Supplemental information for:

Calcium uncaging with visible light.

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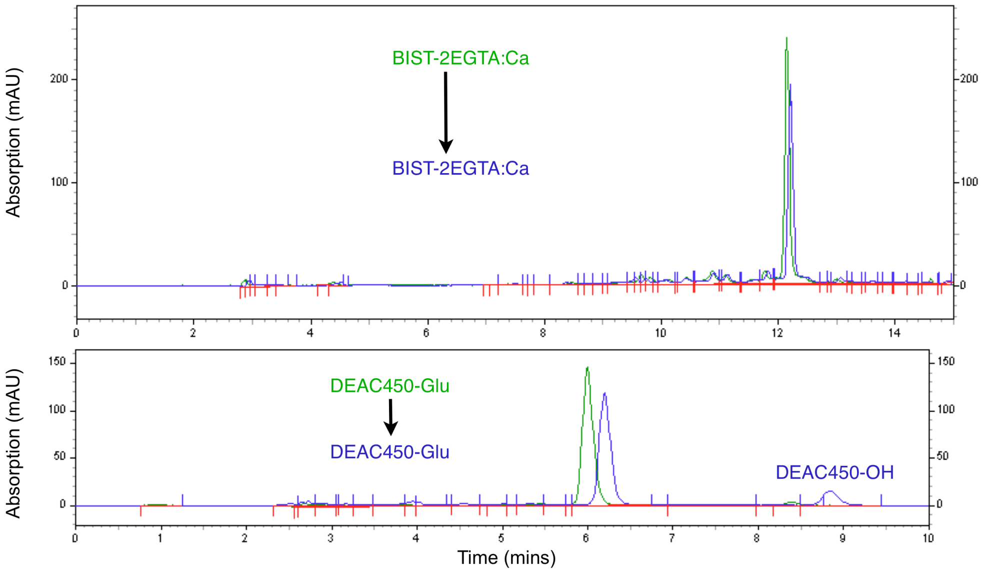
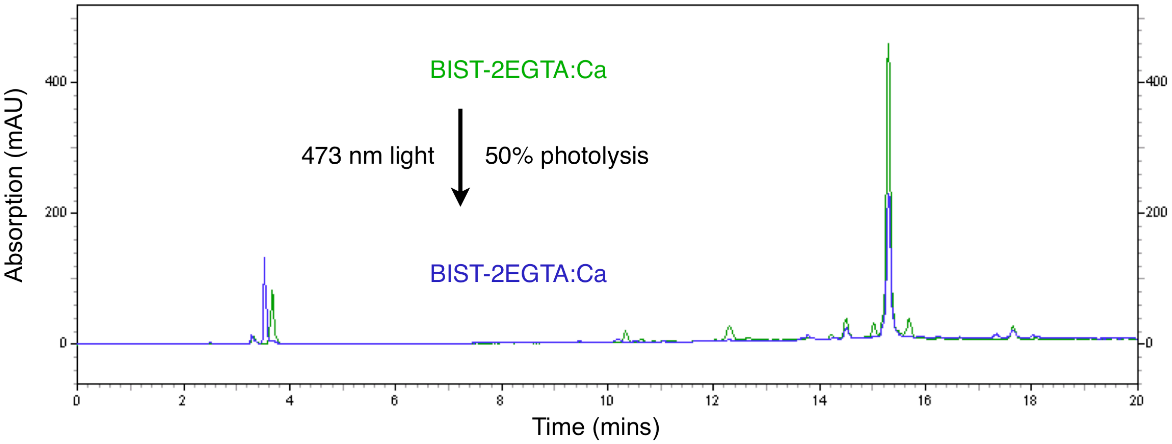
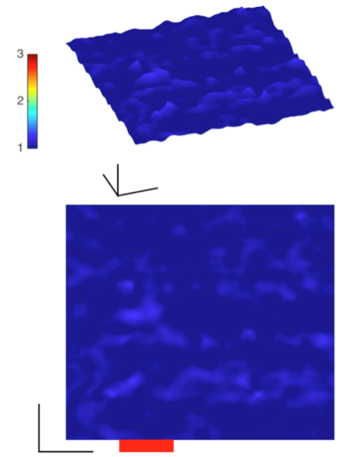


Supplemental Figure 1. Representative HPLC chromatograms from the photolysis of BIST-2EGTA and DEAC450-Glu. Each compound initially had the same absorption at 410 nm. A 410nm-laser was used for photolysis. Chromatograms were monitored at 410 nm.



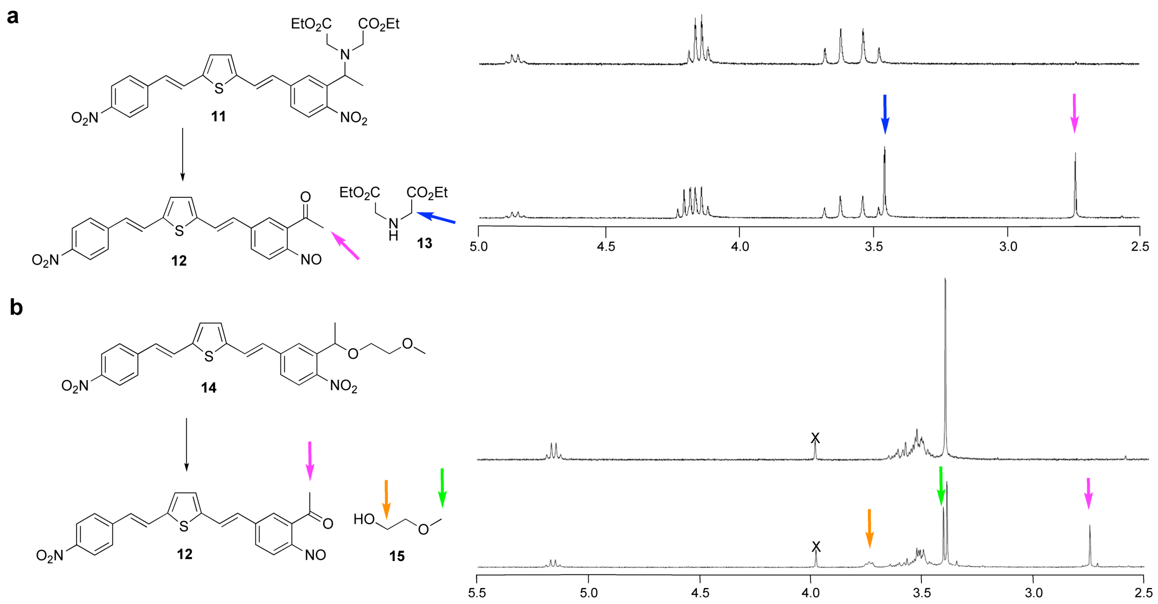
Supplemental Figure 2. HPLC chromatogram from the photolysis of BIST-2EGTA with visible light. Before photolysis a Ca^{2+}-selective electrode showed the free [Ca^{2+}] to be 0.2 μM. After 50% photolysis of BIST-2EGTA the free [Ca^{2+}] increased to 20 μM. Chromatograms were monitored at 473 nm.



Supplemental Figure 3. Control experiment showing photolysis with EGTA in place of BIST-2EGTA does not release Ca.

Cardiac myocyte was patch-clamped as in Fig. 3 with the following solution (mM): 2 EGTA, 1.5 $CaCl_2$, 0.1 X-rhod-5F, 1 GSH, 5 K_2ATP, 10 HEPES, 20 TEA-Cl, 120 L-Aspartic acid, 120 CsOH, 8 NaCl, pH = 7.20. Point 2P irradiation at 810 nm with a much higher energy than used with BIST-2EGTA (~17 mW, 50 ms, red bar) in the middle of the scanning line did not produce any fluorescence signal.

Scale bars for units of 1 F/F_0, 5 μm and 50 ms.



Supplemental Figure 4. NMR spectra of photolysis of a BIST-caged amine and alcohol.

(**a**) NMR analysis of the photolysis of BIST-caged amine **11** in $CDCl_3$ showed the appearance of singlets corresponding to signals from the ketone **12** (pink arrow) and secondary amine **13** photoproducts (blue arrow).

(**b**) NMR analysis of the photolysis of BIST-caged alcohol **14** in $CDCl_3$ showed the appearance of singlets corresponding to signals from the ketone **12** (pink arrow) and primary alcohol **15** photoproducts (green arrow). The alcohol methylene is indicated with the orange arrow. X indicates a small impurity.

BIST-2EGTA.

2-(5-Bromo-2-nitrophenyl)oxirane (2).

A supension of 5-Bromo-2-nitrobenzaldehyde (10.0 g, 43.7 mmol) and cesium carbonate (21.5 g, 66.0 mmol) in tetrahydrofuran (200 mL) was heated at 60 °C for 10 min, then a suspension of carboxymethyl-4-cyanophenylmethylsulfonium trifluoromethanesulfonate (23.4 g, 65.5 mmol) in THF (150 mL) was slowly added to the reaction mixture over a period of 30 min and the reaction was heated for 2 h. The solution was cooled to room temperature, filtered through celite, concentrated and dried under reduced pressure and purified by flash chromatography (3% ethyl acetate in hexanes, v/v) to give 7.90 g (74%) of **2** as white crystals. Melting point: 77 °C. ^{1}H NMR: (300 MHz, CDCl$_3$) δ 8.03 (d, *J* = 8.7 Hz, 1H, Ar H-3), 7.76 (s, 1H, Ar H-6), 7.60 (dd, *J* = 8.7 and 2.4 Hz, 1H, Ar H-4), 4.47 (dd, *J* = 3.9 and 2.4 Hz, 1H, H-1′), 3.31 (t, *J* = 5.1 Hz, 1H, H-2′), 2.68 (dd, *J* = 6.0 and 2.4 Hz, 1H, H-2′′). ^{13}C NMR (75 MHz, CDCl$_3$) δ 146.35, 136.51, 131.69, 130.12, 129.69, 126.13, 50.69, 50.34. HRMS (m/z) for $C_8H_7BrNO_3$. Calcd. 243.9609. Found: m/z 243.9608 (M+H)$^+$.

2-[2{2-Hydroxy-2-(5-bromo-2-nitrophenyl)-ethoxy}ethoxy]ethanol (3).

Sodium hydride (60% dispersion, 0.700 g, 17.1 mmol) was slowly added to diethylene glycol (100 mL) over 30 min. and then heated at 60 °C for 2 h. A warm solution of **2** (4.10 g, 16.8 mmol) in diethylene glycol (50 mL) was added to the reaction mixture, which was then heated at 60 °C for 20 h. Brine (250 mL) was added to the reaction mixture, which was then extracted with dichloromethane (5 x 100 mL). The organic layer was concentrated and dried under reduced pressure and the residue was purified by flash chromatography (3% methanol in dichloromethane, v/v) to give 3.00 g (80%) of **3** as white solid. Unreacted starting material (0.6 g) was also recovered from the reaction. ^{1}H NMR: (300 MHz, CDCl$_3$) δ 8.08 (d, *J* = 2.1 Hz, 1H, Ar H-6), 7.85 (d, *J* = 8.7 Hz, 1H, Ar H-3), 7.55 (dd, *J* = 8.7 and 2.1 Hz, 1H, Ar H-4), 5.53 (dd, *J* = 2.7 and 8.0 Hz, 1H, benzylic-C*H*), 3.84 (dd, *J* = 2.8 and 10.3 Hz, 1H, -CH_2-), 3.60-3.80 (m, 8H, -CH_2-), 3.20 (s, 2H, 1′-OH and 6′-OH), 3.47 (dd, *J* = 8.1 and 10.3 Hz, 1H, -CH_2-). ^{13}C NMR (75 MHz, CDCl$_3$) δ 146.23, 138.17, 132.05, 131.38, 129.77, 125.87, 75.53, 72.59, 70.28, 70.18, 67.78, 61.59. HRMS (m/z) for $C_{12}H_{16}BrNNaO_6$. Clad. 374.0038. Found: m/z 374.0038 (M+Na)$^+$.

2-[2{2-(2-Bromoethoxy)ethoxy}-1-bromoethyl-4-bromonitrobenzene (4).

To a cold solution of **3** (2.29 g, 6.54 mmol) and triphenylphosphene (6.90 g, 26.2 mmol) in anhydrous dichloromethane (80 mL) was added a solution of carbontetrabormide (9.50 g, 28.8 mmol) in dichloromethane (20 mL). The reaction mixture was stirred for 1 h at 4°C and then stirred at room temperature for 2 h. The solvent was evaporated under reduced pressure and the residue was purified by flash chromatography (10% ethyl acetate in hexanes, v/v) to give 2.50 g (80%) of dibromide **4** as yellow oil. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 2.1 Hz, 1H, Ar H-3), 7.50 (d, *J* = 8.7 Hz, 1H, Ar H-6), 7.58 (dd, *J* = 8.7 and 2.1 Hz, 1H, Ar H-5), 5.80 (t, *J* = 6.5 Hz, 1H, benzylic-C*H*), 4.03 (d, *J* = 7.0 Hz, 2H, -CH_2-), 3.77 (t, *J* = 6.1 Hz, 2H, -CH_2-), 3.66-3.72 (m, 2H, -CH_2-), 3.61-3.66 (m, 2H, -CH_2-), 3.44 (t, *J* = 6.1 Hz, 2H, -CH_2-). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.10, 135.42, 133.96, 132.20, 127.89, 125.85, 74.70, 71.12, 70.79, 70.44, 42.91, 30.46. HRMS (m/z) for $C_{12}H_{14}Br_3NO_4Na$. Calcd. 497.8350. Found: m/z 497.8351 $(M+Na)^+$.

2-[2{2-(2-Azidoethoxy)ethoxy}-1-azidoethyl-4-bromonitrobenzene (5).

Sodium Azide (2.4 g, 36.8 mmol) and sodium iodide (4.70 g, 31.2 mmol) and a solution of **4** (2.50 g, 5.2 mmol) in DMF (50 mL) were stirred at room temperature for 18h. The solvent was evaporated under reduced pressure and the residue was purified by flash chromatography (10% ethyl acetate in hexanes, v/v) to give 1.93 g (92%) of **5** as yellow oil. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 7.86-7.90 (m, 2H, Ar H-3, Ar H-6), 7.61 (dd, *J* = 8.7 and 2.1 Hz, 1H, Ar H-5), 5.54 (dd, *J* = 3.8 and 7.7 Hz, 1H, benzylic-C*H*), 3.85 (dd, *J* = 2.8 and 10.4 Hz, 1H, -CH_2-), 3.65-3.78 (m, 7H, -CH_2-), 3.29 (t, *J* = 5.0 Hz, 2H, -CH_2-). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.98, 134.35, 132.85, 132.42, 128.92, 126.51, 74.97, 71.23, 71.00, 70.45, 60.11, 51.06. HRMS (m/z) for $C_{12}H_{14}BrN_7O_4Na$. Calcd. 422.01888. Found: m/z 422.0188 $(M+Na)^+$.

3-[2-{2-(2-Azidoethoxy)ethoxy}-1-azidoethyl]-4-nitrostyrene (6).

Compound **5** (3.95 g, 9.9 mmol) and tetrakis(triphenylphosphine)palladium (0.250 g, 0.220 mmol) were dissolved in ethylene glycol dimethyl ether (90 mL). A solution of potassium carbonate (1.40 g, 10.0 mmol) in water (10 mL) was added to the reaction mixture followed by 2,4,6-trivinyl-boroxin pyridine complex (1.2 g, 5 mmol). The reaction mixture was heated at reflux temperature for 18 h. The solvents were evaporated under reduced pressure and the residue was purified by flash chromatography (20% ethyl acetate in hexanes, v/v) to give 2.50 g (73%) of **6** as yellow oil. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.5 Hz, 1H, Ar H-5), 7.67 (d, *J* = 1.9 Hz, 1H, Ar H-2), 7.48 (dd, *J* = 8.5 and 1.9 Hz, 1H, Ar H-6), 6.76 (dd, *J* = 10.9 and 6.7 Hz, 1H, vinyl-C*H*), 5.94 (d, *J* = 17.6 Hz, 1H, vinyl-C*H*), 5.55 (dd, *J* = 3.5 and 8.1 Hz, 1H, benzylic-C*H*), 5.52 (d, *J* = 10.9 Hz, 1H, vinyl-C*H*), 3.87 (dd, *J* = 3.5 and 10.5 Hz, 1H, -CH_2-), 3.65-3.78 (m, 7H, -CH_2-), 3.39 (t, *J* = 5.0 Hz, 2H, -CH_2-). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.59, 142.78, 134.48, 132.49, 126.95, 125.99, 118.82, 76.58, 74.91, 70.75, 70.63, 70.06, 60.24, 50.70. HRMS (m/z) for $C_{14}H_{17}N_7O_4Na$. Calcd. 370.1240. Found: m/z 370.1241 $(M+Na)^+$.

2,5-Bis[3-{2-(2-(2-azidoethoxy)ethoxy)-1-azidoethyl}-4-nitrostyryl]thiophene (7).
2,5-Dibromothiophene (0.250 mL, 2.20 mmol), **6** (2.30 g, 6.70 mmol), lithium chloride (600 mg, 14.0 mmol), sodium bicarbonate (1.50 g, 18.0 mmol), and tetrabutylammonium chloride (1.20 g, 4.40 mmol) were dissolved in DMF (50 mL) and purged with N_2 for 20 min. Palladium (II) acetate (0.200 g, 0.90 mmol) was added to the reaction mixture, which was then heated at 110 °C for 1 h. Water (100 mL) was added to the reaction mixture, which was then extracted with ethyl acetate (3 x 100 mL). The organic layer was separated, concentrated under reduced pressure and the residue was purified by flash chromatography (30% ethyl acetate in hexanes, v/v) to give 1.20 g (71%) of **7** as amorphous red solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.5 Hz, 2H, Ar H-5), 7.72 (s, 2H, Ar H-2), 7.50 (d, *J* = 8.5 Hz, 2H, Ar H-6), 7.30 (d, *J* = 16 Hz, 2H, vinyl C*H*), 7.10 (s, 2H, thiophene-C*H*), 6.90 (d, *J* = 16 Hz, 2H, vinyl-C*H*), 5.62 (dd, *J* = 3.3 and 7.9 Hz, 2H, benzylic-C*H*), 3.90 (dd, *J* = 3.4 and 10.5 Hz, 2H, -CH_2-), 3.60-3.82 (m, 14H, -CH_2-), 3.38 (t, *J* = 4.9 Hz, 4H, -CH_2-). ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.95, 142.18, 142.06, 132.87, 129.23, 126.80, 126.07, 125.92, 125.85, 125.65, 74.93, 70.71, 70.62, 70.03, 60.31, 50.67. HRMS (m/z) for $C_{32}H_{34}N_{14}O_8SNa$. Calcd. 797.2302. Found: m/z 797.2306 $(M+Na)^+$.

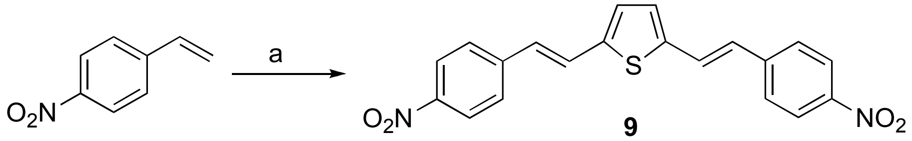
2,5-Bis[3-{2-(2-(2-(*N,N*-diethoxycarboxyl)aminoethoxy)ethoxy)-1-(*N,N*-dicarboxyl)aminoethyl}-4-nitrostyryl]thiophene (8).
To a solution of **7** (1.05 g, 1.36 mmol) in THF (50 mL) and water (1 mL) was added triphenylphosphene (14.3 g, 54.5 mmol), and the reaction mixture was stirred at room temperature for 2 h. Sodium hydroxide solution (2.5 M, 20 mL) was added to the reaction mixture, which was then stirred at room temperature for 18 h. Water (100 mL) was added and the reaction mixture was extracted with dichloromethane (3 x 100 mL). The organic layer was separated and extracted with acidic water (3 x 100 mL 0.1% TFA). The aqueous layer was separated and washed with dichloromethane (100 mL) and dried by lyophilization to give 0.630 g (70%) of tetraamine intermediate, which was used in the next synthetic step. A small amount of this material was purified by reverse phase HPLC using 35% acetonitrile in water (0.1% TFA) on an Altima C_{18} column to yield an analytically pure sample for spectroscopic characterization. ^{1}H NMR: (300 MHz, CD_3OD) δ 8.14 (d, *J* = 8.6 Hz, 2H, Ar H-5), 8.00 (s, 2H, Ar H -2), 7.81 (d, *J* = 8.6 Hz, 2H, Ar H-6), 7.66 (d, *J* = 16 Hz, 2H, vinyl C*H*), 7.26 (s, 2H, thiophene-C*H*), 7.09 (d, *J* = 16 Hz, 2H, vinyl-C*H*), 5.23 (dd, *J* = 4.9 and 7.0 Hz, 2H, benzylic-C*H*), 4.0-4.1 (m, 4H, -CH_2-), 3.67-3.87 (m, 12H, -CH_2-), 3.13 (t, *J* = 5.0 Hz, 4H, -CH_2-). ^{13}C NMR (75 MHz, CD_3OD) δ 146.79, 141.89, 141.76, 132.11, 129.74, 127.16, 126.24, 125.88, 125.59, 117.90, 71.78, 69.78, 69.28, 66.62, 49.22, 38.50. HRMS (m/z) for $C_{32}H_{43}N_6O_8S$. Calcd. 671.2863. Found: m/z 671.2852 $(M+H)^+$.

The tetraamine (0.500 g, 0.750 mmol) and pentamethylpiperidine (1.35 mL, 7.50 mmol) were dissolved in anhydrous acetonitrile (25 mL) and sodium iodide (11.5 g, 75.0 mmol) was added to the solution, followed by ethyl bromoacetate (8.4 mL, 75 mmol) in four equal portions to the reaction mixture over a period of 72 h. During this period the reaction mixture was heated at 60 °C. After completion of the reaction, the solvent was evaporated and the residue was purified by flash chromatography (5% methanol in dichloromethane, v/v) to give an amorphous red solid. This residue was dissolved in methanol and purified by reverse phase HPLC using 75% acetonitrile in water (0.1 % TFA). The solvents were removed under reduced pressure to give 0.450 g (44%) of **8**. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 1.6 Hz, 2H, Ar H-2), 7.82 (d, *J* = 8.5 Hz, 2H, Ar H-5), 7.43 (dd, *J* = 1.6 and 8.5 Hz, 2H, Ar H-6), 7.36 (d, *J* = 16 Hz, 2H, vinyl C*H*), 7.09 (s, 2H, thiophene-C*H*), 6.90 (d, *J* = 16 Hz, 2H, vinyl-C*H*), 5.23 (dd, *J* = 3.2 and 6.6 Hz, 2H, benzylic-C*H*), 4.05-4.23 (m, 16H, $-CH_2-$), 3.89 (s, 8H, $-CH_2-$), 3.41-3.85 (m, 24H, $-CH_2-$), 3.25 (t, *J* = 4.5 Hz, 4H, $-CH_2-$), 1.20-1.30 (m, 24H, $-CH_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.31, 168.43, 148.01, 142.08, 141.56, 136.51, 128.87, 127.77, 126.46, 125.58, 125.51, 125.02, 73.25, 69.99, 68.33, 61.29, 60.49, 59.09, 54.50, 53.69, 53.13, 14.27, 14.13. HRMS (m/z) for $C_{64}H_{91}N_6O_{24}S$. Calcd. 1359.5805. Found: m/z 1359.5804 $(M+H)^+$.

2,5-Bis[3-{2-(2-(2-(*N*,*N*-dicarbonyl)aminoethoxy)ethoxy)-1-(*N*,*N*-diethoxycarbonyl)aminoethyl}-4-nitrostyryl]thiophene (1).

