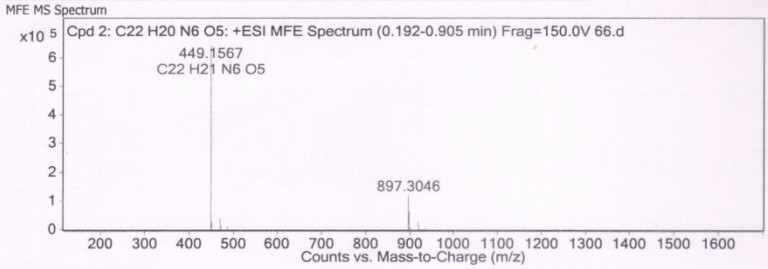


Compound Table

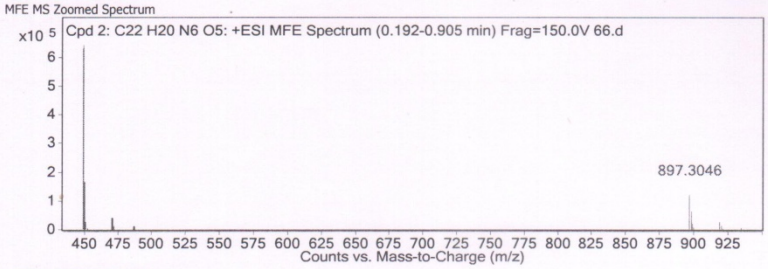
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C22 H20 N6 O5	0.303	448.1494	C22 H20 N6 O5	C22 H20 N6 O5	0.16	C22 H20 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C22 H20 N6 O5	449.1567	0.303	Find by Molecular Feature	448.1494

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

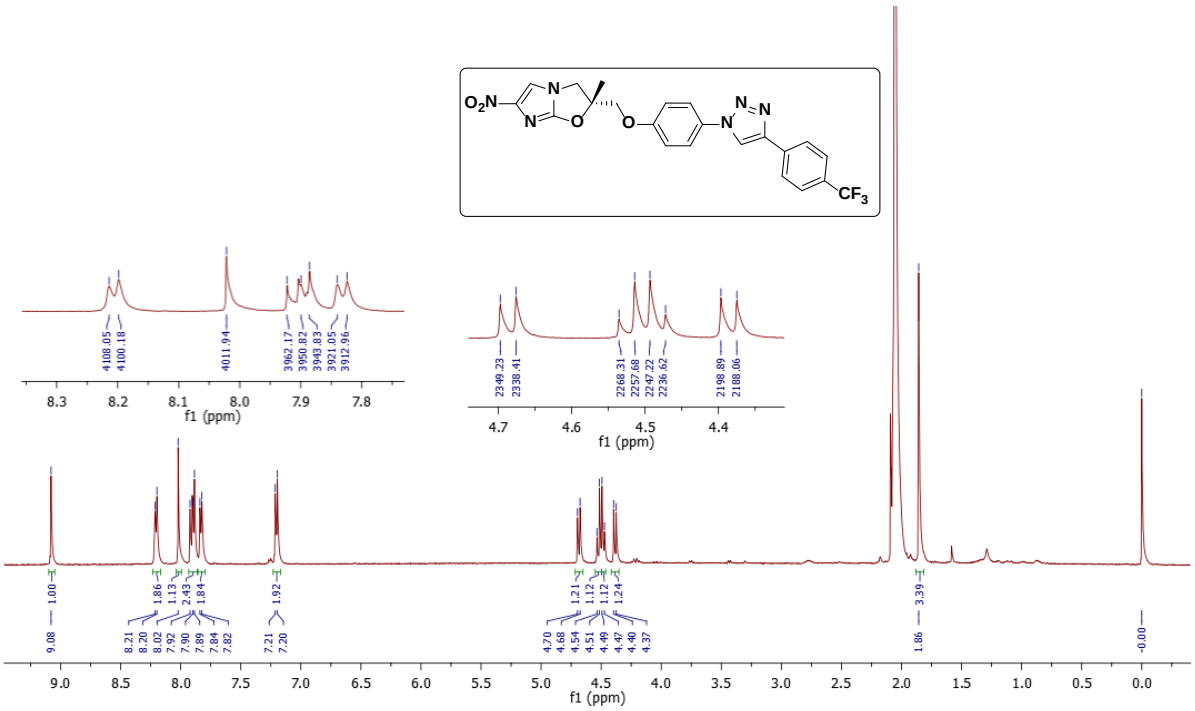
m/z	z	Abund	Formula	Ion
449.1567	1	641743.2	C22 H21 N6 O5	(M+H)+
450.1591	1	154431.4	C22 H21 N6 O5	(M+H)+
451.1613	1	25730.2	C22 H21 N6 O5	(M+H)+
471.1375	1	38784.7	C22 H20 N6 Na O5	(M+Na)+
472.1405	1	11919.6	C22 H20 N6 Na O5	(M+Na)+
897.3046	1	117468.2		(2M+H)+
898.3071	1	62266.8		(2M+H)+
899.3097	1	18730.4		(2M+H)+
919.2857	1	25567.6		(2M+Na)+
920.2893	1	13700.1		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	449.1567	449.1568	0.14	100	100	77.64	76.13
2	450.1591	450.1597	1.3	24.06	26.42	18.68	20.11
3	451.1613	451.1622	1.81	4.01	4.38	3.11	3.34
4	452.1629	452.1646	3.69	0.72	0.54	0.56	0.41

--- End Of Report ---

^{1}H NMR (400 MHz, Acetone-d_6) of compound **1p** (**IIIM/MCD-067):**

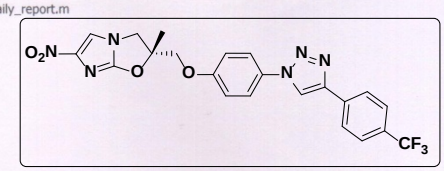


HRMS (ESI-TOF) of compound **1p** (**IIIM/MCD-067)**:

Qualitative Compound Report

Data File	67.d	**Sample Name**	67
Sample Type	Sample	**Position**	Vial 46
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 1:33:49
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)

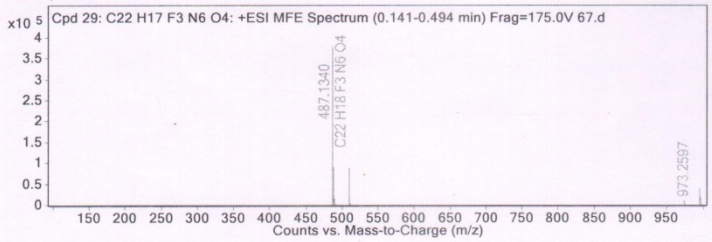


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C22 H17 F3 N6 O4	0.188	486.1266	C22 H17 F3 N6 O4	C22 H17 F3 N6 O4	-0.58	C22 H17 F3 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 29: C22 H17 F3 N6 O4	487.134	0.188	Find by Molecular Feature	486.1266

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
487.134	1	377842.75	C22 H18 F3 N6 O4	(M+H)+
488.1364	1	89091.57	C22 H18 F3 N6 O4	(M+H)+
489.1388	1	14893.67	C22 H18 F3 N6 O4	(M+H)+
509.1155	1	87308.6	C22 H17 F3 N6 Na O4	(M+Na)+
510.1183	1	23297.14	C22 H17 F3 N6 Na O4	(M+Na)+
973.2597	1	10166.56		(2M+H)+
974.2633	1	6208.33		(2M+H)+
995.2419	1	38018.64		(2M+Na)+
996.2453	1	18914.61		(2M+Na)+
997.2482	1	5191.13		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	487.134	487.1336	-0.82	100	100	78.02	76.34
2	488.1364	488.1365	0.06	23.58	26.35	18.4	20.11
3	489.1388	489.139	0.48	3.94	4.16	3.08	3.18
4	490.1383	490.1415	6.54	0.66	0.49	0.51	0.37

--- End Of Report ---

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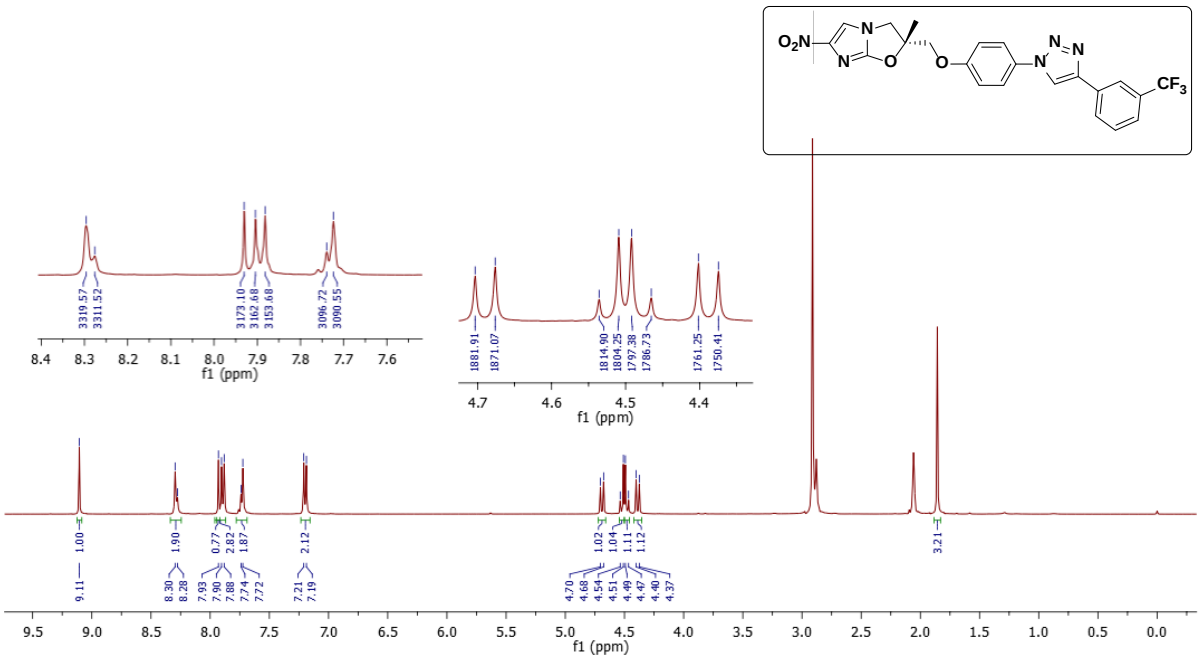
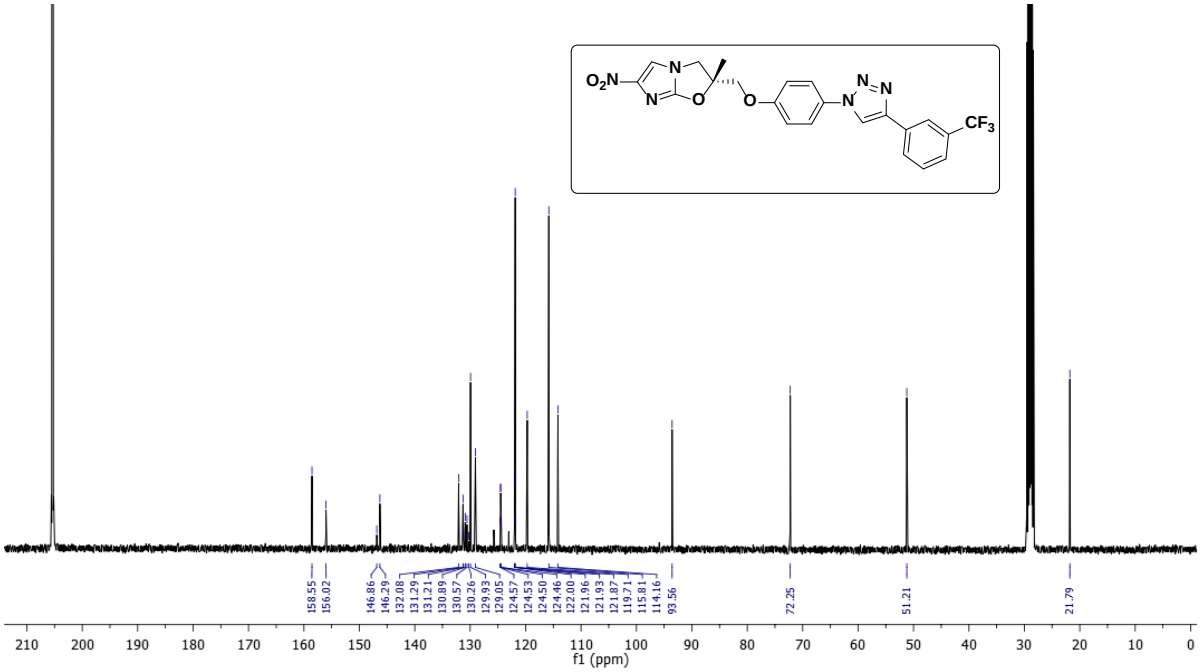
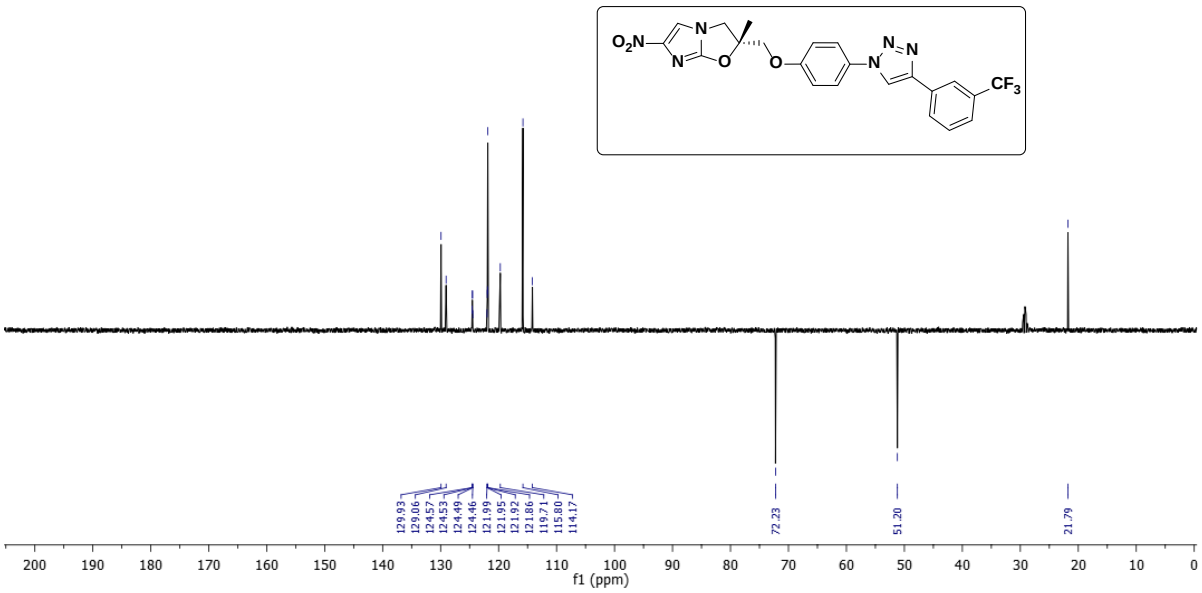
^{1}H NMR (400 MHz, Acetone-d_6) of compound **1q (IIIM/MCD-178):**



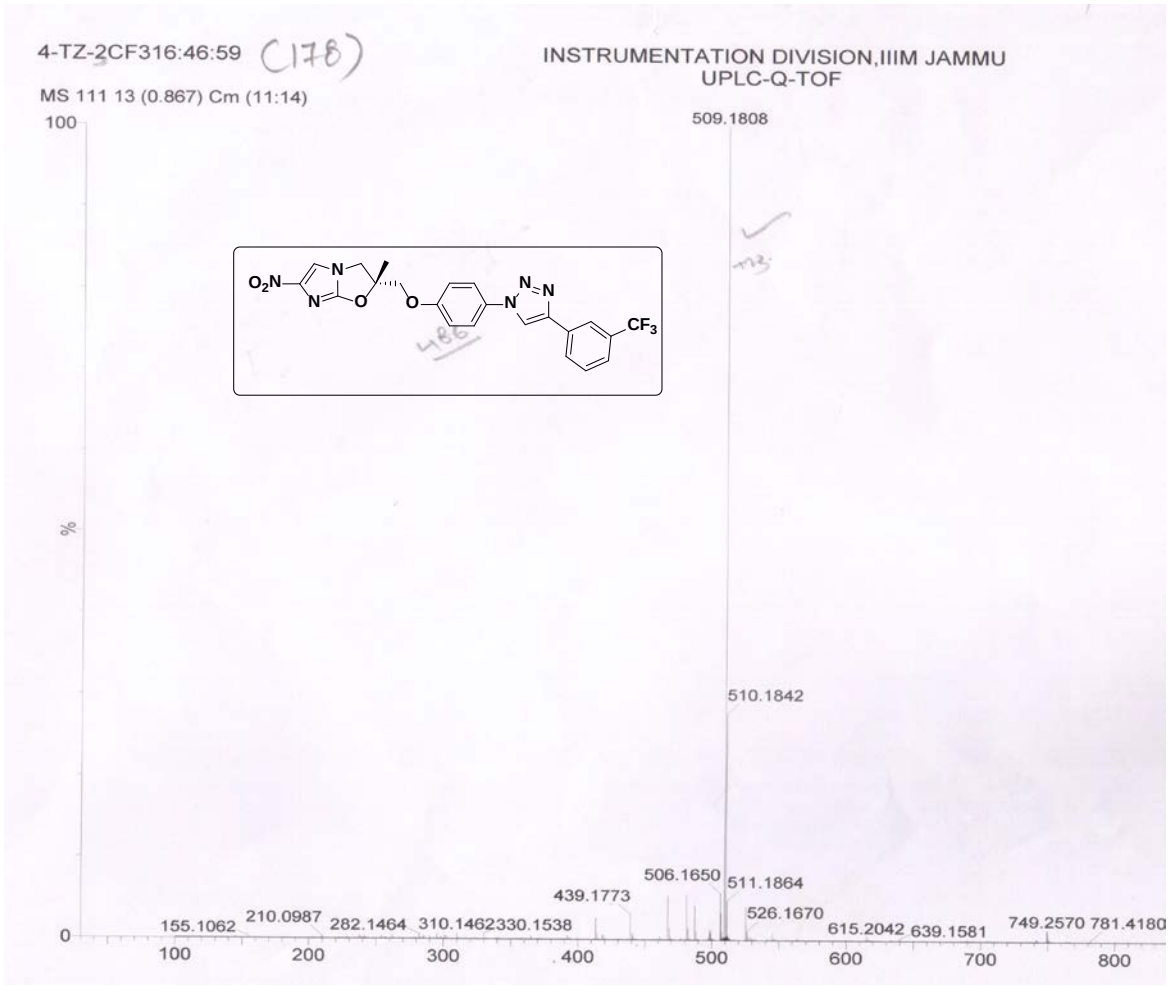
^{13}C NMR (101 MHz, Acetone-d_6) of compound **1q (IIIM/MCD-178):**



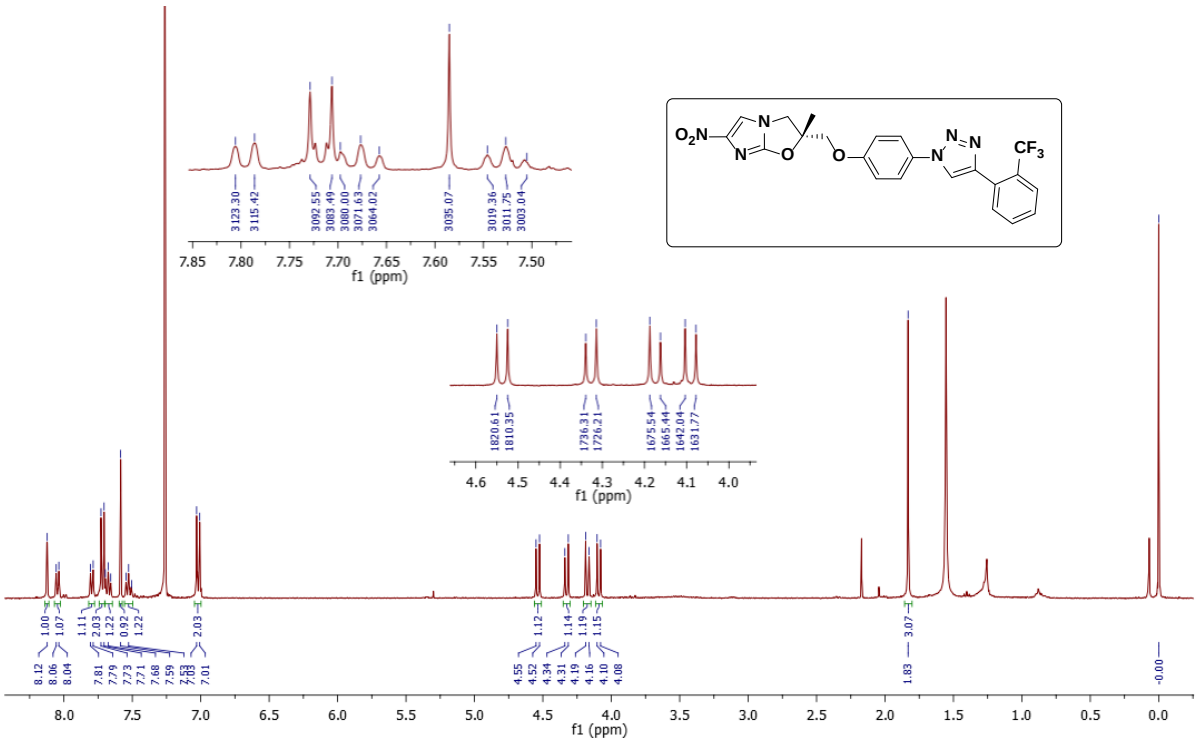
DEPT (101 MHz, Acetone-d_6) of compound **1q (IIIM/MCD-178):**



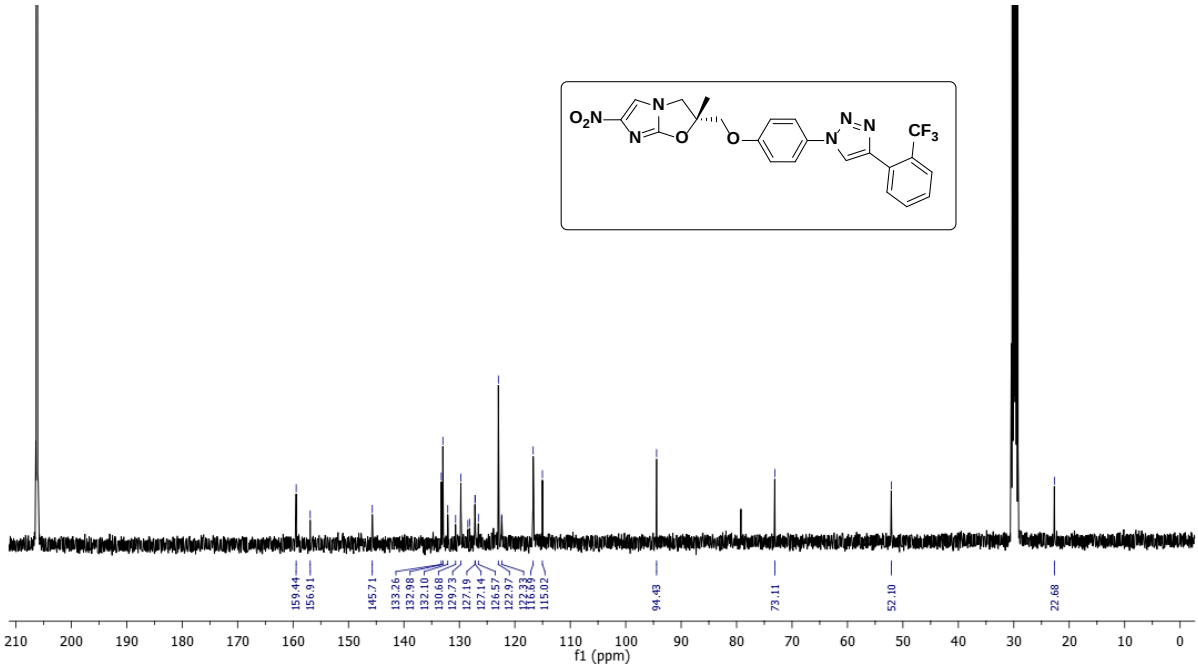
LC-MS (ESI-TOF) of compound **19 (IIIM/MCD-178)**:



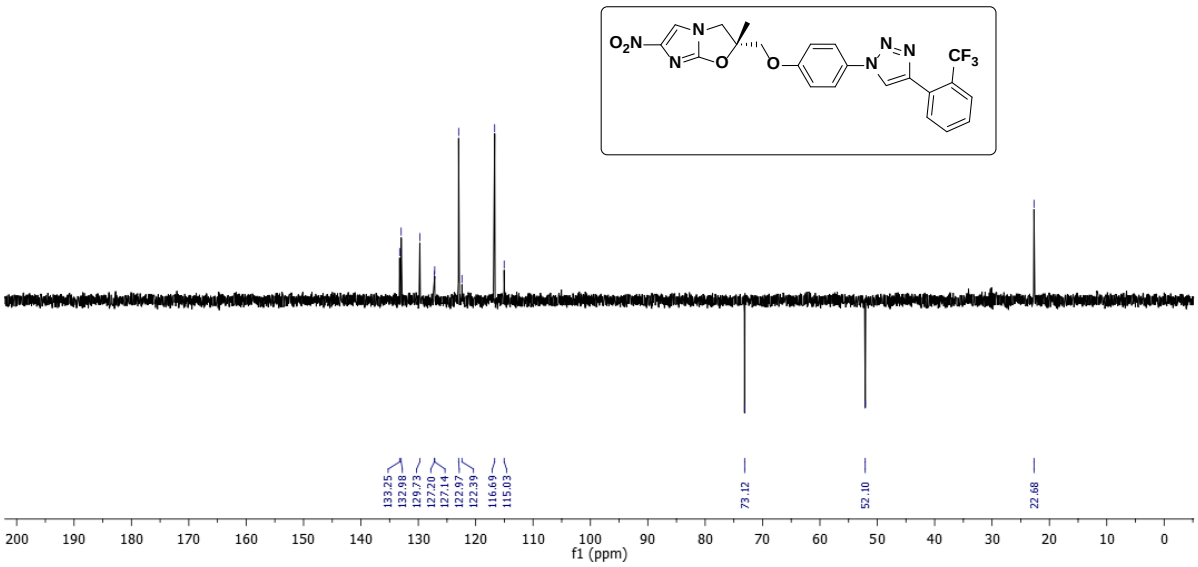
^{1}H NMR (400 MHz, Acetone-d_6) of compound **1r (IIIM/MCD-051):**



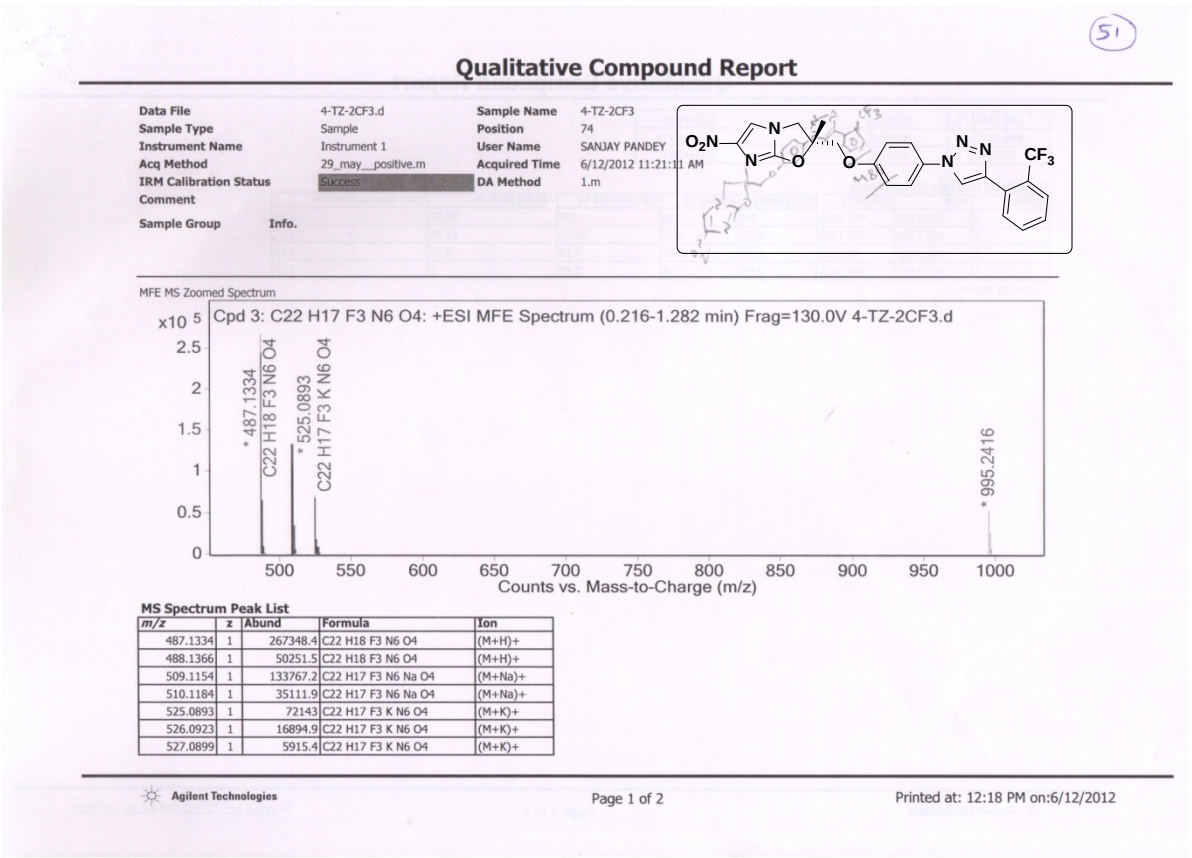
^{13}C NMR (101 MHz, Acetone-d_6) of compound **1r (IIIM/MCD-051):**



DEPT (101 MHz, Acetone-d_6) of compound **1r (IIIM/MCD-051):**



HRMS (ESI-TOF) of compound **1r (IIIM/MCD-051)**:



Qualitative Compound Report

Data File	4-TZ-2CF3.d	Sample Name	4-TZ-2CF3
Sample Type	Sample	Position	74
Instrument Name	Instrument 1	User Name	SANJAY PANDEY
Acq Method	29_may__positive.m	Acquired Time	6/12/2012 11:21:11 AM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group	Info.		