Compound **7** (0.370 g, 0.270 mmol) was dissolved in methanol (25 mL) and potassium hydroxide (1 M, 0.82 mL) was added to the solution. The reaction mixture was stirred at room temperature for 18 h. The solvent was evaporated and residue was purified by reverse phase HPLC using 35% acetonitrile in water (0.1 % TFA) as the solvent system. Solvents were removed by lyophilyzation to give 0.162 g (53%) of **1** as an amorphous red solid. ^{1}H NMR: (300 MHz, D_2O) δ 7.97 (s, 2H, Ar H-2), 7.75 (d, *J* = 8.5 Hz, 2H, Ar H-5), 7.36-7.49 (m, 4H, Ar H-6 and vinyl C*H*), 7.12 (s, 2H, thiophene-C*H*), 6.96 (d, *J* = 16 Hz, 2H, vinyl-C*H*), 4.97 (t, *J* = 5.4 Hz, 2H, benzylic-C*H*), 3.67-3.87 (m, 4H, $-CH_2-$), 3.36-3.51 (m, 12H, $-CH_2-$), 3.19-3.22 (m, 16H, $-CH_2-$), 2.74-2.87 (m, 4H, $-CH_2-$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.76, 167.75, 148.09, 141.93, 141.17, 136.11, 129.67, 127.69, 126.63, 126.05, 125.64, 125.03, 72.56, 72.46, 69.50,69.37,65.55, 63.16, 58.69, 55.02, 52.85. HRMS (m/z) for $C_{48}H_{59}N_6O_{24}S$. Calcd. 1135.3301. Found: m/z 1135.3297 $(M+H)^+$.

Synthesis of compound 9.

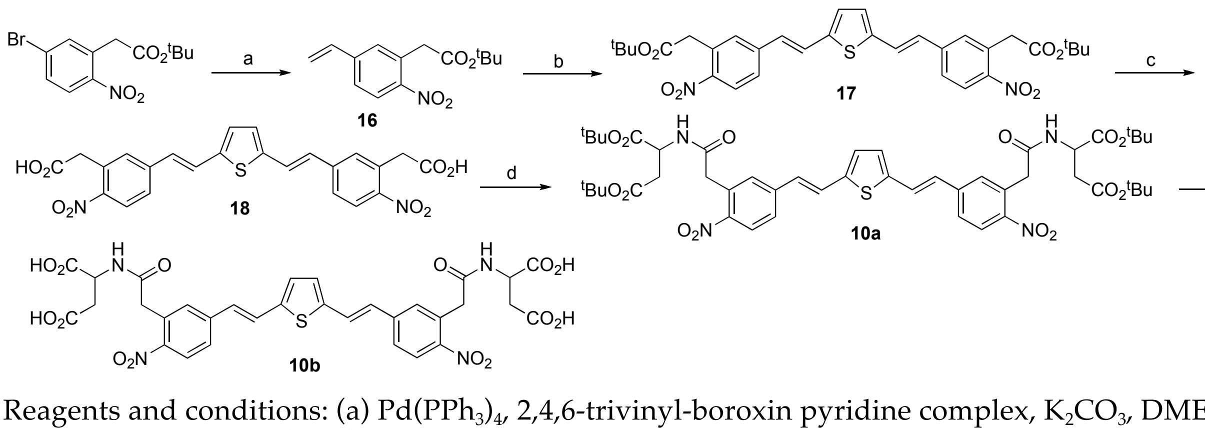


Reagents and conditions: (a) 2,5-Dibromothiophene, Pd(OAc)$_2$, LiCl, TBACl, NaHCO$_3$, TPGS-750-M, DMF. Note this is a known compound.

2,5-Bis-4-nitrostyrylthiophene (9).

2,5-Dibromothiophene (50.0 mg, 0.207 mmol), 4-nitrostyrene (123 mg, 0.825 mmol), lithium chloride (100 mg, 2.38 mmol), sodium bicarbonate (200 mg, 2.38 mmol), and tetrabutylammonium chloride (120 mg, 0.43 mmol) were dissolved in DMF (5 mL) and purged with N$_2$ for 20 min. TPGS-750M (DL-α-Tocopherol methoxypolyethylene glycol succinate solution, 5 wt % in water, 200 μL) and palladium (II) acetate (10.0 mg, 0.045 mmol) were added to the reaction mixture, which was then heated at 110 °C for 1 h. Water (100 mL) was added to the reaction mixture, which was extracted with ethyl acetate (3 x 100 mL). The organic layer was separated, concentrated under reduced pressure and the residue was purified by flash chromatography (50% ethyl acetate and 10% THF in hexanes, v/v) to give 50.0 mg (64%) of **9** as an amorphous red solid. ^{1}H NMR: (300 MHz, DMSO-d$_6$) δ 8.23 (d, *J* = 8.6 Hz, 4H, Ar H-3,5), 7.86 (d, *J* = 8.6 Hz, 4H, Ar H-2,6), 7.76 (d, *J* = 16.2 Hz, 2H, vinyl C*H*), 7.34 (s, 2H, thiophene-C*H*), 7.14 (d, *J* = 16.2 Hz, 2H, vinyl-C*H*). ^{13}C NMR (75 MHz, DMSO-d$_6$) δ 145.88, 143.22, 141.99, 129.78, 127.01, 126.24, 126.16, 123.84.

Synthesis of compound 10.



Reagents and conditions: (a) Pd(PPh$_3$)$_4$, 2,4,6-trivinyl-boroxin pyridine complex, K$_2$CO$_3$, DME, H$_2$O; (b) 2,5-dibromothiophene, Pd(OAc)$_2$, LiCl, TBACl, NaHCO$_3$, TPGS-750-M, DMF; (c) DCM, TFA; (d) L-aspartic acid di-*tert*-butyl ester hydrochloride, EDC hydrochloride, THF; (e) DCM, TFA.

tert-Butyl 2-(2-nitro-5-vinylphenyl)acetate (**16**).

tert-Butyl 2-(5-bromo-2-nitrophenyl)acetate (330 mg, 1 mmol) and tetrakis(triphenylphosphine)palladium (24.0 mg, 0.021 mmol) were dissolved in ethylene glycol dimethyl ether (10 mL) and a solution of potassium carbonate (145 mg, 1 mmol) in water (3 mL) was added to the reaction mixture followed by 2,4,6-trivinyl-boroxin pyridine complex (125 mg, 0.52 mmol). The reaction mixture was heated at reflux temperature for 18 h and then the solvents were evaporated under reduced pressure. The residue was purified by flash chromatography (10% ethyl acetate in hexanes, v/v) to give 242 mg (88%) of **16** as colorless oil. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.5 Hz, 1H, Ar H-5), 7.39 (dd, *J* = 8.5 and 1.9 Hz, 1H, Ar H-2), 7.27 (d, *J* = 1.9 Hz, 1H, Ar H-6), 6.67 (dd, *J* = 10.9 and 17.5 Hz, 1H, vinyl-C*H*), 5.85 (d, *J* = 17.5 Hz, 1H, vinyl-C*H*), 5.42 (dd, *J* = 10.9 Hz, 1H, vinyl-C*H*), 3.90 (s, 2H, -CH_2-), 1.41 (s, 9H, -CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.74, 147.27, 142.34, 134.37, 130.81, 130.62, 125.39, 125.32, 118.18, 81.48, 41.12, 27.83. HRMS (m/z) for $C_{14}H_{17}NO_4Na$. Calcd. 286.1055. Found: m/z 286.1050 $(M+Na)^+$.

Di-tert-butyl 2,2'-(((1E,1'E)-thiophene-2,5-diylbis(ethene-2,1-diyl))bis(6-nitro-3,1-phenylene))diacetate (**17**).

2,5-Dibromothiophene (73.0 mg, 0.300 mmol), **16** (240 mg, 0.910 mmol), lithium chloride (42.0 mg, 1.00 mmol), sodium bicarbonate (84.0 mg, 1.00 mmol), and tetrabutylammonium chloride (140 mg, 0.500 mmol) were dissolved in DMF (5 mL) and purged with N_2 for 20 min. TPGS-750-M (5 wt % in water, 200 μL) and palladium (II) acetate (15.0 mg, 0.070 mmol) were added to the reaction mixture, which was then heated at 110 °C for 1 h. Water (100 mL) was added to the reaction mixture, which was extracted with ethyl acetate (3 x 100 mL). The organic layer was separated and concentrated under reduced pressure. The residue was purified by flash chromatography (20% ethyl acetate in hexanes, v/v) to give 140 mg (70%) of **17** as an amorphous red solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.6 Hz, 2H, Ar H-5), 7.46 (dd, *J* = 1.6 and 8.6 Hz, 2H, Ar H-4), 7.34 (d, *J* = 1.6 Hz,), 7.27 (d, *J* = 16.0 Hz, 2H, vinyl C*H*), 7.03 (s, 2H, thiophene-C*H*), 6.84 (d, *J* = 16.0 Hz, 2H, vinyl-C*H*), 3.95 (s, 4H, -CH_2-), 1.45 (s, 18H, -CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.91, 146.90, 142.00, 141.88, 131.10, 130.87, 129.00, 126.07, 125.85, 125.54, 125.35, 81.72, 41.40, 27.99. HRMS (m/z) for $C_{32}H_{34}N_2O_8SNa$. Calcd. 629.1934. Found: m/z 629.1917 $(M+H)^+$.

2,2'-(((1E,1'E)-Thiophene-2,5-diylbis(ethene-2,1-diyl))bis(6-nitro-3,1-phenylene))diacetic acid (18).

Compound **17** (140 mg, 0.23 mmol) was dissolved in dichloromethane (5 mL) and TFA (5 mL) was added to the solution. The reaction mixture was stirred at room temperature for 1 h. The solvents were removed using nitrogen gas to give 113 mg (96 %) of **18** as an amorphous red solid. ^{1}H NMR: (300 MHz, DMSO-d$_6$) δ 8.11 (d, *J* = 8.5 Hz, 2H, Ar H-5), 7.66-7.80 (m, 6H, Ar H, vinyl-C*H*), 7.32 (s, 2H, thiophene-C*H*), 7.06 (d, *J* = 16.0 Hz, 2H, vinyl-C*H*), 4.01 (s, 4H, -C*H*$_2$-). ^{13}C NMR (75 MHz, DMSO-d$_6$) δ 171.08, 146.63, 141.95, 141.90, 131.29, 131.06, 129.72, 126.06, 125.98, 125.87, 125.55. HRMS (m/z) for $C_{24}H_{19}N_2O_8S$. Calcd. 495.0862. Found: m/z 495.0847 (M+H)$^+$.

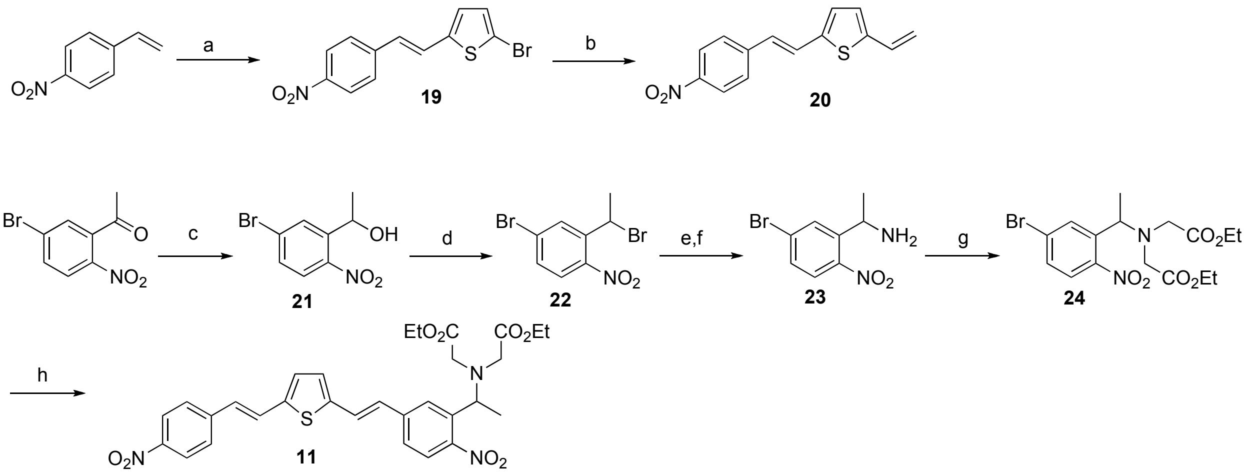
Tetra-tert-butyl 2,2'-((2,2'-(((1E,1'E)-thiophene-2,5-diylbis(ethene-2,1-diyl))bis(6-nitro-3,1-phenylene))bis(acetyl))bis(azanediyl))disuccinate 10a.

Compound **18** (78 mg, 0.16 mmol), L-aspartic acid di-*tert*-butyl ester hydrochloride (158 mg, 0.800 mmol) and EDC hydrochloride (158 mg, 0.800 mmol) were dissolved in THF (10 mL) and then stirred at room temperature for 20 h. 1N HCl (100 mL) was added to the reaction mixture, which was extracted with ethyl acetate (100 mL). The organic layer was separated and washed with saturated sodium bicarbonate solution (2 x 100 mL). The organic layer was concentrated under reduced pressure and the residue was purified by flash chromatography (50% ethyl acetate in hexanes, v/v) to give 133 mg (89%) of **10a** as an amorphous red solid. ^{1}H NMR: (300 MHz, CDCl$_3$) δ 8.04 (d, *J* = 8.4 Hz, 2H, Ar H-5), 7.40-7.50 (m, 4H, Ar H-2 and H-4), 7.28 (d, *J* = 16.0 Hz, 2H, vinyl-C*H*), 7.03 (s, 2H, thiophene-C*H*), 6.77-6.92 (m, 4H, -CON*H*-, vinyl-C*H*), 4.63-4.75 (m, 2H, -C*H*-), 3.92 (dd, *J* = 15.3 and 26.8 Hz, 4H, -C*H*$_2$-), 2.88 (dd, *J* = 4.3 and 17.2 Hz, 2H, -C*H*2-), 2.73 (dd, *J* = 4.3 and 17.2 Hz, 2H, -C*H*2-), 1.42 (s, 36H, -C*H*$_3$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 170.02, 169.44, 168.39, 146.84, 142.07, 142.03, 130.92, 130.85, 129.06, 125.98, 125.86, 125.73, 125.51, 82.22, 81.45, 49.33, 41.26, 37.35, 28.02, 27.89. HRMS (m/z) for $C_{48}H_{60}N_4O_{14}SNa$. Calcd. 971.3724. Found: m/z 971.3721 (M+Na)$^+$.

2,2'-((2,2'-(((1E,1'E)-thiophene-2,5-diylbis(ethene-2,1-diyl))bis(6-nitro-3,1-phenylene))bis(acetyl))bis(azanediyl))disuccinic acid (10b).

Compound **10a** (103 mg, 0.11 mmol) was dissolved in dichloromethane (5 mL), TFA (5 mL) was added to the solution, which was then stirred at room temperature for 1 h. The solvents were removed with nitrogen gas to give 78.0 mg (99 %) of **10b** as an amorphous red solid. ^{1}H NMR: (300 MHz, CD$_3$OD) δ 8.04 (d, *J* = 9.0 Hz, 2H, Ar H-5), 7.56-7.66 (m, 4H, Ar H-2 and H-4), 7.52 (d, *J* = 16.1 Hz, 2H, vinyl-C*H*), 7.15 (s, 2H, thiophene-C*H*), 7.00 (d, *J* = 16.1 Hz, 2H, vinyl-C*H*), 4.75 (t, *J* = 5.5 Hz, 2H, -C*H*-), 4.00 (dd, *J* = 16.3 and 23.3 Hz, 4H, -C*H*$_2$-), 2.84 (d, *J* = 4.4 Hz, 4H, -C*H*2-). ^{13}C NMR (75 MHz, CD$_3$OD) δ 172.07, 171.41, 168.24, 147.17, 141.17, 141.88, 141.44, 131.52, 130.69, 129.60, 126.02, 125.82, 125.53, 125.26, 48.75, 36.12. HRMS (m/z) for $C_{32}H_{29}N_4O_{14}S$. Calcd. 725.1401. Found: m/z 725.1395 (M+H)$^+$.

Synthesis of compound 11.



Reagents and conditions: (a) 2-Bromothiophene, benzoquinone, acetic acid, $Pd(OAc)_2$; (b) $Pd(PPh_3)_4$, 2,4,6-trivinyl-boroxin pyridine complex, K_2CO_3, DME, H_2O. (c) $NaBH_4$, THF, H_2O, 10 min, RT; (d) CBr_4, PPh_3, DCM, 3 h, RT; (e) potassium phthalimide, DMF, 3h, 60 °C; (f) hydrazine hydrate, MeOH, 2h, RT; (g) $BrCH_2COOEt$, K_2CO_3, pentamethyl piperidine, acetonitrile, 48 h, 65 °C; (h) 9, $Pd(OAc)_2$, LiCl, TBACl, $NaHCO_3$, TPGS750-M, DMF, 1 h, 110 °C.

2-(4-Nitrostyryl)-5-bromothiophene (**19**).

4-Nitrostyrene (2.1 g, 14.1 mmol) and 2-bromothiophene (2.70 mL, 28.2 mmol) were dissolved in DMSO (30 mL) and acetic acid (30 mL), then benzophenone and palladium(II) acetate (500 mg, 2.24 mmol) were added and the solution stirred at room temperature for 72 h. Sodium hydroxide (5 N, 50 mL) was added to the reaction mixture, which was then extracted with ethyl acetate (3 x 50 mL). The organic layer was separated and the solvents removed under reduced pressure. The residue was purified by column chromatography (silica, 20% ethyl acetate in hexanes, v/v) to give (3.55 g (80%) of **19** as an amorphous red solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.9 Hz, 2H, Ar H), 7.55 (d, *J* = 8.9 Hz, 2H, Ar H), 7.25 (d, *J* = 16 Hz, 1H, vinyl C*H*), 6.99 (d, 1H, *J* = 3.8 Hz, thiophene-C*H*), 6.89 (d, 1H, *J* = 3.8 Hz, thiophene-C*H*), 6.81 (d, *J* = 16 Hz, 1H, vinyl-C*H*). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.63, 143.12, 142.97, 130.73, 128.21, 126.53, 125.89, 125.33, 124.12, 113.25. HRMS (m/z) for $C_{12}H_9BrNO_2S$. Calcd. 309.9537. Found: m/z 309.9532 $(M+H)^+$.

2-(4-Nitrostyryl)-5-vinylthiophene (**20**).

Compound **19** (3.2 g, 10.2 mmol) and tetrakis(triphenylphosphine)palladium (235 mg, 0.2 mmol) were dissolved in ethylene glycol dimethyl ether (40 mL). A solution of potassium carbonate (1.40 g, 10.2 mmol) in water (10 mL) was added to the reaction mixture followed by 2,4,6-trivinyl-boroxin pyridine complex (1.2 g, 5 mmol). The reaction mixture was heated at reflux temperature for 20 h. The solvents were evaporated under reduced pressure and the residue was purified by column chromatography (silica, 20% ethyl acetate in hexanes, v/v) to give 2.35 g (88%) of **20** as an amorphous red solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.9 Hz, 2H, Ar H), 7.55 (d, *J* = 8.9 Hz, 2H, Ar H), 7.31 (d, *J* = 16 Hz, 1H, vinyl C*H*), 7.02 (d, 1H, *J* = 3.8 Hz, thiophene-C*H*), 6.89 (d, 1H, *J* = 3.8 Hz, thiophene-C*H*), 6.88 (d, *J* = 16 Hz, 1H, vinyl-C*H*), 6.78 (dd, *J* = 11.0 and 17.3 Hz, 1H, vinyl-C*H*) 5.60 (d, *J* = 17.3 Hz, 1H, vinyl-C*H*), 5.22 (d, *J* = 11.0 Hz, 1H, vinyl-C*H*). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.72, 143.91, 143.63, 140.70, 129.94, 129.08, 127.11, 126.74, 126.39, 125.87, 124.38, 114.78. HRMS (m/z) for $C_{14}H_{12}NO_2S$. Calcd. 258.0589. Found: m/z 258.0584 $(M+H)^+$.

4-Bromo-2-(1-bromoethyl)nitrobenzene (22).

The known compound **21** was synthesized by reacting 1-(5-bromo-2-nitrophenyl)ethanone with sodium borohydride in THF. Then to a cold solution of **21** (1.00 g, 4.00 mmol) and triphenyl phosphene (2.20 g, 8.10 mmol) in anhydrous dichloromethane (20 mL) was added a solution of carbon tetrabromide (3.00 g, 8.50 mmol) in dichloromethane (10 mL). The reaction mixture was stirred for 1 h at 4ºC, and the stirred at room temperature for 2 h. The solvents were evaporated under reduced pressure and the residue was purified by column chromatography (silica, 5% ethyl acetate in hexanes, v/v) to give 1.20 g (96%) of **22** as colorless oil. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 7.99 (d, *J* = 2.1 Hz, 1H, Ar H-6), 7.73 (d, *J* = 8.7 Hz, 1H, Ar H-3), 7.56 (dd, *J* = 2.1 and 8.7 Hz, 1H, Ar H-5), 5.77 (q, *J* = 6.8 Hz, 1H, benzylic-CH), 2.07 (d, *J* = 6.8 Hz, 3H, CH-C*H*$_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.97, 139.57, 132.97, 131.98, 128.16, 125.85, 40.76, 27.05.

1-(5-Bromo-2-nitrophenyl)ethanamine (23).

A solution of **22** (1.1 g, 3.6 mmol) and potassium phthalimide (1.00 g, 5.40 mmol) in DMF (10 mL) was heated for 3 h at 60 °C. The NaOH solution (0.1 N, 50 mL) was added to the reaction mixture, which was then extracted with DCM (20 mL × 3). The organic layer was separated and the solvents removed under reduced pressure. The residue was dissolved in methanol (20 mL) and reacted with hydrazine hydrate (230 μL, 7.3 mmol) for 2 h at room temperature. Solvent was removed under reduced pressure and residue was redissolved in water (20 mL) and concentrated HCl (10 mL) and the solution was heated for 3 h at 60 °C. Precipitates were removed and the pH of the solution was adjusted to 8 with NaOH and extracted with ethyl acetate (3 x 20 mL). The organic layer was separated and the solvents removed under reduced pressure to give 0.680 g (96%) of **23** as an amorphous white solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 7.99 (d, *J* = 2.1 Hz, 1H, Ar H-3), 7.68 (d, *J* = 8.6 Hz, 1H, Ar H-6), 7.49 (dd, *J* = 2.1 and 8.6 Hz, 1H, Ar H-4), 4.56-4.70 (m, 1H, benzylic-CH), 1.44 (d, *J* = 6.5 Hz, 3H, CH-C*H*$_3$). ^{13}C NMR (75 MHz,

$CDCl_3$) δ 147.34, 130.91, 130.58, 128.1, 125.60, 45.98, 24.85. HRMS (m/z) for $C_8H_{10}BrN_2O_2$. Calcd. 244.9926. Found: m/z 244.9926 $(M+H)^+$.

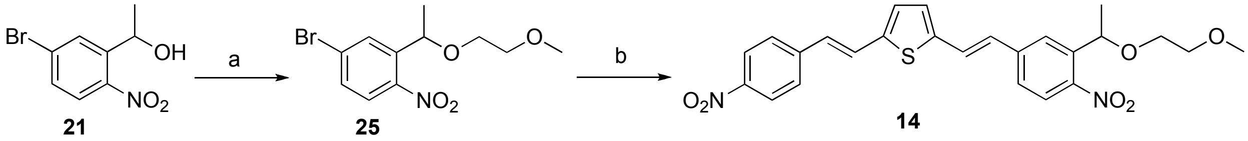
***N,N*-Diethoxycarbonylmethyl-1-(5-bromo-2-nitrophenyl)ethanamine (24).**

A solution of **23** (150 mg, 0.620 mmol) and sodium iodide (0.840 g, 5.60 mmol) in acetonitrile (20 mL), pentamethyl piperidine (350 μL, 2.00 mmol) and bromoethyl acetate (300 mg, 1.80 mmol) was heated for 20 h at 60 °C. The solvent was removed under reduced pressure and the residue was purified by column chromatography (silica, 15% ethyl acetate in hexanes, v/v) to give 0.160 g (62%) of **24** as an amorphous white solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.15 (d, *J* = 2.2 Hz, 1H, Ar H-3), 7.62 (d, *J* = 8.6 Hz, 1H, Ar H-6), 7.48 (dd, *J* = 2.2 and 8.6 Hz, 1H, Ar H-4), 4.74 (q, *J* = 6.6 Hz, 1H, benzylic-CH), 4.13 (q, *J* = 7.1 Hz, 4H, $-CH_2-CH_3$), 1.78-2.22 (br s, 2H, NH_2), 1.38 (d, *J* = 6.6 Hz, 3H, $CH-CH_3$), 1.25 (t, *J* = 7.1 Hz, 3H, $-CH_2-CH_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.94, 148.06, 142.16, 132.30, 130.92, 127.70, 125.33, 60.60, 55.49, 52.65, 21.14, 14.20. HRMS (m/z) for $C_{16}H_{22}BrN_2O_6$. Calcd. 417.0661. Found: m/z 417.0660 $(M+H)^+$.