MFE MS Zoomed Spectrum

Cpd 3: C22 H17 F3 N6 O4: +ESI MFE Spectrum (0.216-1.282 min) Frag=130.0V 4-TZ-2CF3.d

x10 5 2.5 2 1.5 1 0.5 0

* 487.1334 C22 H18 F3 N6 O4

* 525.0893 C22 H17 F3 K N6 O4

* 995.2416

500 550 600 650 700 750 800 850 900 950 1000

Counts vs. Mass-to-Charge (m/z)

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
487.1334	1	267348.4	C22 H18 F3 N6 O4	(M+H)+
488.1366	1	50251.5	C22 H18 F3 N6 O4	(M+H)+
509.1154	1	133767.2	C22 H17 F3 N6 Na O4	(M+Na)+
510.1184	1	35111.9	C22 H17 F3 N6 Na O4	(M+Na)+
525.0893	1	72143	C22 H17 F3 K N6 O4	(M+K)+
526.0923	1	16894.9	C22 H17 F3 K N6 O4	(M+K)+
527.0899	1	5915.4	C22 H17 F3 K N6 O4	(M+K)+

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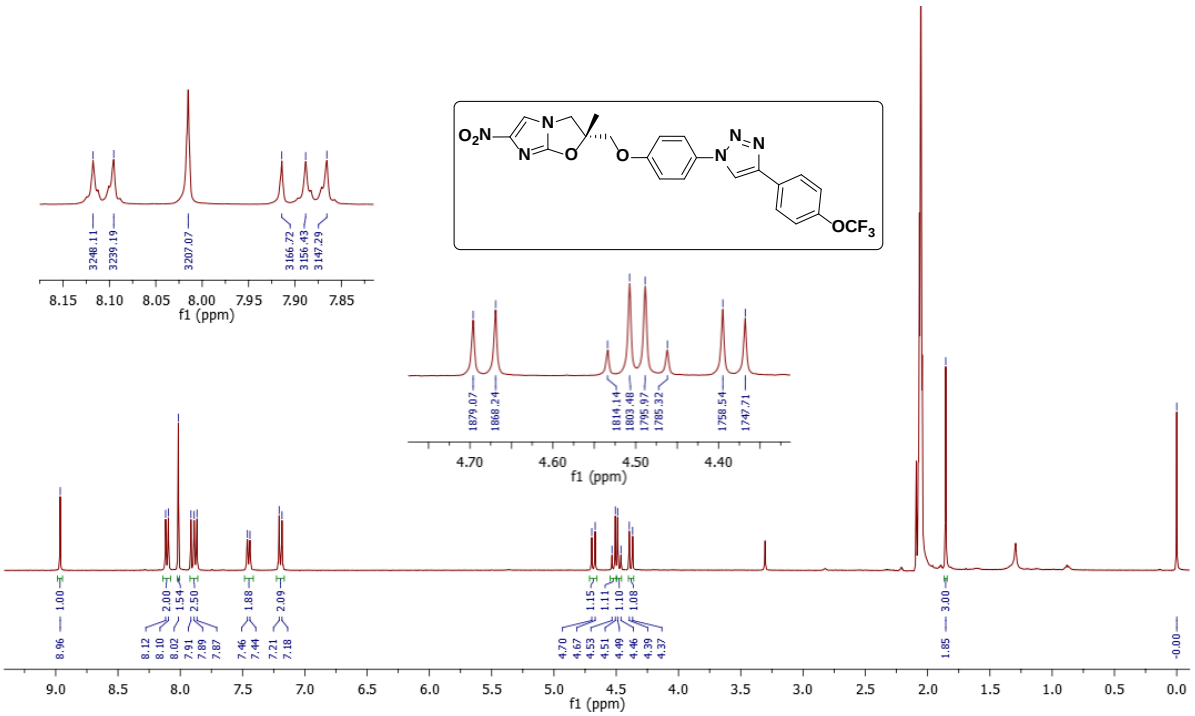
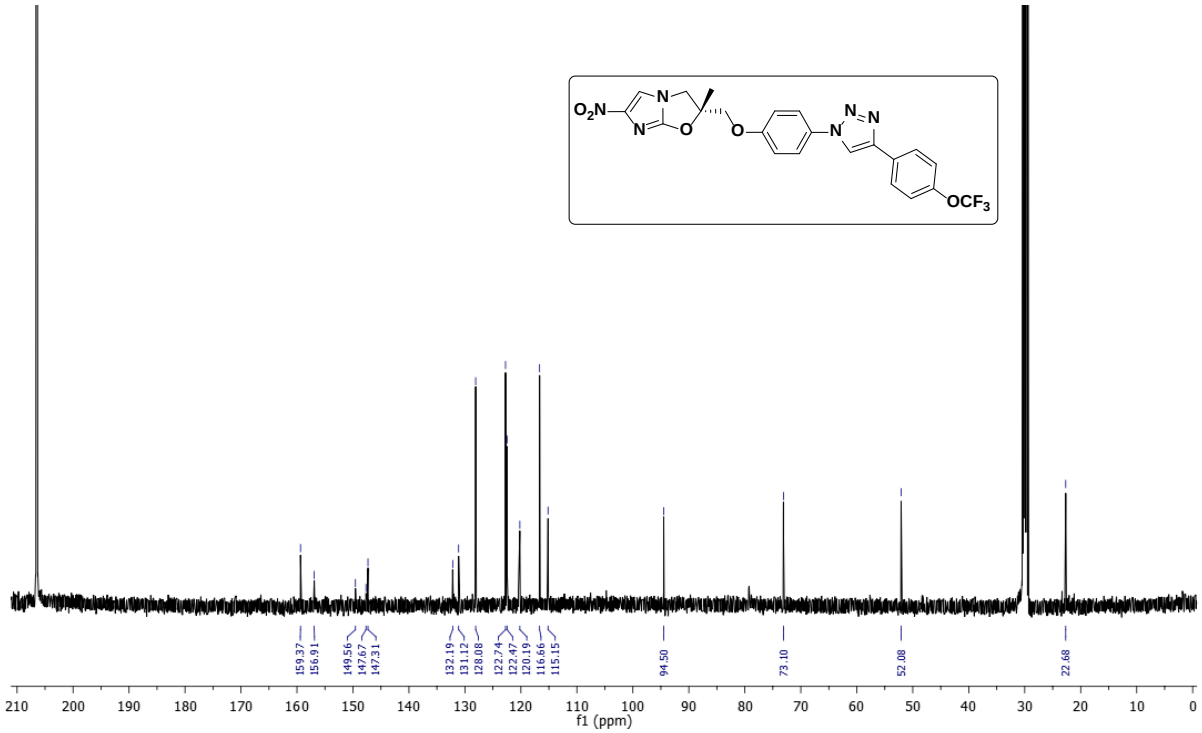
Printed at: 12:18 PM on:6/12/2012

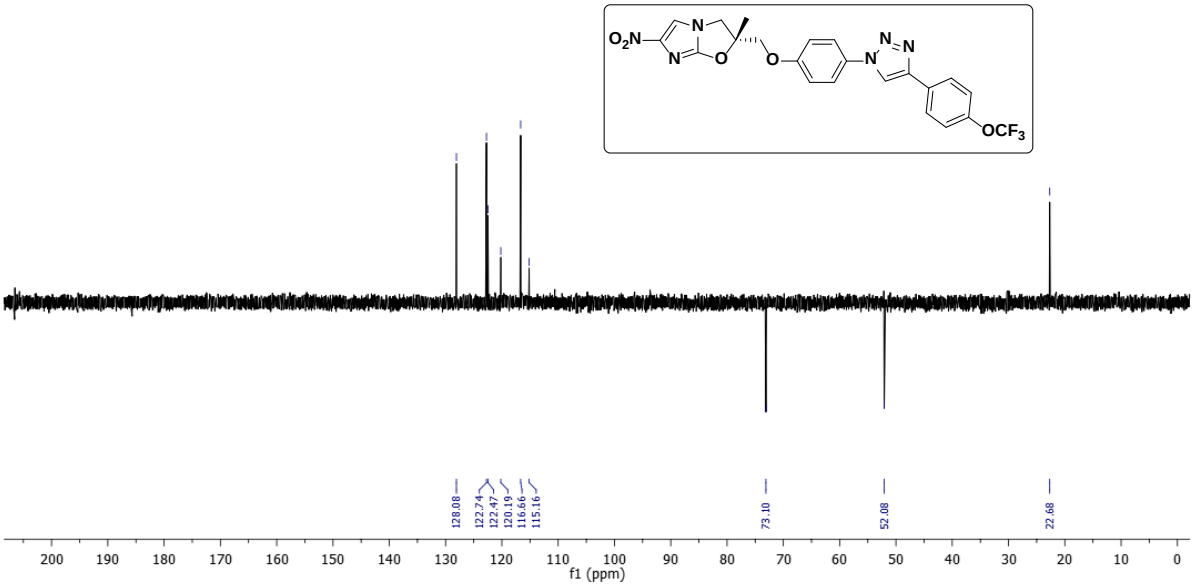
^{1}H NMR (400 MHz, Acetone-d_6) of compound **1s (IIIM/MCD-068):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **1s (IIIM/MCD-068):**



DEPT (126 MHz, Acetone-d_6) of compound **1s (IIIM/MCD-068):**



HRMS (ESI-TOF) of compound **1s (IIIM/MCD-068)**:

Qualitative Compound Report

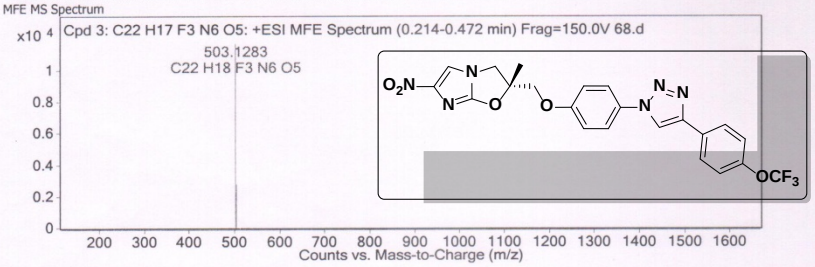
Data File	68.d	**Sample Name**	68
Sample Type	Sample	**Position**	Vial 27
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	27-07-2012 PM 01:07:21
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

Compound Table

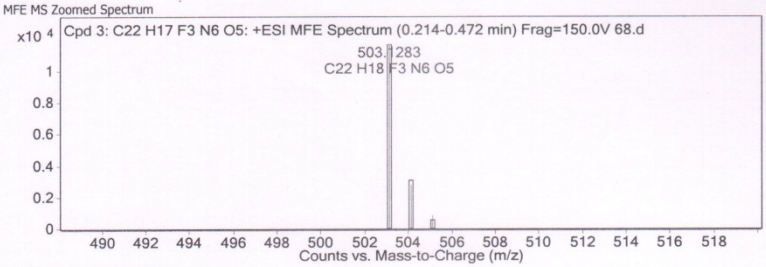
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C22 H17 F3 N6 O5	0.289	502.1211	C22 H17 F3 N6 O5	C22 H17 F3 N6 O5	0.38	C22 H17 F3 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C22 H17 F3 N6 O5	503.1283	0.289	Find by Molecular Feature	502.1211

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

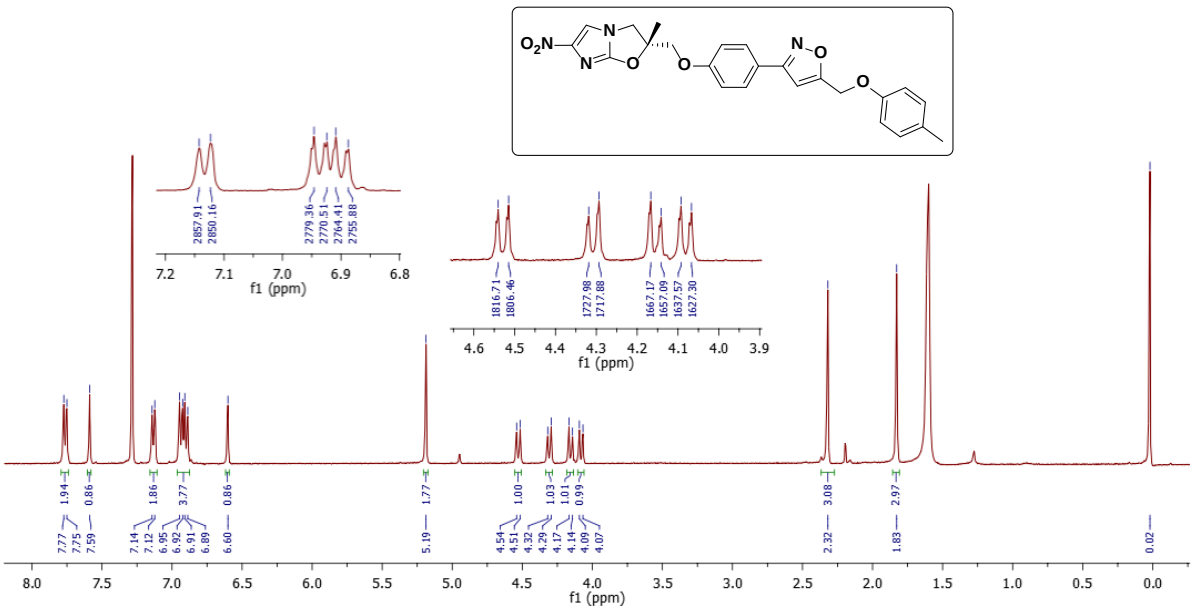
m/z	z	Abund	Formula	Ion
503.1283	1	11679.3	C22 H18 F3 N6 O5	(M+H)+
504.131	1	2756.3	C22 H18 F3 N6 O5	(M+H)+
505.136	1	865.4	C22 H18 F3 N6 O5	(M+H)+

Predicted Isotope Match Table

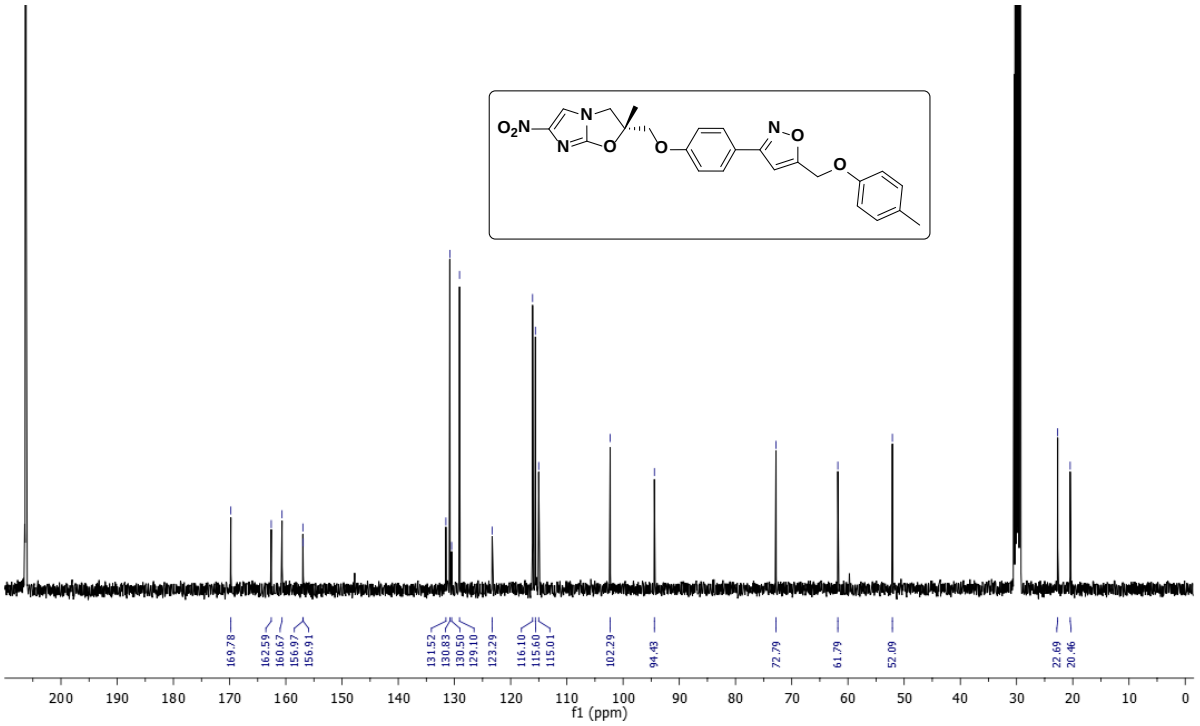
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	503.1283	503.1285	0.38	100	100	76.33	76.48
2	504.131	504.1314	0.67	23.6	26.38	18.01	20.18
3	505.136	505.1339	-4.13	7.41	4.38	5.66	3.35

--- End Of Report ---

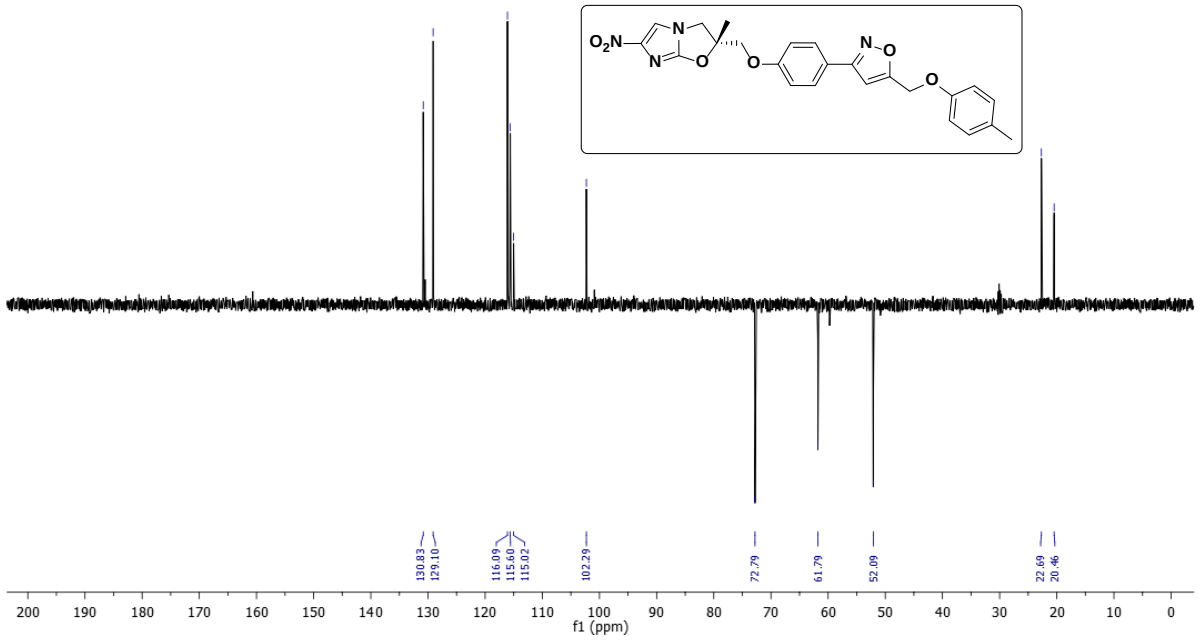
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2a (IIIM/MCD-118):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **2a (IIIM/MCD-118):**



DEPT (101 MHz, Acetone-d_6) of compound **2a (IIIM/MCD-118):**

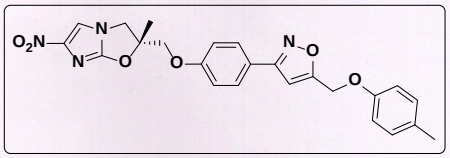


HRMS (ESI-TOF) of compound **2a (IIIM/MCD-118):**

Qualitative Compound Report

Data File	118.d	**Sample Name**	118
Sample Type	Sample	**Position**	Vial 45
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 1:29:17
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)

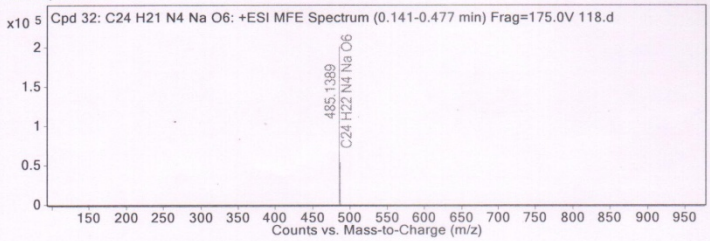


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 32: C24 H21 N4 Na O6	0.19	484.1316	C24 H21 N4 Na O6	C24 H21 N4 Na O6	8.81	C24 H21 N4 Na O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 32: C24 H21 N4 Na O6	485.1389	0.19	Find by Molecular Feature	484.1316

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
485.1389	1	200657.53	C24 H22 N4 Na O6	(M+H)+
486.1418	1	53231.55	C24 H22 N4 Na O6	(M+H)+
487.1447	1	9081.8	C24 H22 N4 Na O6	(M+H)+
488.1493	1	1101.72	C24 H22 N4 Na O6	(M+H)+
489.1476	1	281.95	C24 H22 N4 Na O6	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	485.1389	485.1432	8.73	100	100	75.9	74.84
2	486.1418	486.1462	9.15	26.53	27.9	20.14	20.88
3	487.1447	487.1488	8.42	4.53	4.98	3.44	3.73
4	488.1493	488.1513	4.2	0.55	0.67	0.42	0.5
5	489.1476	489.1538	12.66	0.14	0.07	0.11	0.05

--- End Of Report ---

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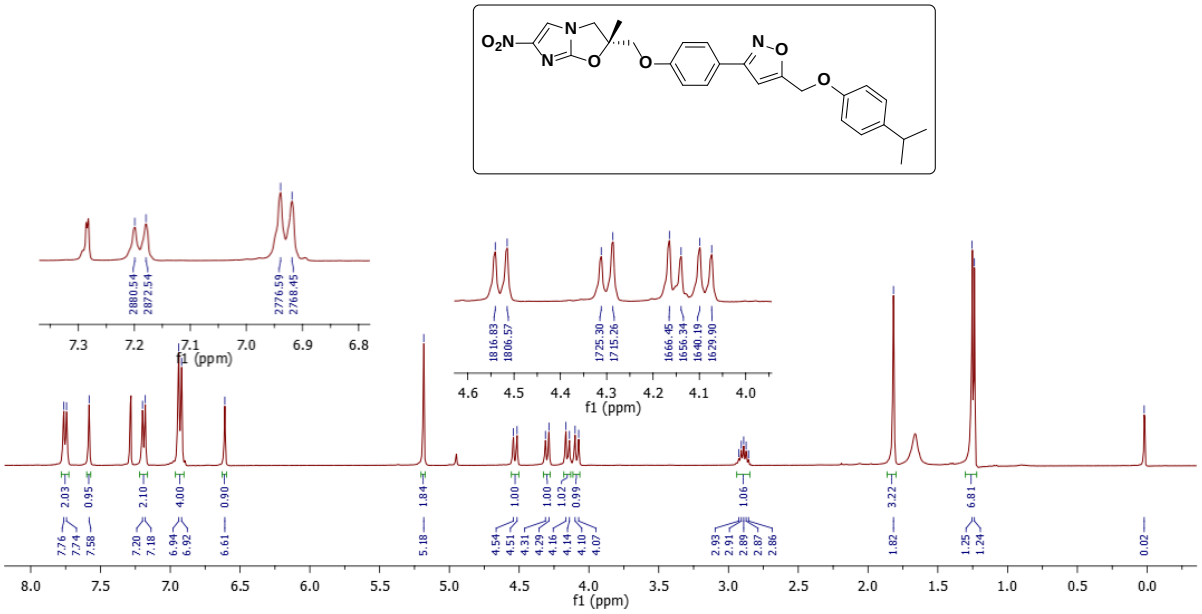
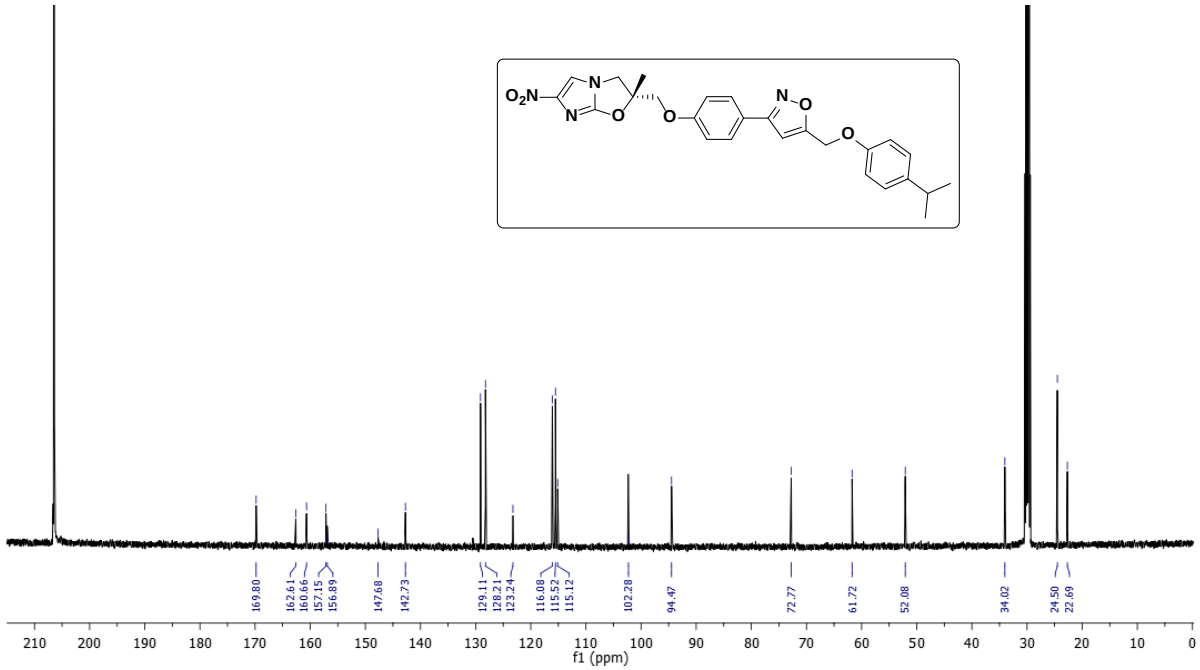
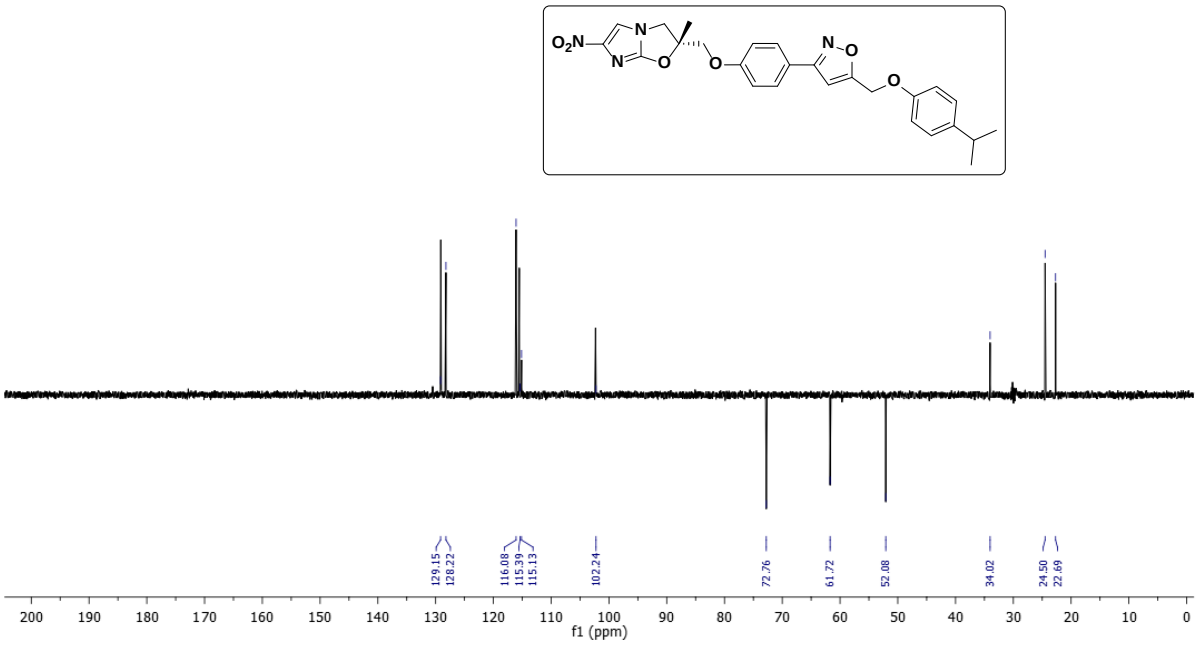
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2b (IIIM/MCD-116):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **2b (IIIM/MCD-116):**



DEPT (126 MHz, Acetone-d_6) of compound **2b (IIIM/MCD-116):**



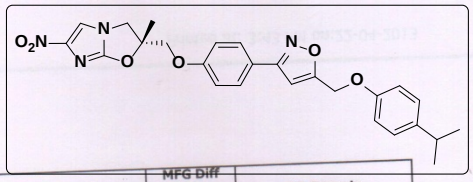
HRMS (ESI-TOF) of compound **2b (IIIM/MCD-116):**

Qualitative Compound Report

Data File	116.d	**Sample Name**	116
Sample Type	Sample	**Position**	Vial 33
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 12:25:04
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

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

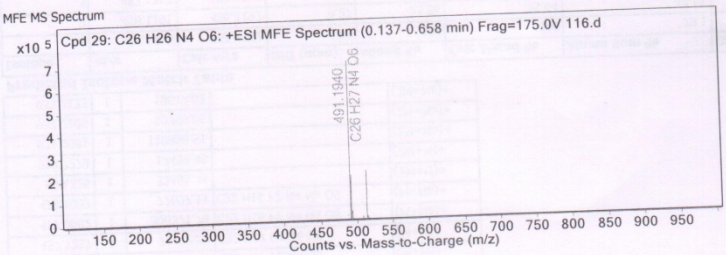


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C26 H26 N4 O6	0.191	490.1865	C26 H26 N4 O6	C26 H26 N4 O6	-2.55	C26 H26 N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 29: C26 H26 N4 O6	491.194	0.191	Find by Molecular Feature	490.1865

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
491.194	1	701826.5	C26 H27 N4 O6	(M+H)+
492.1963	1	192840.44	C26 H27 N4 O6	(M+H)+
493.1987	1	35753.47	C26 H27 N4 O6	(M+H)+
494.2015	1	5000.45	C26 H27 N4 O6	(M+H)+
508.2191	1	10525.7	C26 H30 N5 O6	(M+NH4)+
509.2219	1	3174.05	C26 H30 N5 O6	(M+NH4)+
513.1752	1	214633.56	C26 H26 N4 Na O6	(M+Na)+
514.1778	1	63898.27	C26 H26 N4 Na O6	(M+Na)+
515.1801	1	12696.37	C26 H26 N4 Na O6	(M+Na)+
516.1824	1	2273.56	C26 H26 N4 Na O6	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	491.194	491.1925	-2.96	100	100	74.96	73.2
2	492.1963	492.1956	-1.35	27.48	30.12	20.6	22.05
3	493.1987	493.1982	-1	5.09	5.61	3.82	4.11
4	494.2015	494.2008	-1.27	0.71	0.78	0.53	0.57
5	495.2077	495.2034	-8.72	0.13	0.09	0.1	0.06

--- End Of Report ---

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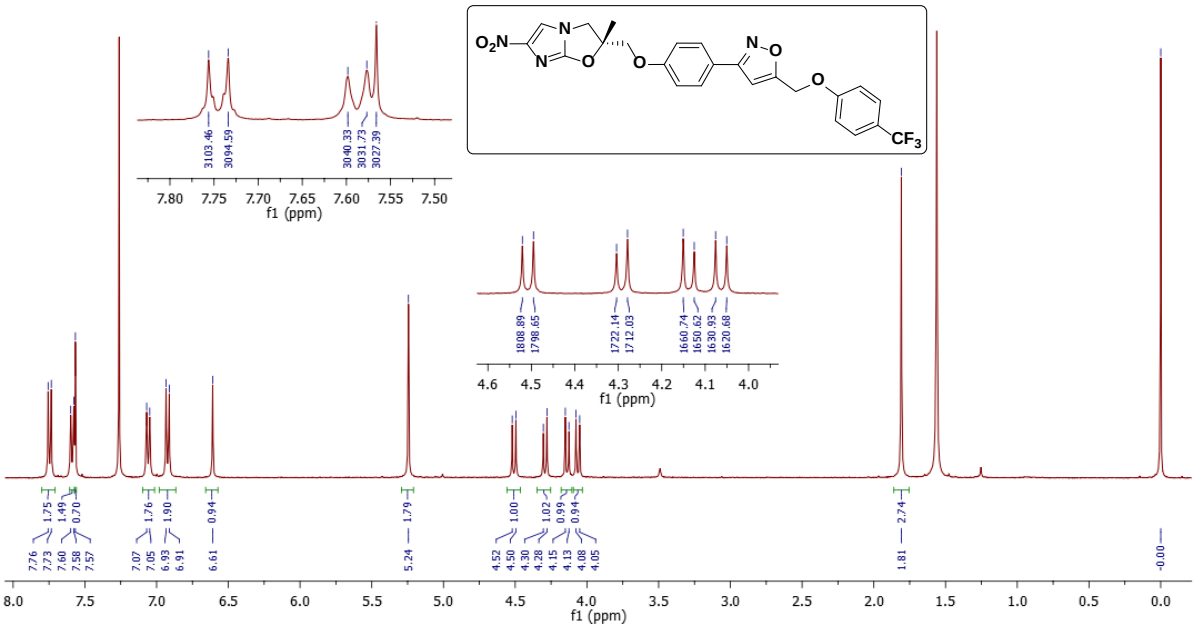
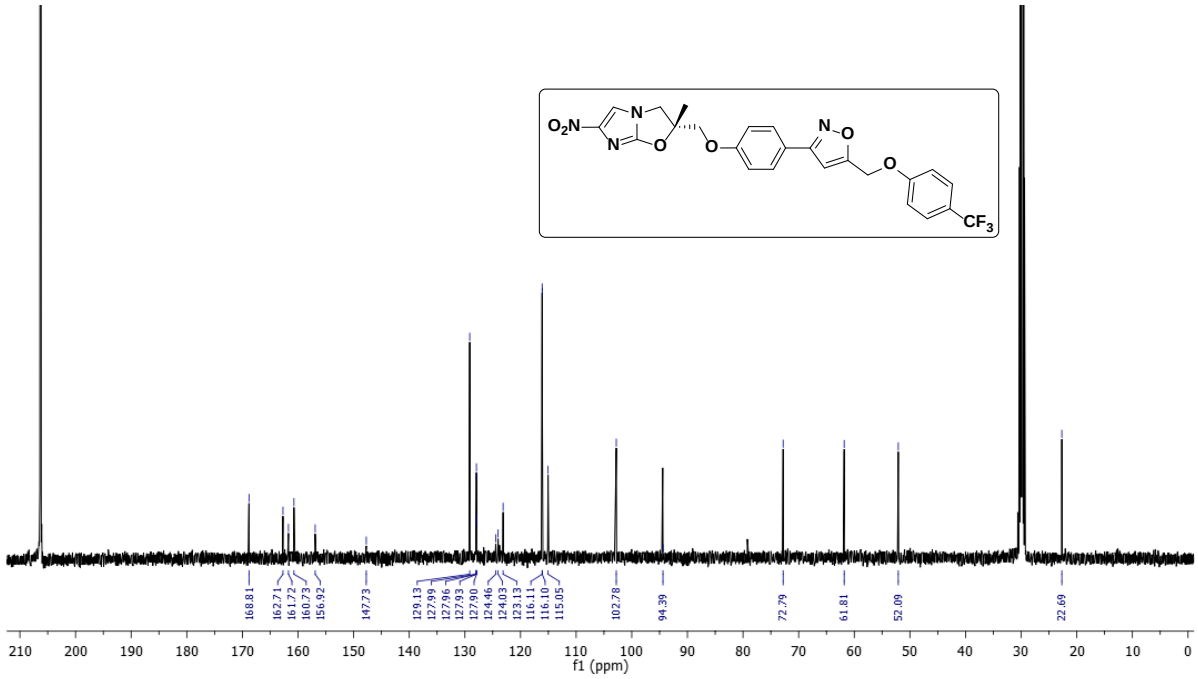
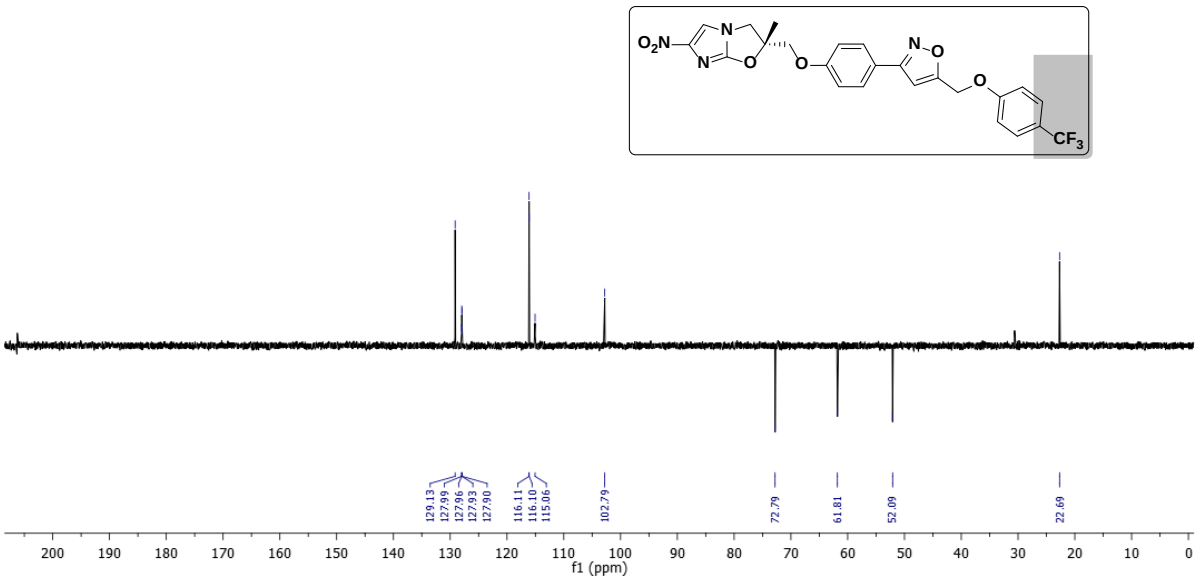
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2c (IIIM/MCD-115):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **2c (IIIM/MCD-115):**



DEPT (126 MHz, Acetone-d_6) of compound **2c (IIIM/MCD-115):**

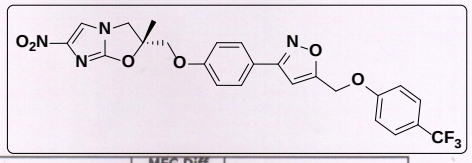


HRMS (ESI-TOF) of compound **2c (IIIM/MCD-115):**

Qualitative Compound Report

Data File	115.d	**Sample Name**	115
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	26-04-2013 PM 1:51:48
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)

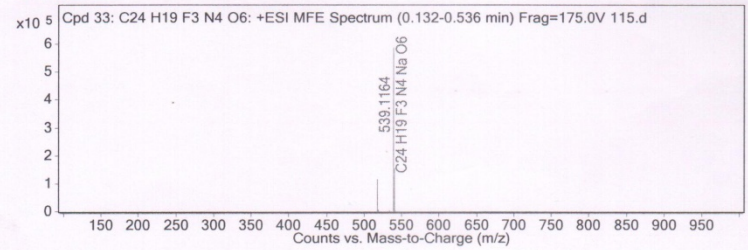


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C24 H19 F3 N4 O6	0.188	516.127	C24 H19 F3 N4 O6	C24 H19 F3 N4 O6	-2.53	C24 H19 F3 N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C24 H19 F3 N4 O6	539.1164	0.188	Find by Molecular Feature	516.127

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
517.1333	1	117501	C24 H20 F3 N4 O6	(M+H)+
518.1364	1	30969.21	C24 H20 F3 N4 O6	(M+H)+
519.1394	1	5188.86	C24 H20 F3 N4 O6	(M+H)+
520.1442	1	772.91	C24 H20 F3 N4 O6	(M+H)+
534.1595	1	4360.68	C24 H23 F3 N5 O6	(M+NH4)+
535.1643	1	1491.41	C24 H23 F3 N5 O6	(M+NH4)+
539.1164	1	586815.75	C24 H19 F3 N4 Na O6	(M+Na)+
540.1187	1	155128.55	C24 H19 F3 N4 Na O6	(M+Na)+
541.1205	1	24116.08	C24 H19 F3 N4 Na O6	(M+Na)+
542.1234	1	3842.85	C24 H19 F3 N4 Na O6	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	517.1333	517.1329	-0.62	100	100	76.09	74.9
2	518.1364	518.136	-0.75	26.36	27.88	20.05	20.88
3	519.1394	519.1386	-1.59	4.42	4.98	3.36	3.73
4	520.1442	520.1411	-5.89	0.66	0.67	0.5	0.5

--- End Of Report ---

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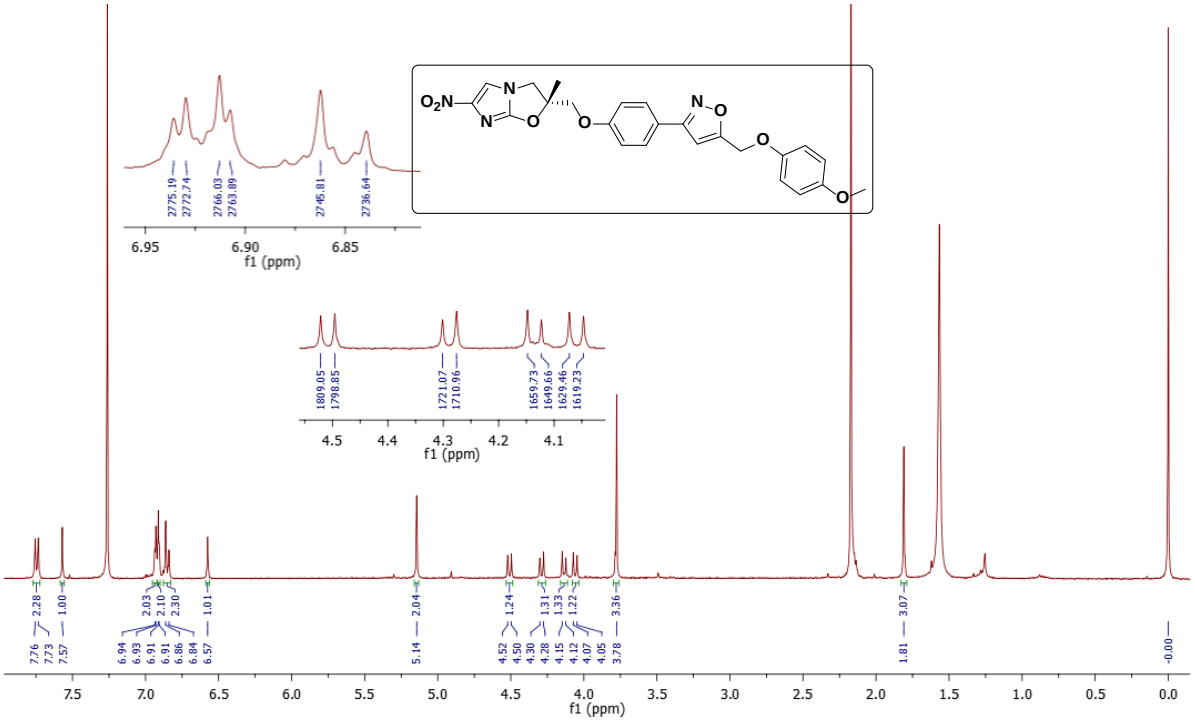
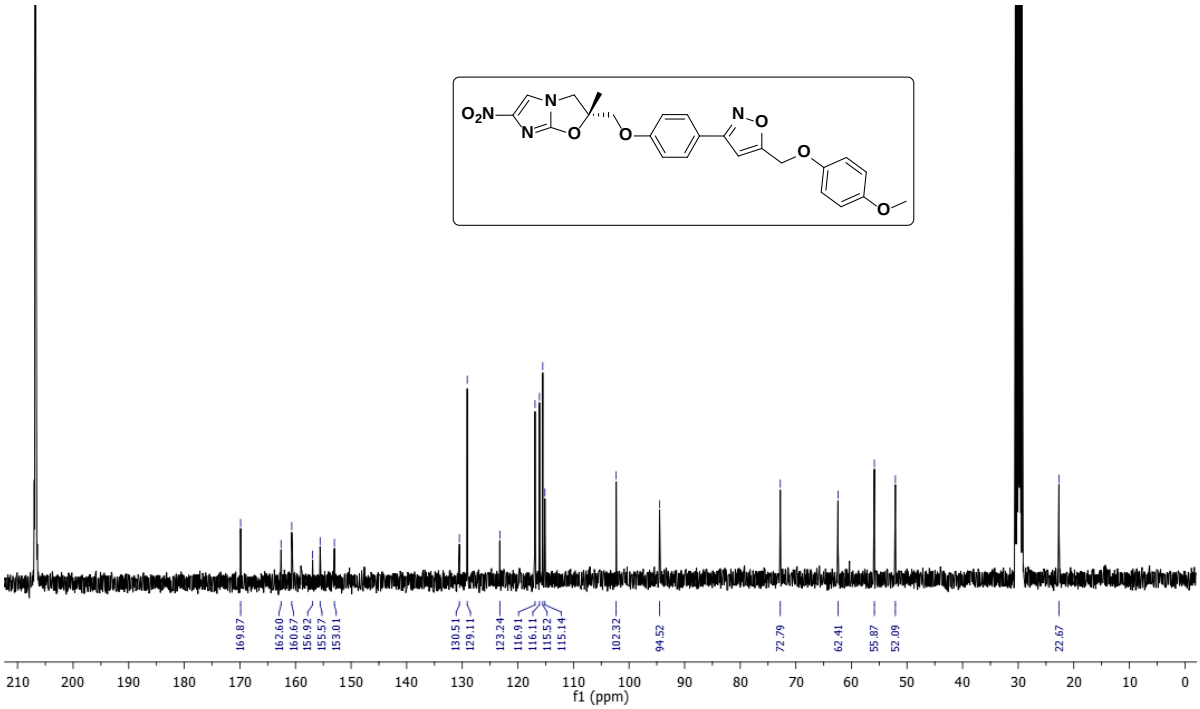
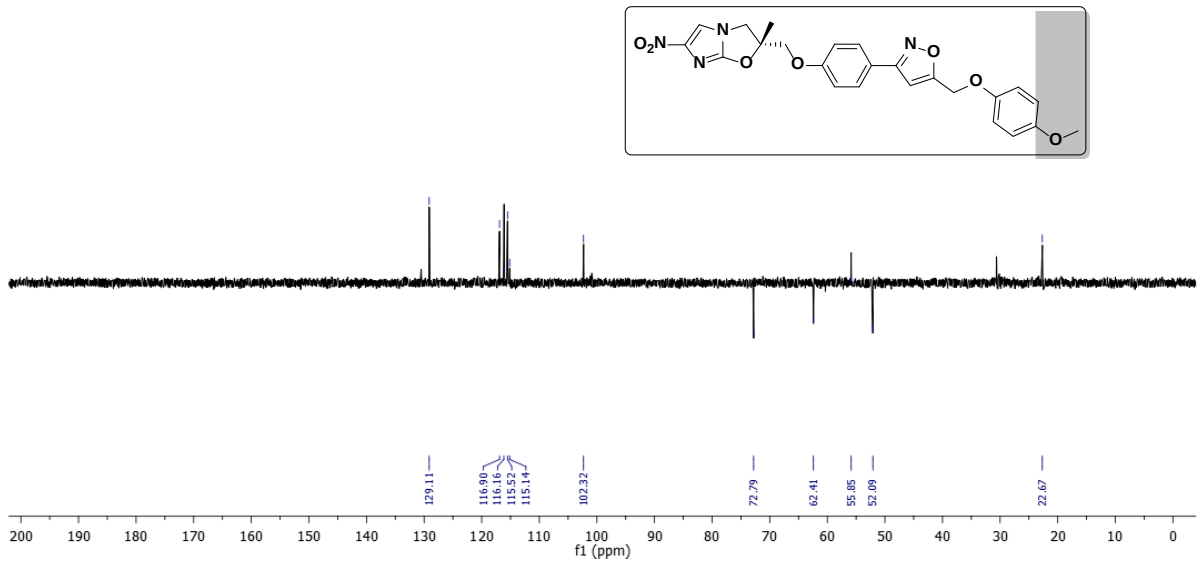
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2d (IIIM/MCD-128):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **2d (IIIM/MCD-128):**



DEPT (101 MHz, Acetone-d_6) of compound **2d (IIIM/MCD-128):**

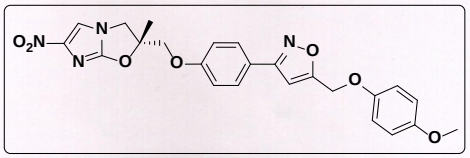


HRMS (ESI-TOF) of compound **2d (IIIM/MCD-128):**

Qualitative Compound Report

Data File	128.d	**Sample Name**	128
Sample Type	Sample	**Position**	Vial 30
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	04-03-2013 PM 2:58:51
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

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

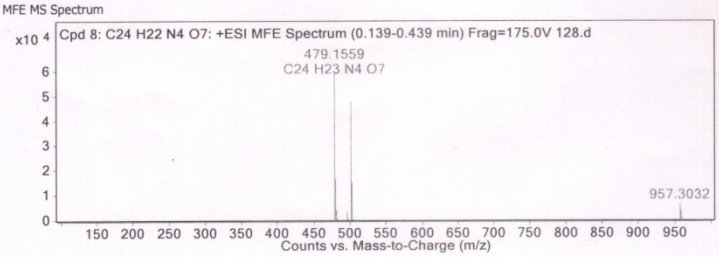


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C24 H22 N4 O7	0.192	478.1486	C24 H22 N4 O7	C24 H22 N4 O7	0.44	C24 H22 N4 O7

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C24 H22 N4 O7	479.1559	0.192	Find by Molecular Feature	478.1486

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
479.1559	1	60041.71	C24 H23 N4 O7	(M+H)+
480.1589	1	16531.63	C24 H23 N4 O7	(M+H)+
481.1615	1	4009.54	C24 H23 N4 O7	(M+H)+
496.1829	1	3356.4	C24 H26 N5 O7	(M+NH4)+
501.1382	1	47570.77	C24 H22 N4 Na O7	(M+Na)+
502.1401	1	15183.67	C24 H22 N4 Na O7	(M+Na)+
503.1461	1	2882.35	C24 H22 N4 Na O7	(M+Na)+
957.3032	1	6431.53		(2M+H)+
958.3062	1	4033.15		(2M+H)+
959.3107	1	1317.64		(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	479.1559	479.1561	0.4	100	100	73.95	74.69
2	480.1589	480.1592	0.66	27.53	27.95	20.36	20.88
3	481.1615	481.1617	0.46	6.68	5.2	4.94	3.89
4	482.1653	482.1643	-2.26	1.02	0.73	0.76	0.54

--- End Of Report ---

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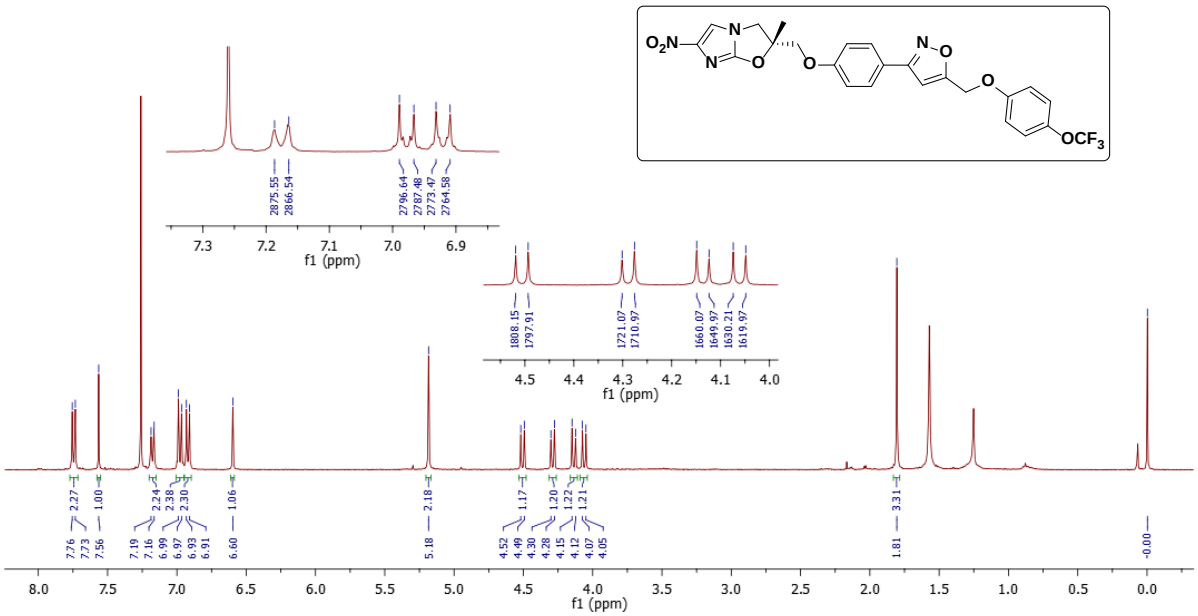
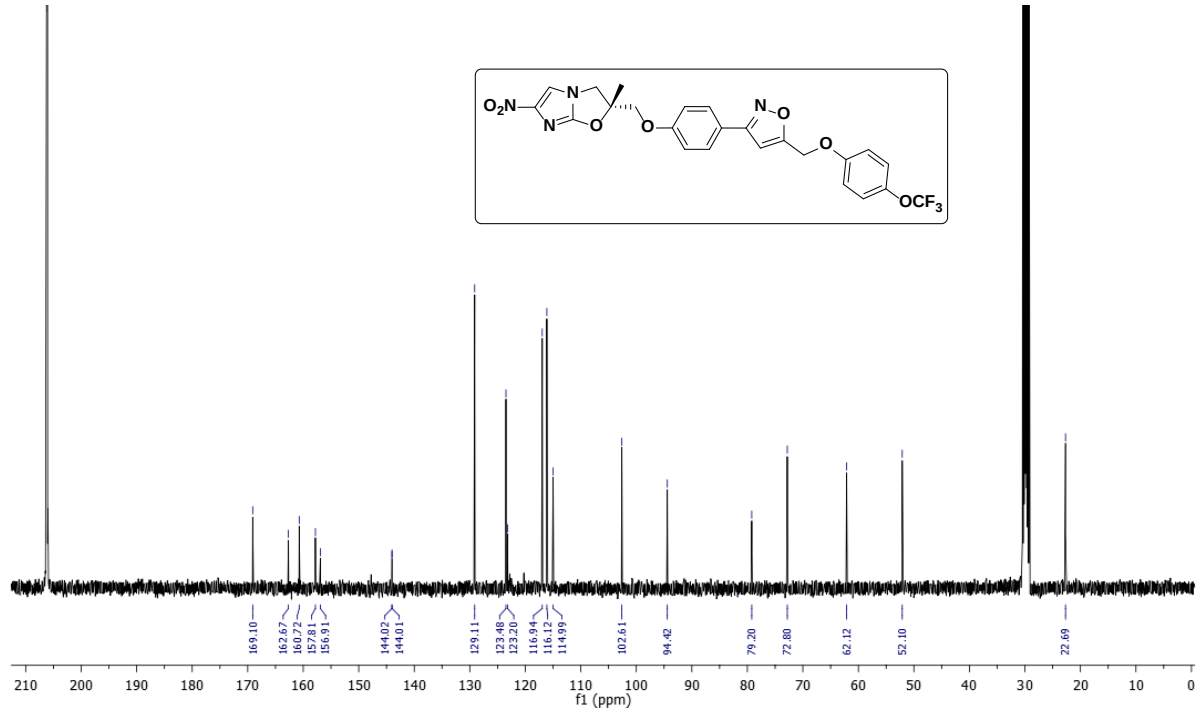
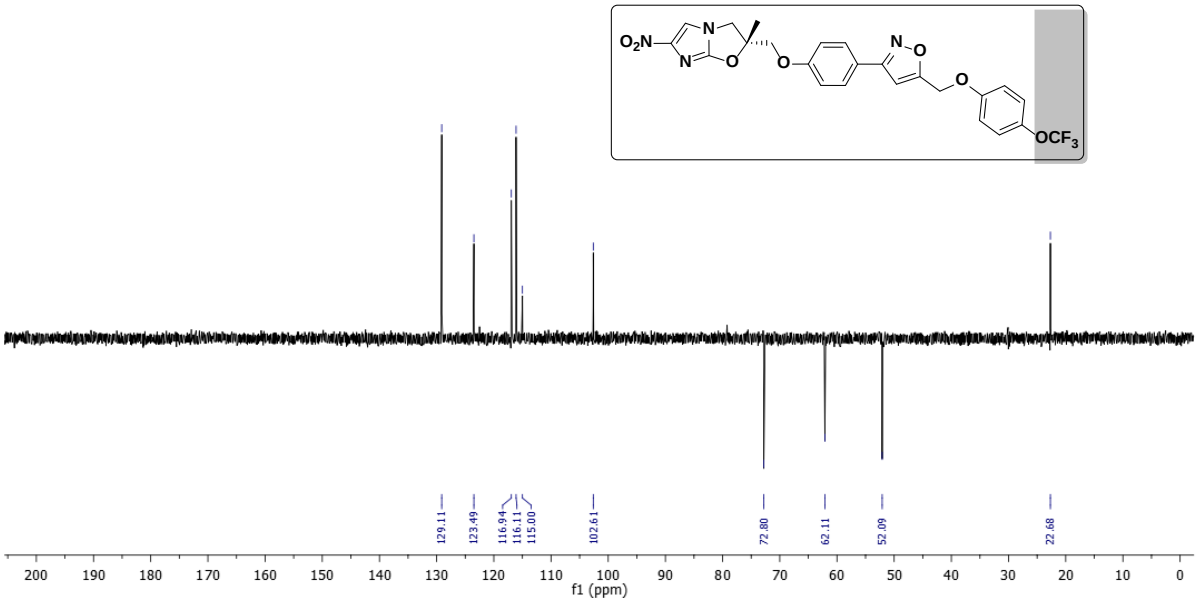
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2e (IIIM/MCD-069):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **2e (IIIM/MCD-069):**



DEPT (101 MHz, Acetone-d_6) of compound **2e (IIIM/MCD-069):**

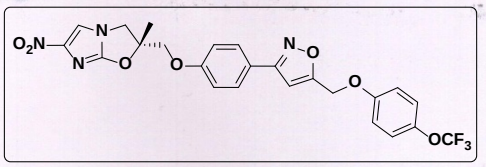


HRMS (ESI-TOF) of compound **2e (IIIM/MCD-069)**:

Qualitative Compound Report

Data File	69.d	**Sample Name**	69
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:48:42
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)