2-[3-{1-(*N,N*-Diethoxycarbonylmethyl)aminoethyl}-4-nitrostyryl]-5-(4-nitrostyryl)-thiophene (11).

Compound **24** (150 mg, 0.36 mmol), **20** (185 mg, 0.72 mmol), lithium chloride (45.0 mg, 1.10 mmol), sodium bicarbonate (100 mg, 1.20 mmol), and tetrabutylammonium chloride (100 mg, 0.360 mmol) were dissolved in DMF (5 mL) and purged with N_2 for 20 min. TPGS-750-M (5% wt in water, 200 μL) and palladium(II) acetate (16 mg, 0.07 mmol) were added to the reaction mixture, which was heated at 110 °C for 1 h. Water (100 mL) was added to the reaction mixture, which was then extracted with ethyl acetate (3 x 100 mL). The organic layer was separated and dried under reduced pressure. The residue was purified by column chromatography (silica, 40% ethyl acetate in hexanes, v/v) to give 43.0 mg (21%) of **11** as an amorphous red solid. ^{1}H NMR: (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.9 Hz, 2H, Ar H), 8.10 (d, *J* = 1.9 Hz, 1H, Ar H), 7.78 (d, *J* = 8.5 Hz, 2H, Ar H), 7.57 (d, *J* = 8.9 Hz, 2H, Ar H), 7.41 (dd, *J* = 1.9 and 8.5 Hz, 1H, Ar H), 7.35 (d, *J* = 16 Hz, 1H, vinyl C*H*), 7.33 (d, *J* = 16 Hz, 1H, vinyl C*H*), 7.08 (s, 2H, thiophene-C*H*), 6.99 (d, *J* = 16 Hz, 2H, vinyl-C*H*), 5.23 (dd, *J* = 3.2 and 6.6 Hz, 2H, benzylic-C*H*), 4.05-4.23 (m, 16H, $-CH_2-$), 3.89 (s, 8H, $-CH_2-$), 3.41-3.85 (m, 24H, $-CH_2-$), 3.25 (t, *J* = 4.5 Hz, 4H, $-CH_2-$), 1.20-1.30 (m, 24H, $-CH_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.30, 147.87, 146.58, 143.12, 142.52, 141.75, 141.62, 141.07, 129.12, 128.77, 126.96, 126.91, 126.58, 126.29, 125.82, 125.17, 125.06, 124.89, 124.14, 60.66, 55.62, 52.81, 21.51, 14.34. HRMS (m/z) for $C_{30}H_{32}N_3O_8S$. Calcd. 594.1910. Found: m/z 594.1910 $(M+H)^+$.

Synthesis of compound 14.



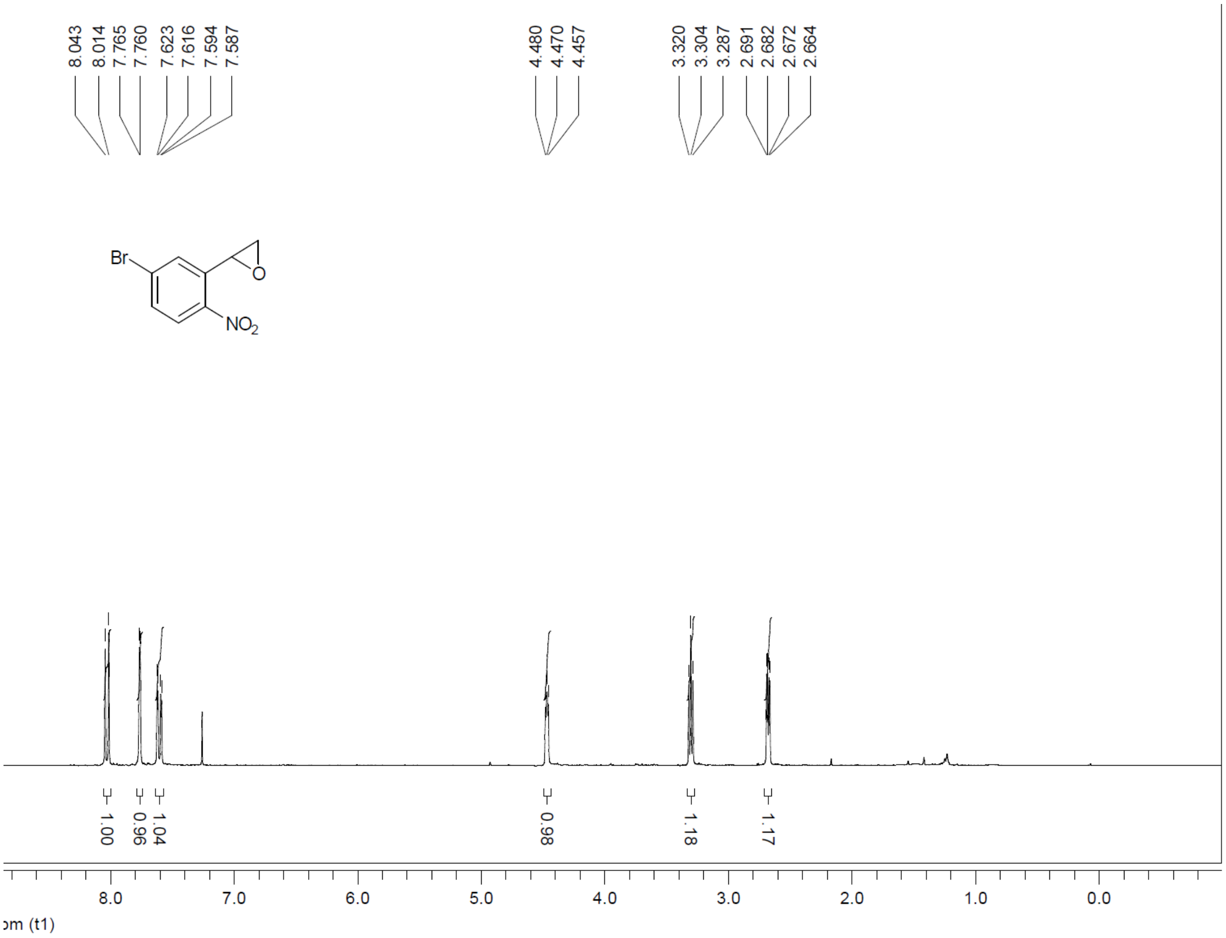
Reagents and conditions: (a) 2-Bromoethyl methyl ether, NaH, DMF, 20 h, RT; (b) **16**, Pd(OAc)$_2$, LiCl, TBACl, NaHCO$_3$, TPGS-750-M, DMF, 1 h, 110 °C.

4-Bromo-2-{1-(2-methoxyethoxy)ethyl}nitrobenzene (25).

Compound **21** (90 mg, 0.36 mmol) and 2-bromoethyl methyl ether (50.0 mg, 0.370 mmol) were dissolved in DMF (5 mL) and a suspension of NaH (30.0 mg, 0.750 mmol) in DMF (5 mL) was added and the reaction mixture was stirred at room temperature for 20 h. The solvent was evaporated and the residue purified by column chromatography (silica, 10% ethyl acetate in hexanes, v/v) to give 56.0 mg (51%) of **25** as an amorphous white solid. ^{1}H NMR: (300 MHz, CDCl$_3$) δ 7.97 (d, *J* = 2.2 Hz, 1H, Ar H-3), 7.79 (d, *J* = 8.7 Hz, 1H, Ar H-6), 7.52 (dd, *J* = 2.2 and 8.7 Hz, 1H, Ar H-5), 5.04 (q, *J* = 6.3 Hz, 1H, benzylic-CH), 3.36-3.56 (m, 4H, -C*H*$_2$-), 3.33 (s, 3H, -C*H*$_3$), 1.50 (d, *J* = 6.3 Hz, 3H, -C*H*$_3$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 146.79, 142.10, 131.02, 128.73, 125.77, 73.40, 71.79, 68.58, 58.94, 23.56. HRMS (m/z) for $C_{11}H_{15}BrNO_4$. Calcd. 304.0184. Found: m/z 304.0151 (M+H)$^+$.

2-**[3-{1-(2-methoxyethoxy)ethyl}-4-nitrostyryl]-5-(4-nitrostyryl)-thiophene (14).**

Compound **25** (50.0 mg, 0.160 mmol), **16** (85.0 mg, 0.330 mmol), lithium chloride (21.0 mg, 0.500 mmol), sodium bicarbonate (42 mg, 0.5 mmol), and tetrabutylammonium chloride (47.0 mg, 0.170 mmol) were dissolved in DMF (5 mL) and the solution was purged with N$_2$ for 20 min. TPGS-750-M (5% wt in water, 100 μL) and palladium(II) acetate (10.0 mg, 0.045 mmol) were added to the reaction mixture, which was then heated at 110 °C for 1 h. Water (100 mL) was added to the cooled reaction mixture, which was then extracted with ethyl acetate (3 x 100 mL). The organic layer was separated and dried under reduced pressure. The residue was purified by column chromatography (silica, 20% ethyl acetate in hexanes, v/v) to give 71.0 mg (90%) of **14** as an amorphous red solid. ^{1}H NMR: (300 MHz, CDCl$_3$) δ 8.21 (d, *J* = 8.9 Hz, 2H, Ar H), 7.99 (d, *J* = 8.6 Hz, 1H, Ar H-5), 7.96 (d, *J* = 2.0 Hz, 1H, Ar H-2), 7.59 (d, *J* = 8.9 Hz, 2H, Ar H), 7.45 (dd, *J* = 2.0 and 8.6 Hz, 1H, Ar H-6), 7.38 (d, *J* = 16.0 Hz, 1H, vinyl C*H*), 7.35 (d, *J* = 16.0 Hz, 1H, vinyl C*H*), 7.10 (s, 2H, thiophene C*H*), 6.95 (d, *J* = 16.0 Hz, 2H, vinyl C*H*), 5.16 (q, *J* = 6.3 Hz, 1H, benzylic-CH), 3.43-3.66 (m, 4H, -C*H*$_2$-), 3.39 (s, 3H, -C*H*$_3$), 1.57 (d, *J* = 6.3 Hz, 3H, -C*H*$_3$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 146.49, 146.44, 143.01, 142.34, 142.20, 141.87, 140.92, 129.12, 128.82, 126.74, 126.52, 126.30, 125.71, 125.41, 125.30, 125.06, 124.05, 73.73, 71.92, 68.43, 58.99, 23.74. HRMS (m/z) for $C_{25}H_{26}N_2O_7S$. Calcd. 498.1461. Found: m/z 498.1689 (M+H$_2$O)$^+$.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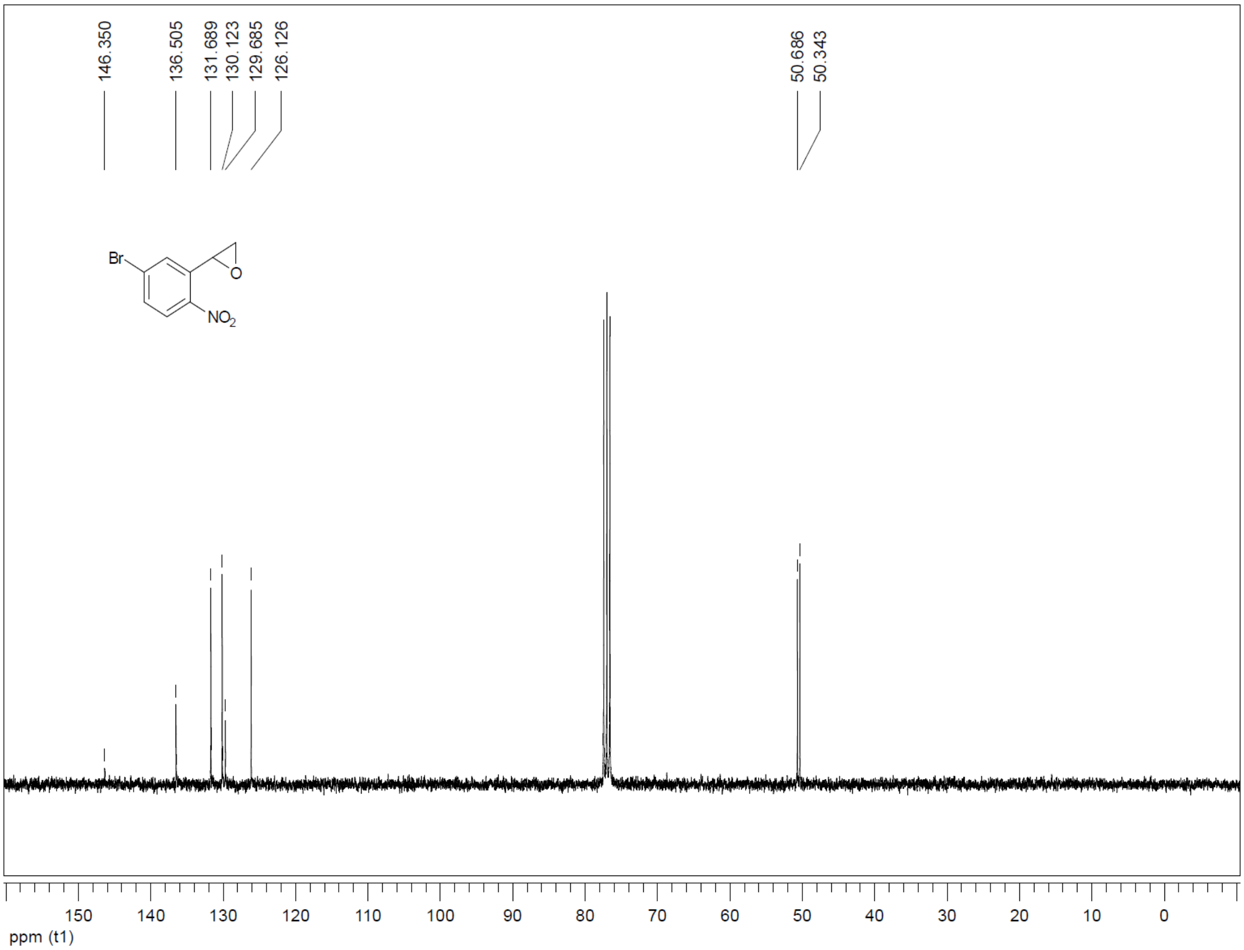
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Compound Table

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Compound Label	*m/z*	RT	Algorithm	Mass
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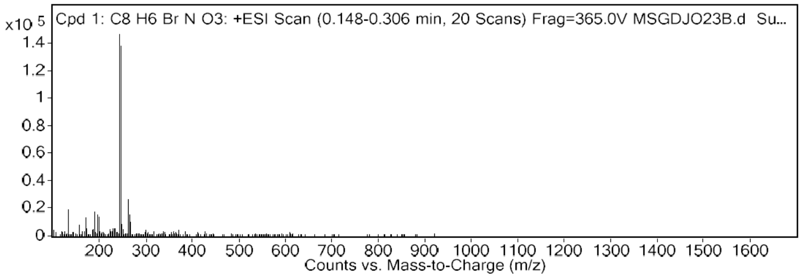
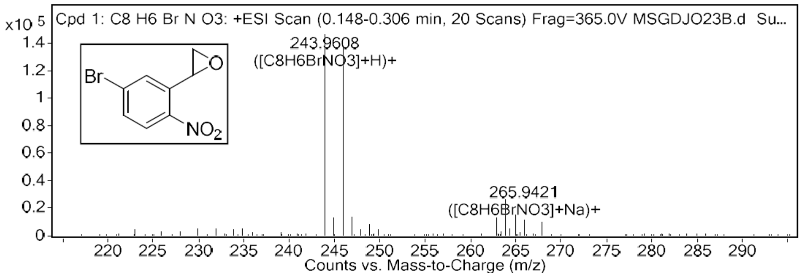
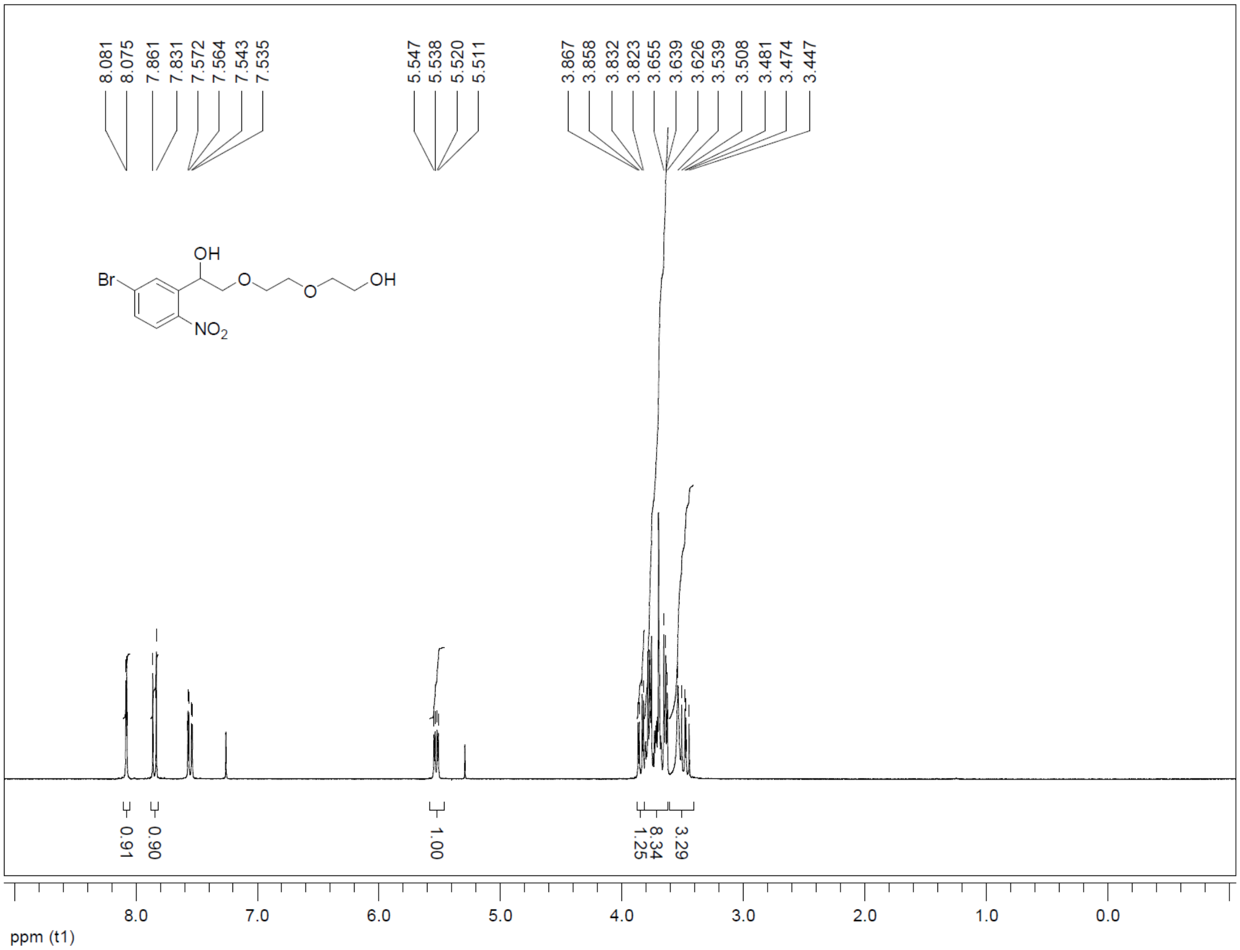


MS Zoomed Spectrum

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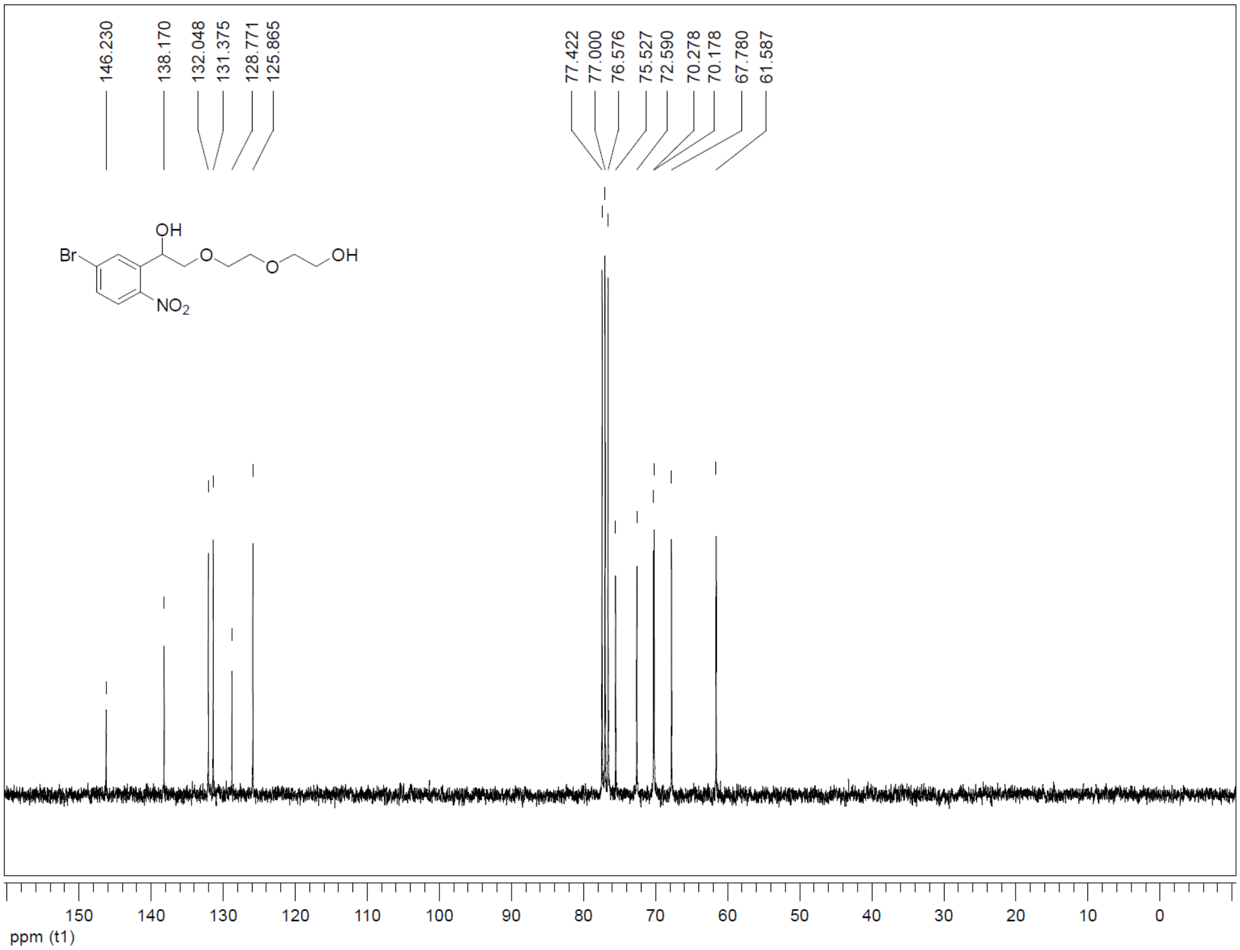
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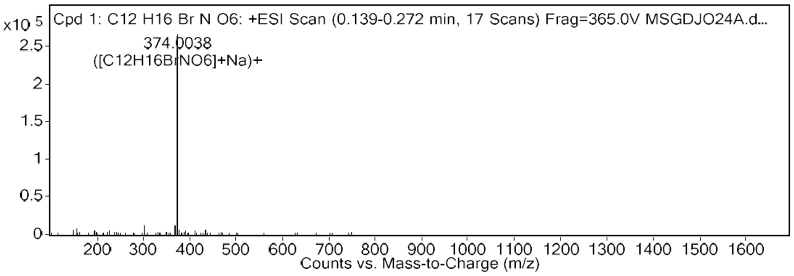
77.422
77.000
76.576
75.527
72.590
70.278
70.178
67.780
61.587
Br
OH
O
O
OH
NO$_2$
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