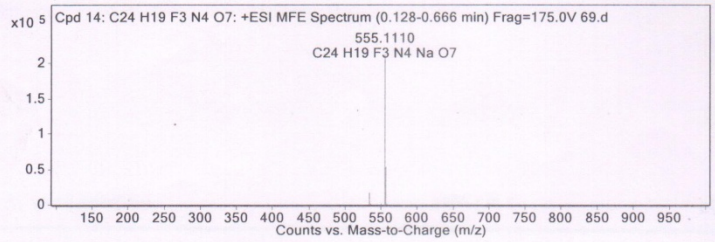


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C24 H19 F3 N4 O7	0.188	532.1215	C24 H19 F3 N4 O7	C24 H19 F3 N4 O7	-1.74	C24 H19 F3 N4 O7

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C24 H19 F3 N4 O7	555.111	0.188	Find by Molecular Feature	532.1215

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
533.1277	1	16662.8	C24 H20 F3 N4 O7	(M+H)+
534.1311	1	4643.86	C24 H20 F3 N4 O7	(M+H)+
535.1328	1	1436.28	C24 H20 F3 N4 O7	(M+H)+
550.1538	1	994.31	C24 H23 F3 N5 O7	(M+NH4)+
555.111	1	211875.69	C24 H19 F3 N4 Na O7	(M+Na)+
556.1129	1	53332.46	C24 H19 F3 N4 Na O7	(M+Na)+
557.1151	1	9635.07	C24 H19 F3 N4 Na O7	(M+Na)+
558.1168	1	1639.74	C24 H19 F3 N4 Na O7	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	533.1277	533.1279	0.23	100	100	73.27	75.13
2	534.1311	534.1309	-0.36	27.87	27.92	20.42	20.97
3	535.1328	535.1334	1.24	8.62	5.19	6.32	3.9

--- End Of Report ---

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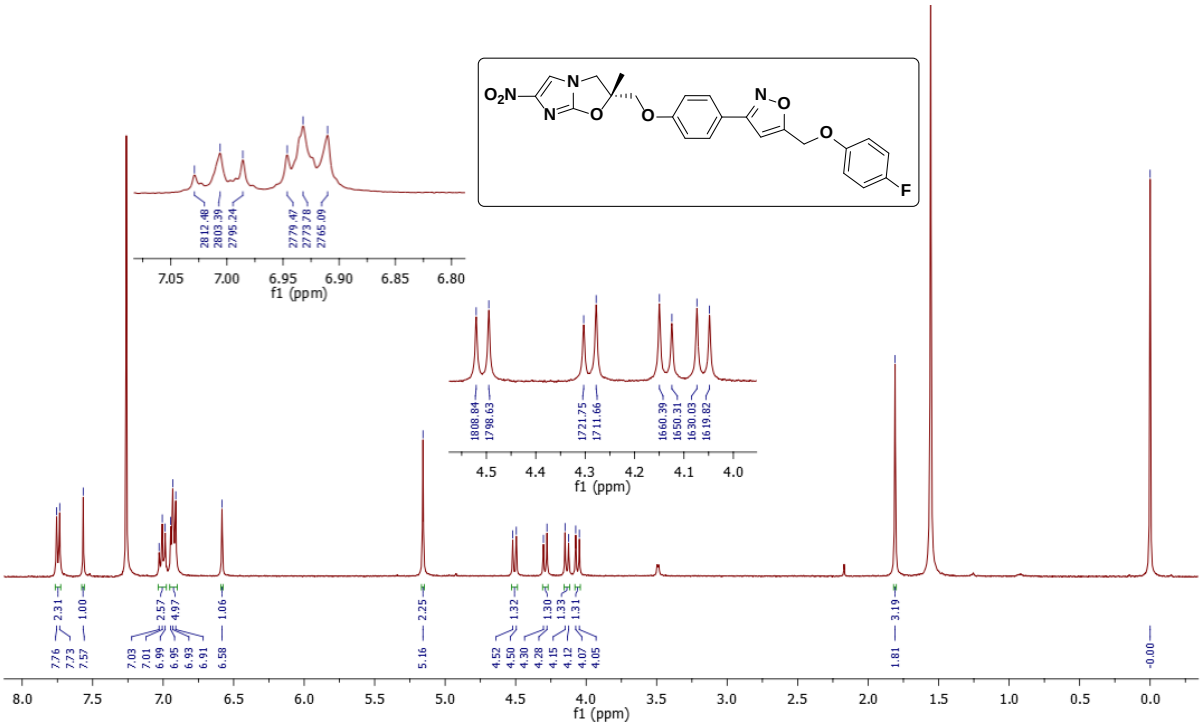
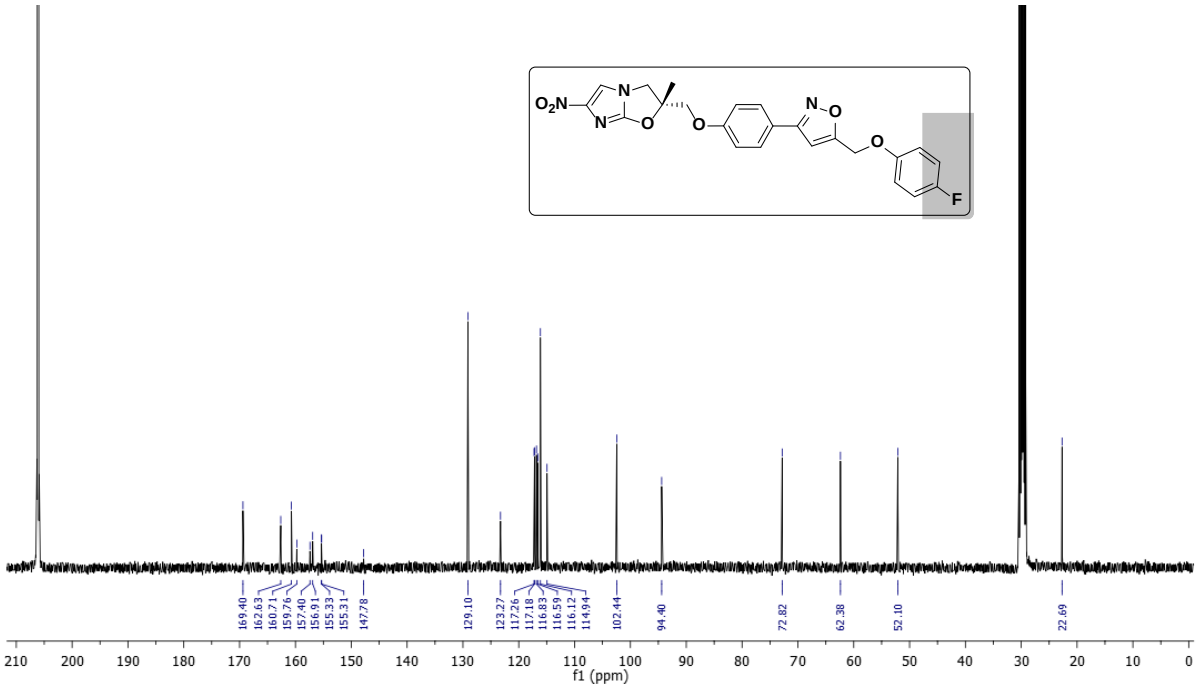
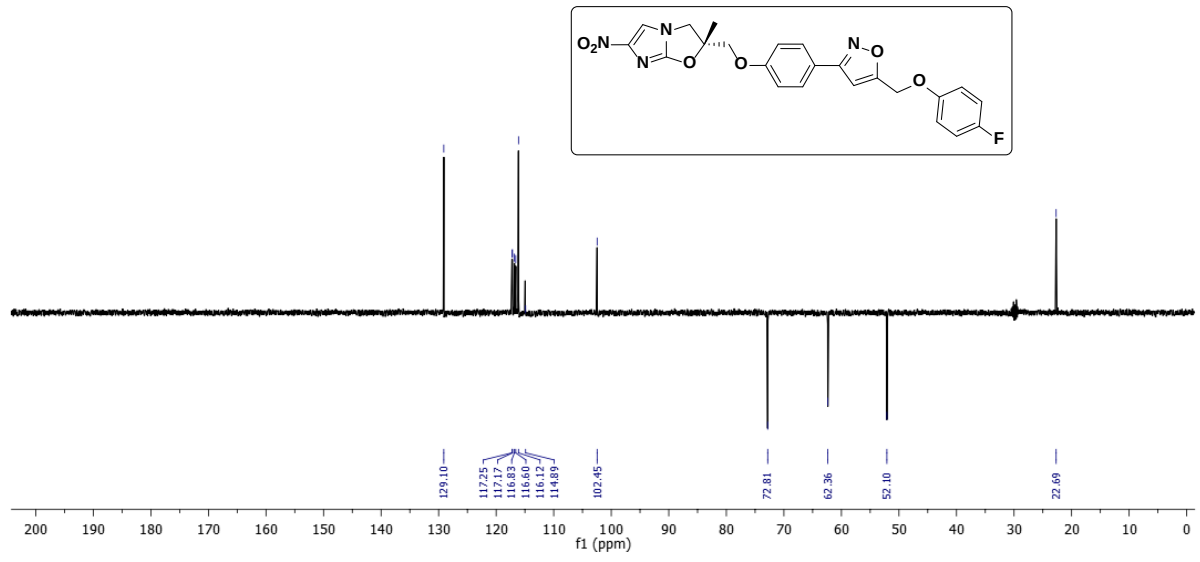
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2f (IIIM/MCD-114):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **2f (IIIM/MCD-114):**



DEPT (101 MHz, Acetone-d_6) of compound **2f (IIIM/MCD-114):**

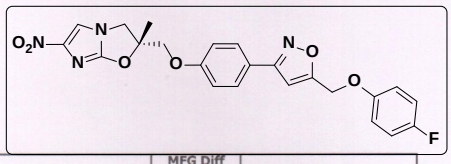


HRMS (ESI-TOF) of compound **2f (IIIM/MCD-114)**:

Qualitative Compound Report

Data File	114.d	**Sample Name**	114
Sample Type	Sample	**Position**	Vial 8
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-04-2013 PM 1:33:25
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)

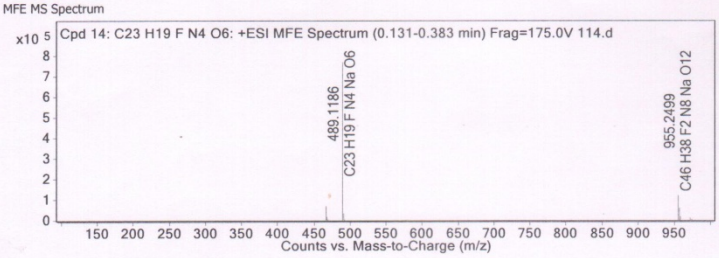


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C23 H19 F N4 O6	0.191	466.129	C23 H19 F N4 O6	C23 H19 F N4 O6	-0.33	C23 H19 F N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C23 H19 F N4 O6	489.1186	0.191	Find by Molecular Feature	466.129

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
467.1364	1	71133.53	C23 H20 F N4 O6	(M+H)+
468.1394	1	18972.37	C23 H20 F N4 O6	(M+H)+
489.1186	1	769131	C23 H19 F N4 Na O6	(M+Na)+
490.1206	1	201429.91	C23 H19 F N4 Na O6	(M+Na)+
491.1207	1	35261.13	C23 H19 F N4 Na O6	(M+Na)+
955.2499	1	121049.98	C46 H38 F2 N8 Na O12	(2M+Na)+
956.2518	1	60082.35	C46 H38 F2 N8 Na O12	(2M+Na)+
957.2536	1	17433.57	C46 H38 F2 N8 Na O12	(2M+Na)+
971.2216	1	11439.14	C46 H38 F2 K N8 O12	(2M+K)+
972.2253	1	6334.54	C46 H38 F2 K N8 O12	(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	467.1364	467.1361	-0.61	100	100	76.31	76.06
2	468.1394	468.1392	-0.46	26.67	26.8	20.35	20.38
3	469.1426	469.1417	-1.85	4.37	4.69	3.33	3.56

--- End Of Report ---

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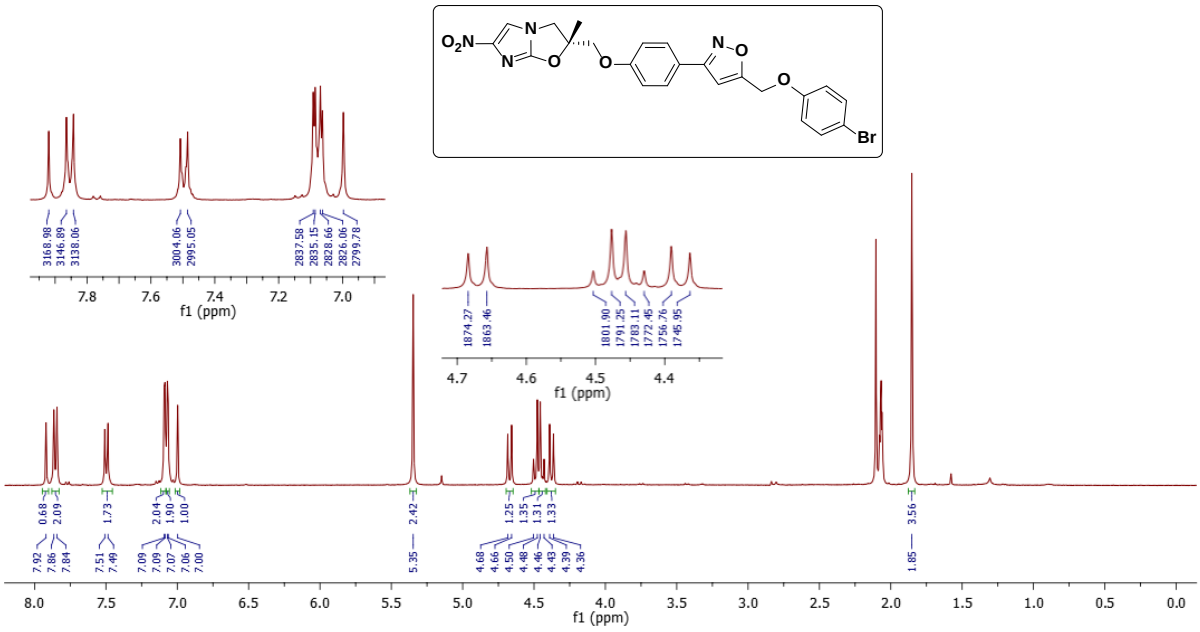
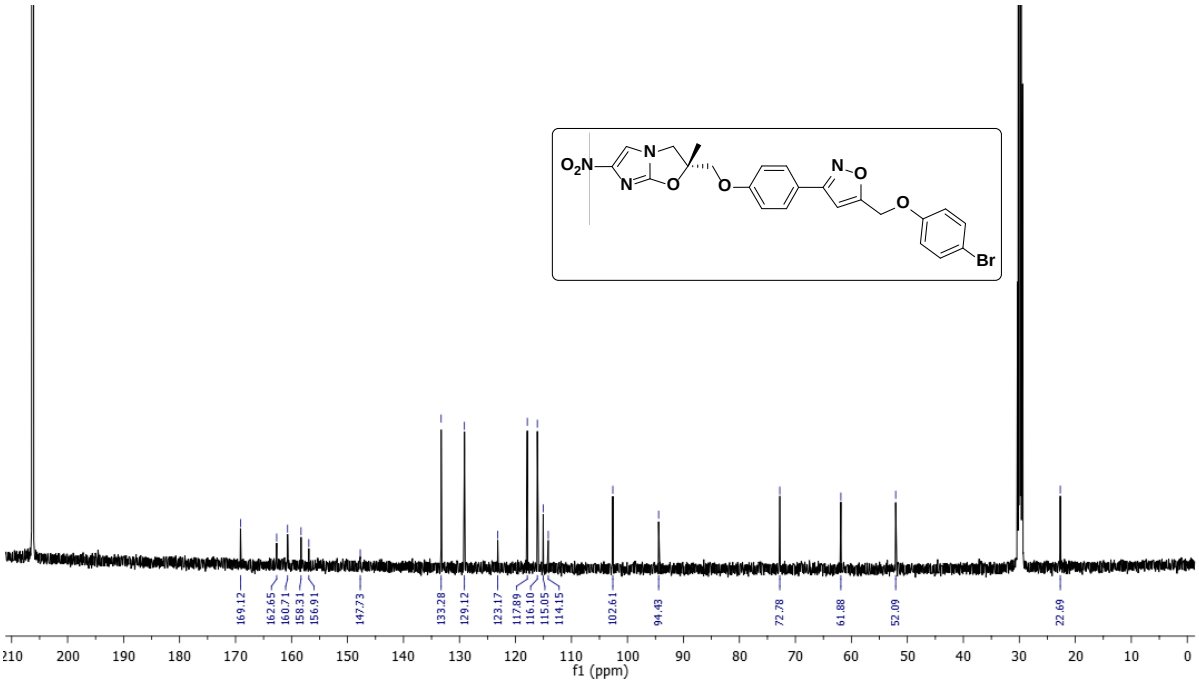
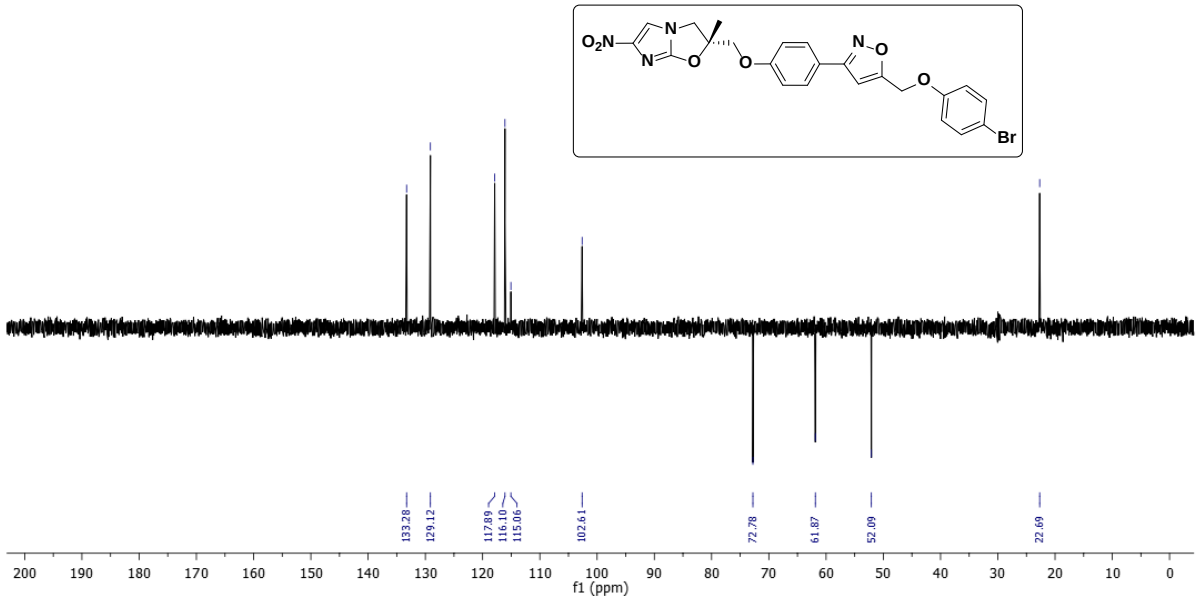
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2g (IIIM/MCD-127):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **2g (IIIM/MCD-127):**



DEPT (126 MHz, Acetone-d_6) of compound **2g (IIIM/MCD-127):**

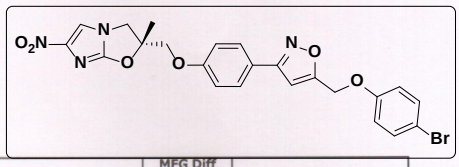


HRMS (ESI-TOF) of compound **2g (IIIM/MCD-127)**:

Qualitative Compound Report

Data File	127.d	**Sample Name**	127
Sample Type	Sample	**Position**	Vial 27
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	04-03-2013 PM 2:45:21
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

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

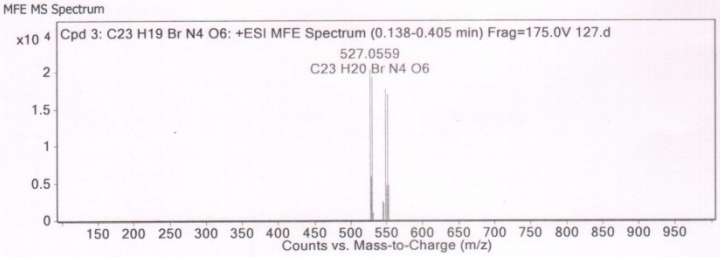


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C23 H19 Br N4 O6	0.194	526.0484	C23 H19 Br N4 O6	C23 H19 Br N4 O6	0.82	C23 H19 Br N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C23 H19 Br N4 O6	527.0559	0.194	Find by Molecular Feature	526.0484

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
527.0559	1	20273.5	C23 H20 Br N4 O6	(M+H)+
528.0571	1	5902.68	C23 H20 Br N4 O6	(M+H)+
529.0541	1	19295.58	C23 H20 Br N4 O6	(M+H)+
530.0569	1	6271.41	C23 H20 Br N4 O6	(M+H)+
544.0814	1	2510.14		(M+NH4)+
546.0798	1	2243.65		(M+NH4)+
549.0378	1	17752.14	C23 H19 Br N4 Na O6	(M+Na)+
550.0412	1	4551.3	C23 H19 Br N4 Na O6	(M+Na)+
551.0355	1	16970	C23 H19 Br N4 Na O6	(M+Na)+
552.0373	1	4755.94	C23 H19 Br N4 Na O6	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	527.0559	527.0561	0.25	100	98.07	38.43	38.45
2	528.0571	528.0591	3.88	29.12	26.28	11.19	10.3
3	529.0541	529.0544	0.51	95.18	100	36.58	39.21
4	530.0569	530.0572	0.59	30.93	26.17	11.89	10.26
5	531.0588	531.0597	1.64	4.96	4.53	1.91	1.78

--- End Of Report ---

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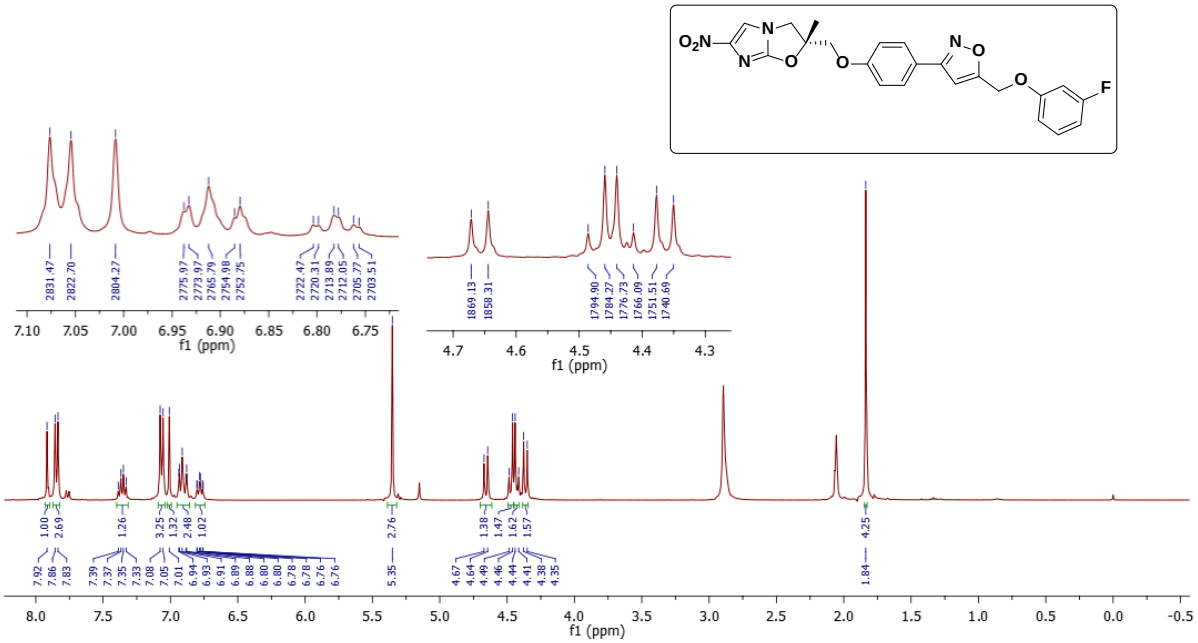
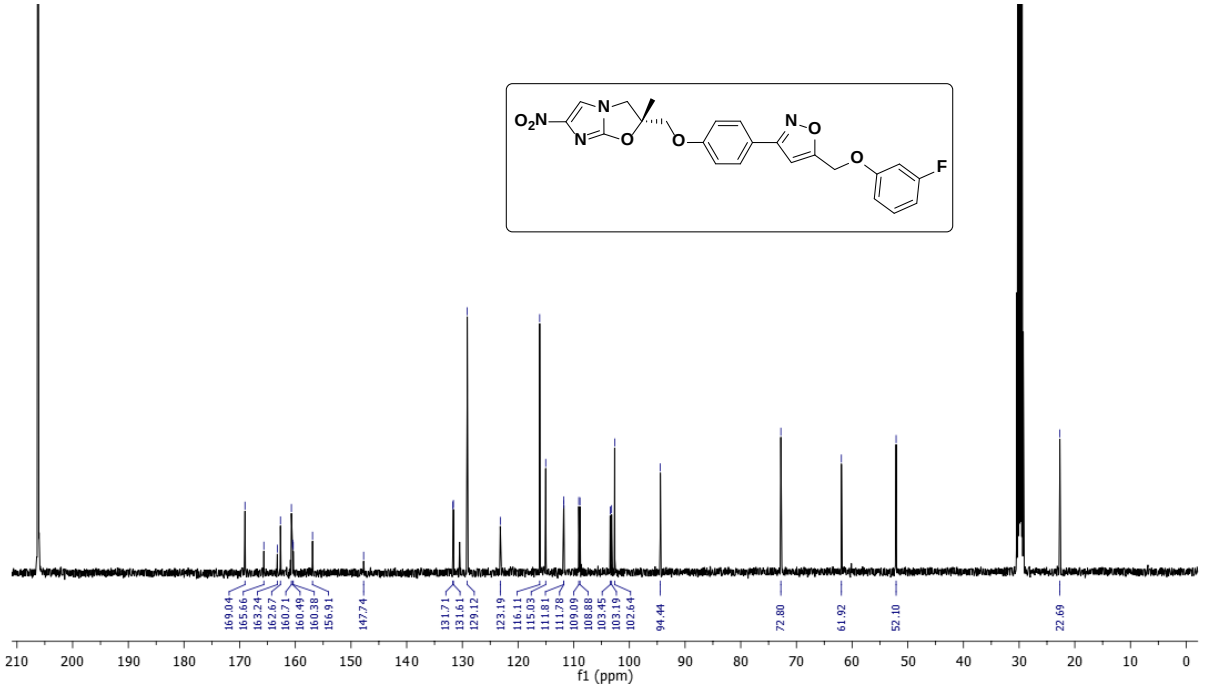
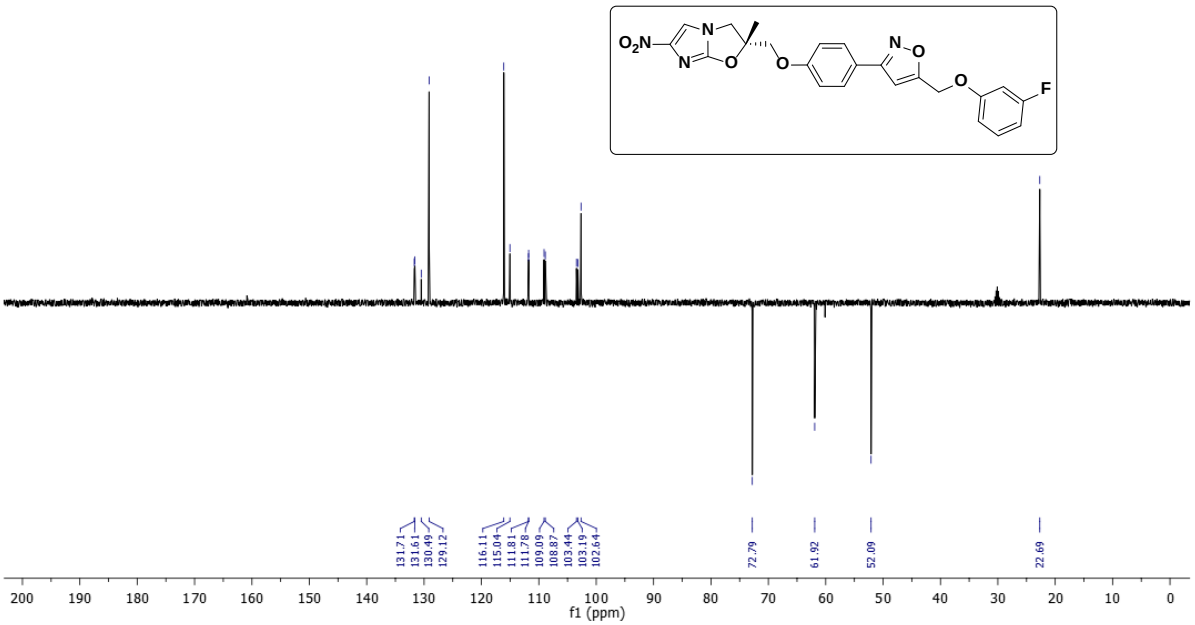
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2h (IIIM/MCD-175):**