Compound Table

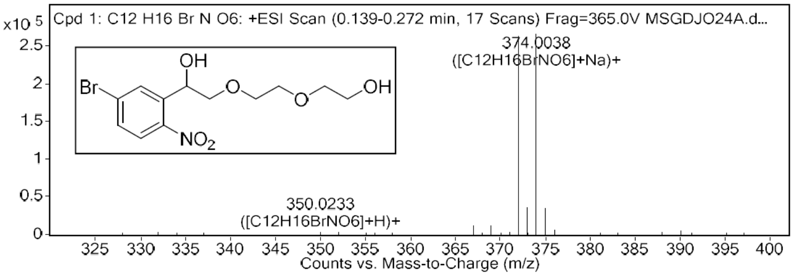
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C12 H16 Br N O6	0.18	349.0164	10917	C12 H16 Br N O6	349.0161	0.87	C12 H16 Br N O6	C12 H16 Br N O6

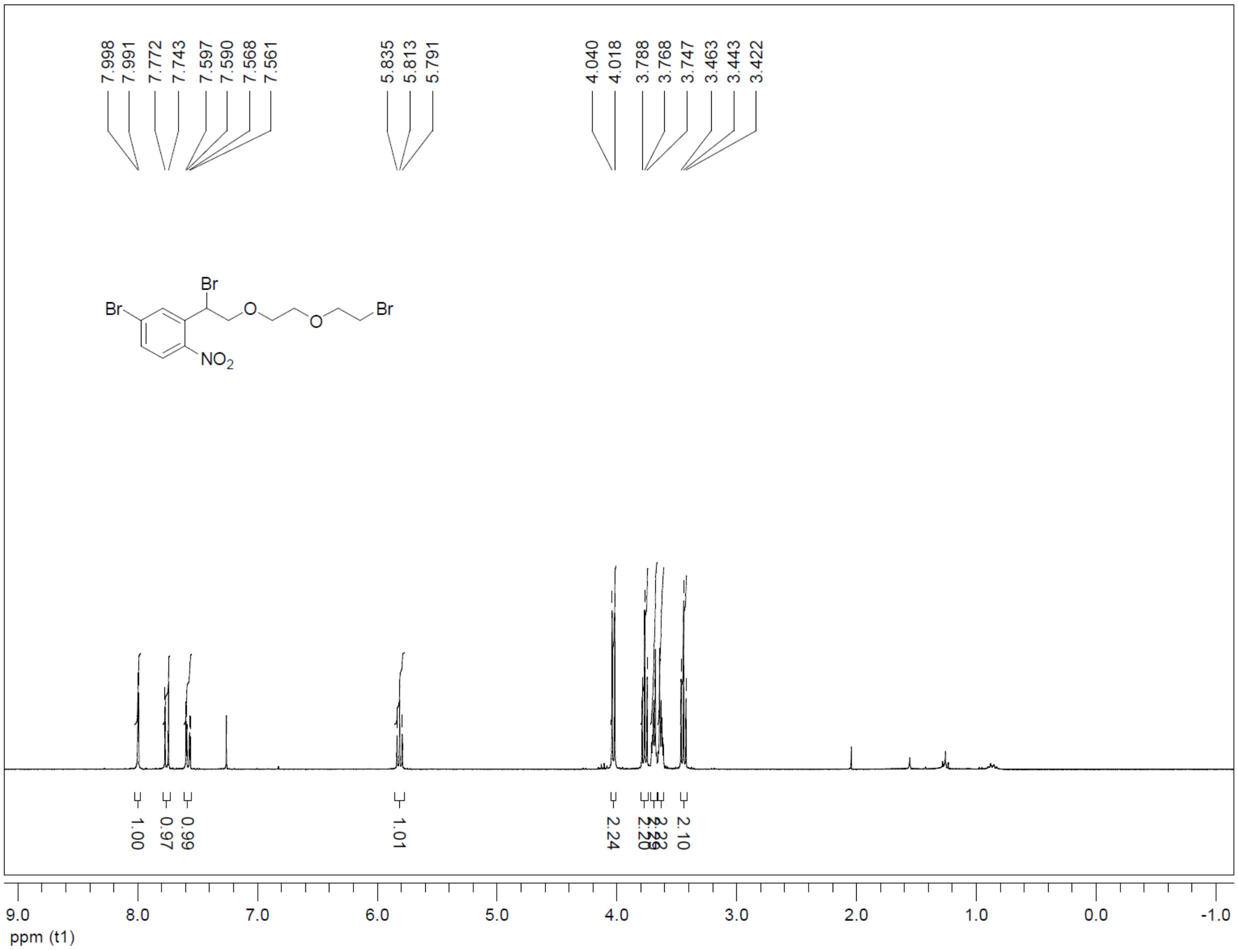
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C12 H16 Br N O6	369.048	0.18	Find By Formula	349.0164

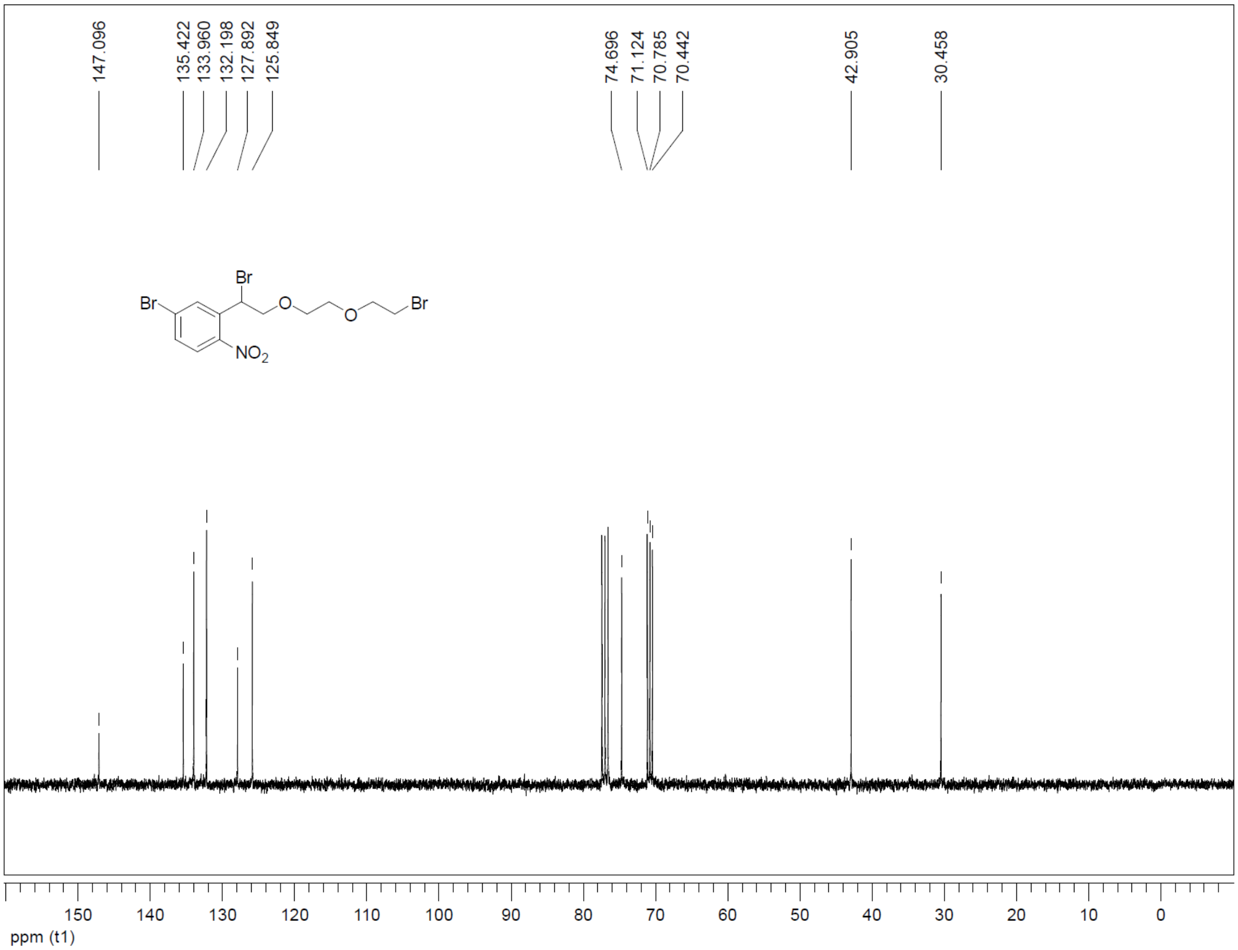
MS Spectrum



MS Zoomed Spectrum




7.998
7.991
7.772
7.743
7.597
7.590
7.568
7.561
5.835
5.813
5.791
4.040
4.018
3.788
3.768
3.747
3.463
3.443
3.422
Br
Br
O
O
Br
NO2
1.00
0.97
0.99
1.01
2.24
2.20
2.29
2.23
2.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (t1)

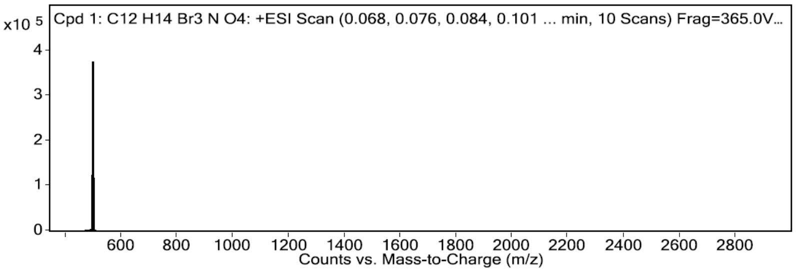

147.096
135.422
133.960
132.198
127.892
125.849
74.696
71.124
70.785
70.442
42.905
30.458
Br
Br
O
O
Br
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

Compound Table

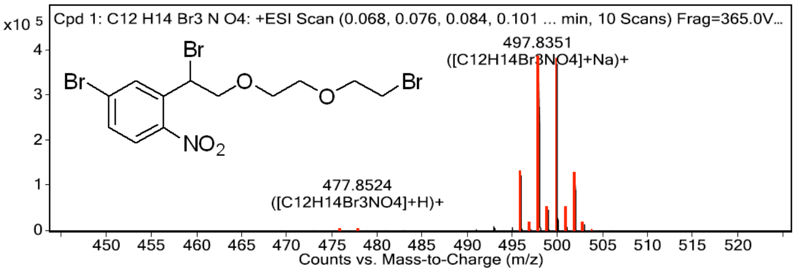
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C12 H14 Br3 N O4	0.093	472.8479	387207	C12 H14 Br3 N O4	472.8473	1.28	C12 H14 Br3 N O4	C12 H14 Br3 N O4

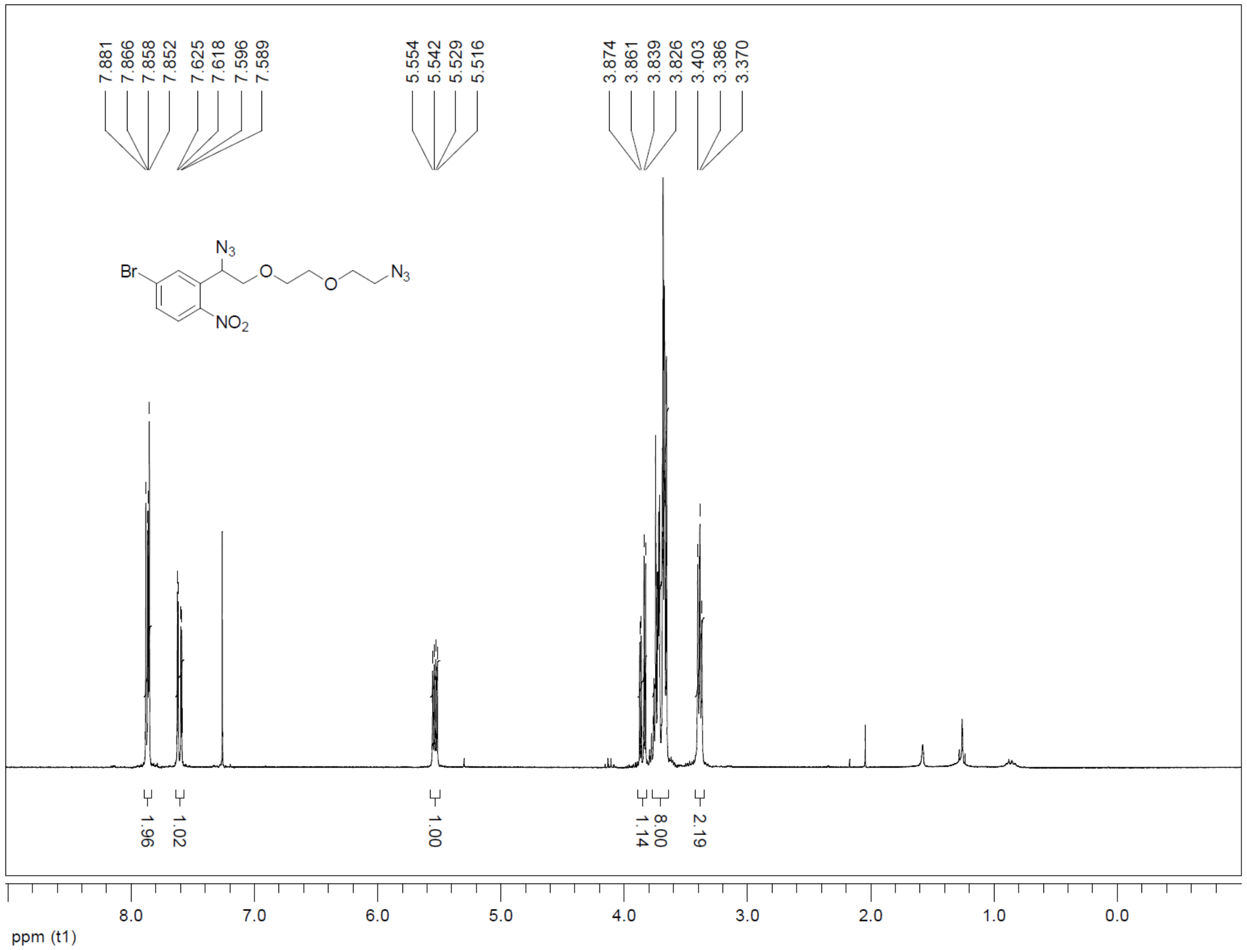
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C12 H14 Br3 N O4	497.8351	0.093	Find By Formula	472.8479

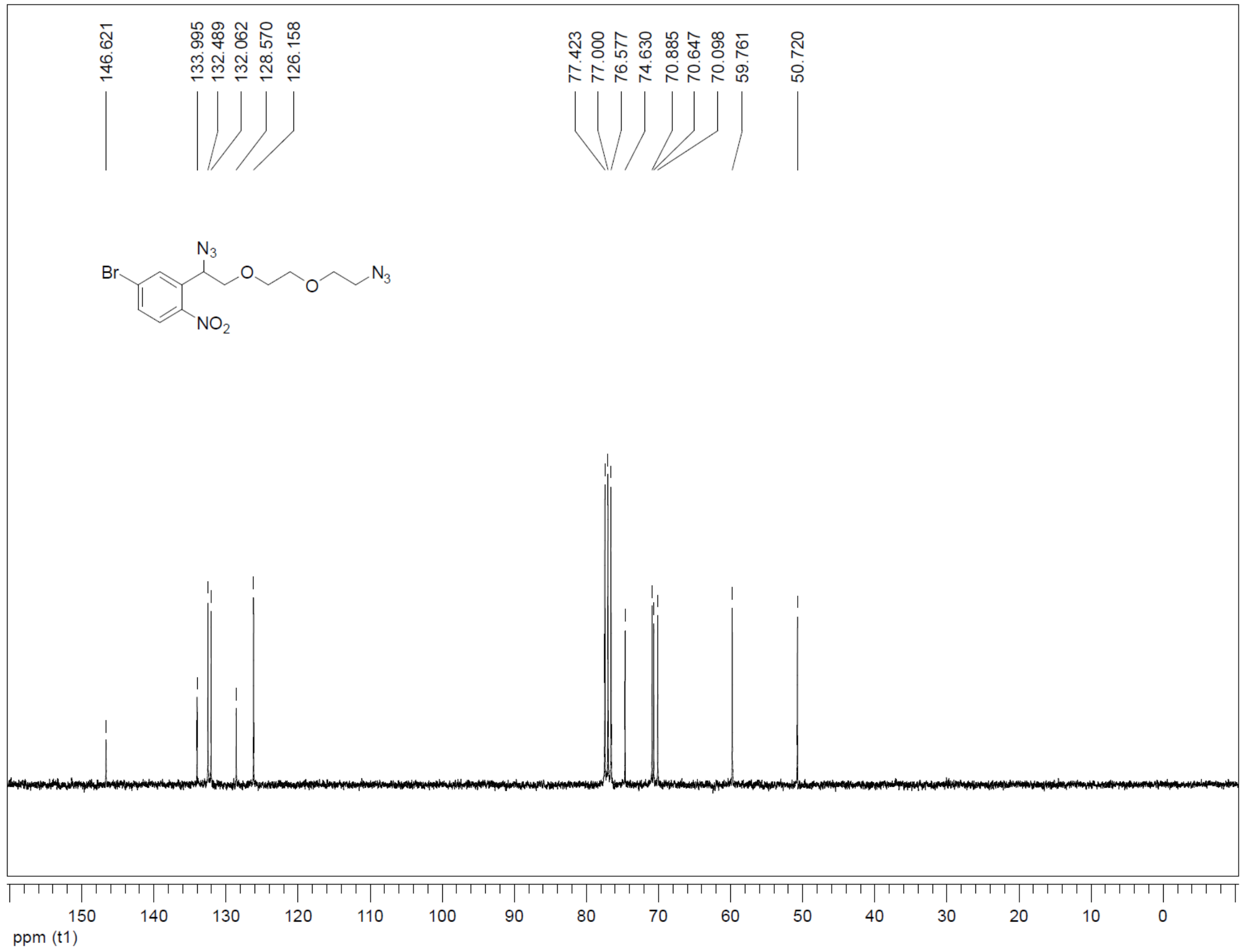
MS Spectrum



MS Zoomed Spectrum




7.881
7.866
7.858
7.852
7.625
7.618
7.596
7.589
5.554
5.542
5.529
5.516
3.874
3.861
3.839
3.826
3.403
3.386
3.370
Br
N3
O
O
N3
NO2
1.96
1.02
1.00
1.14
8.00
2.19
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

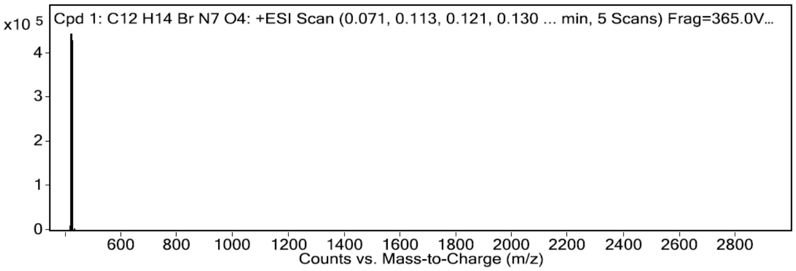

146.621
133.995
132.489
132.062
128.570
126.158
77.423
77.000
76.577
74.630
70.885
70.647
70.098
59.761
50.720
Br
N3
O
O
N3
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

Compound Table

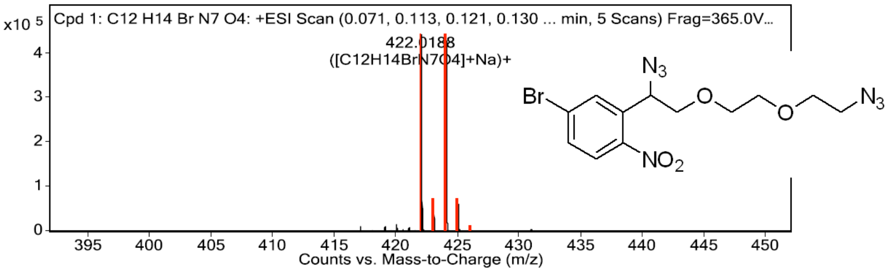
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C12 H14 Br N7 O4	0.088	399.0297	447573	C12 H14 Br N7 O4	399.0291	1.47	C12 H14 Br N7 O4	C12 H14 Br N7 O4

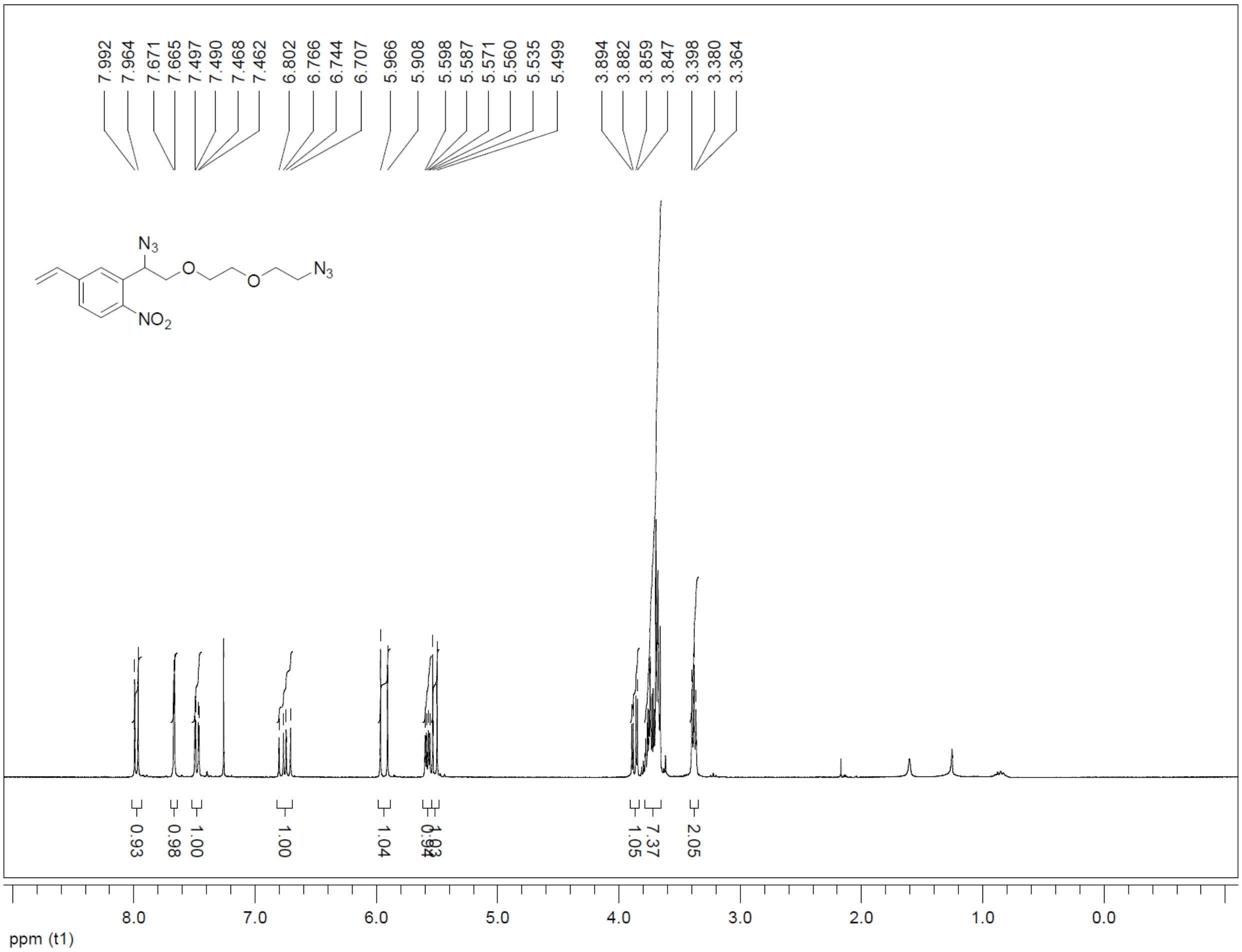
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C12 H14 Br N7 O4	422.0188	0.088	Find By Formula	399.0297

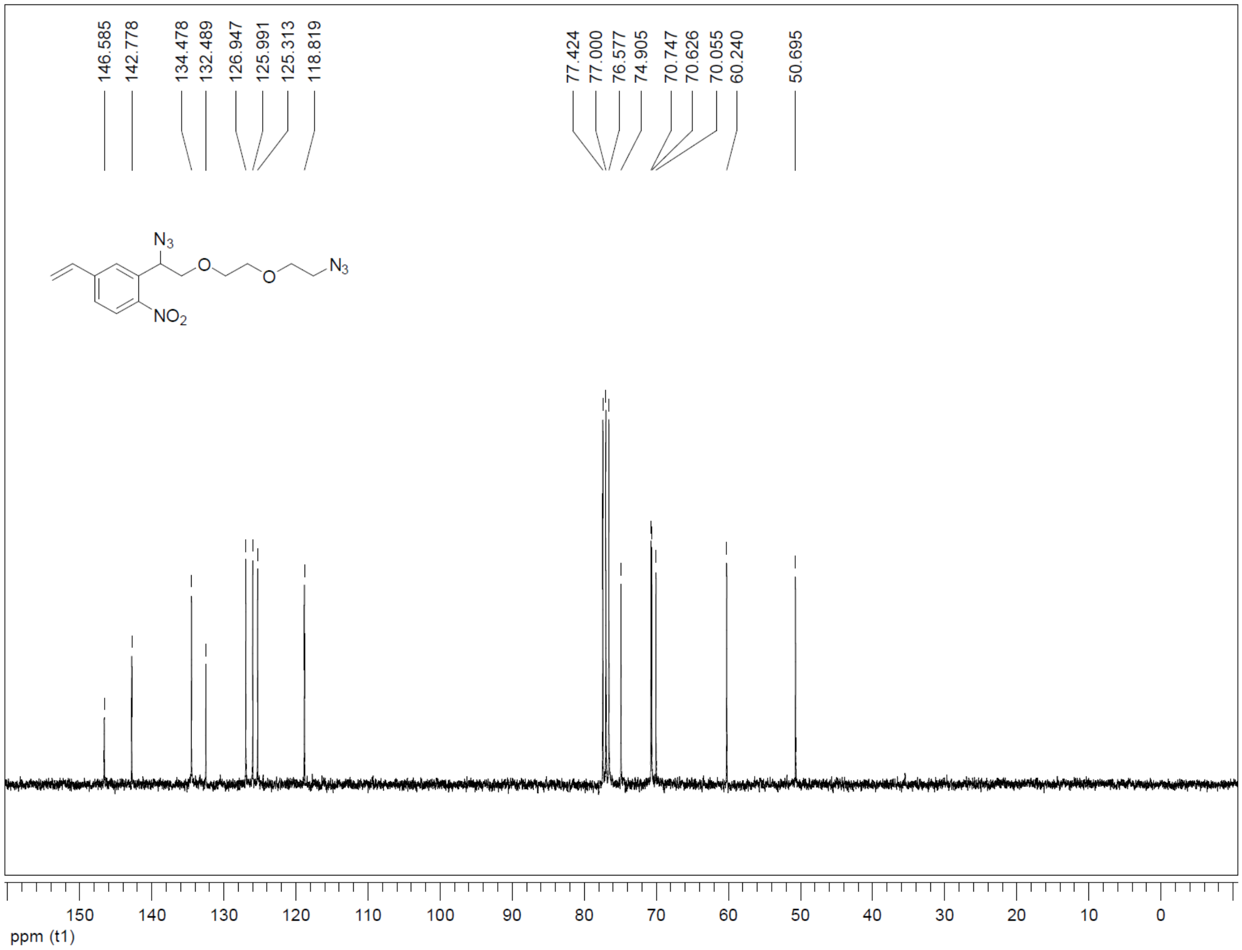
MS Spectrum



MS Zoomed Spectrum




7.992
7.964
7.671
7.665
7.497
7.490
7.468
7.462
6.802
6.766
6.744
6.707
5.966
5.908
5.598
5.587
5.571
5.560
5.535
5.499
3.894
3.882
3.859
3.847
3.398
3.380
3.364
N3
O
O
N3
NO2
0.93
0.98
1.00
1.00
1.04
0.94
1.03
1.05
7.37
2.05
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

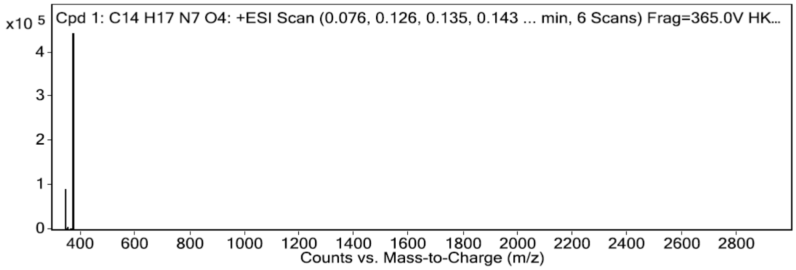

146.585
142.778
134.478
132.489
126.947
125.991
125.313
118.819
77.424
77.000
76.577
74.905
70.747
70.626
70.055
60.240
50.695
N3
O
O
N3
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

Compound Table

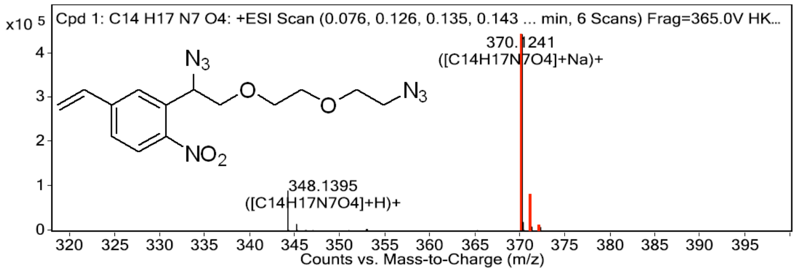
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H17 N7 O4	0.093	347.1349	448217	C14 H17 N7 O4	347.1342	2.15	C14 H17 N7 O4	C14 H17 N7 O4

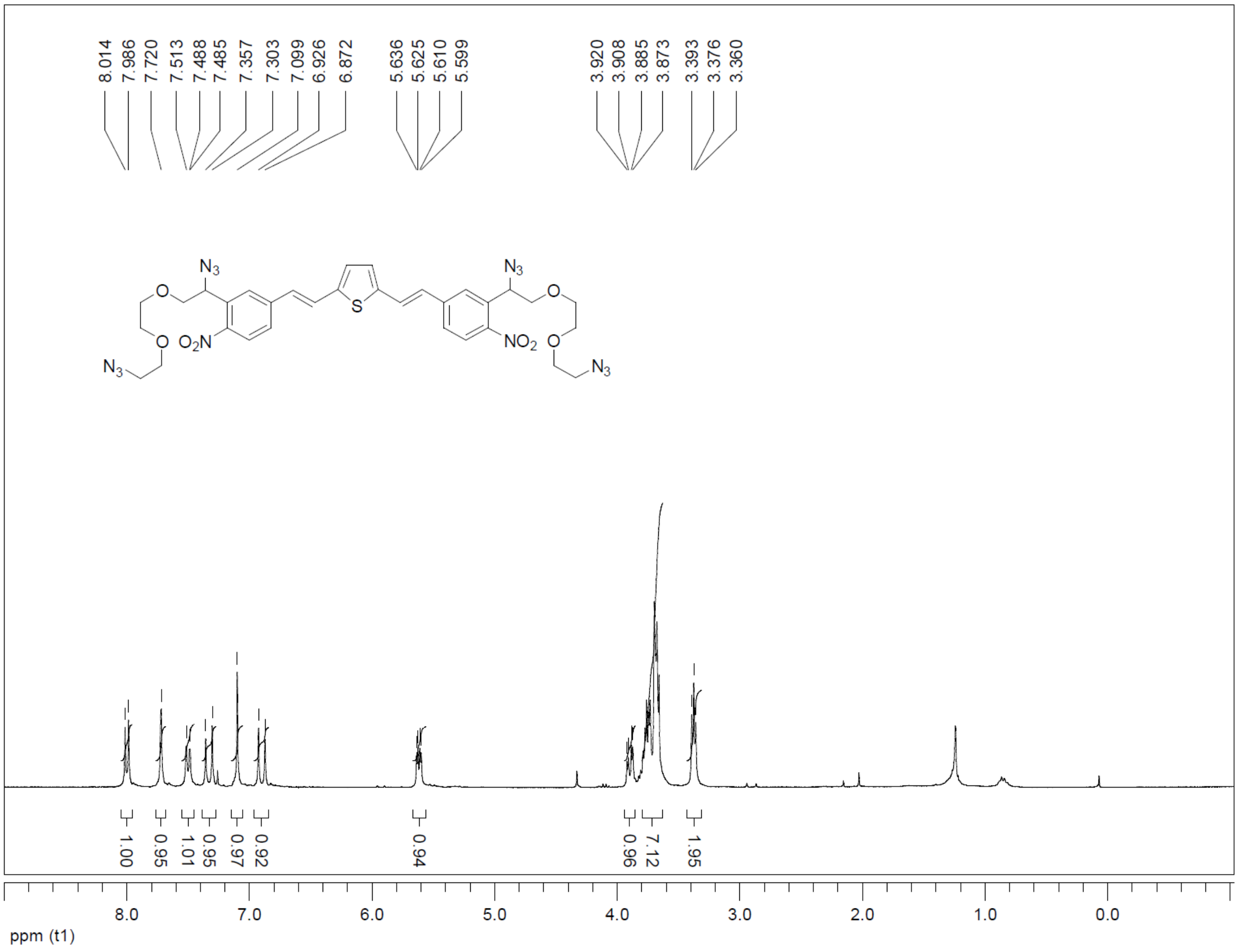
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H17 N7 O4	370.1241	0.093	Find By Formula	347.1349

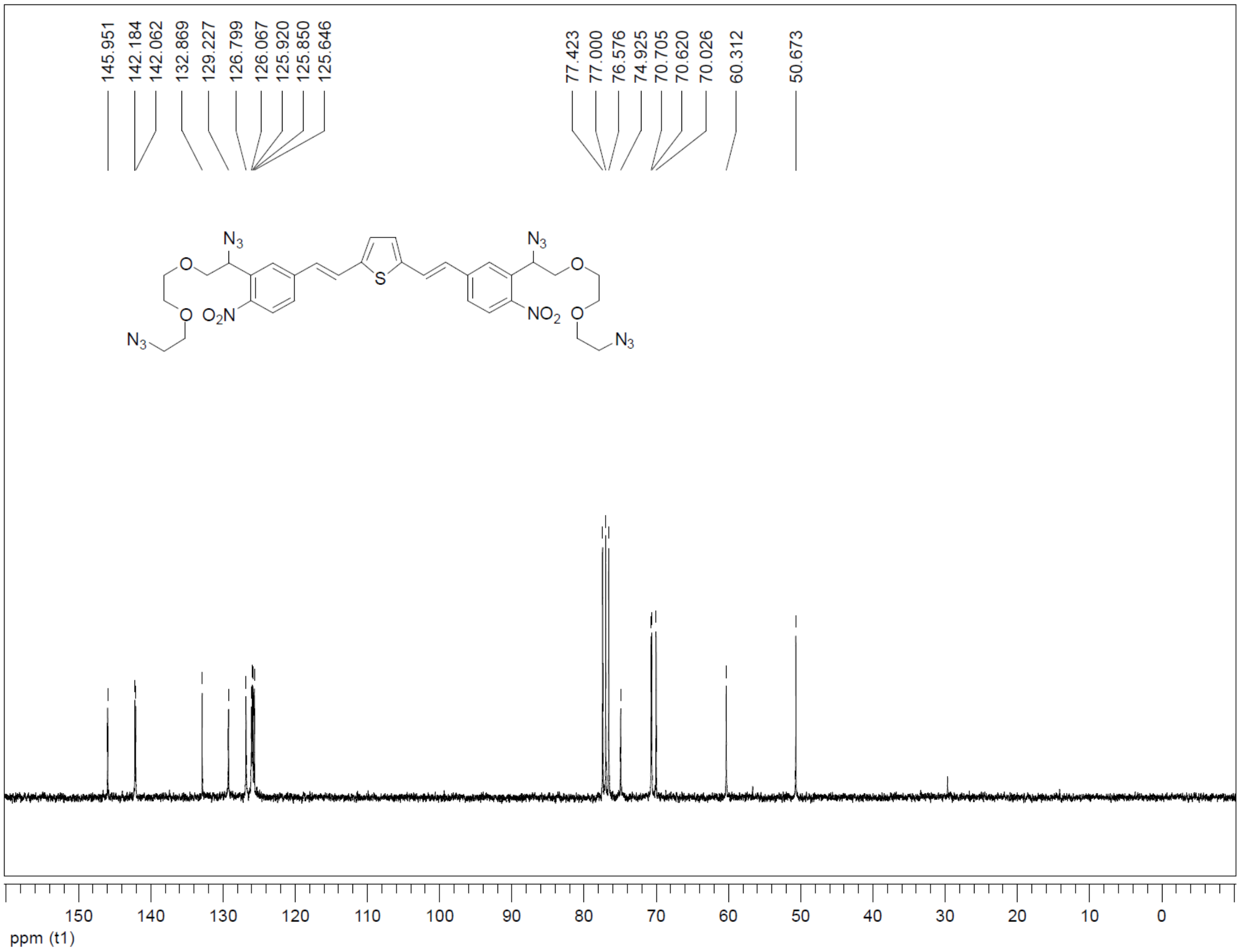
MS Spectrum



MS Zoomed Spectrum




8.014
7.986
7.720
7.513
7.488
7.485
7.357
7.303
7.099
6.926
6.872
5.636
5.625
5.610
5.599
3.920
3.908
3.885
3.873
3.393
3.376
3.360
N_3
N_3
O_2N
NO_2
O
O
O
O
S
N_3
N_3
1.00
0.95
1.01
0.95
0.97
0.92
0.94
0.96
7.12
1.95
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

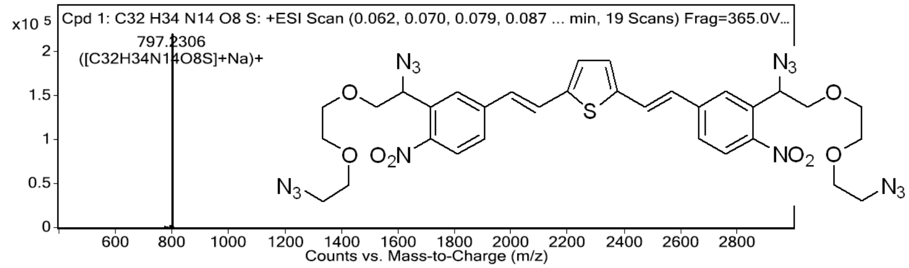

145.951
142.184
142.062
132.869
129.227
126.799
126.067
125.920
125.850
125.646
77.423
77.000
76.576
74.925
70.705
70.620
70.026
60.312
50.673
N3
O
O2N
NO2
S
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

Compound Table

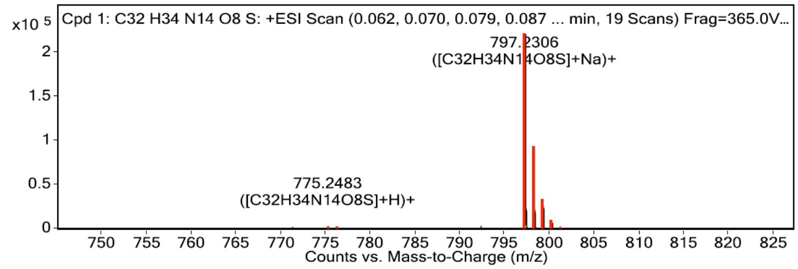
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C32 H34 N14 O8 S	0.095	774.2414	223129	C32 H34 N14 O8 S	774.2405	1.15	C32 H34 N14 O8 S	C32 H34 N14 O8 S

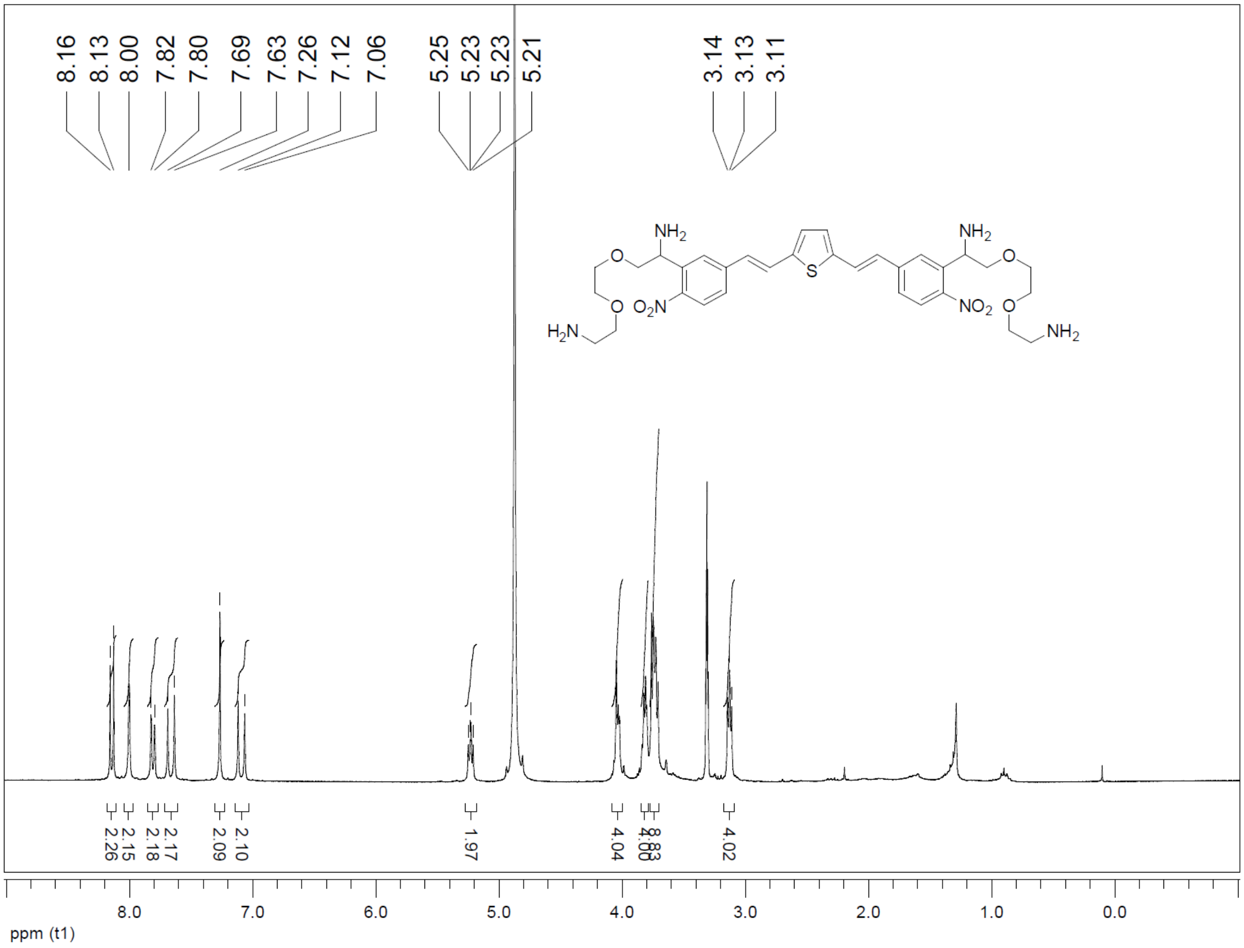
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C32 H34 N14 O8 S	797.2306	0.095	Find By Formula	774.2414