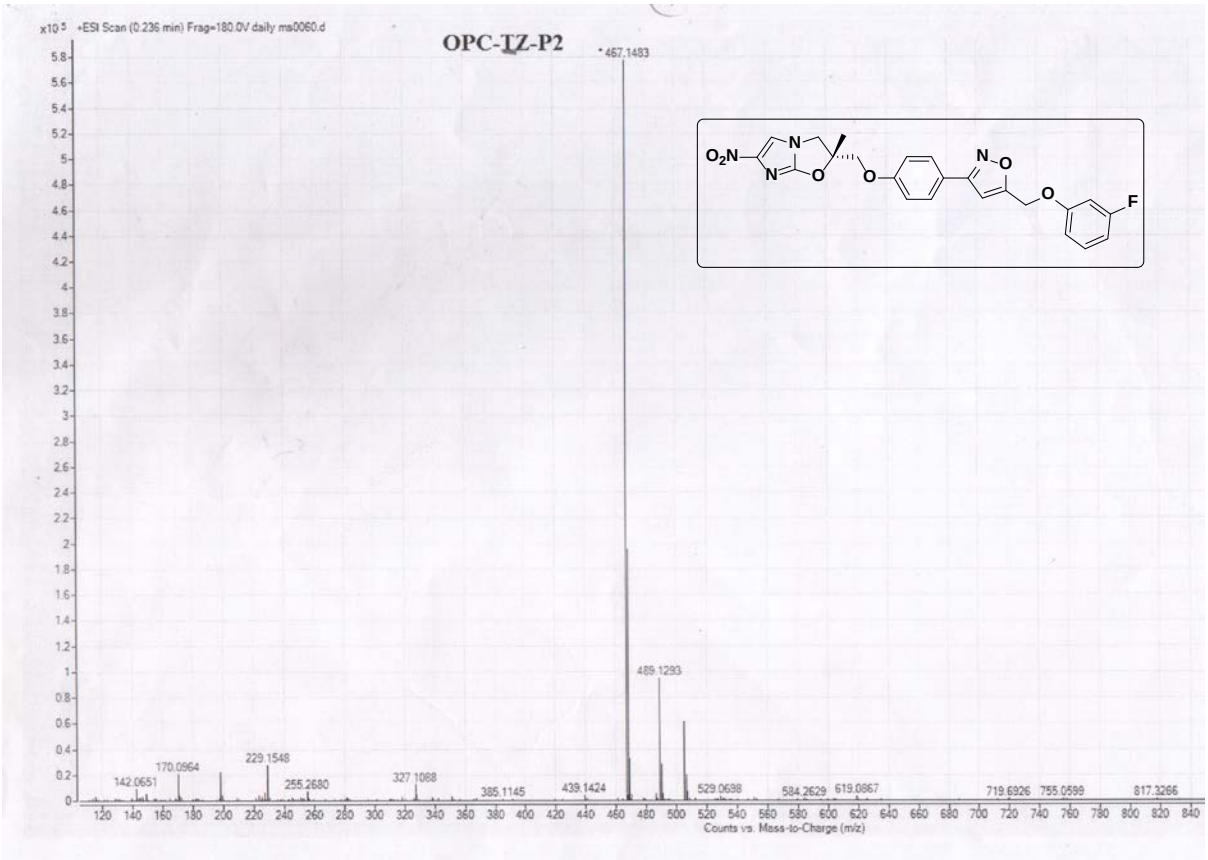
^{13}C NMR (101 MHz, Acetone-d_6) of compound **2h (IIIM/MCD-175):**



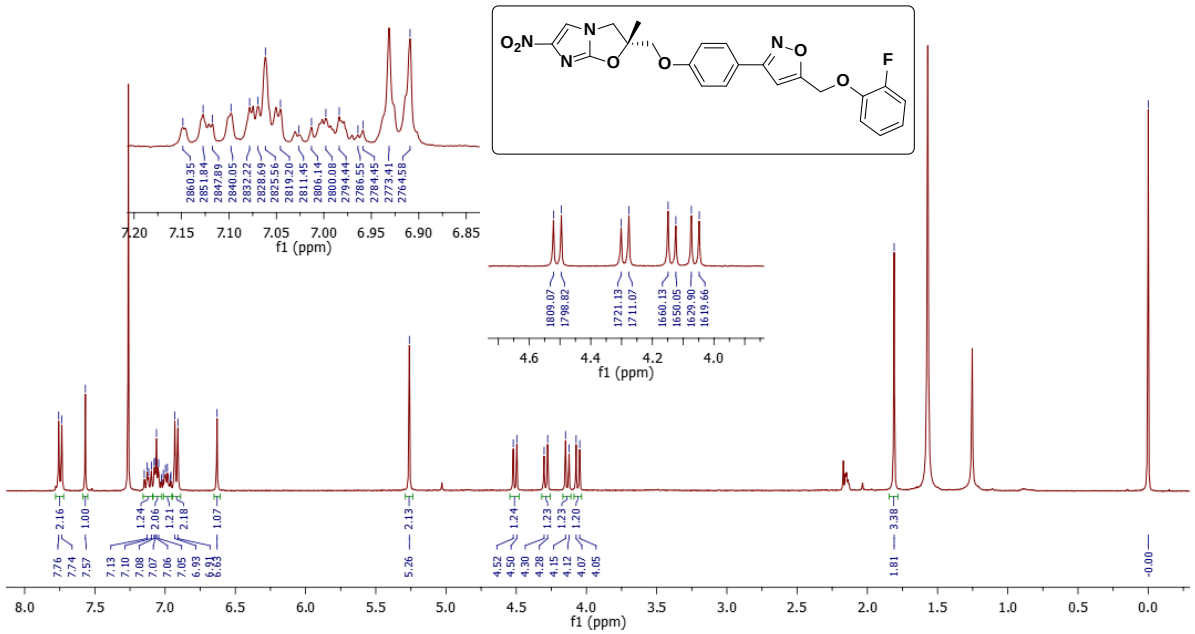
DEPT (101 MHz, Acetone-d_6) of compound **2h (IIIM/MCD-175):**



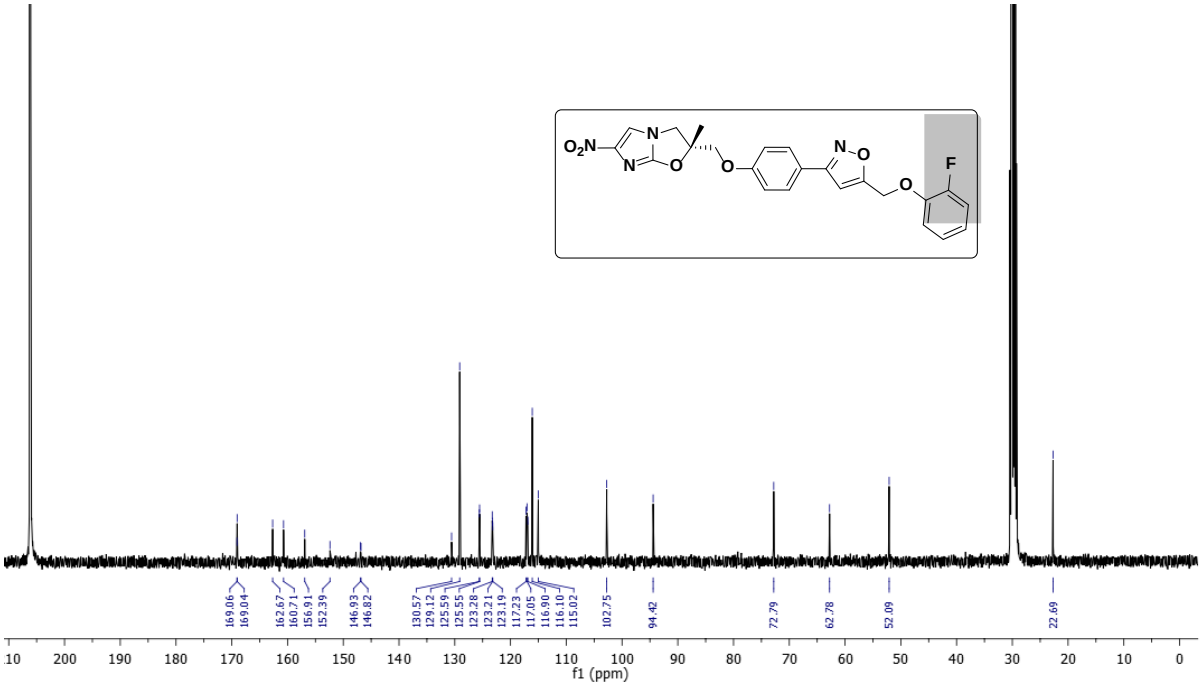
LC-MS (ESI-TOF) of compound **2h (IIIM/MCD-175)**:



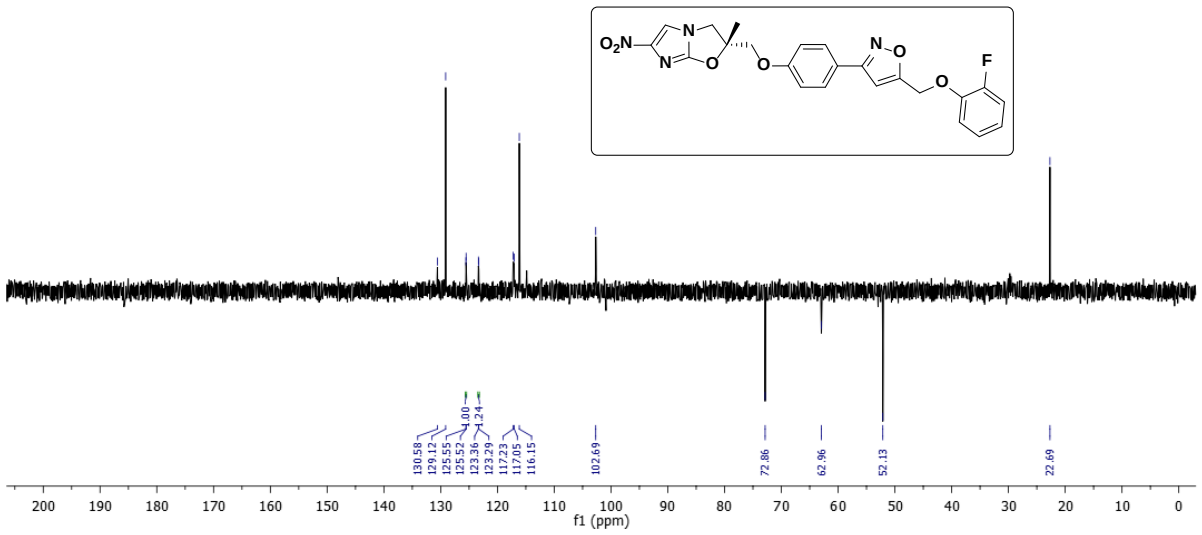
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2i (IIIM/MCD-117):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **2i (IIIM/MCD-117):**



DEPT (101 MHz, Acetone-d_6) of compound **2i (IIIM/MCD-117):**

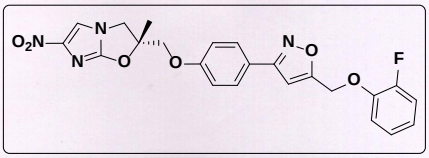


HRMS (ESI-TOF) of compound **2i (IIIM/MCD-117)**:

Qualitative Compound Report

Data File	117.d	**Sample Name**	117
Sample Type	Sample	**Position**	Vial 44
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 1:24:41
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)

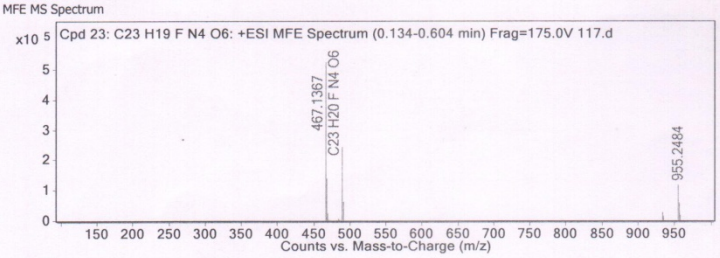


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C23 H19 F N4 O6	0.188	466.1293	C23 H19 F N4 O6	C23 H19 F N4 O6	-0.94	C23 H19 F N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 23: C23 H19 F N4 O6	467.1367	0.188	Find by Molecular Feature	466.1293

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
467.1367	1	523453.91	C23 H20 F N4 O6	(M+H)+
468.1392	1	137779.28	C23 H20 F N4 O6	(M+H)+
469.1414	1	22338.29	C23 H20 F N4 O6	(M+H)+
489.1183	1	241457.91	C23 H19 F N4 Na O6	(M+Na)+
490.1208	1	61329.18	C23 H19 F N4 Na O6	(M+Na)+
933.2655	1	26416.05		(2M+H)+
934.2678	1	14538.44		(2M+H)+
955.2484	1	119231.13		(2M+Na)+
956.2509	1	60181.14		(2M+Na)+
957.2525	1	18027.18		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	467.1367	467.1361	-1.25	100	100	76.1	75.66
2	468.1392	468.1392	-0.03	26.32	26.8	20.03	20.28
3	469.1414	469.1417	0.73	4.27	4.69	3.25	3.55
4	470.1445	470.1443	-0.42	0.72	0.61	0.55	0.47
5	471.1484	471.1467	-3.5	0.09	0.07	0.07	0.05

--- End Of Report ---

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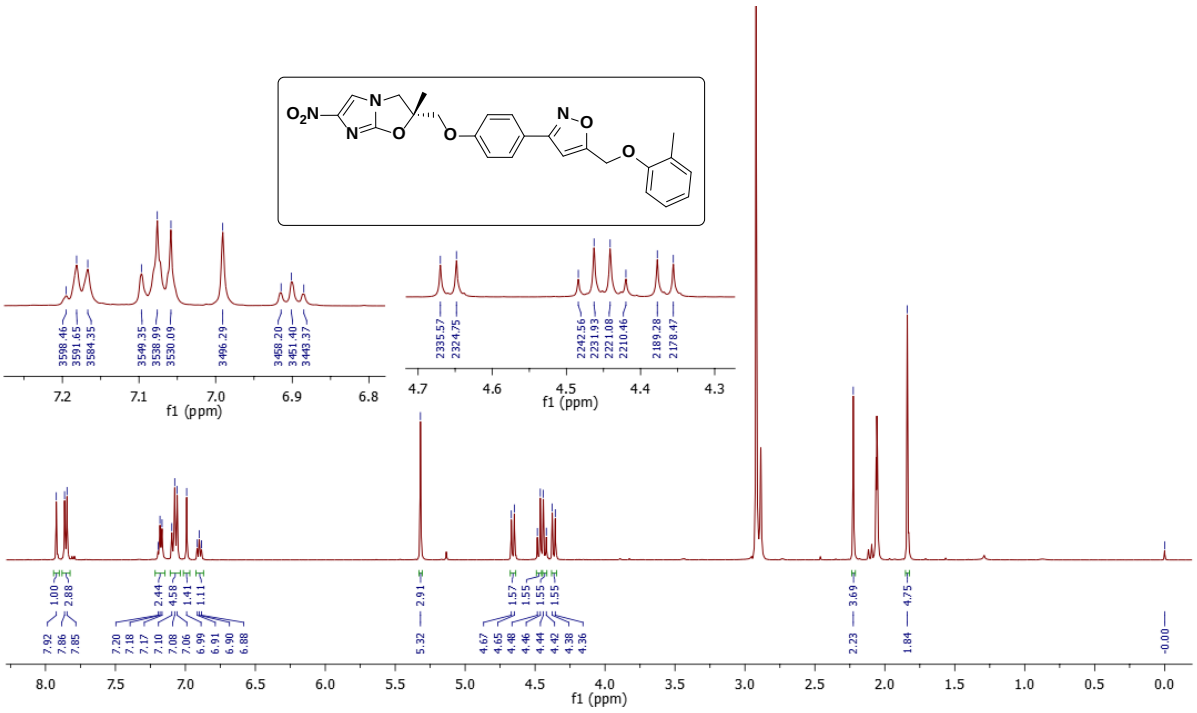
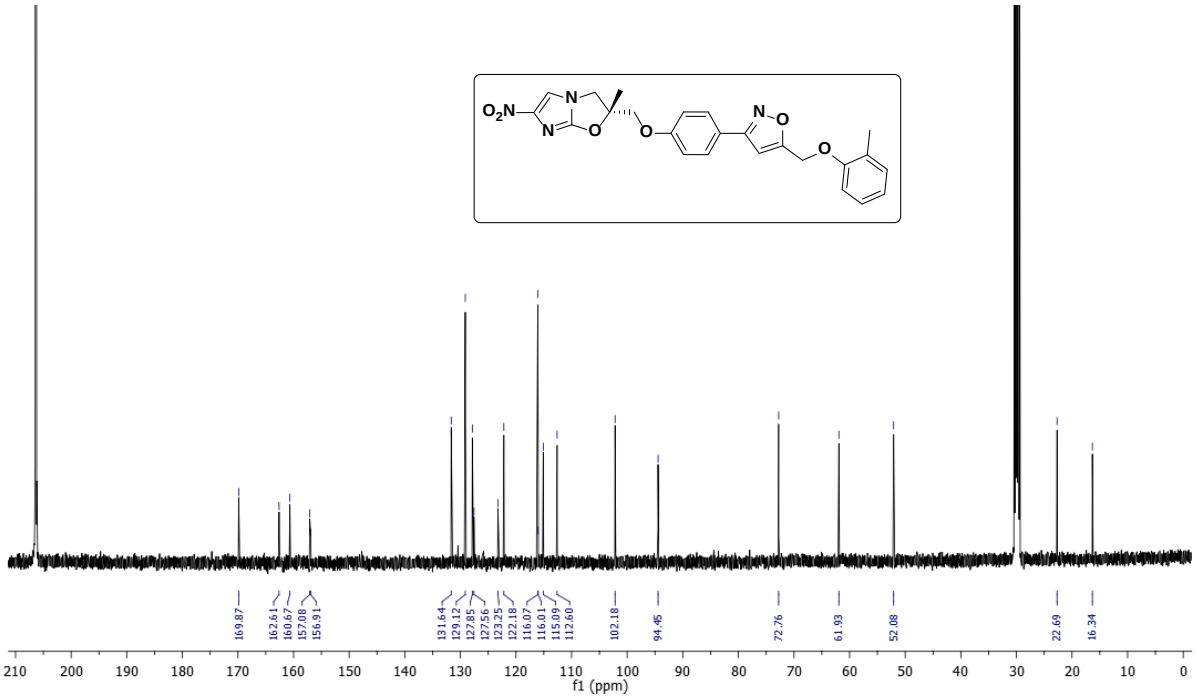
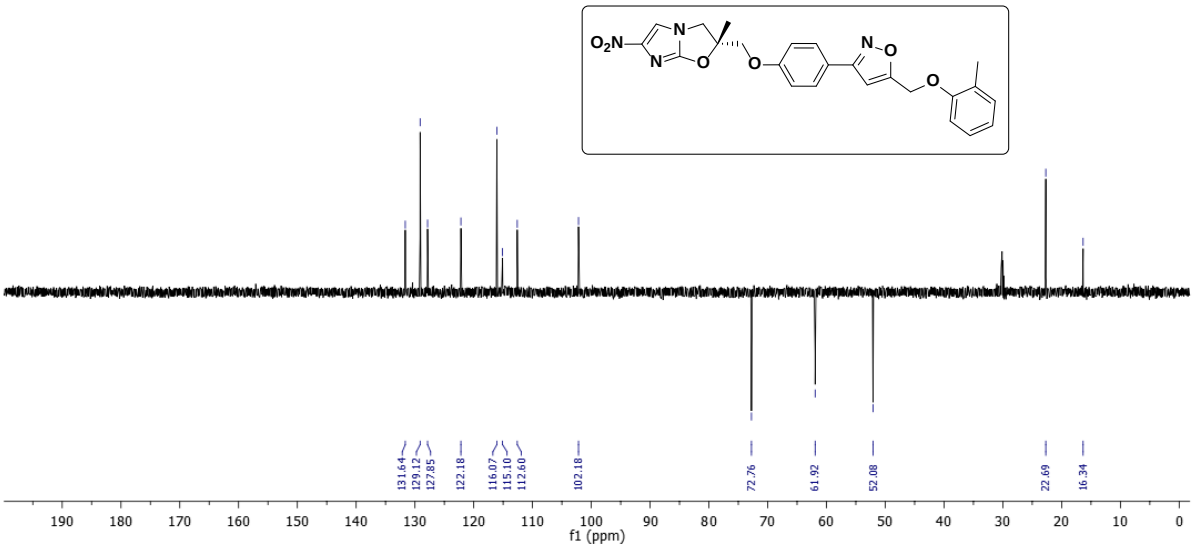
^{1}H NMR (500 MHz, Acetone-d_6) of compound **2j (IIIM/MCD-177):**



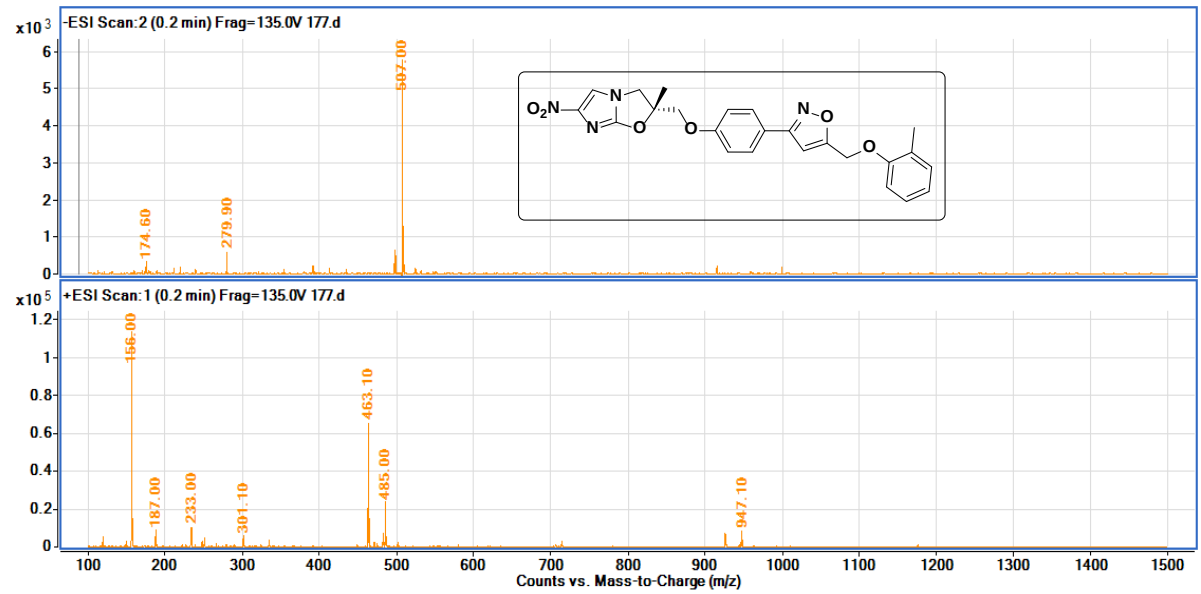
^{13}C NMR (126 MHz, Acetone-d_6) of compound **2j (IIIM/MCD-177):**



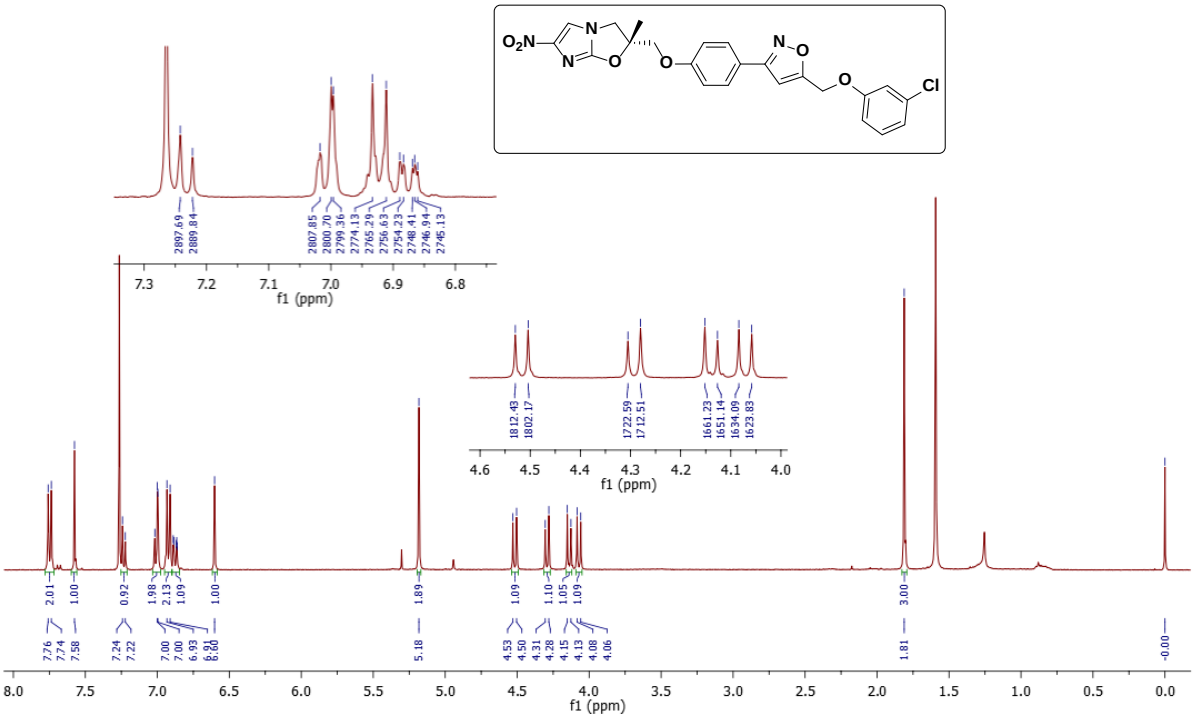
DEPT (126 MHz, Acetone-d_6) of compound **2j (IIIM/MCD-177):**



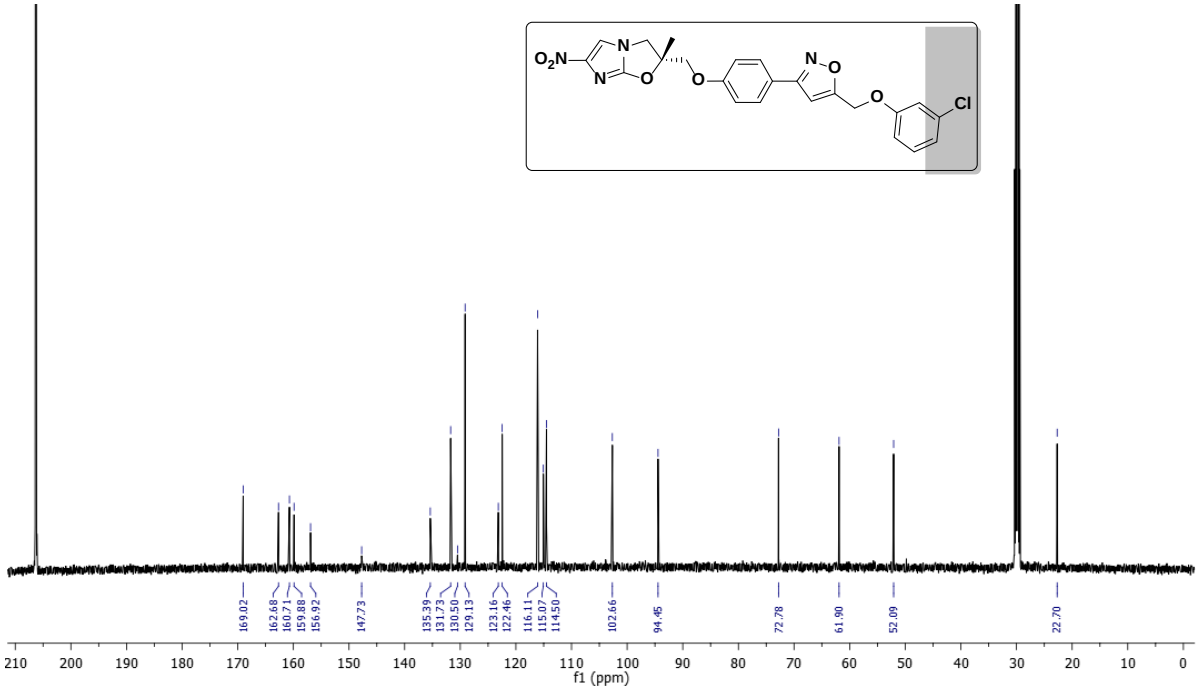
LC-MS (ESI-TOF) of compound **2j (IIIM/MCD-177):**



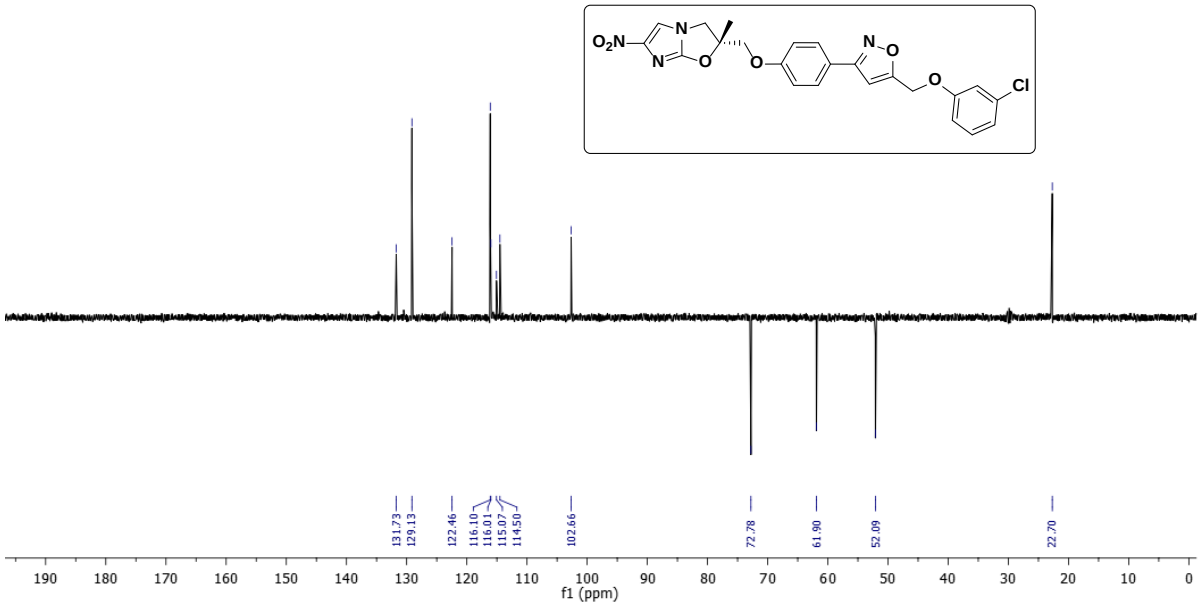
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2k (IIIM/MCD-138):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **2k (IIIM/MCD-138):**



DEPT (126 MHz, Acetone-d_6) of compound **2k (IIIM/MCD-138)**:

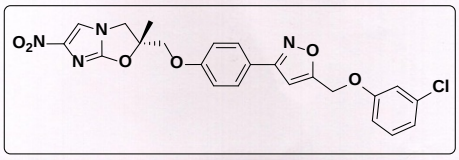


HRMS (ESI-TOF) of compound **2k (IIIM/MCD-138)**:

Qualitative Compound Report

Data File	138.d	**Sample Name**	138
Sample Type	Sample	**Position**	Vial 31
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	05-03-2013 PM 3:38:02
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

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

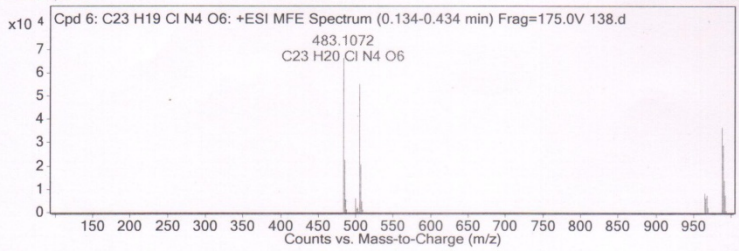


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C23 H19 Cl N4 O6	0.194	482.1	C23 H19 Cl N4 O6	C23 H19 Cl N4 O6	-1.51	C23 H19 Cl N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C23 H19 Cl N4 O6	483.1072	0.194	Find by Molecular Feature	482.1

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
483.1072	1	66364.26	C23 H20 Cl N4 O6	(M+H)+
484.1105	1	16561.47	C23 H20 Cl N4 O6	(M+H)+
485.1055	1	22645.74	C23 H20 Cl N4 O6	(M+H)+
505.089	1	55288.79	C23 H19 Cl N4 Na O6	(M+Na)+
506.092	1	14155.97	C23 H19 Cl N4 Na O6	(M+Na)+
507.0877	1	20617.74	C23 H19 Cl N4 Na O6	(M+Na)+
987.1911	1	36689.49		(2M+Na)+
988.1924	1	18270.32		(2M+Na)+
989.1886	1	28889.01		(2M+Na)+
990.1906	1	13964		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	483.1072	483.1066	-1.32	100	100	58.94	57.4
2	484.1105	484.1096	-1.73	24.96	26.8	14.71	15.38
3	485.1055	485.1047	-1.67	34.12	36.68	20.11	21.05
4	486.1083	486.1072	-2.26	8.6	9.19	5.07	5.27
5	487.1102	487.1096	-1.23	1.98	1.56	1.17	0.9

--- End Of Report ---

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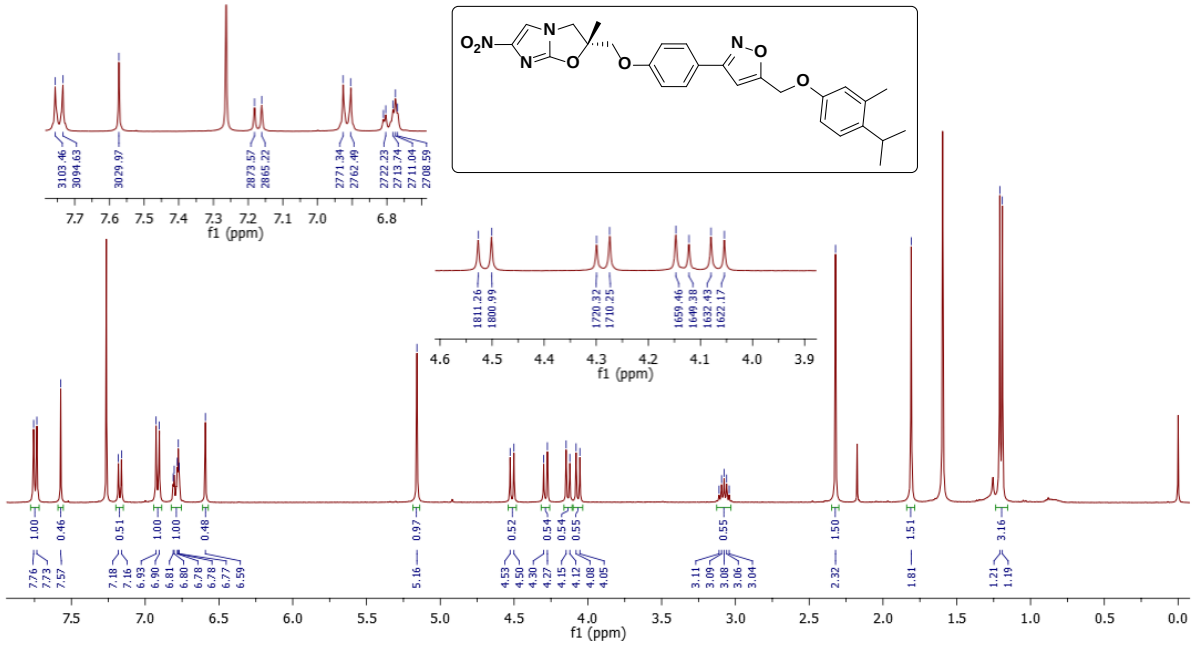
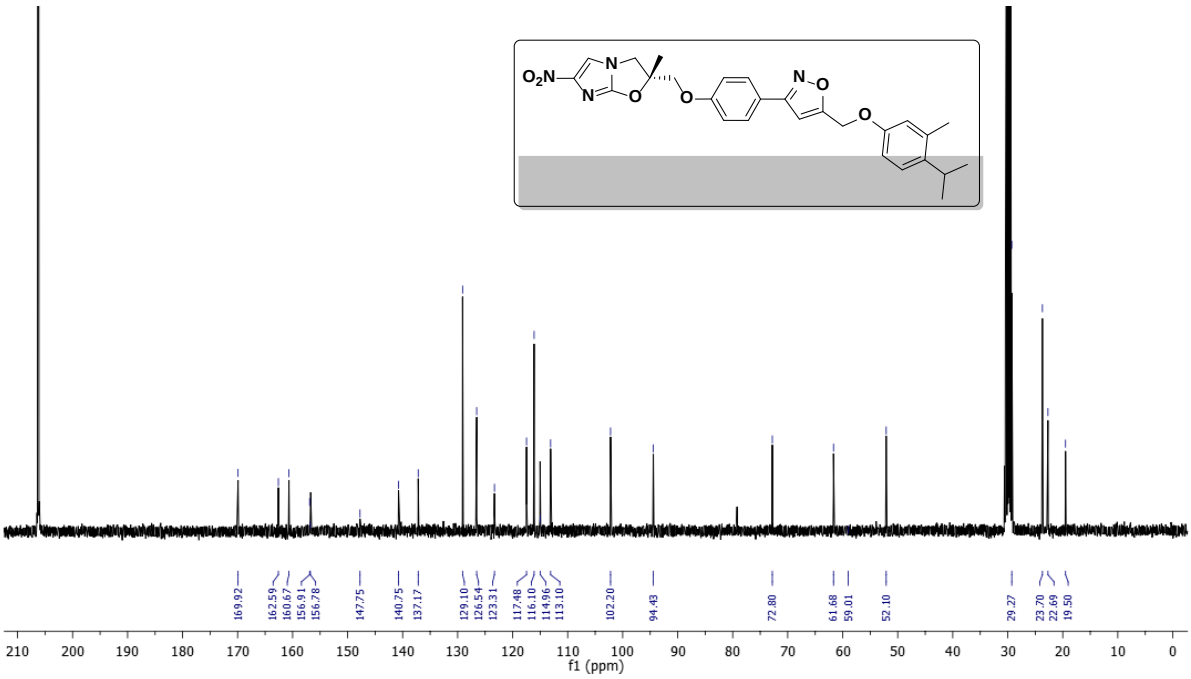
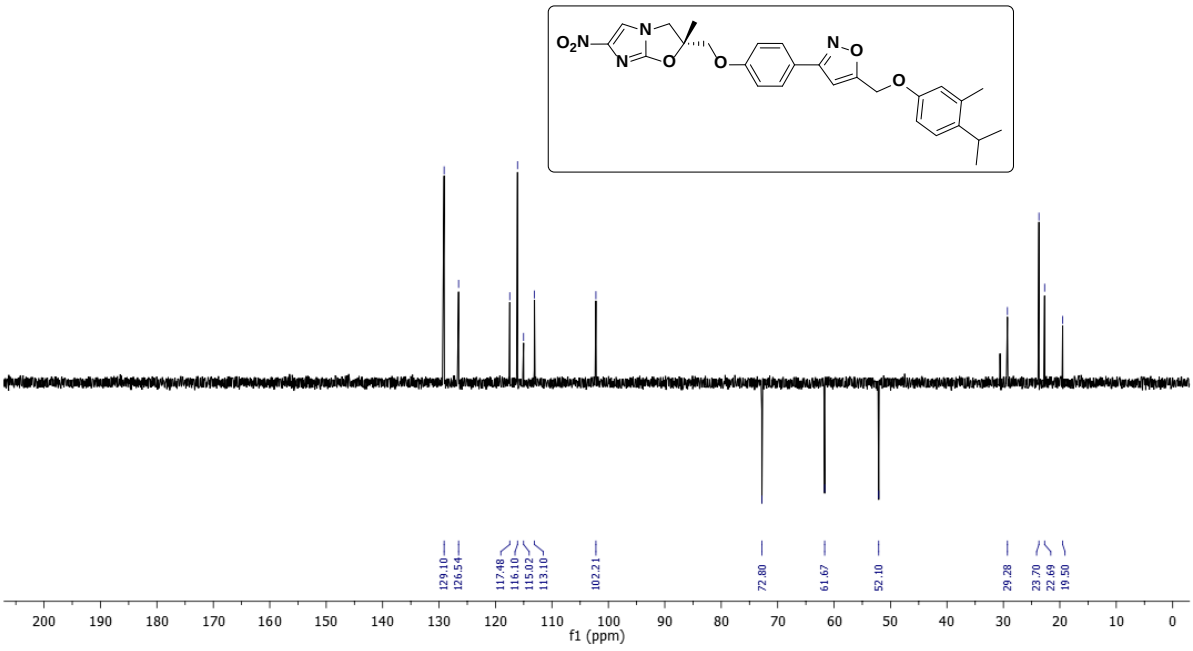
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2l (IIIM/MCD-139):**



^{13}C NMR (101 MHz, Acetone-d_6) of compound **2l (IIIM/MCD-139):**



DEPT (101 MHz, Acetone-d_6) of compound **2l (IIIM/MCD-139)**:

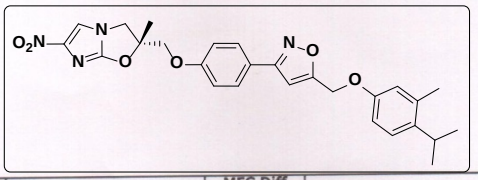


HRMS (ESI-TOF) of compound **2l (IIIM/MCD-139)**:

Qualitative Compound Report

Data File	139.d	**Sample Name**	139
Sample Type	Sample	**Position**	Vial 33
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	05-03-2013 PM 3:54:42
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

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

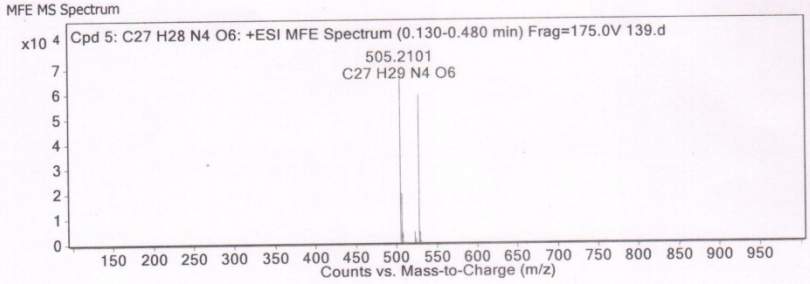


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C27 H28 N4 O6	0.189	504.2029	C27 H28 N4 O6	C27 H28 N4 O6	-3.93	C27 H28 N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C27 H28 N4 O6	505.2101	0.189	Find by Molecular Feature	504.2029

MFE MS Spectrum



MS Spectrum Peak List

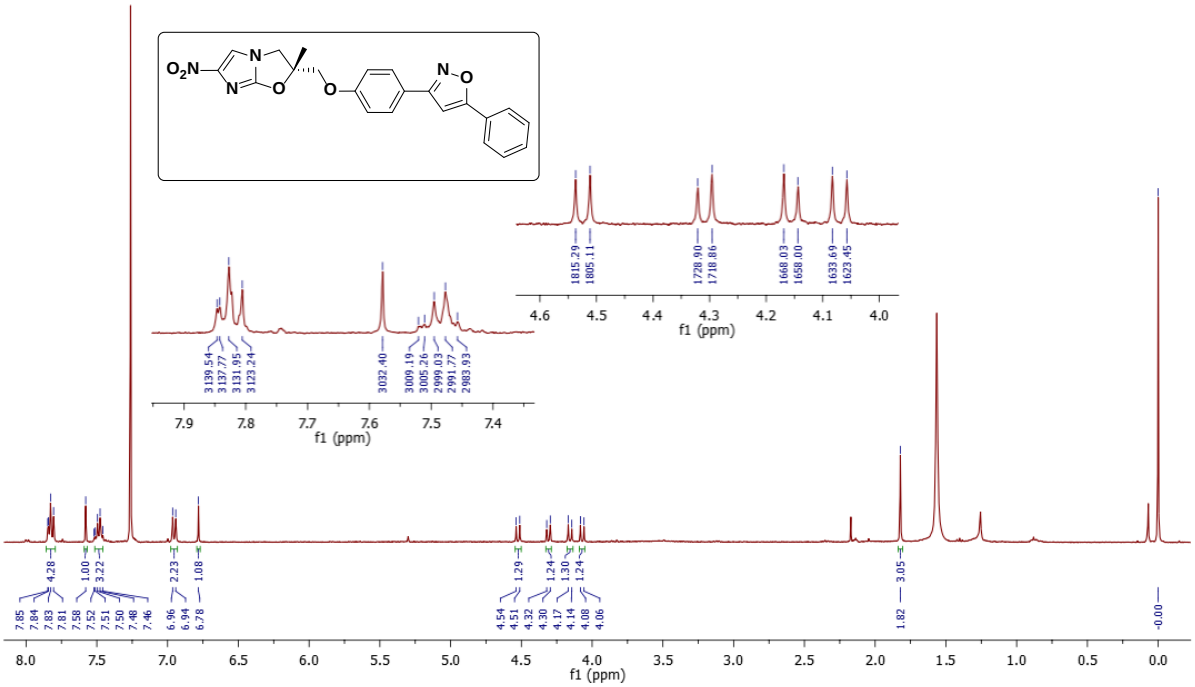
m/z	z	Abund	Formula	Ion
505.2101	1	66789.78	C27 H29 N4 O6	(M+H)+
506.2136	1	19373.52	C27 H29 N4 O6	(M+H)+
507.2157	1	4010.87	C27 H29 N4 O6	(M+H)+
508.216	1	553.01	C27 H29 N4 O6	(M+H)+
522.236	1	4510.39	C27 H32 N5 O6	(M+NH4)+
523.2393	1	1484.27	C27 H32 N5 O6	(M+NH4)+
527.192	1	58944.45	C27 H28 N4 Na O6	(M+Na)+
528.1949	1	16879.33	C27 H28 N4 Na O6	(M+Na)+
529.1976	1	4230.34	C27 H28 N4 Na O6	(M+Na)+
530.1944	1	773.05	C27 H28 N4 Na O6	(M+Na)+

Predicted Isotope Match Table

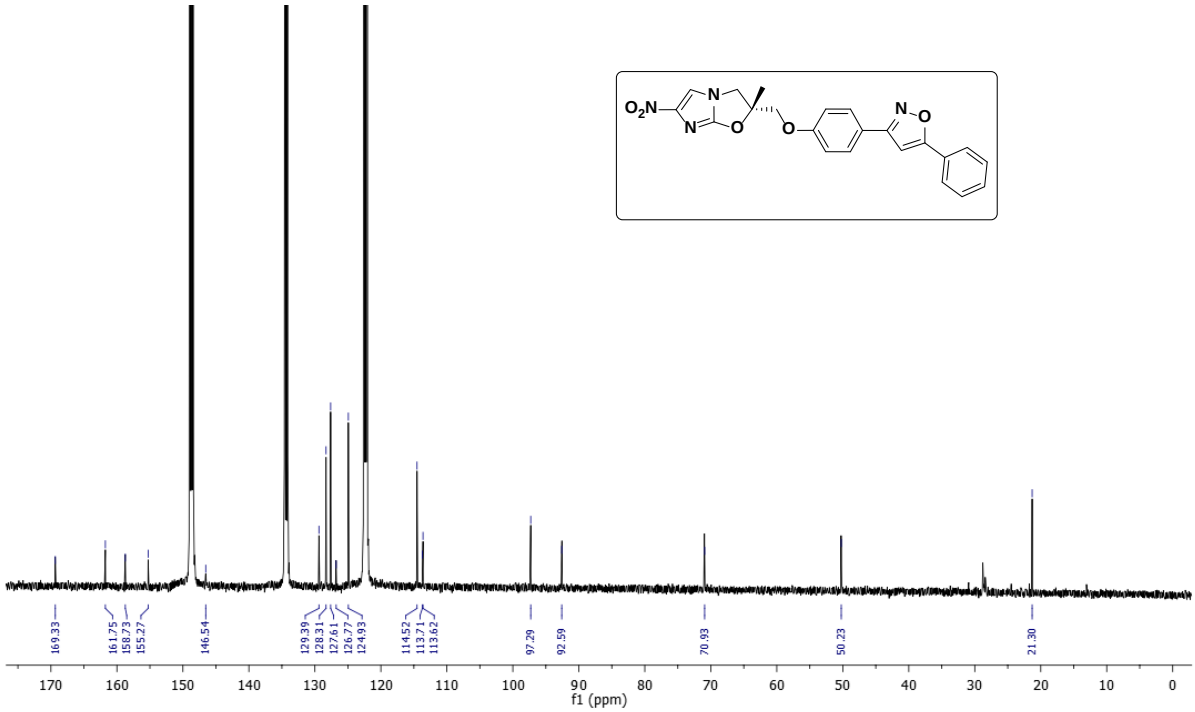
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	505.2101	505.2082	-3.79	100	100	73.62	72.46
2	506.2136	506.2113	-4.6	29.01	31.23	21.35	22.62
3	507.2157	507.2139	-3.52	6.01	5.95	4.42	4.31
4	508.216	508.2165	1.14	0.83	0.84	0.61	0.61

--- End Of Report ---

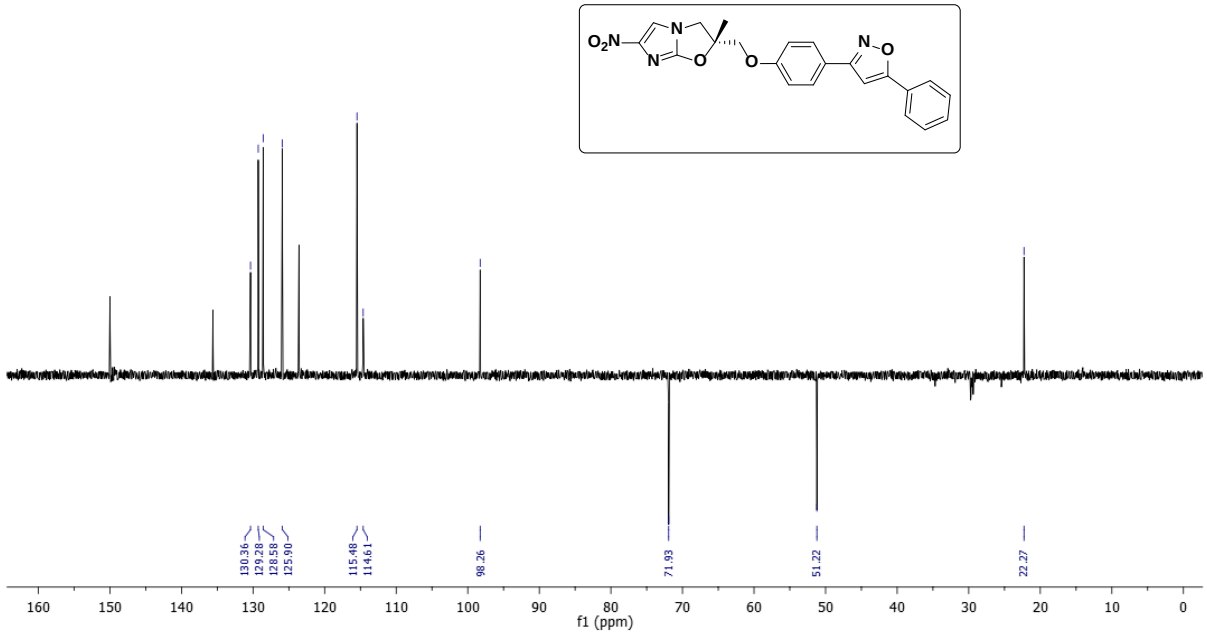
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2m (IIIM/MCD-050):**



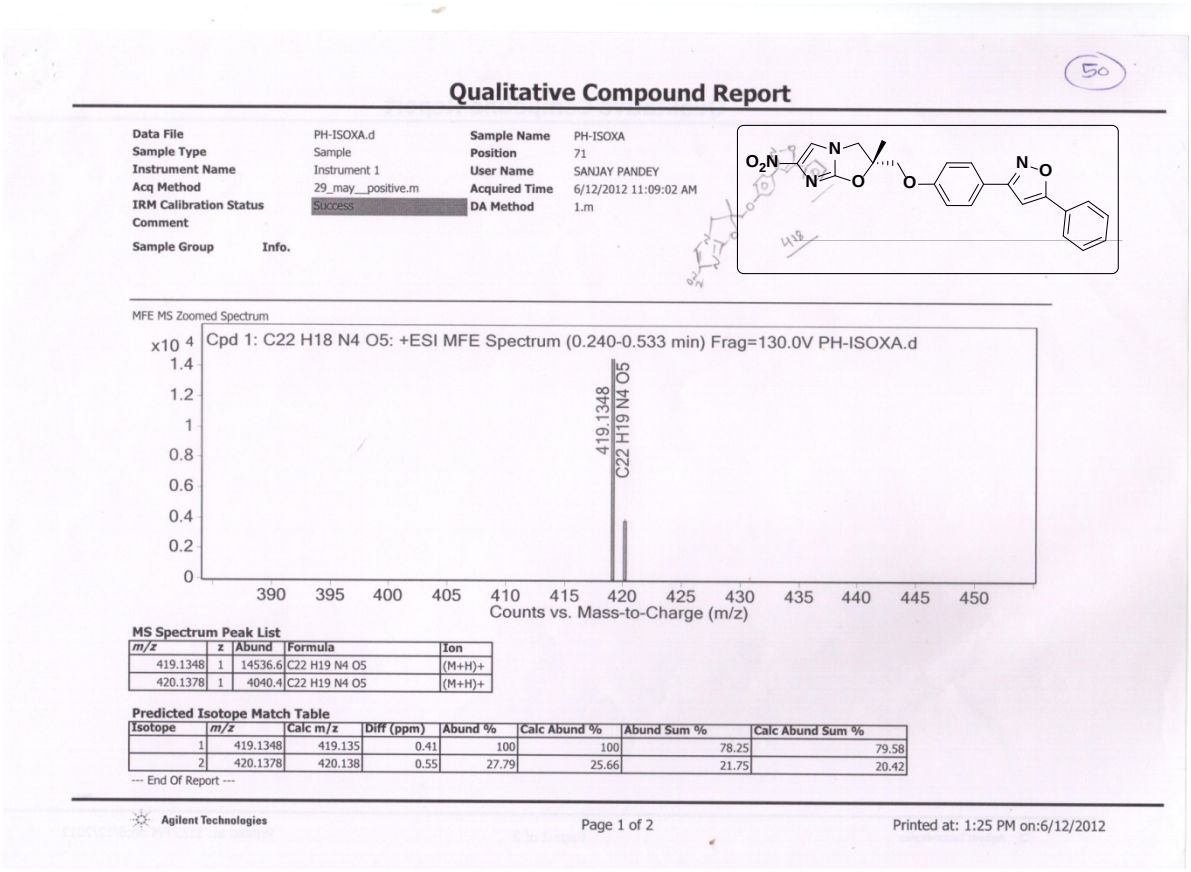
^{13}C NMR (126 MHz, pyridine-d_5) of compound **2m (IIIM/MCD-050):**



DEPT (126 MHz, pyridine-d_5) of compound **2m (IIIM/MCD-050):**



HRMS (ESI-TOF) of compound **2m (IIIM/MCD-050)**:



Qualitative Compound Report

Data File	PH-ISOXA.d	Sample Name	PH-ISOXA
Sample Type	Sample	Position	71
Instrument Name	Instrument 1	User Name	SANJAY PANDEY
Acq Method	29_may__positive.m	Acquired Time	6/12/2012 11:09:02 AM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group	Info.		

MFE MS Zoomed Spectrum

Cpd 1: C22 H18 N4 O5: +ESI MFE Spectrum (0.240-0.533 min) Frag=130.0V PH-ISOXA.d

x10 4 1.4 1.2 1 0.8 0.6 0.4 0.2 0

419.1348 C22 H19 N4 O5

390 395 400 405 410 415 420 425 430 435 440 445 450

Counts vs. Mass-to-Charge (m/z)

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
419.1348	1	14536.6	C22 H19 N4 O5	(M+H)+
420.1378	1	4040.4	C22 H19 N4 O5	(M+H)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	419.1348	419.135	0.41	100	100	78.25	79.58
2	420.1378	420.138	0.55	27.79	25.66	21.75	20.42

--- End Of Report ---

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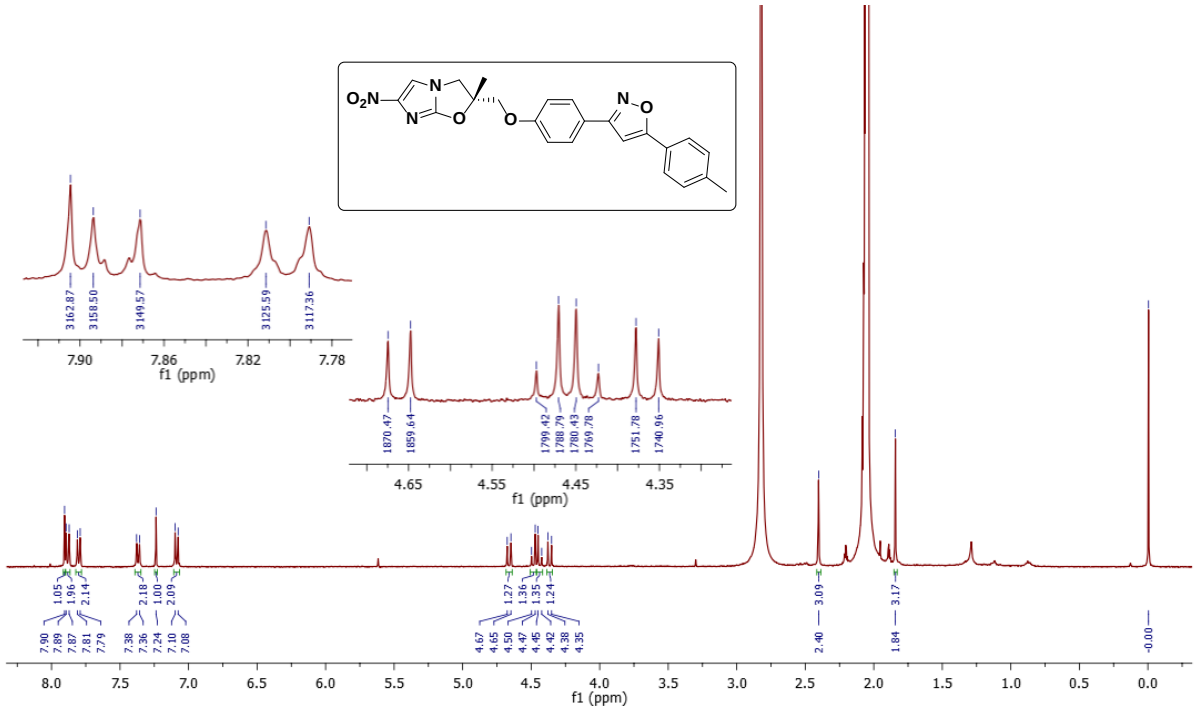
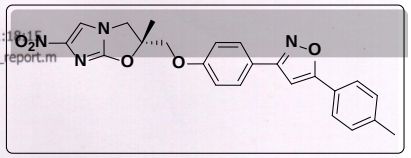
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2n (IIIM/MCD-072):**



HRMS (ESI-TOF) of compound **2n (IIIM/MCD-072)**:

Qualitative Compound Report

Data File	72.d	**Sample Name**	72
Sample Type	Sample	**Position**	Vial 29
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	27-07-2012 PM 01:1[illegible]
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

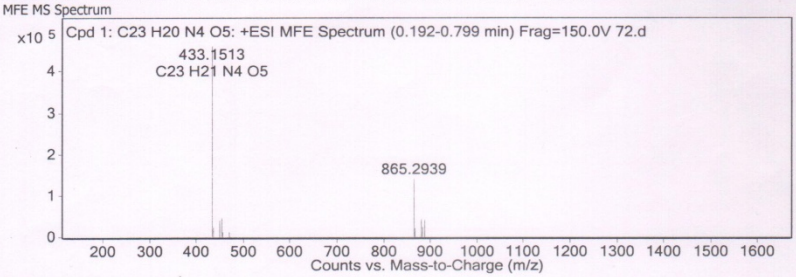


Compound Table

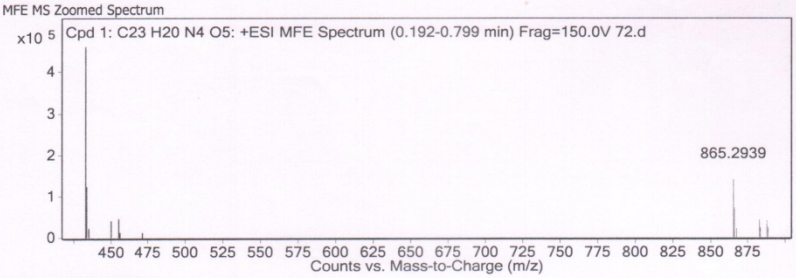
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H20 N4 O5	0.308	432.144	C23 H20 N4 O5	C23 H20 N4 O5	-1.43	C23 H20 N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H20 N4 O5	433.1513	0.308	Find by Molecular Feature	432.144