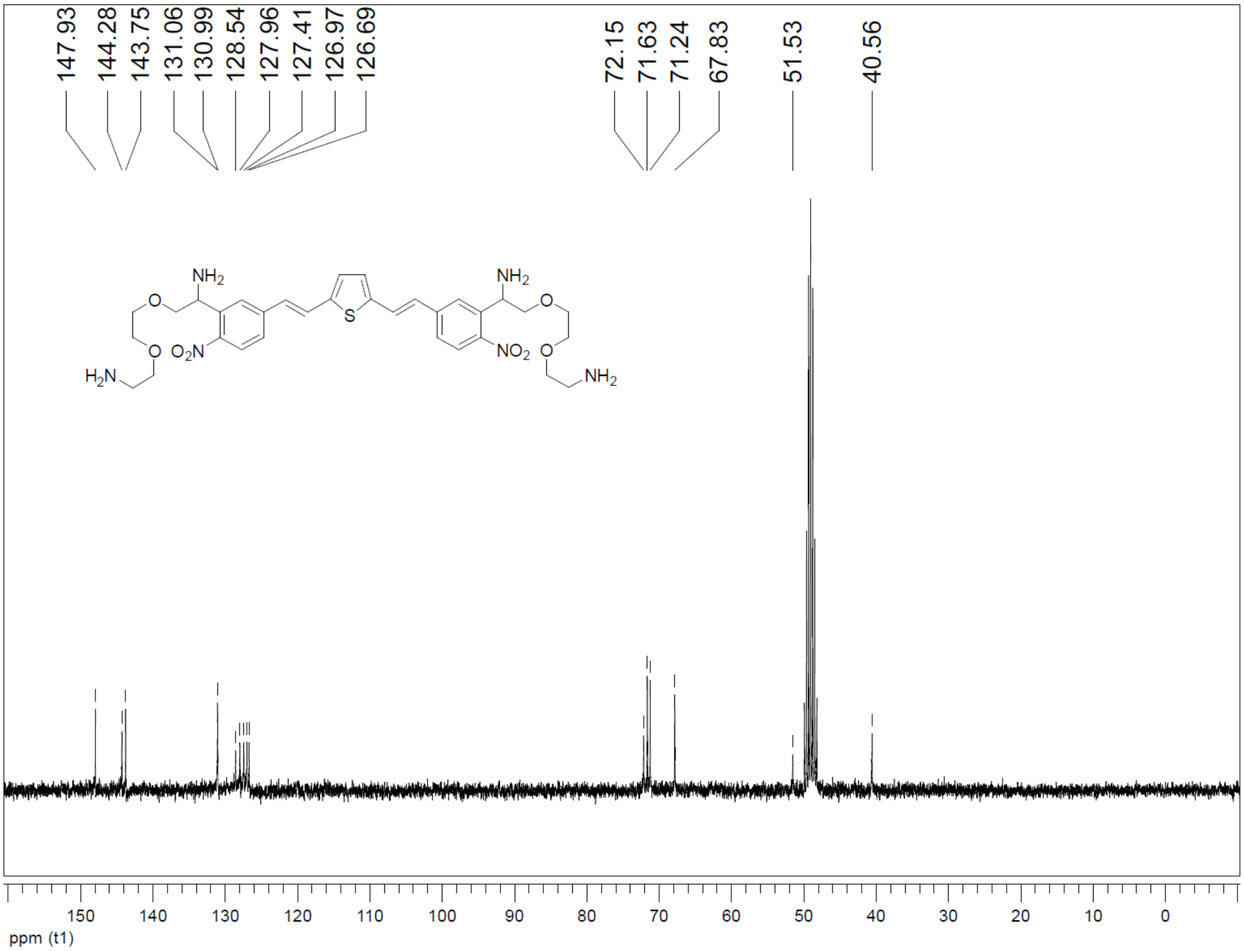
MS Spectrum

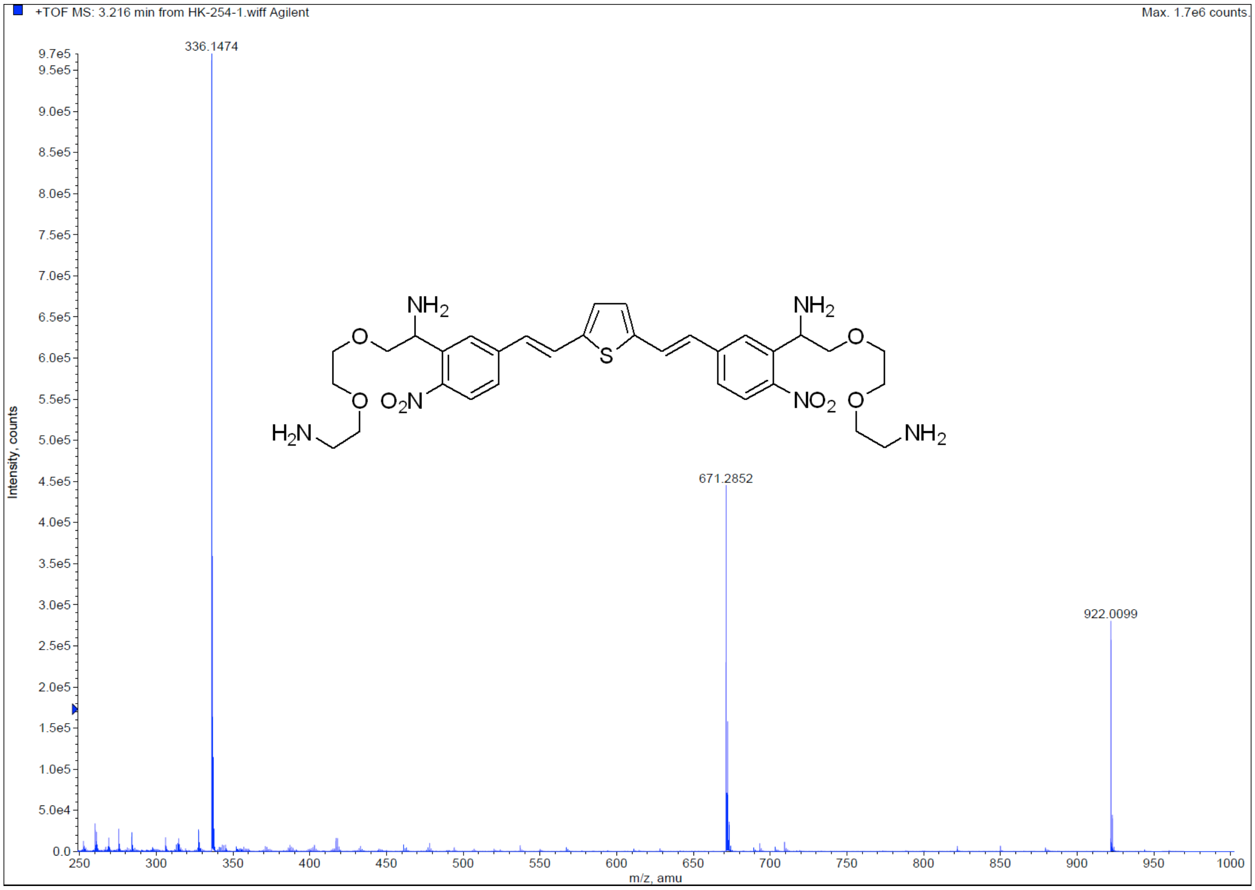


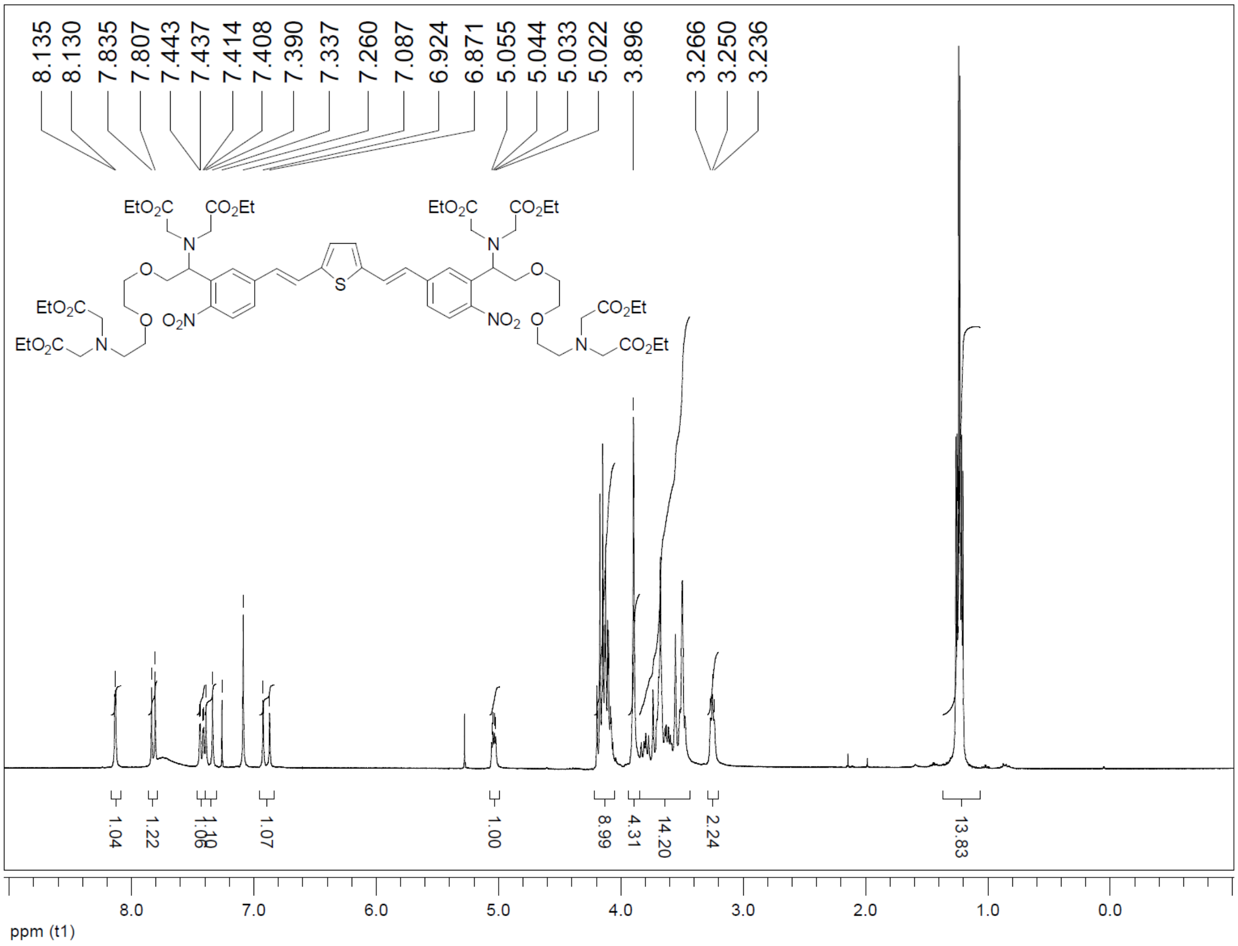
MS Zoomed Spectrum

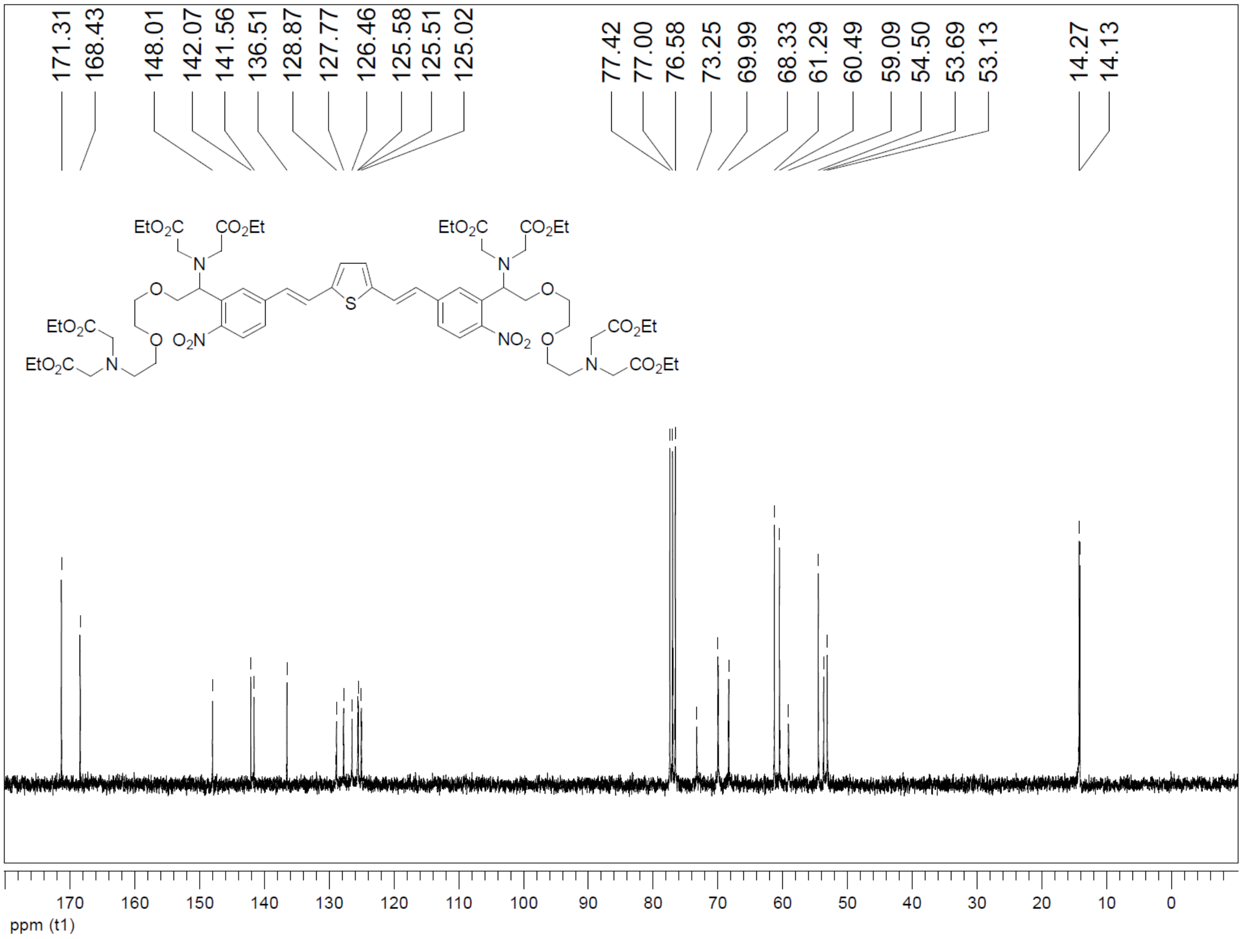


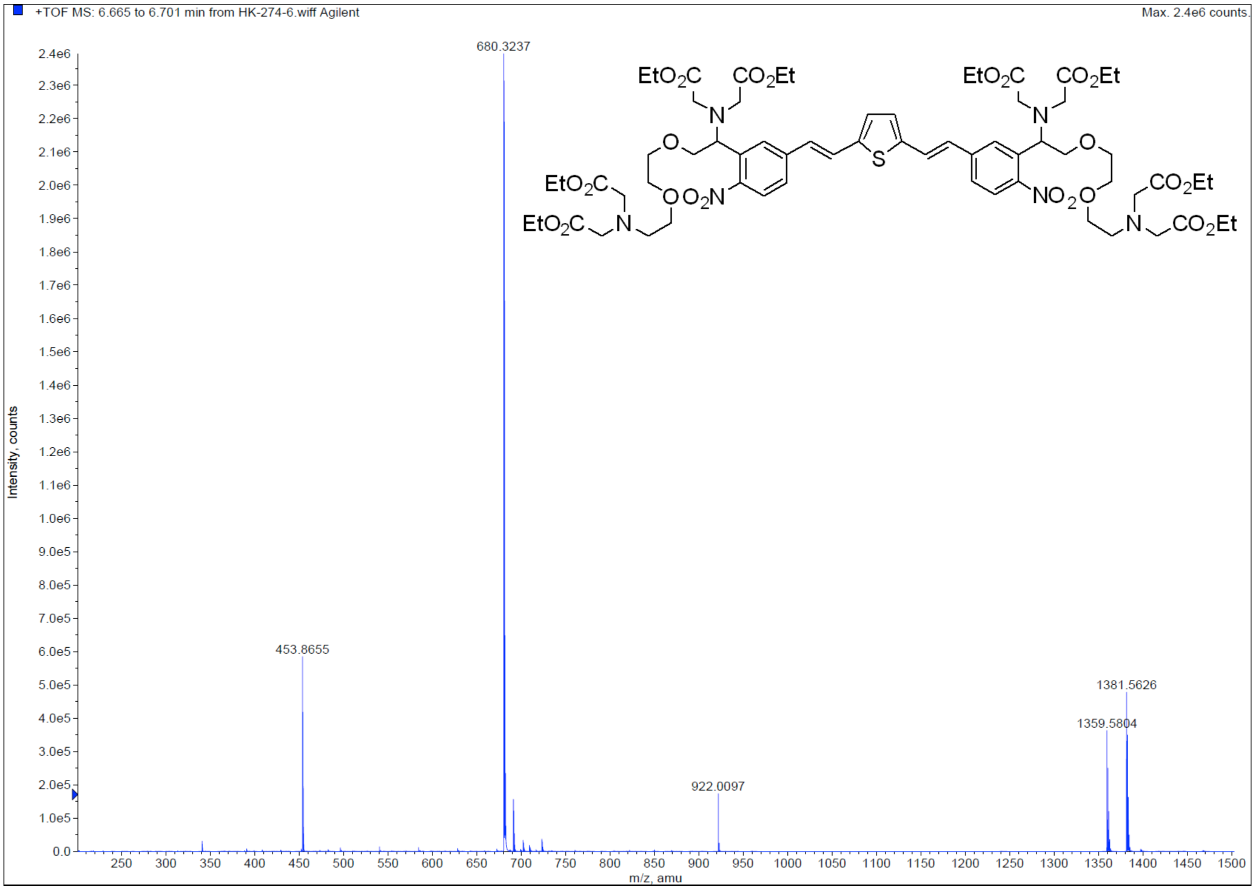

8.16
8.13
8.00
7.82
7.80
7.69
7.63
7.26
7.12
7.06
5.25
5.23
5.23
5.21
3.14
3.13
3.11
NH2
NH2
O
O
S
O
O
H2N
O2N
NO2
NH2
2.26
2.15
2.18
2.17
2.09
2.10
1.97
4.04
4.00
8.83
4.02
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

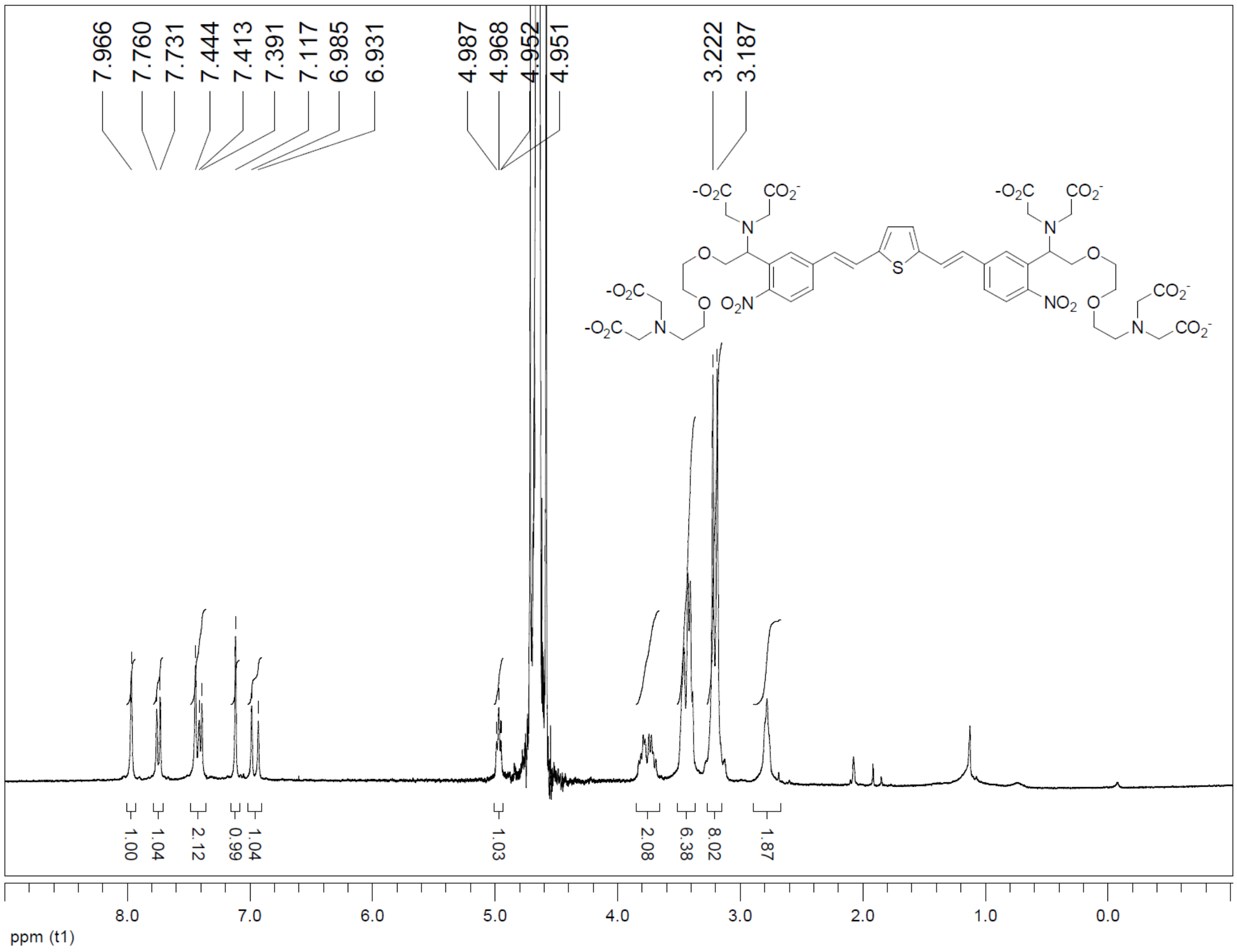

147.93
144.28
143.75
131.06
130.99
128.54
127.96
127.41
126.97
126.69
72.15
71.63
71.24
67.83
51.53
40.56
NH2
O
O
H2N
O2N
S
NH2
O
O
NO2
NH2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

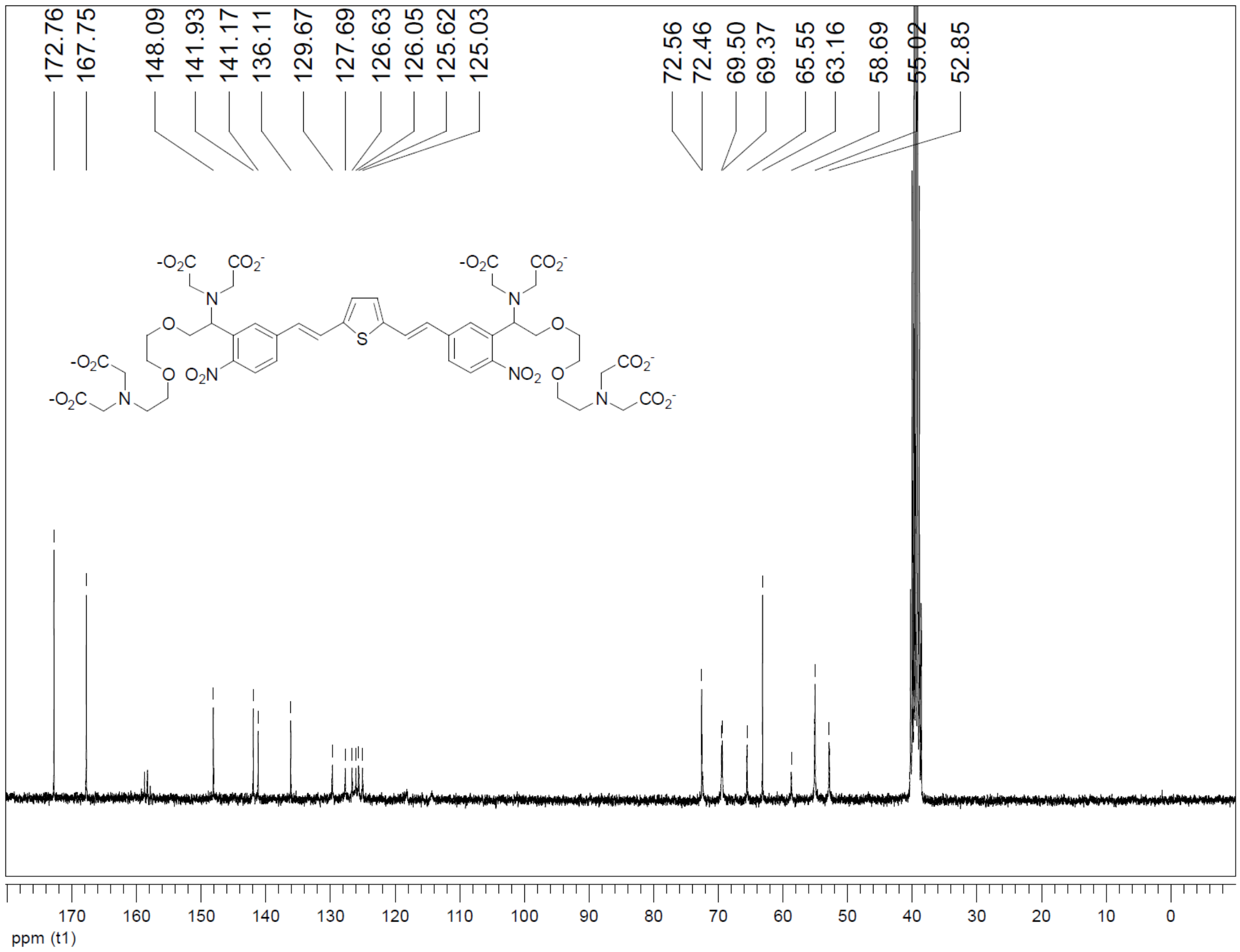

+TOF MS: 3.216 min from HK-254-1.wiff Agilent
Max. 1.7e6 counts.
336.1474
671.2852
922.0099
Intensity, counts
m/z, amu
9.7e5
9.5e5
9.0e5
8.5e5
8.0e5
7.5e5
7.0e5
6.5e5
6.0e5
5.5e5
5.0e5
4.5e5
4.0e5
3.5e5
3.0e5
2.5e5
2.0e5
1.5e5
1.0e5
5.0e4
0.0
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
NH2
O
O
H2N
O2N
S
NH2
NO2
O
O
NH2


8.135
8.130
7.835
7.807
7.443
7.437
7.414
7.408
7.390
7.337
7.260
7.087
6.924
6.871
5.055
5.044
5.033
5.022
3.896
3.266
3.250
3.236
EtO2C
CO2Et
N
O
S
O2N
NO2
1.04
1.22
1.06
1.10
1.07
1.00
8.99
4.31
14.20
2.24
13.83
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