MFE MS Spectrum



MFE MS Zoomed Spectrum

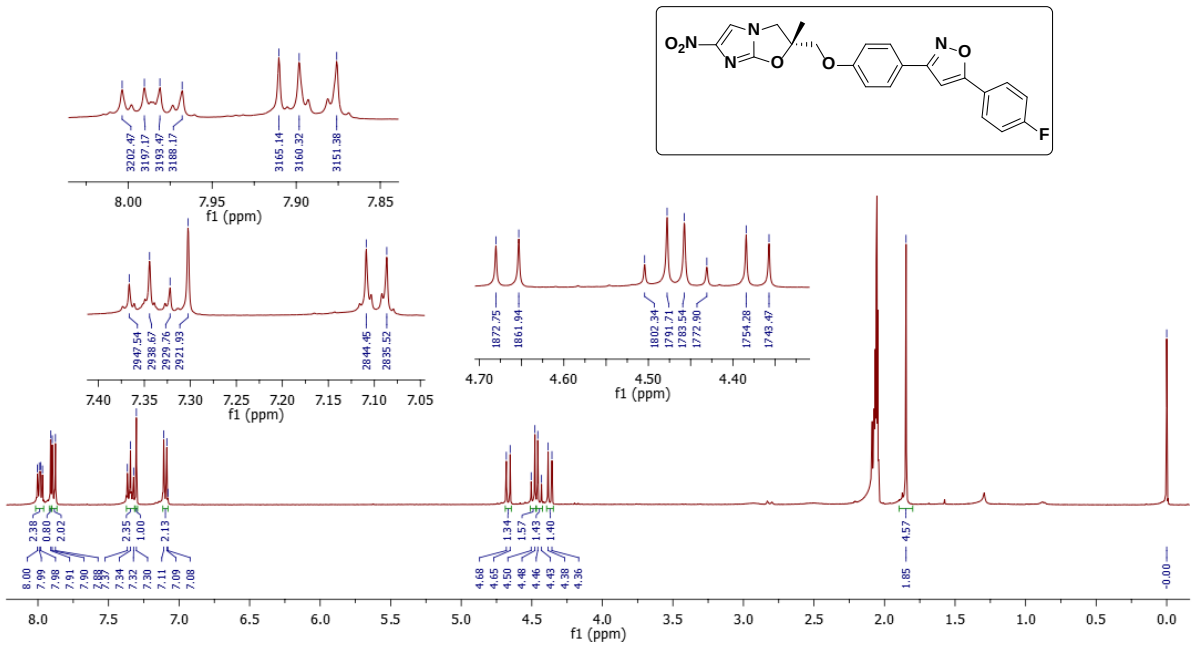


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
433.1513	1	460177.5	C23 H21 N4 O5	(M+H)+
434.1538	1	122191.3	C23 H21 N4 O5	(M+H)+
435.1562	1	23402.9	C23 H21 N4 O5	(M+H)+
450.1768	1	39931.6	C23 H24 N5 O5	(M+NH4)+
455.1323	1	45582.4	C23 H20 N4 Na O5	(M+Na)+
865.2939	1	140161.9		(2M+H)+
866.2966	1	71468		(2M+H)+
882.3199	1	43307.9		(2M+NH4)+
883.3227	1	23191.7		(2M+NH4)+
887.2751	1	40748.1		(2M+Na)+

--- End Of Report ---

^{1}H NMR (400 MHz, Acetone-d_6) of compound **2o (IIIM/MCD-119):**

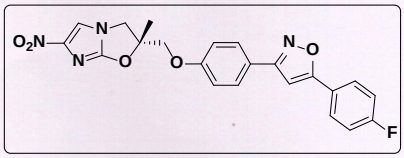


HRMS (ESI-TOF) of compound **2o (IIIM/MCD-119):**

Qualitative Compound Report

Data File	119.d	**Sample Name**	119
Sample Type	Sample	**Position**	Vial 43
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 1:20:08
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)

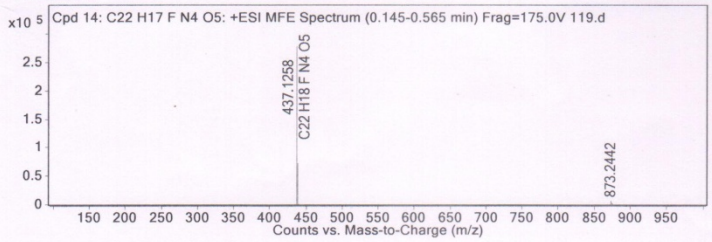


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C22 H17 F N4 O5	0.189	436.1184	C22 H17 F N4 O5	C22 H17 F N4 O5	-0.28	C22 H17 F N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C22 H17 F N4 O5	437.1258	0.189	Find by Molecular Feature	436.1184

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
437.1258	1	278006.16	C22 H18 F N4 O5	(M+H)+
438.1282	1	72282.92	C22 H18 F N4 O5	(M+H)+
439.1316	1	10867.85	C22 H18 F N4 O5	(M+H)+
440.1315	1	1615.42	C22 H18 F N4 O5	(M+H)+
873.2442	1	6637.77		(2M+H)+
874.2468	1	2725.23		(2M+H)+
875.25	1	1082.4		(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	437.1258	437.1256	-0.6	100	100	76.63	76.72
2	438.1282	438.1286	0.93	26	25.65	19.93	19.68
3	439.1316	439.1312	-0.9	3.91	4.19	3	3.21
4	440.1315	440.1337	4.96	0.58	0.51	0.45	0.39

--- End Of Report ---

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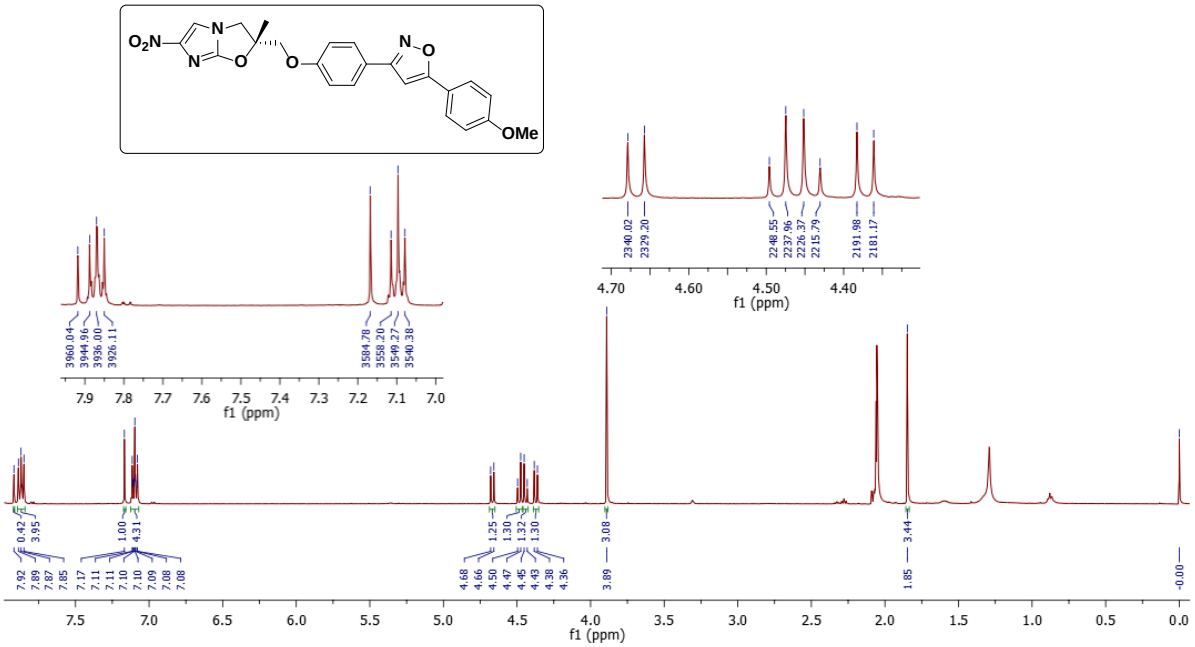
^{1}H NMR (500 MHz, Acetone-d_6) of compound **2p (IIIM/MCD-071):**

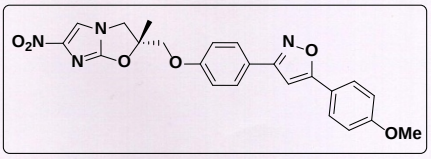


HRMS (ESI-TOF) of compound **2p (IIIM/MCD-071)**:

Qualitative Compound Report

Data File	71.d	**Sample Name**	71
Sample Type	Sample	**Position**	Vial 32
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 12:20:30
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)

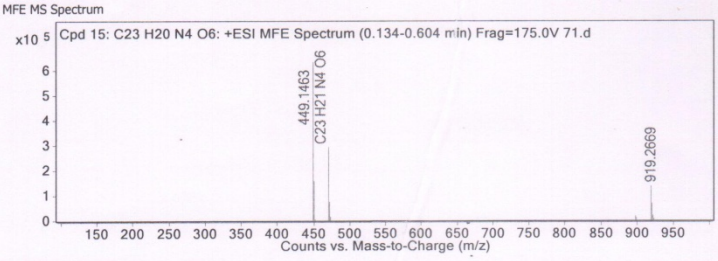


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C23 H20 N4 O6	0.189	448.1388	C23 H20 N4 O6	C23 H20 N4 O6	-1.23	C23 H20 N4 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C23 H20 N4 O6	449.1463	0.189	Find by Molecular Feature	448.1388

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
449.1463	1	633103.38	C23 H21 N4 O6	(M+H)+
450.1487	1	158954.63	C23 H21 N4 O6	(M+H)+
451.1512	1	25778.15	C23 H21 N4 O6	(M+H)+
471.1278	1	294201.56	C23 H20 N4 Na O6	(M+Na)+
472.1306	1	75298.01	C23 H20 N4 Na O6	(M+Na)+
473.1327	1	14525.27	C23 H20 N4 Na O6	(M+Na)+
897.2836	1	18051		(2M+H)+
919.2669	1	136455.23		(2M+Na)+
920.2697	1	68398.34		(2M+Na)+
921.2714	1	20884.12		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	449.1463	449.1456	-1.56	100	100	76.9	75.66
2	450.1487	450.1486	-0.14	25.11	26.81	19.31	20.28
3	451.1512	451.1512	-0.04	4.07	4.69	3.13	3.55
4	452.1535	452.1537	0.31	0.75	0.62	0.57	0.47
5	453.1586	453.1562	-5.41	0.12	0.07	0.09	0.05

--- End Of Report ---

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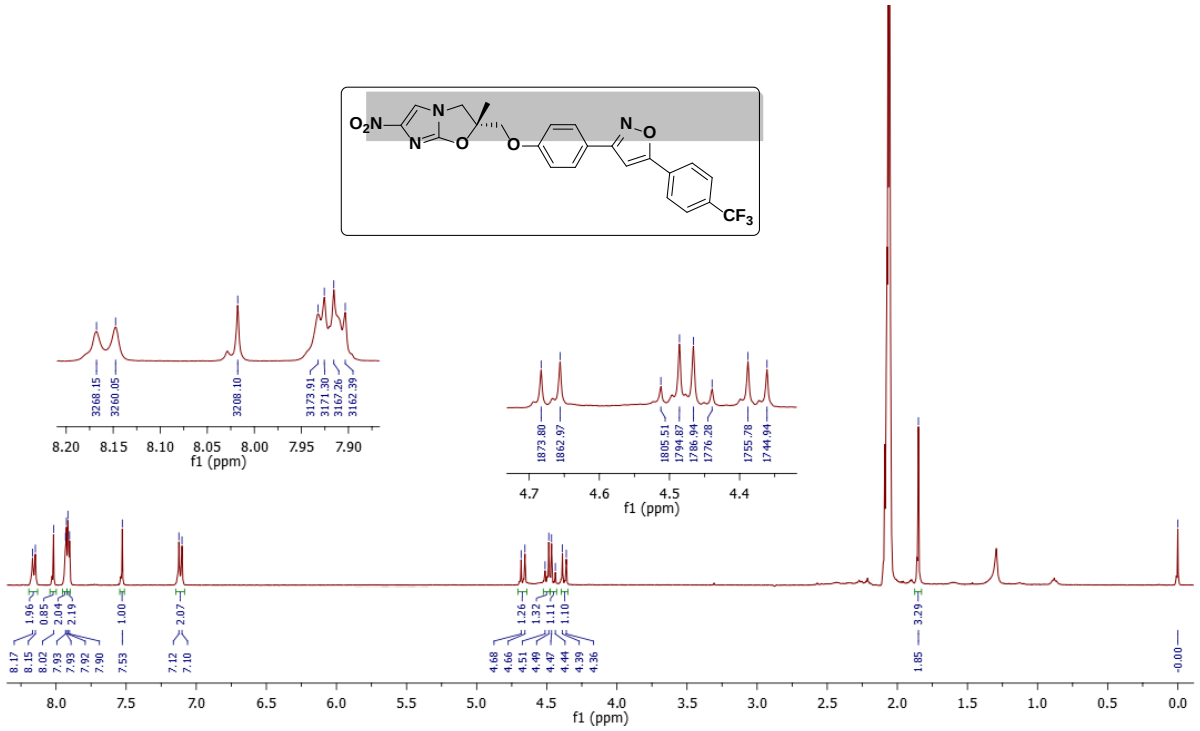
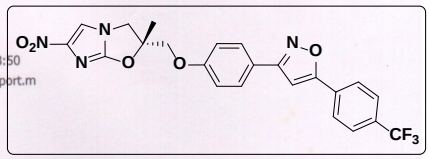
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2q (IIIM/MCD-073):**



HRMS (ESI-TOF) of compound **2q (IIIM/MCD-073)**:

Qualitative Compound Report

Data File	73.d	**Sample Name**	73
Sample Type	Sample	**Position**	Vial 30
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	27-07-2012 PM 01:23:50
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		

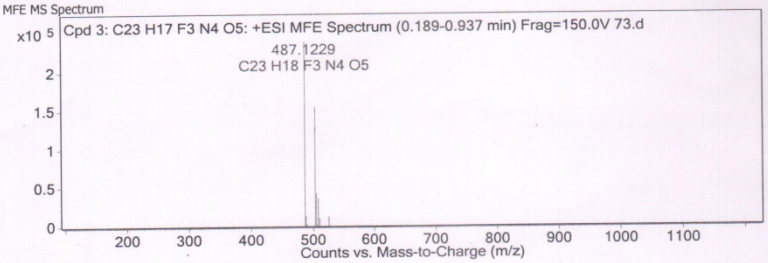


Compound Table

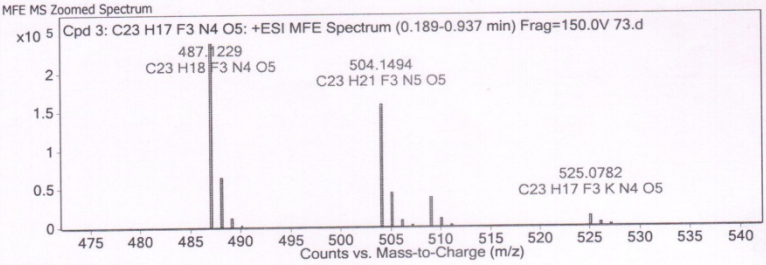
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C23 H17 F3 N4 O5	0.309	486.1156	C23 H17 F3 N4 O5	C23 H17 F3 N4 O5	-1.08	C23 H17 F3 N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C23 H17 F3 N4 O5	487.1229	0.309	Find by Molecular Feature	486.1156

MFE MS Spectrum



MFE MS Zoomed Spectrum

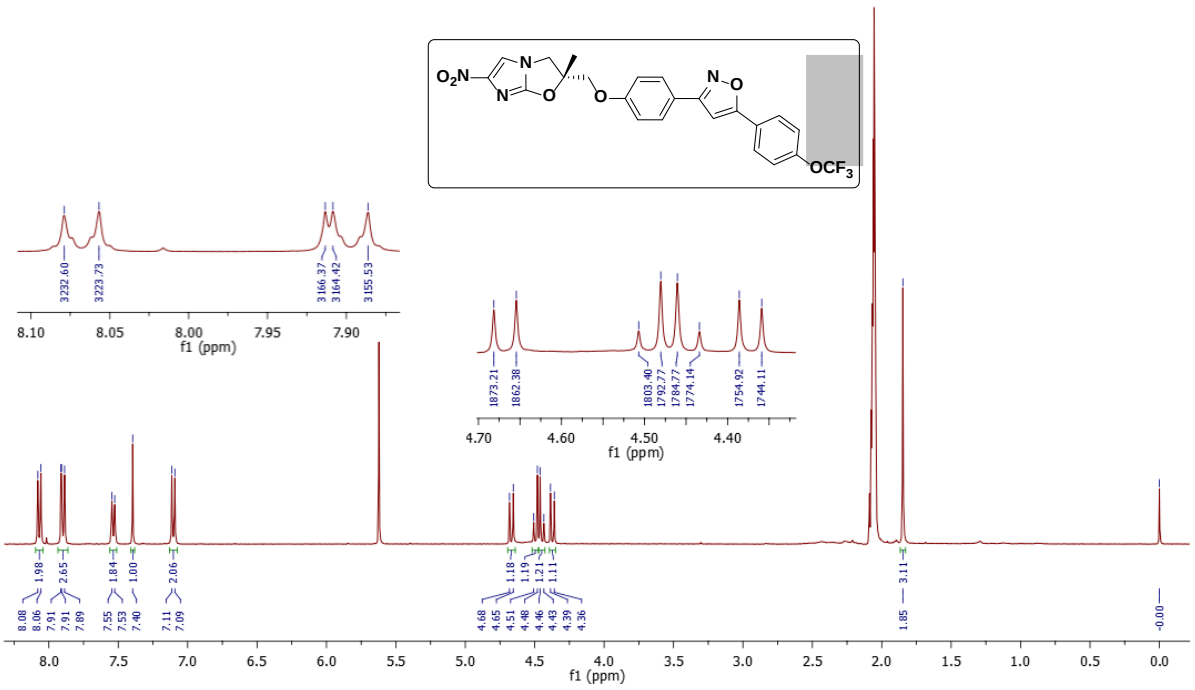


MS Spectrum Peak List

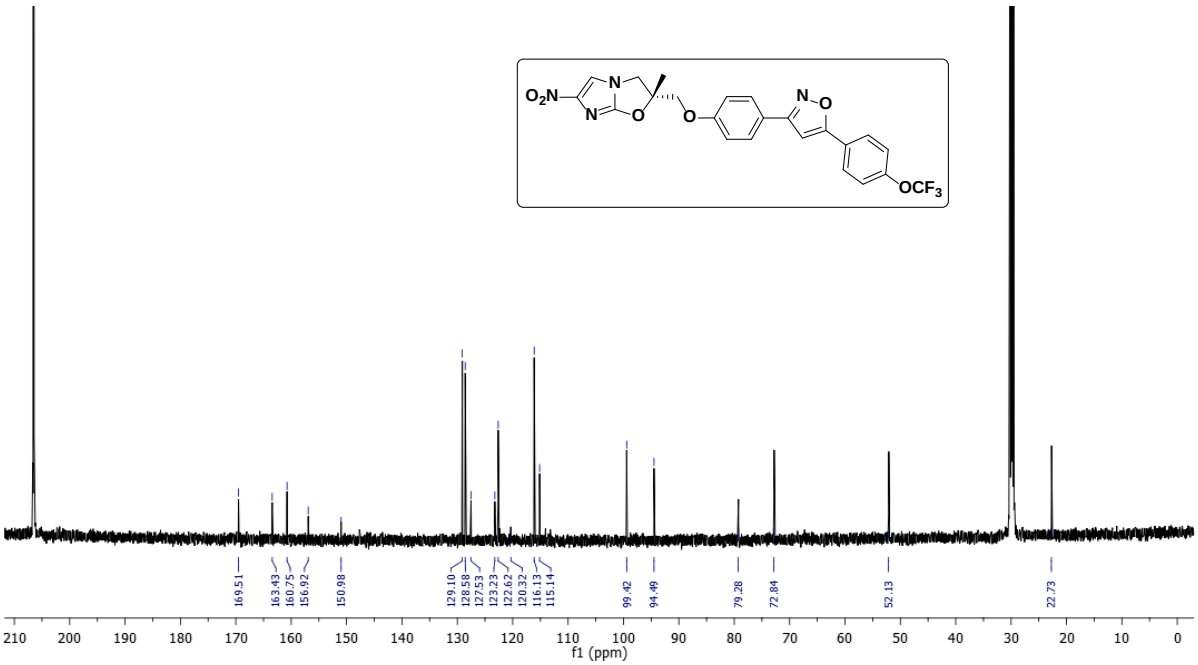
m/z	z	Abund	Formula	Ion
487.1229	1	238775.1	C23 H18 F3 N4 O5	(M+H)+
488.1257	1	63360	C23 H18 F3 N4 O5	(M+H)+
489.1284	1	12572	C23 H18 F3 N4 O5	(M+H)+
504.1494	1	155304.3	C23 H21 F3 N5 O5	(M+NH4)+
505.1522	1	42535.1	C23 H21 F3 N5 O5	(M+NH4)+
506.1547	1	8618.5	C23 H21 F3 N5 O5	(M+NH4)+
509.1045	1	35474	C23 H17 F3 N4 Na O5	(M+Na)+
510.1071	1	10296.7	C23 H17 F3 N4 Na O5	(M+Na)+
525.0782	1	11909.7	C23 H17 F3 K N4 O5	(M+K)+
526.0814	1	3268.6	C23 H17 F3 K N4 O5	(M+K)+

--- End Of Report ---

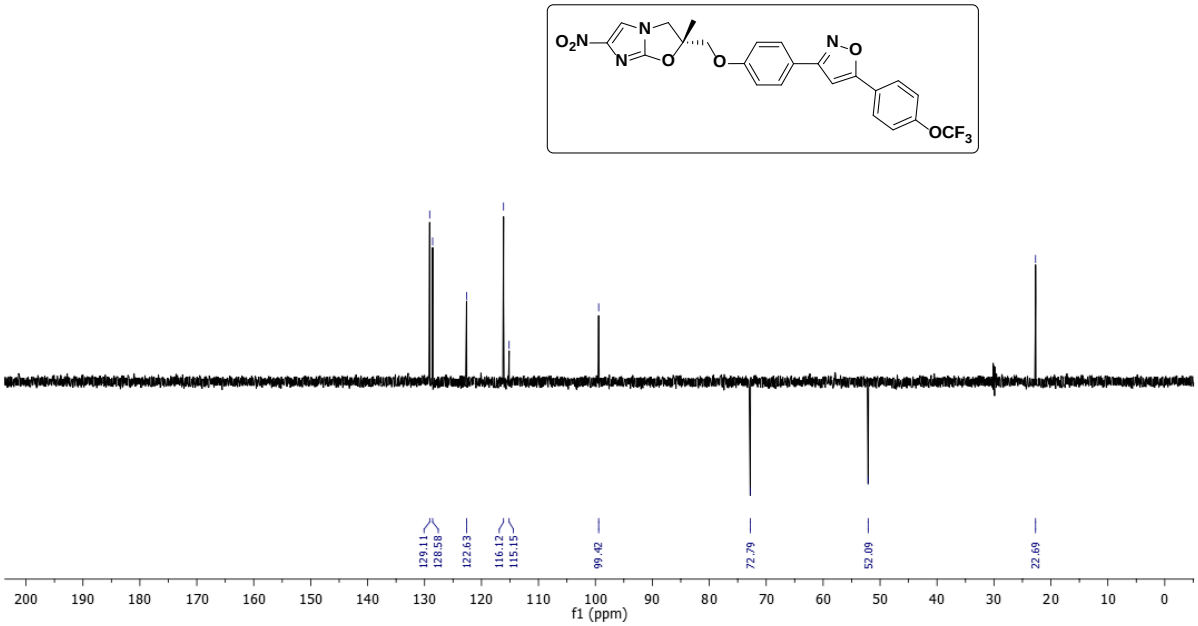
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2r (IIIM/MCD-074):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **2r (IIIM/MCD-074):**



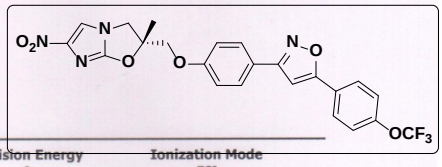
DEPT (126 MHz, Acetone-d_6) of compound **2r (IIIM/MCD-074):**



HRMS (ESI-TOF) of compound **2r (IIIM/MCD-074)**:

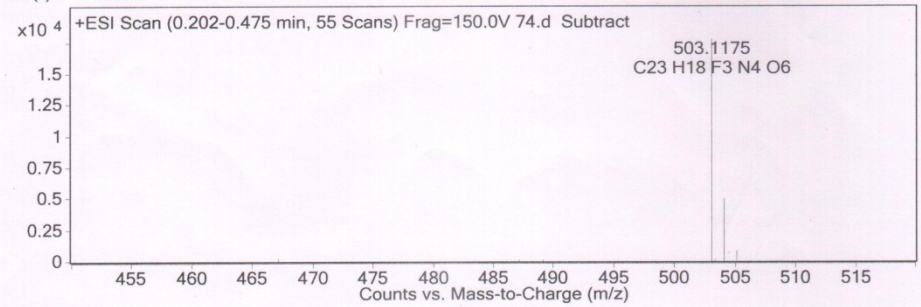
Qualitative Analysis Report

Data Filename	74.d	**Sample Name**	74
Sample Type	Sample	**Position**	Vial 31
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	27-07-2012 PM 01:29:16
IRM Calibration Status	Success	**DA Method**	Vishal_Compound_report.m
Comment			
Sample Group	**Info.**		



User Spectra

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



Peak List

m/z	z	Abund	Formula	Ion
288.2896		968		
503.1175	1	17748.6	C23 H18 F3 N4 O6	(M+H)+
504.1208	1	4901	C23 H18 F3 N4 O6	(M+H)+
520.144	1	8320.7		
521.1469	1	2337.7		
525.0996	1	4871.5		
526.1027	1	1235.1		
541.0734		2349.5		

Formula Calculator Element Limits

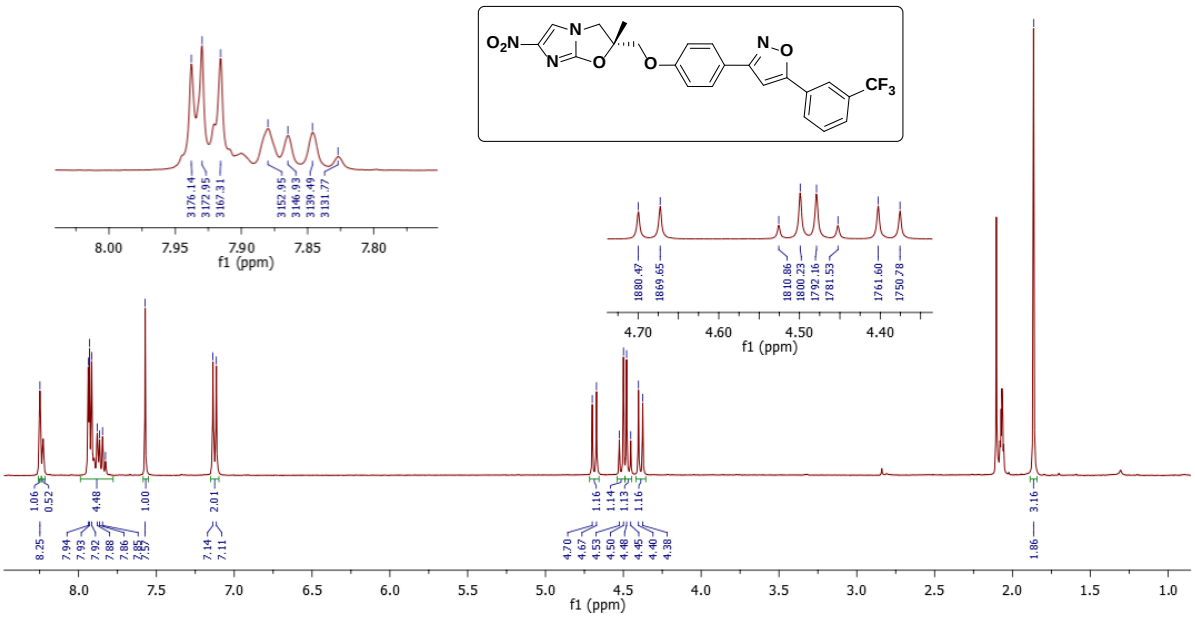
Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	10
F	0	6