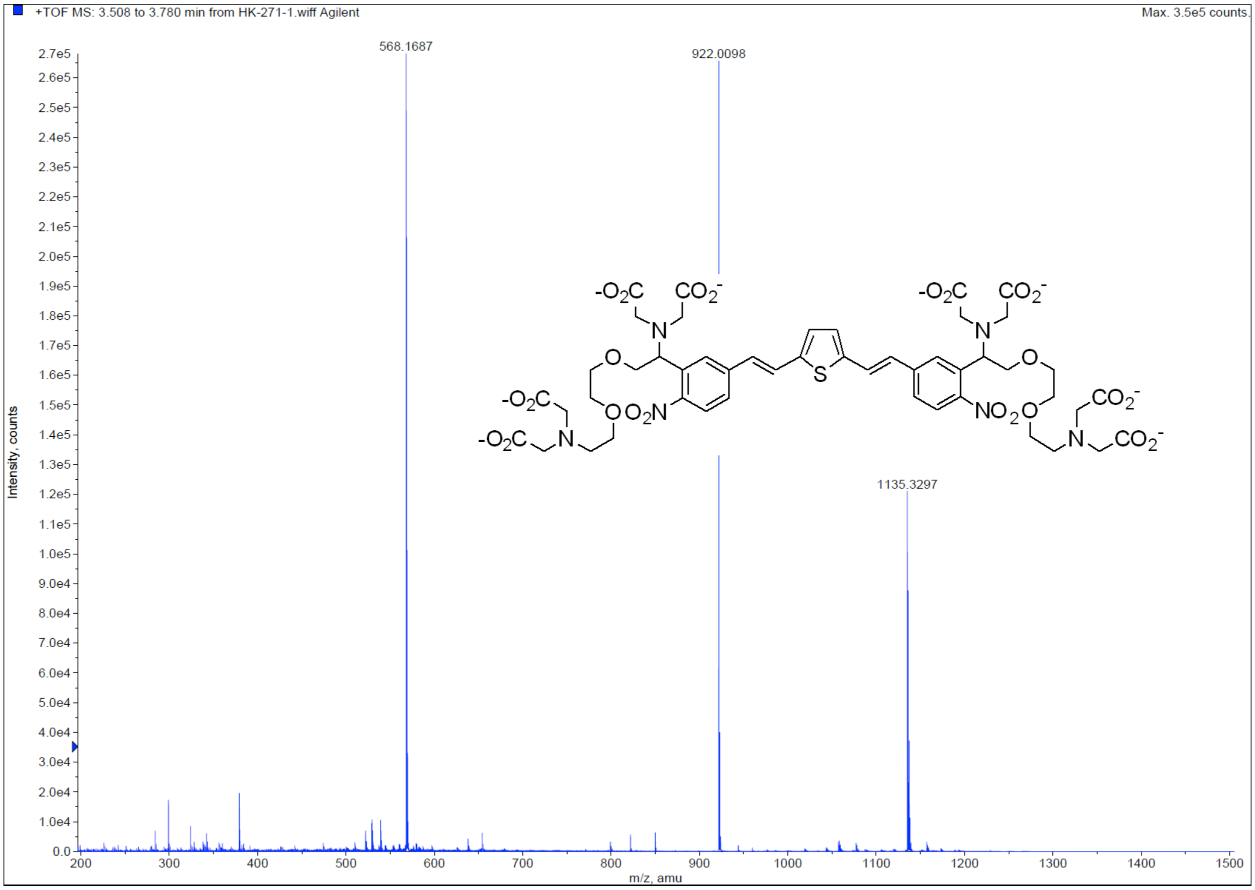

171.31
168.43
148.01
142.07
141.56
136.51
128.87
127.77
126.46
125.58
125.51
125.02
77.42
77.00
76.58
73.25
69.99
68.33
61.29
60.49
59.09
54.50
53.69
53.13
14.27
14.13
EtO2C
CO2Et
N
O
S
O2N
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

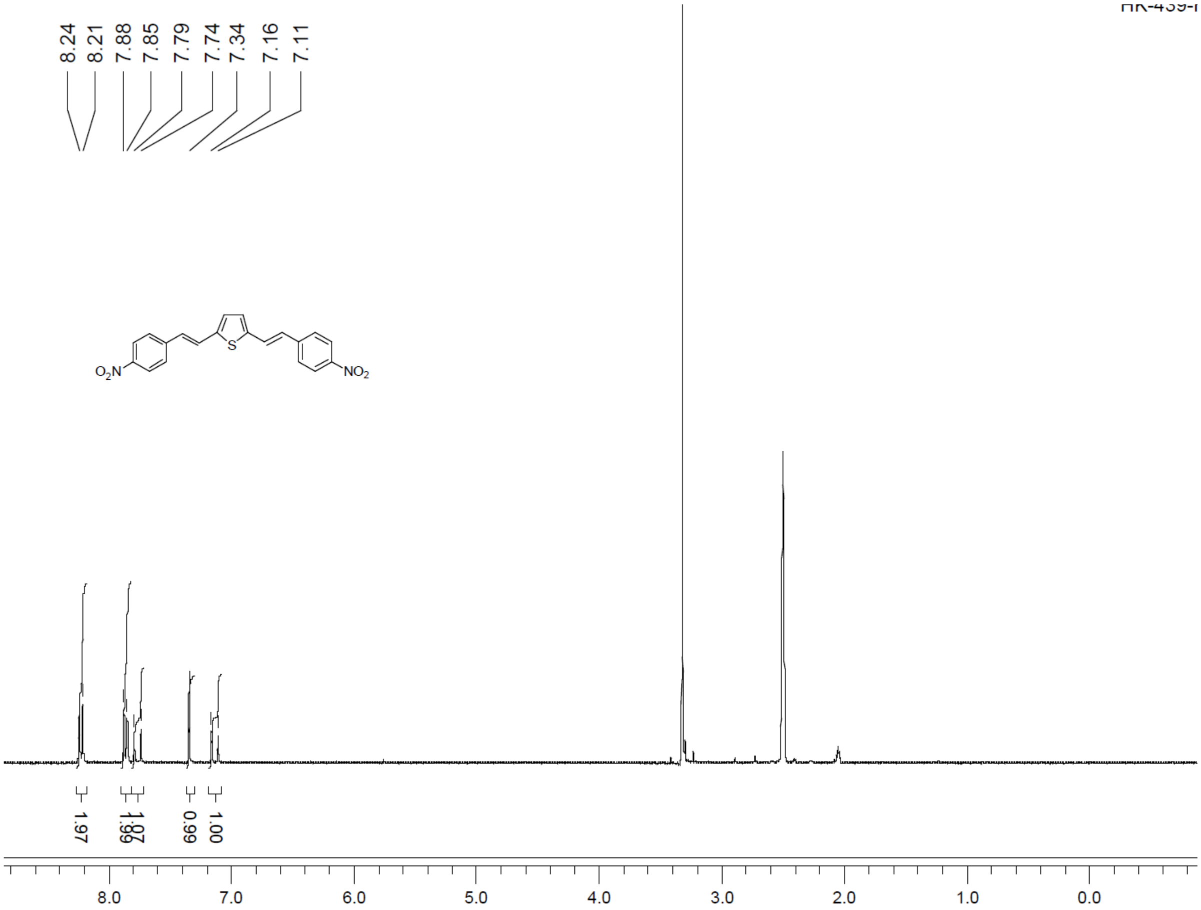

+TOF MS: 6.665 to 6.701 min from HK-274-6.wiff Agilent
Max. 2.4e6 counts.
680.3237
453.8655
922.0097
1359.5804
1381.5626
Intensity, counts
m/z, amu
0.0
1.0e5
2.0e5
3.0e5
4.0e5
5.0e5
6.0e5
7.0e5
8.0e5
9.0e5
1.0e6
1.1e6
1.2e6
1.3e6
1.4e6
1.5e6
1.6e6
1.7e6
1.8e6
1.9e6
2.0e6
2.1e6
2.2e6
2.3e6
2.4e6
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
1100
1150
1200
1250
1300
1350
1400
1450
1500
EtO2C
CO2Et
N
O
S
O2N
NO2
EtO2C
CO2Et
N

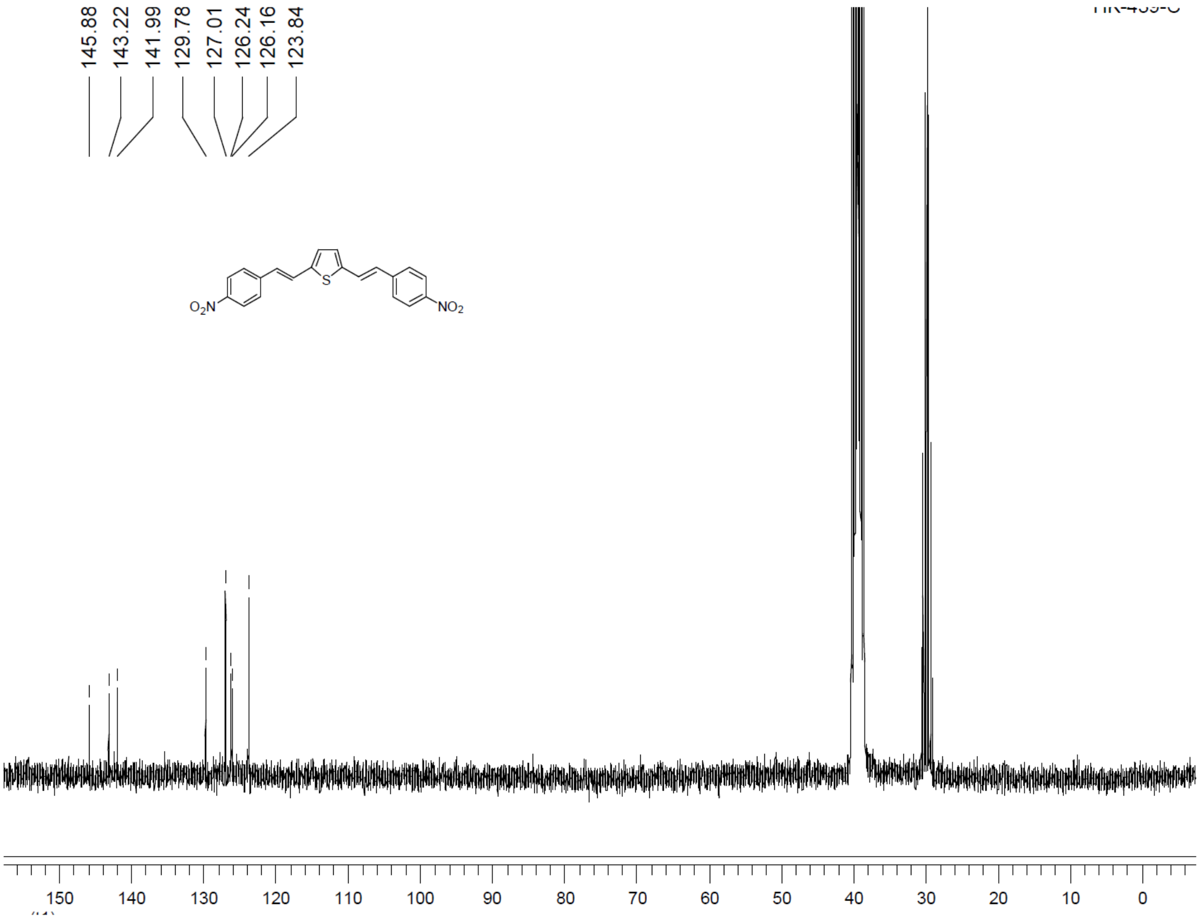

7.966
7.760
7.731
7.444
7.413
7.391
7.117
6.985
6.931
4.987
4.968
4.952
4.951
3.222
3.187
-O$_2$C
CO$_2^-$
N
O
S
O$_2$N
NO$_2$
1.00
1.04
2.12
0.99
1.04
1.03
2.08
6.38
8.02
1.87
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)



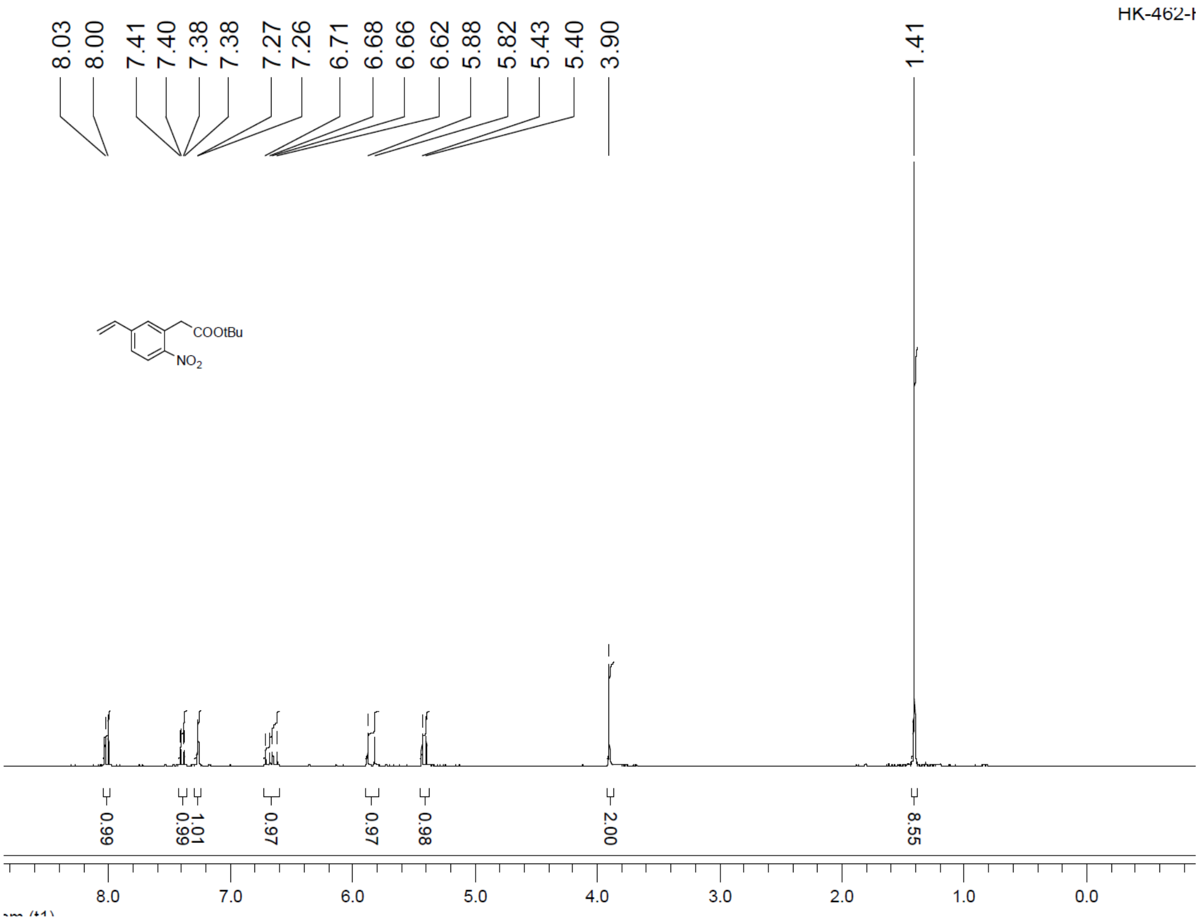
172.76
167.75
148.09
141.93
141.17
136.11
129.67
127.69
126.63
126.05
125.62
125.03
72.56
72.46
69.50
69.37
65.55
63.16
58.69
55.02
52.85
-O2C
CO2-
N
O
S
O2N
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

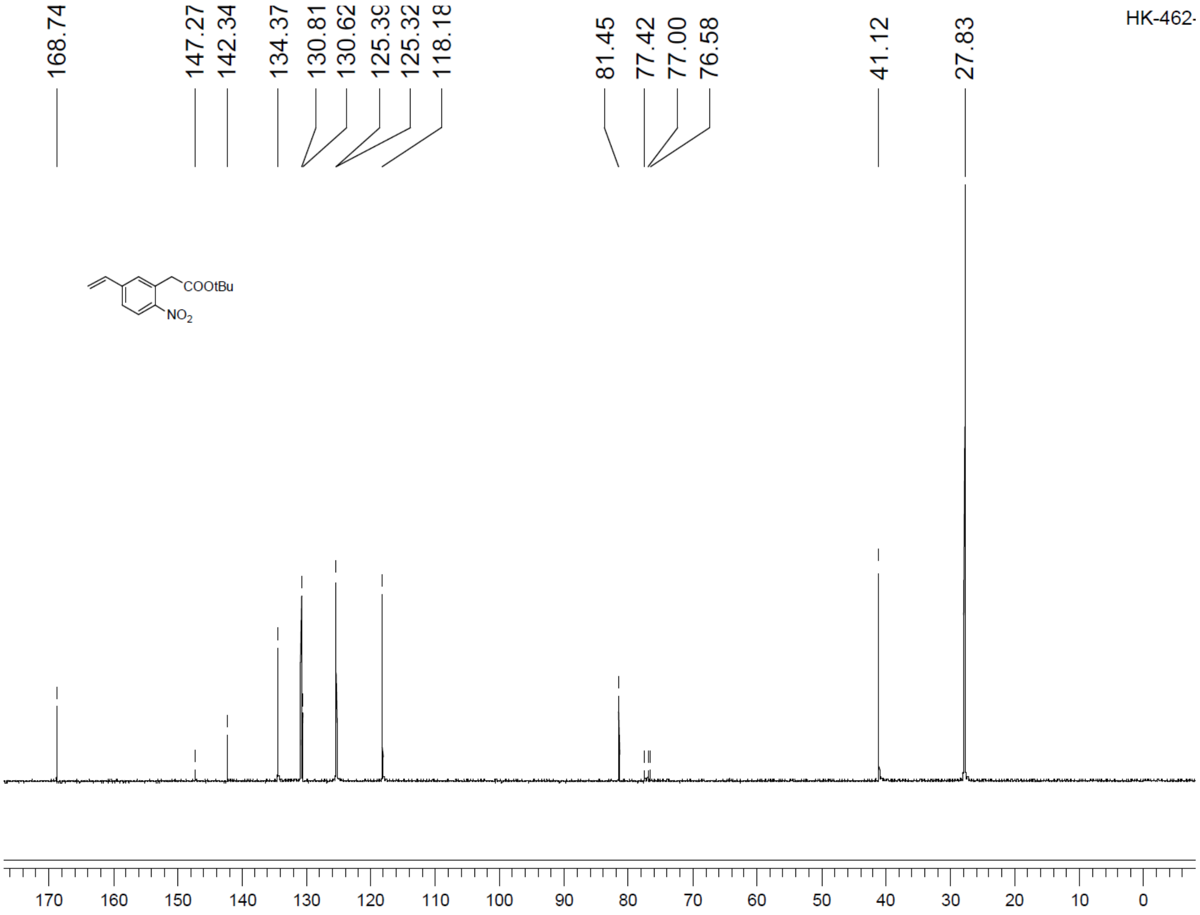

+TOF MS: 3.508 to 3.780 min from HK-271-1.wiff Agilent
Max. 3.5e5 counts.
568.1687
922.0098
1135.3297
Intensity, counts
m/z, amu
2.7e5
2.6e5
2.5e5
2.4e5
2.3e5
2.2e5
2.1e5
2.0e5
1.9e5
1.8e5
1.7e5
1.6e5
1.5e5
1.4e5
1.3e5
1.2e5
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
-O2C
CO2-
N
O
S
O2N
NO2
O
N


8.24
8.21
7.88
7.85
7.79
7.74
7.34
7.16
7.11
O_2N
S
NO_2
1.97
1.96
1.07
0.99
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0



HR-459-C
145.88
143.22
141.99
129.78
127.01
126.24
126.16
123.84
S
O_2N
NO_2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


HK-462-
8.03
8.00
7.41
7.40
7.38
7.38
7.27
7.26
6.71
6.68
6.66
6.62
5.88
5.82
5.43
5.40
3.90
1.41
COOtBu
NO_2
0.99
0.99
1.01
0.97
0.97
0.98
2.00
8.55
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

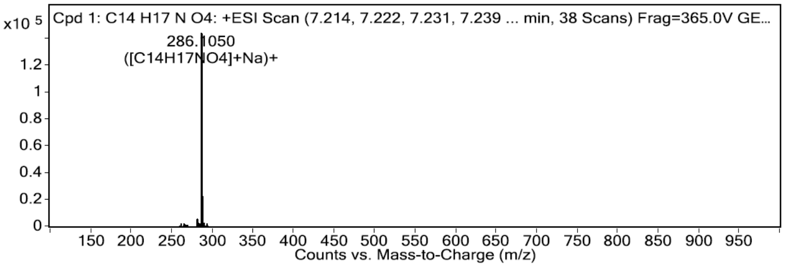

HK-462-
168.74
147.27
142.34
134.37
130.81
130.62
125.39
125.32
118.18
81.45
77.42
77.00
76.58
41.12
27.83
COOtBu
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound Table

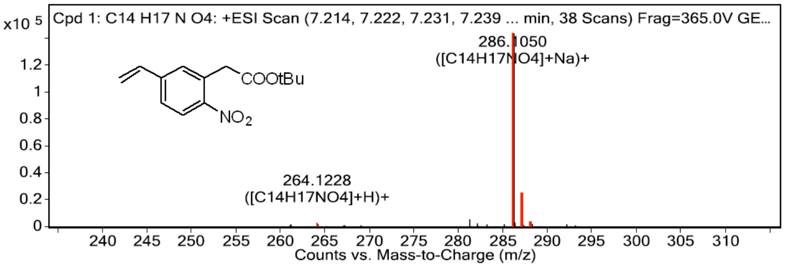
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H17 N O4	7.322	263.1158	151386	C14 H17 N O4	263.1158	-0.01	C14 H17 N O4	C14 H17 N O4

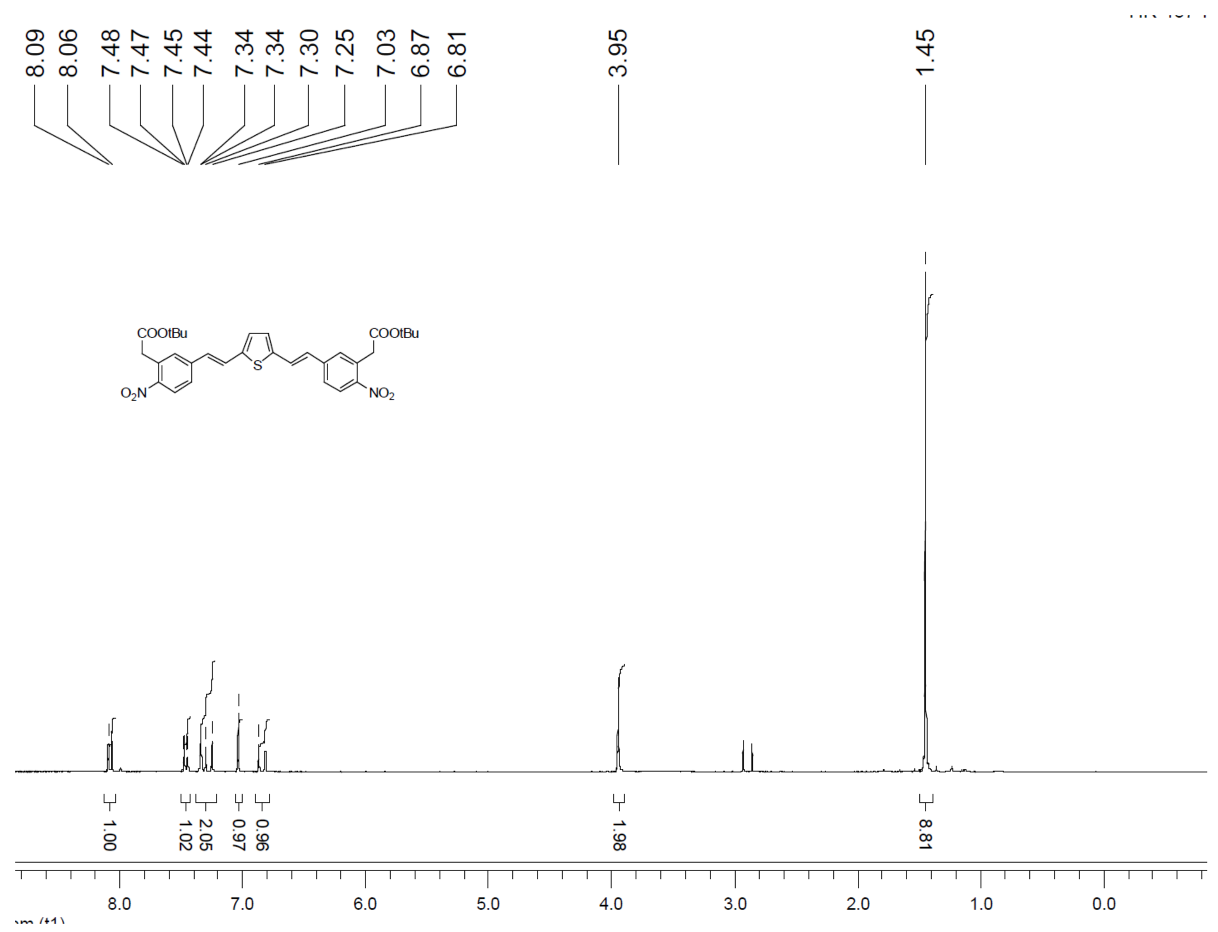
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H17 N O4	286.105	7.322	Find By Formula	263.1158