Formula Calculator Results

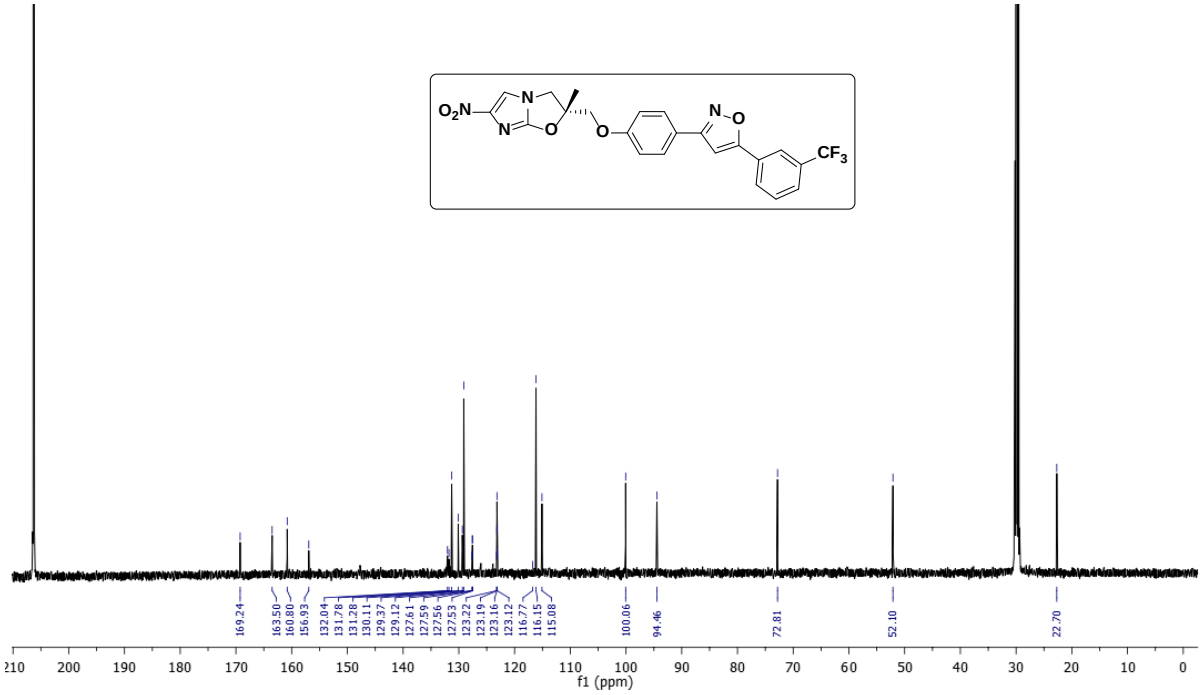
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C23 H17 F3 N4 O6	TRUE	502.1102	502.11	-0.39	C23 H18 F3 N4 O6	99.58
C21 H14 N10 O6		502.1102	502.1098	-0.9	C21 H15 N10 O6	98.75
C24 H22 O12		502.1102	502.1111	1.83	C24 H23 O12	97.37
C24 H13 F3 N8 O2		502.1102	502.1114	2.26	C24 H14 F3 N8 O2	96.69
C29 H15 F5 N2 O		502.1102	502.1105	0.48	C29 H16 F5 N2 O	96.62
C27 H12 F2 N8 O		502.1102	502.1102	-0.02	C27 H13 F2 N8 O	96.6
C22 H12 F6 N8		502.1102	502.1089	-2.61	C22 H13 F6 N8	95.73
C26 H16 F6 N2 O2		502.1102	502.1116	2.76	C26 H17 F6 N2 O2	95.7
C26 H16 F2 N4 O5		502.1102	502.1089	-2.67	C26 H17 F2 N4 O5	95.52
C18 H15 F N10 O7		502.1102	502.1109	1.38	C18 H16 F N10 O7	95.21

--- End Of Report ---

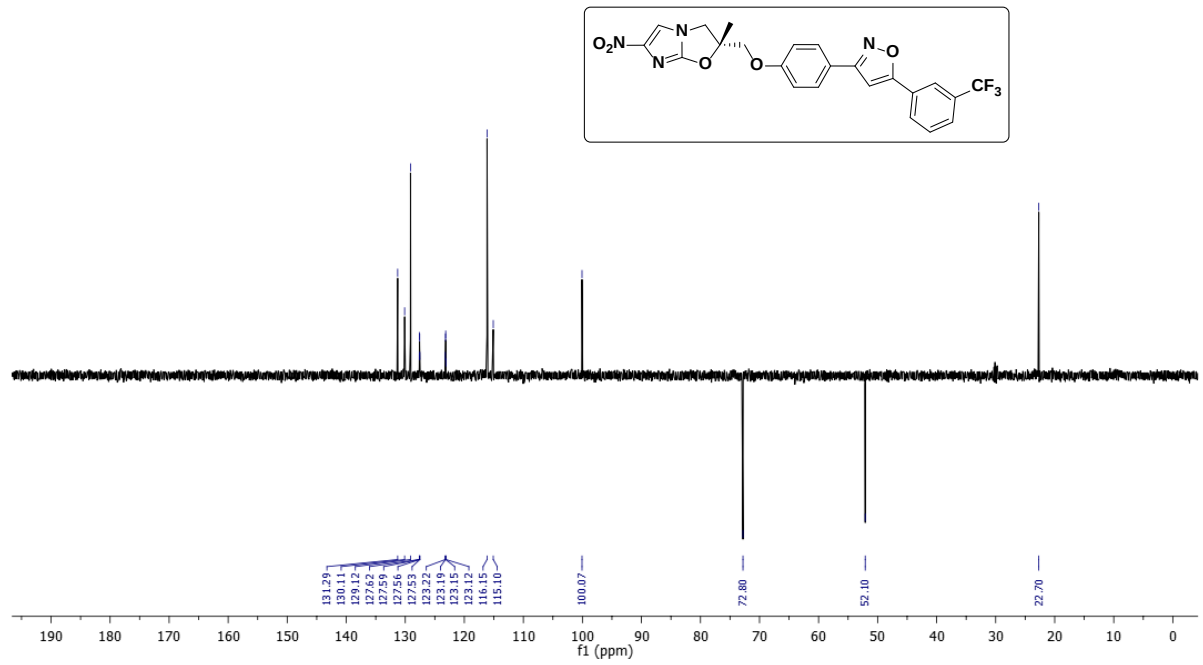
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2s (IIIM/MCD-125):**



^{13}C NMR (126 MHz, Acetone-d_6) of compound **2s (IIIM/MCD-125):**



DEPT (126 MHz, Acetone-d_6) of compound **2s (IIIM/MCD-125):**

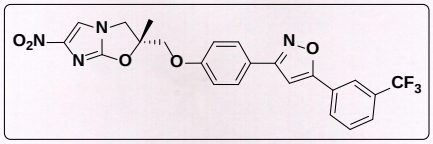


HRMS (ESI-TOF) of compound **2s (IIIM/MCD-125)**:

Qualitative Compound Report

Data File	125.d	**Sample Name**	125
Sample Type	Sample	**Position**	Vial 25
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	04-03-2013 PM 2:39:23
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

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

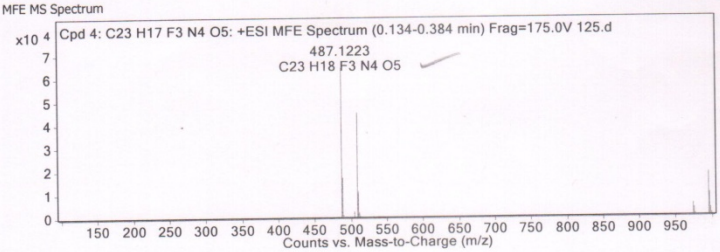


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C23 H17 F3 N4 O5	0.192	486.1149	C23 H17 F3 N4 O5	C23 H17 F3 N4 O5	0.41	C23 H17 F3 N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C23 H17 F3 N4 O5	487.1223	0.192	Find by Molecular Feature	486.1149

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
487.1223	1	64273.68	C23 H18 F3 N4 O5	(M+H)+
488.1251	1	16923.33	C23 H18 F3 N4 O5	(M+H)+
489.1272	1	3450.28	C23 H18 F3 N4 O5	(M+H)+
509.104	1	44775.54	C23 H17 F3 N4 Na O5	(M+Na)+
510.1072	1	11174.5	C23 H17 F3 N4 Na O5	(M+Na)+
973.2376	1	5185.26		(2M+H)+
974.2366	1	2962.2		(2M+H)+
995.2204	1	18278.33		(2M+Na)+
996.2211	1	9595.55		(2M+Na)+
997.2244	1	3231.42		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	487.1223	487.1224	0.17	100	100	75.37	75.9
2	488.1251	488.1254	0.75	26.33	26.73	19.85	20.29
3	489.1272	489.128	1.68	5.37	4.46	4.05	3.39
4	490.1261	490.1306	9.2	0.97	0.56	0.73	0.42

--- End Of Report ---

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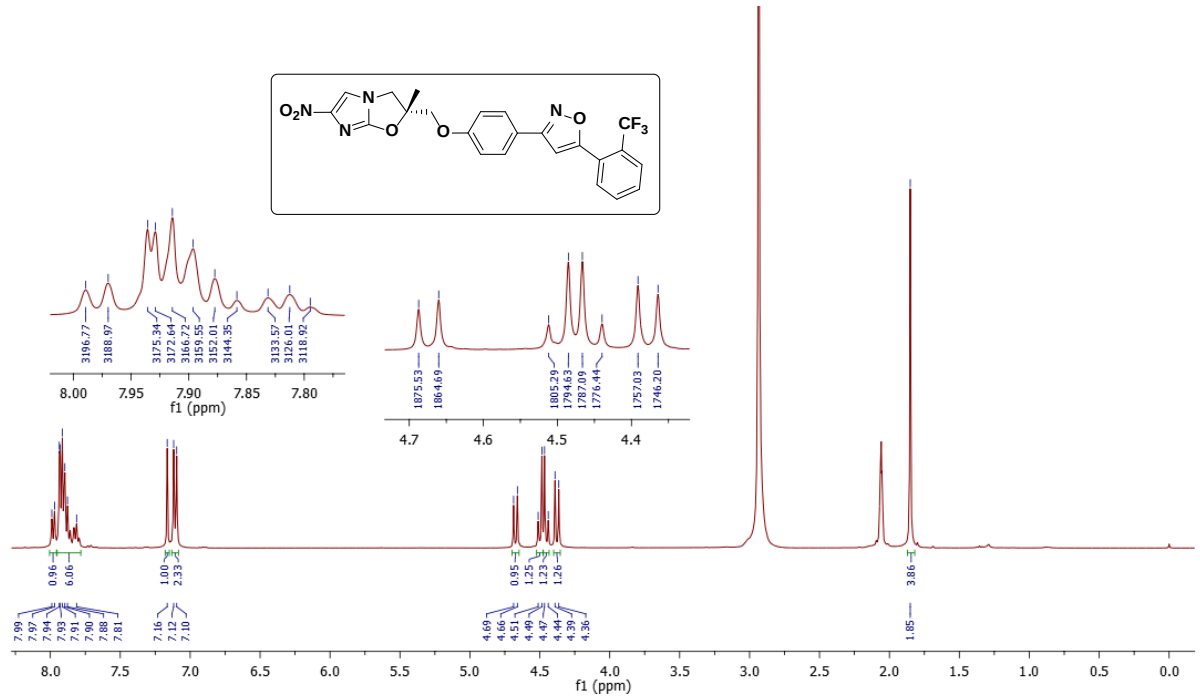
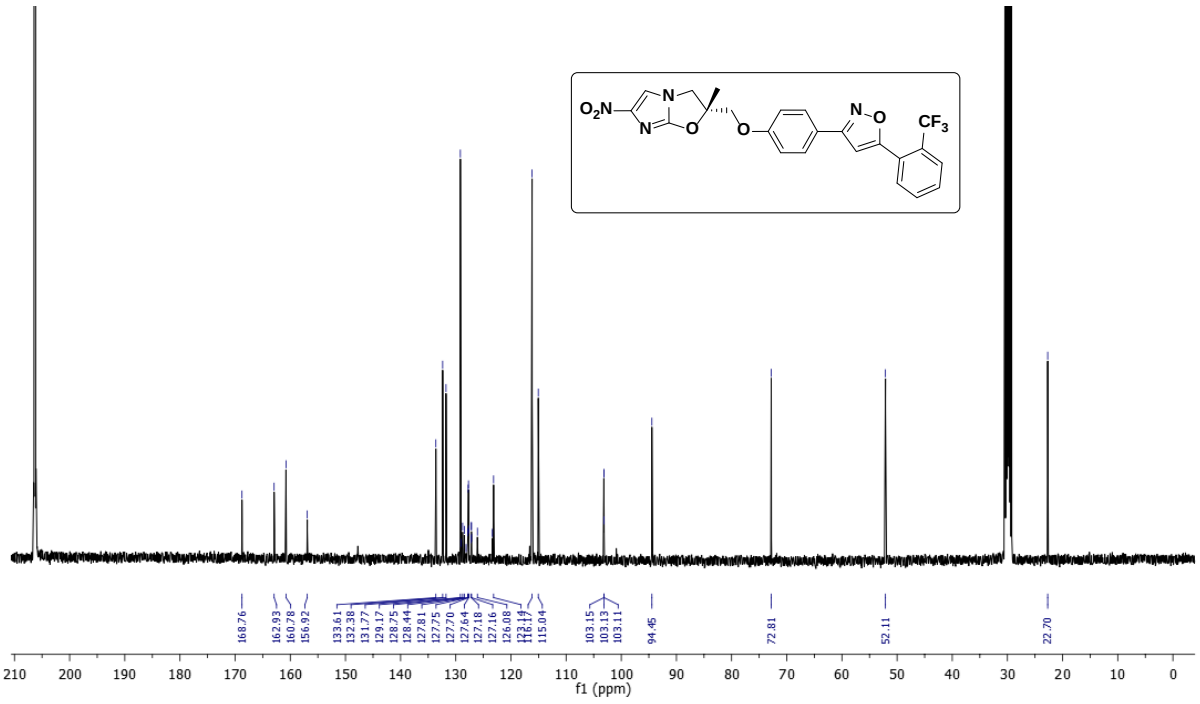
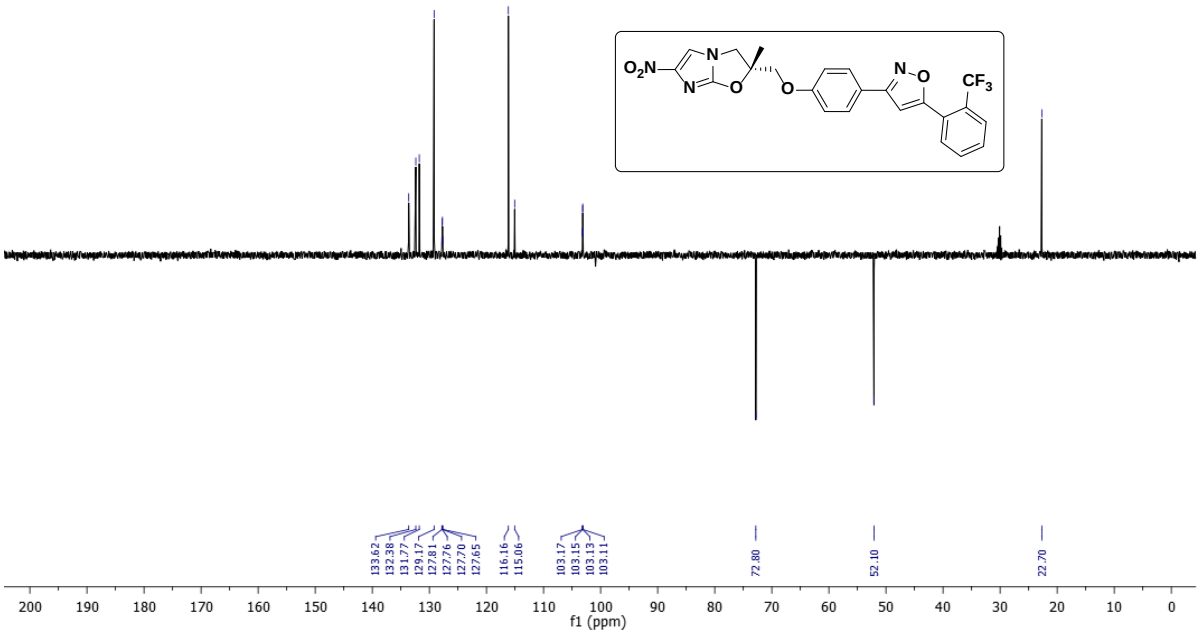
^{1}H NMR (400 MHz, Acetone-d_6) of compound **2t (IIIM/MCD-176):**



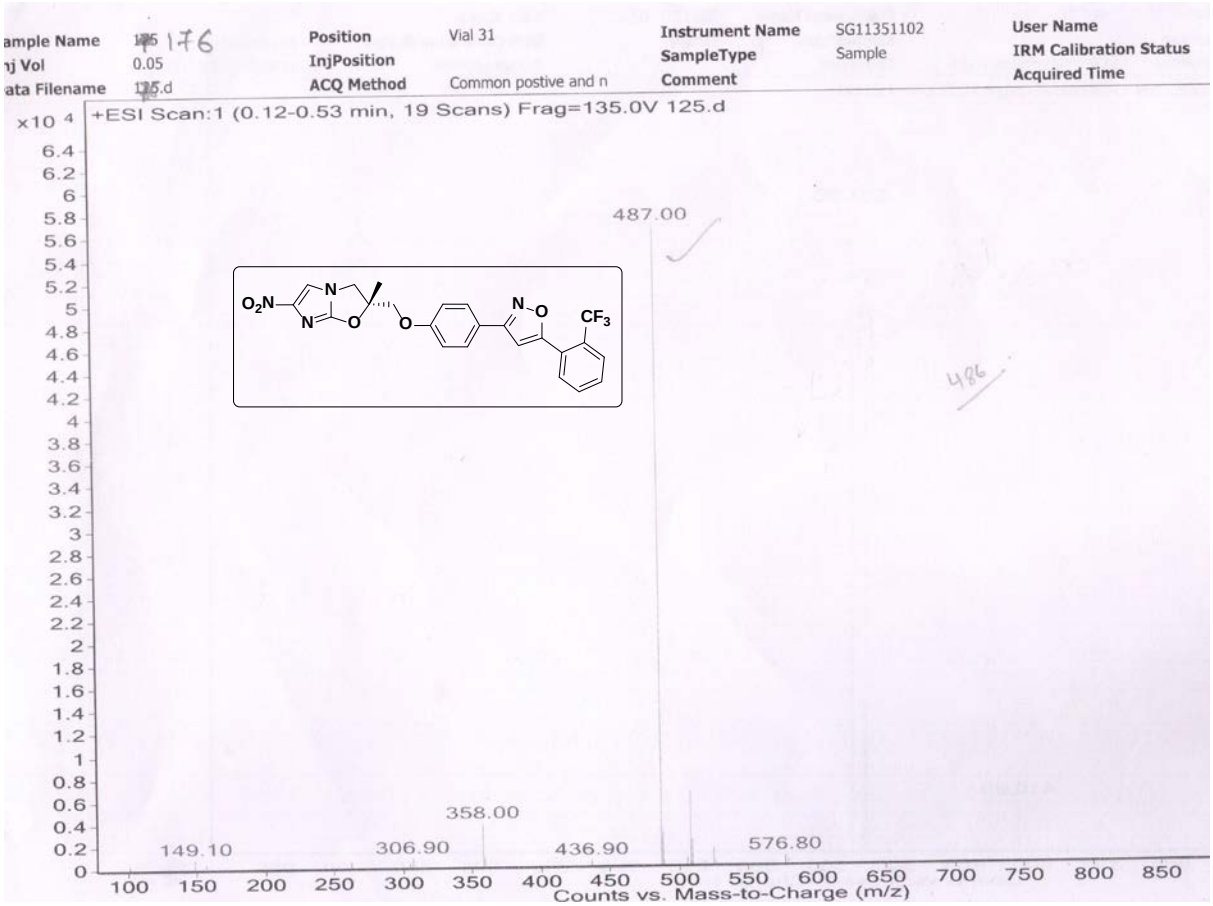
^{13}C NMR (101 MHz, Acetone-d_6) of compound **2t (IIIM/MCD-176):**



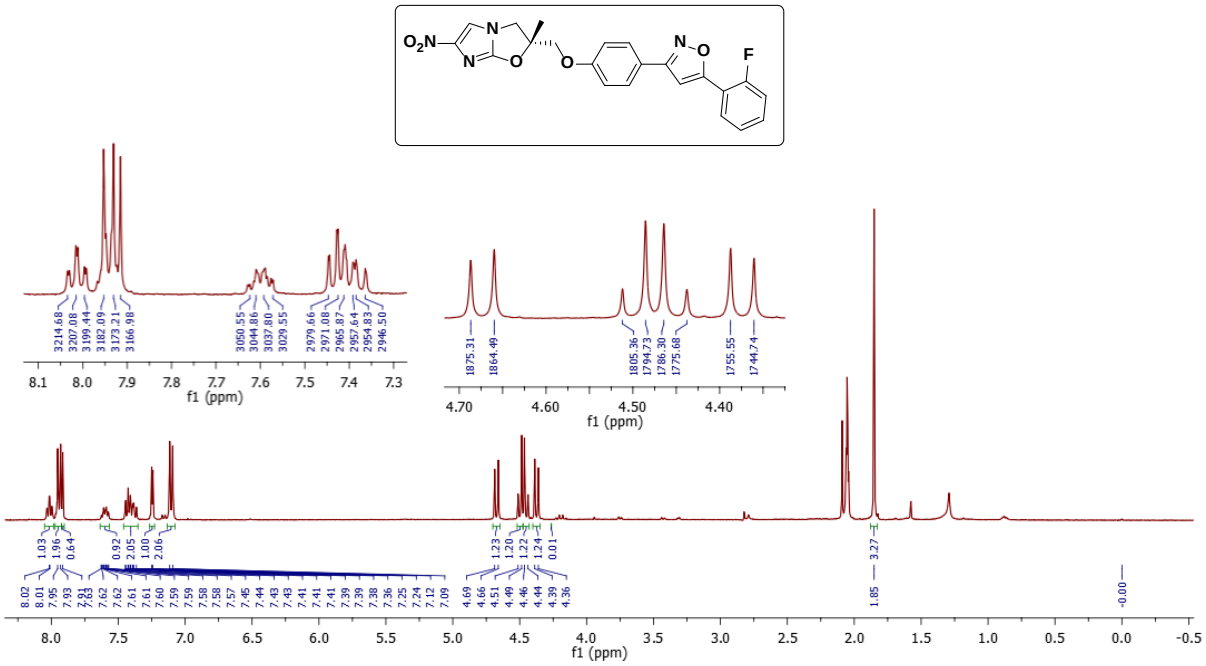
DEPT (101 MHz, Acetone-d_6) of compound **2t (IIIM/MCD-176):**



LC-MS (ESI-TOF) of compound **2t (IIIM/MCD-176)**:



^{1}H NMR (400 MHz, Acetone-d_6) of compound **2u (IIIM/MCD-126):**

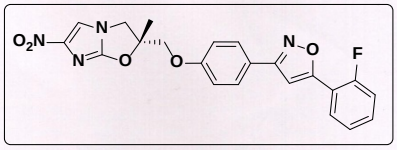


HRMS (ESI-TOF) of compound **2u (IIIM/MCD-126)**:

Qualitative Compound Report

Data File	126.d	**Sample Name**	126
Sample Type	Sample	**Position**	Vial 26
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	04-03-2013 PM 2:40:52
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

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

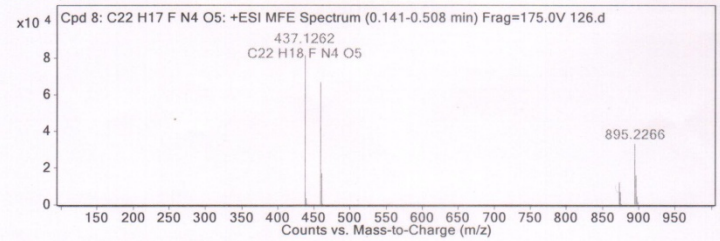


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C22 H17 F N4 O5	0.192	436.1188	C22 H17 F N4 O5	C22 H17 F N4 O5	-1.23	C22 H17 F N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C22 H17 F N4 O5	437.1262	0.192	Find by Molecular Feature	436.1188

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
437.1262	1	81529.41	C22 H18 F N4 O5	(M+H)+
438.1289	1	22530.55	C22 H18 F N4 O5	(M+H)+
459.1084	1	66613.77	C22 H17 F N4 Na O5	(M+Na)+
460.1114	1	17086.86	C22 H17 F N4 Na O5	(M+Na)+
461.1123	1	3821.33	C22 H17 F N4 Na O5	(M+Na)+
873.2444	1	12324.99		(2M+H)+
874.2464	1	7032.78		(2M+H)+
895.2266	1	33251.28		(2M+Na)+
896.2309	1	15949.37		(2M+Na)+
897.2317	1	4547.14		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	437.1262	437.1256	-1.43	100	100	75.6	76.72
2	438.1289	438.1286	-0.7	27.63	25.65	20.89	19.68
3	439.131	439.1312	0.4	4.04	4.19	3.05	3.21
4	440.1343	440.1337	-1.48	0.6	0.51	0.45	0.39

--- End Of Report ---

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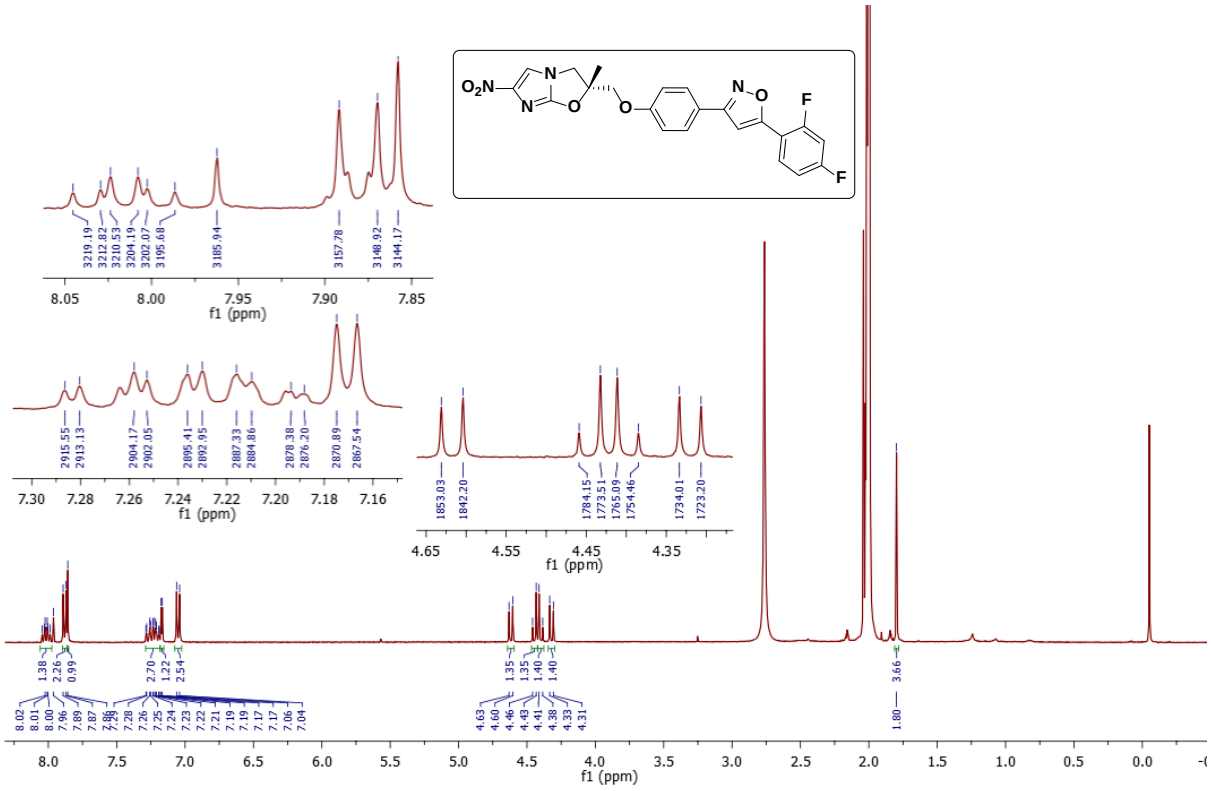
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2v (IIIM/MCD-070):**

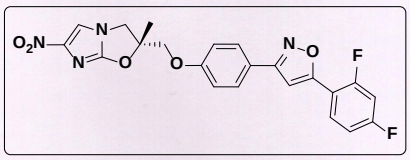


HRMS (ESI-TOF) of compound **2v (IIIM/MCD-070)**:

Qualitative Compound Report

Data File	70.d	**Sample Name**	70
Sample Type	Sample	**Position**	Vial 40
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-04-2013 PM 1:01:42
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)

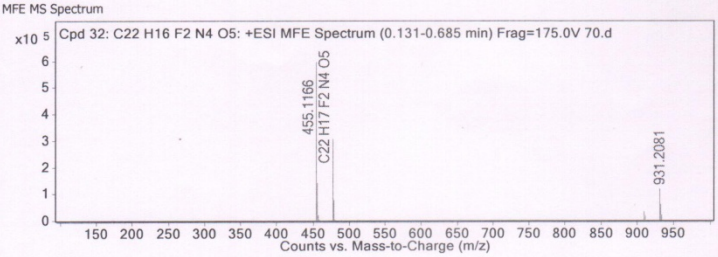


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 32: C22 H16 F2 N4 O5	0.189	454.1092	C22 H16 F2 N4 O5	C22 H16 F2 N4 O5	-0.71	C22 H16 F2 N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 32: C22 H16 F2 N4 O5	455.1166	0.189	Find by Molecular Feature	454.1092

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
455.1166	1	594639.81	C22 H17 F2 N4 O5	(M+H)+
456.1191	1	141999.67	C22 H17 F2 N4 O5	(M+H)+
457.1217	1	21452.59	C22 H17 F2 N4 O5	(M+H)+
477.0982	1	306321.78	C22 H16 F2 N4 Na O5	(M+Na)+
478.1007	1	77607.11	C22 H16 F2 N4 Na O5	(M+Na)+
909.225	1	32465.74		(2M+H)+
910.2279	1	17499.49		(2M+H)+
931.2081	1	118956.51		(2M+Na)+
932.2105	1	60755.06		(2M+Na)+
933.2132	1	19647.02		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	455.1166	455.1162	-0.98	100	100	78.1	76.69
2	456.1191	456.1192	0.27	23.88	25.64	18.65	19.67
3	457.1217	457.1217	0	3.61	4.18	2.82	3.21
4	458.1239	458.1243	0.85	0.44	0.51	0.34	0.39
5	459.1208	459.1268	12.9	0.11	0.05	0.08	0.04

--- End Of Report ---

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