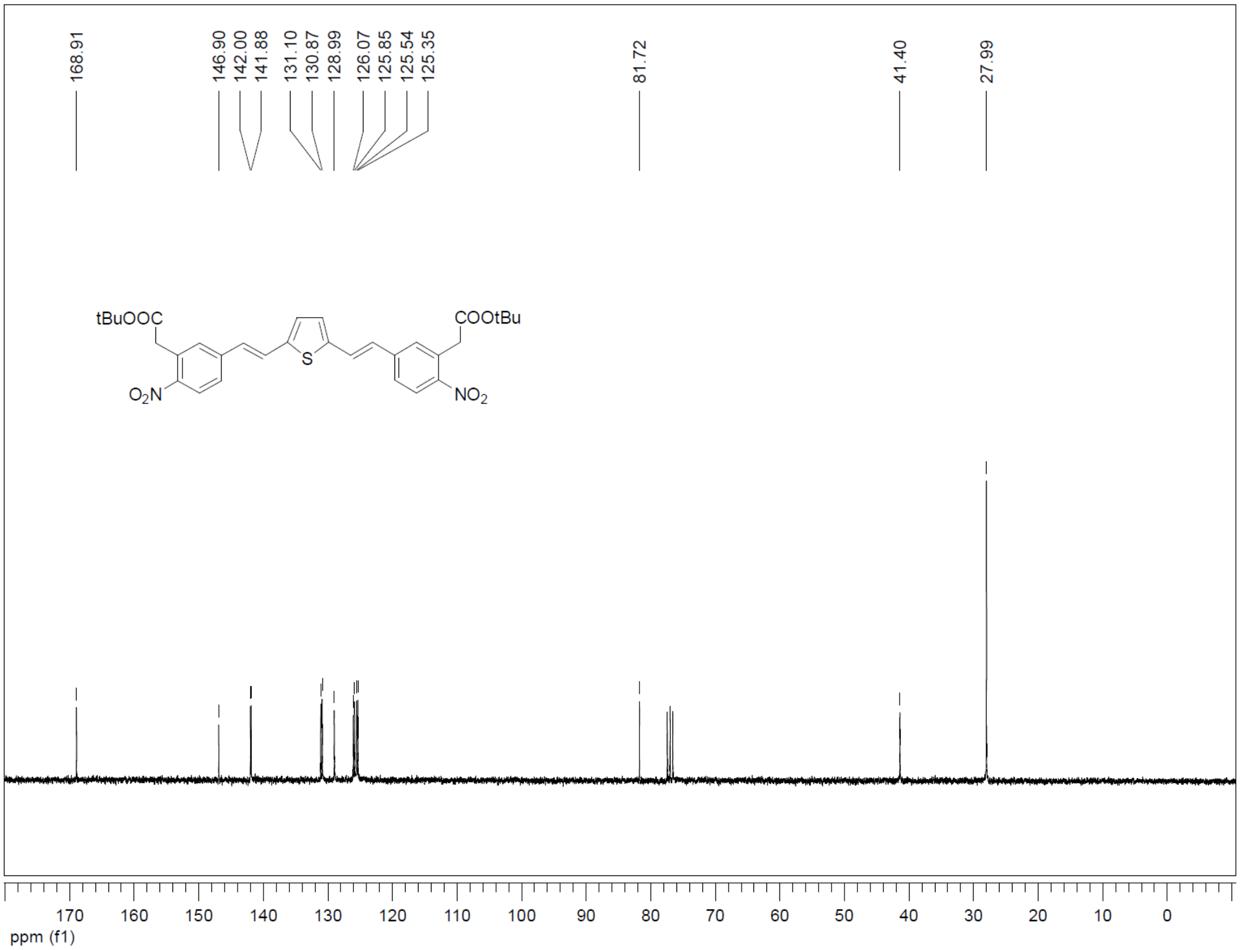
MS Spectrum



MS Zoomed Spectrum




8.09
8.06
7.48
7.47
7.45
7.44
7.34
7.34
7.30
7.25
7.03
6.87
6.81
3.95
1.45
COOtBu
COOtBu
S
O_2N
NO_2
1.00
1.02
2.05
0.97
0.96
1.98
8.81
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

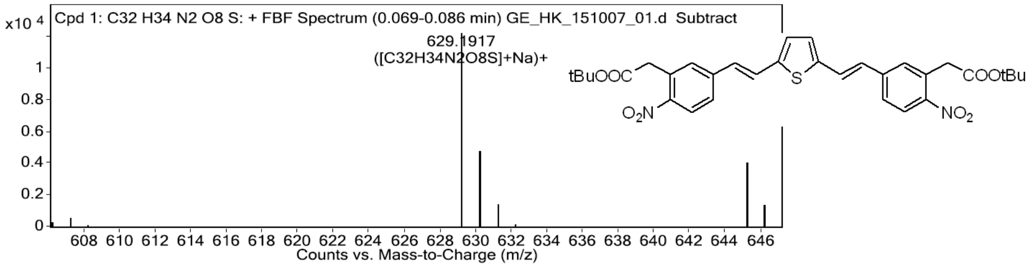

168.91
146.90
142.00
141.88
131.10
130.87
128.99
126.07
125.85
125.54
125.35
81.72
41.40
27.99
tBuOOC
COOtBu
S
O2N
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)

Compound Table

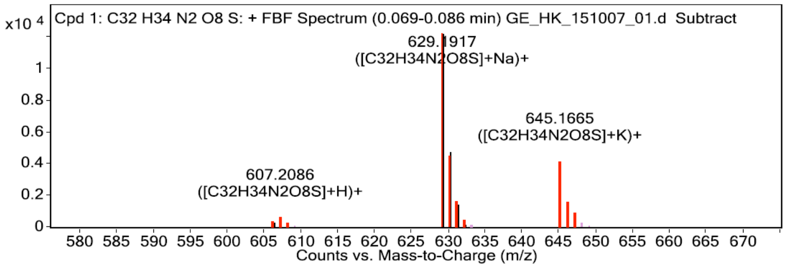
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C32 H34 N2 O8 S	0.078	606.2032	12216	C32 H34 N2 O8 S	606.2036	-0.58	C32 H34 N2 O8 S	C32 H34 N2 O8 S

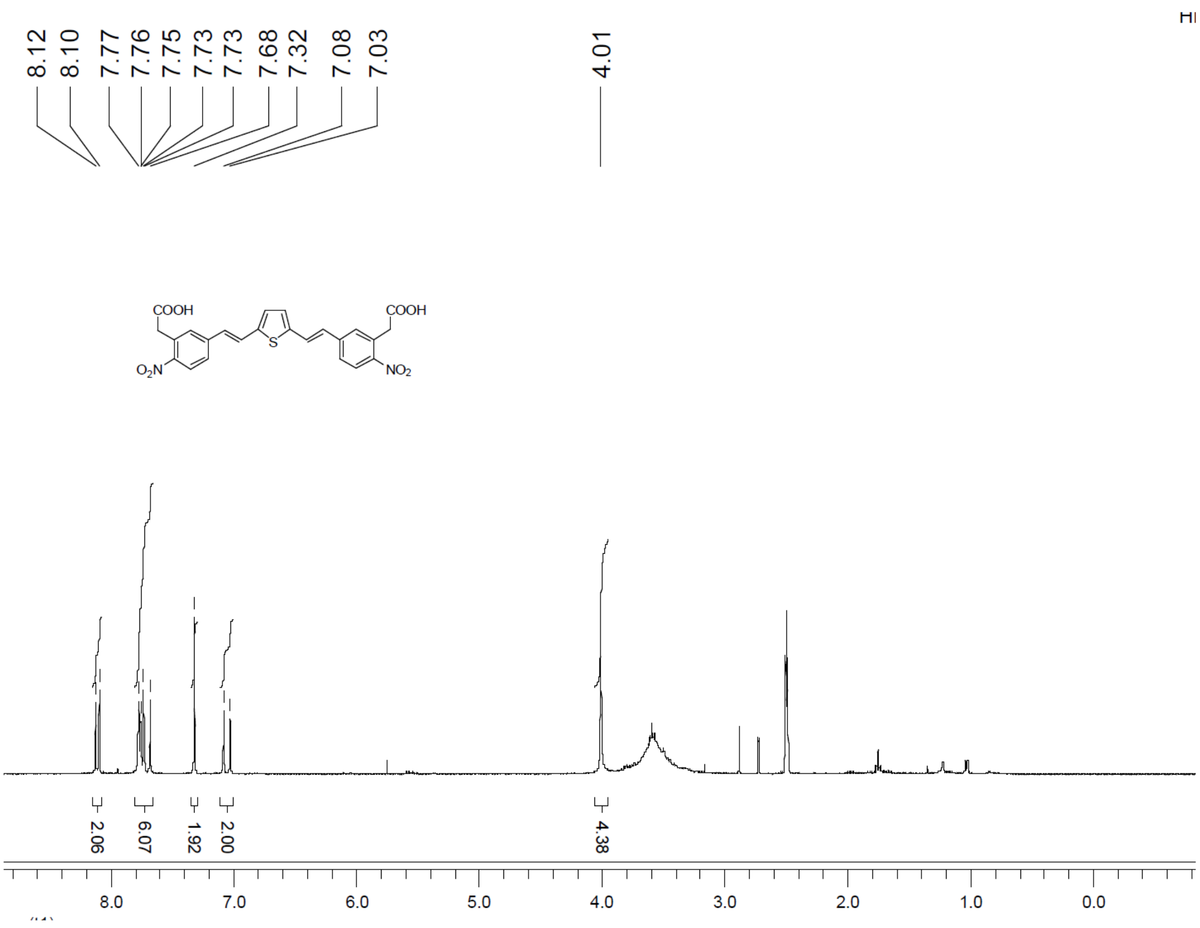
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C32 H34 N2 O8 S	629.1917	0.078	Find By Formula	606.2032

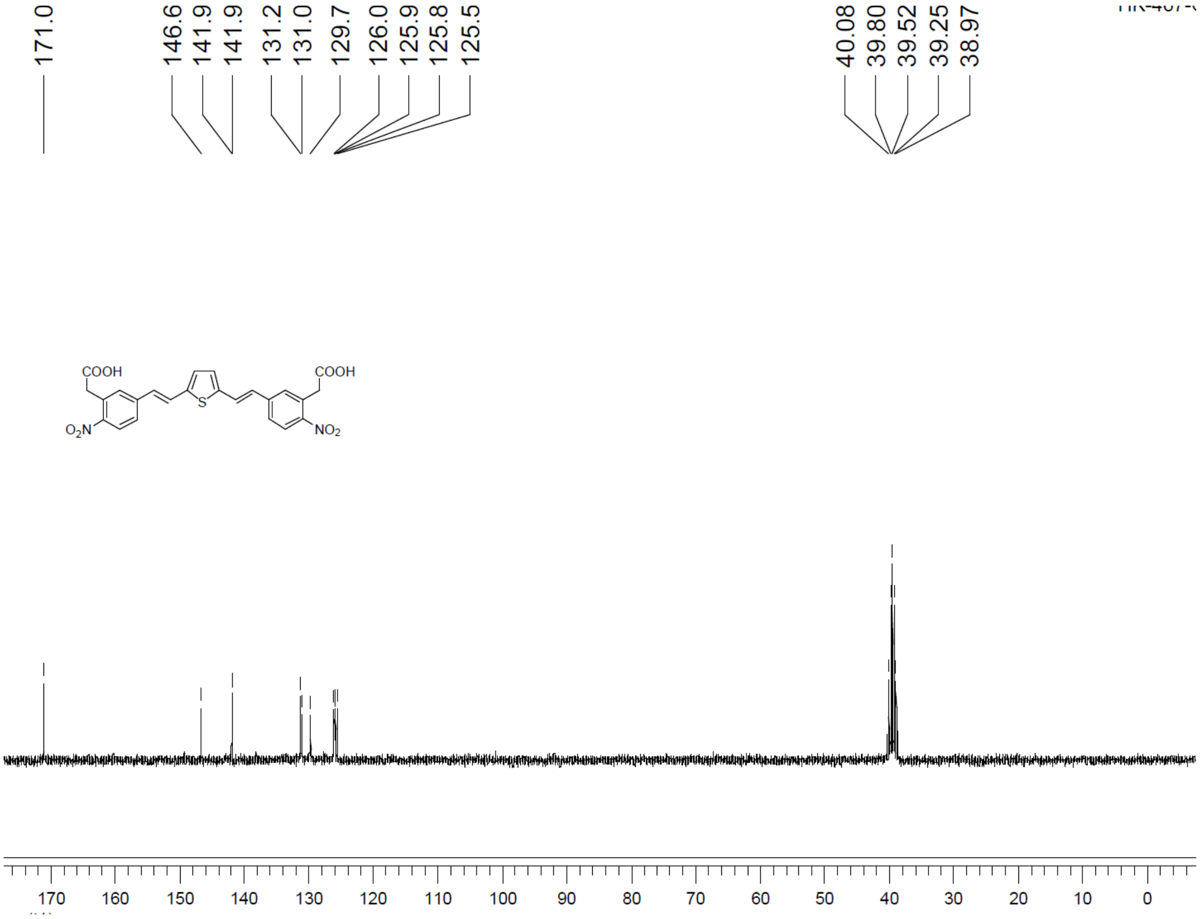
MS Spectrum



MS Zoomed Spectrum




HI
8.12
8.10
7.77
7.76
7.75
7.73
7.73
7.68
7.32
7.08
7.03
4.01
COOH
COOH
S
O2N
NO2
2.06
6.07
1.92
2.00
4.38
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0



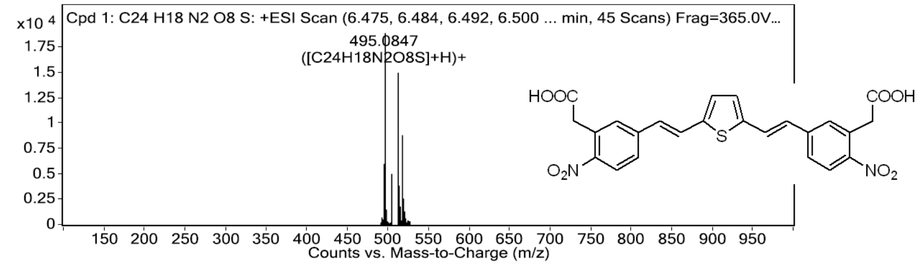
171.0
146.6
141.9
141.9
131.2
131.0
129.7
126.0
125.9
125.8
125.5
40.08
39.80
39.52
39.25
38.97
COOH
COOH
S
O_2N
NO_2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound Table

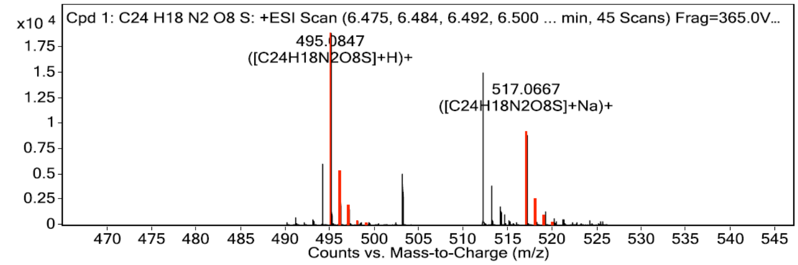
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C24 H18 N2 O8 S	6.559	494.0776	18945	C24 H18 N2 O8 S	494.0784	-1.67	C24 H18 N2 O8 S	C24 H18 N2 O8 S

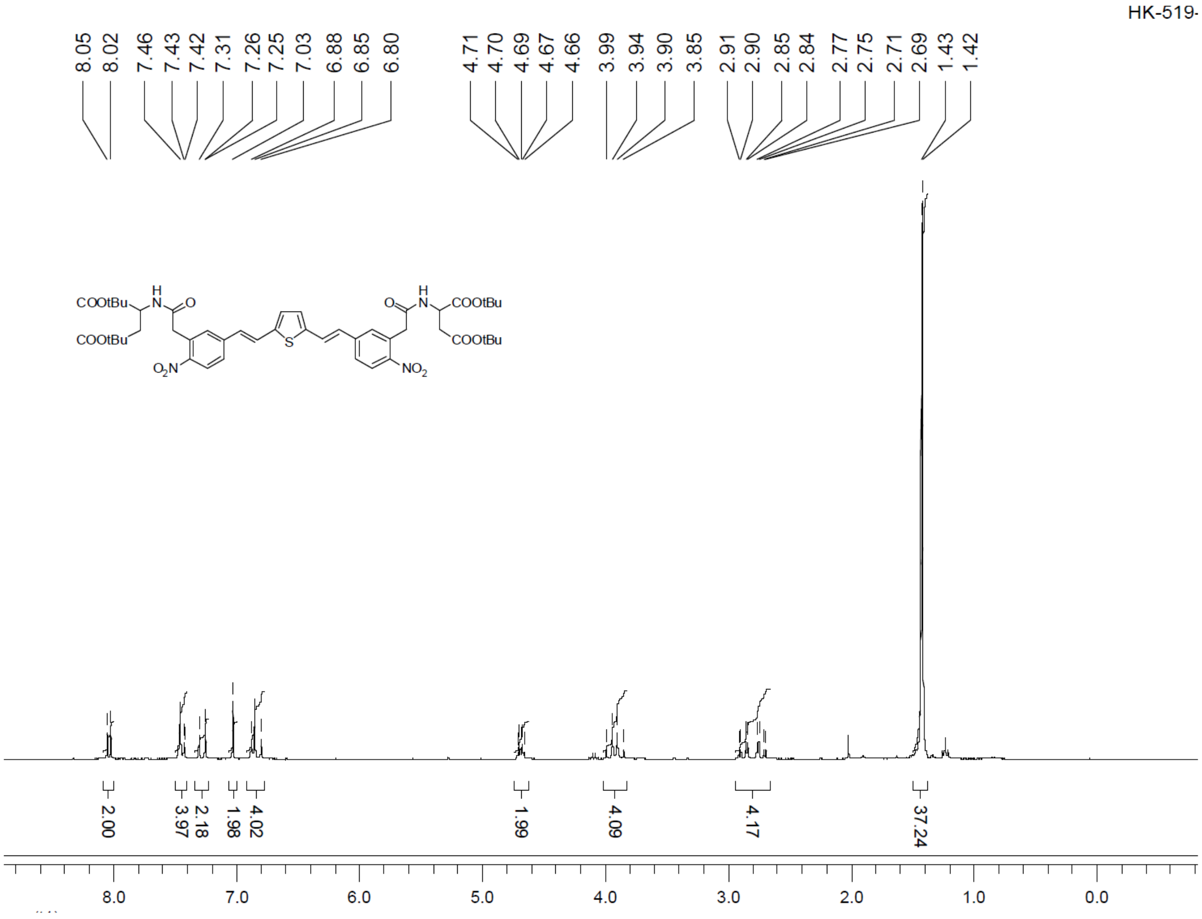
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H18 N2 O8 S	495.0847	6.559	Find By Formula	494.0776

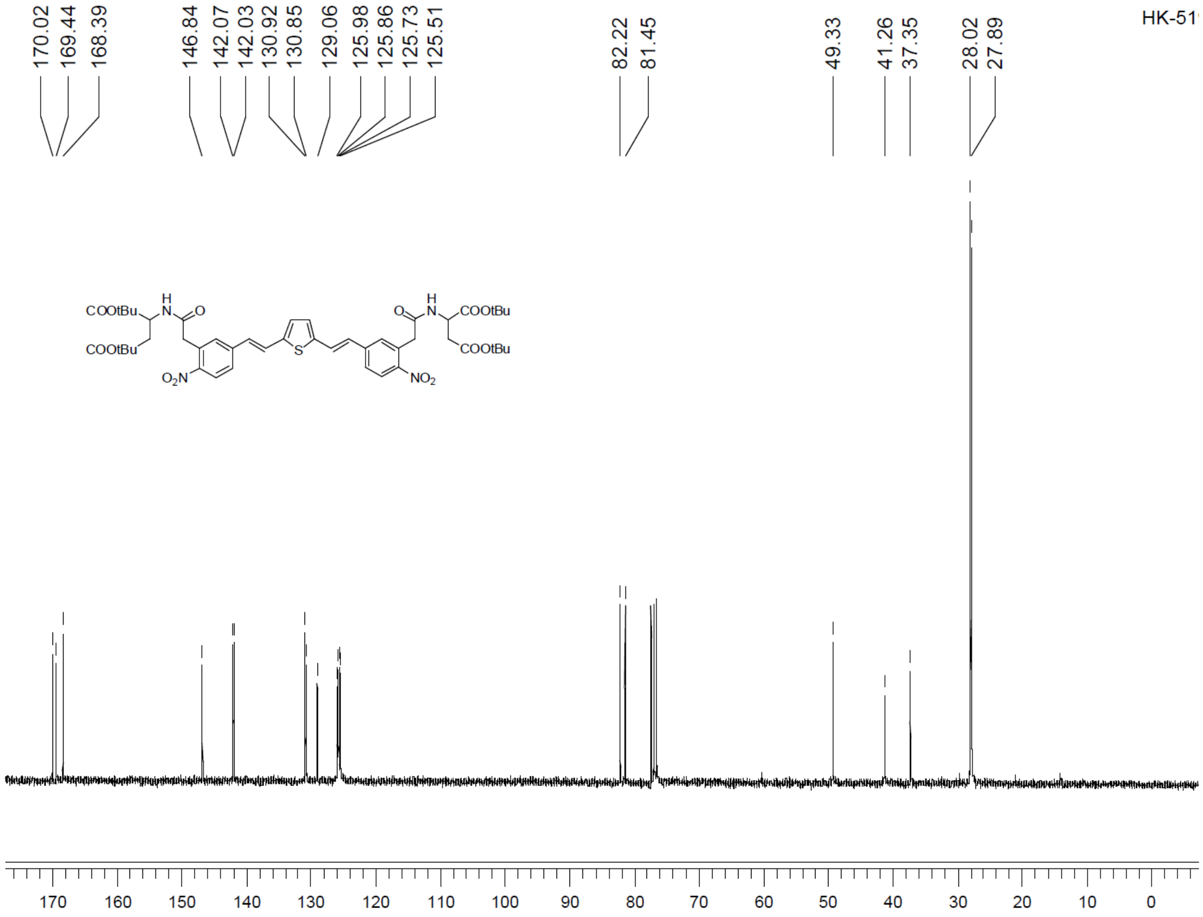
MS Spectrum



MS Zoomed Spectrum




HK-519-
8.05
8.02
7.46
7.43
7.42
7.31
7.26
7.25
7.03
6.88
6.85
6.80
4.71
4.70
4.69
4.67
4.66
3.99
3.94
3.90
3.85
2.91
2.90
2.85
2.84
2.77
2.75
2.71
2.69
1.43
1.42
COOtBu
H
N
O
COOtBu
O$_2$N
S
O
H
N
COOtBu
COOtBu
NO$_2$
2.00
3.97
2.18
1.98
4.02
1.99
4.09
4.17
37.24
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

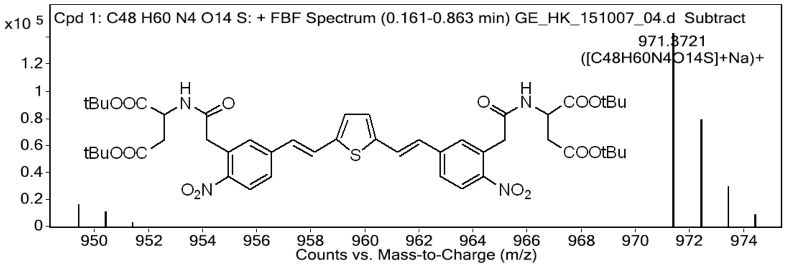

170.02
169.44
168.39
146.84
142.07
142.03
130.92
130.85
129.06
125.98
125.86
125.73
125.51
82.22
81.45
49.33
41.26
37.35
28.02
27.89
HK-51
COOtBu
COOtBu
H
N
O
O_2N
S
O
H
N
COOtBu
COOtBu
NO_2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound Table

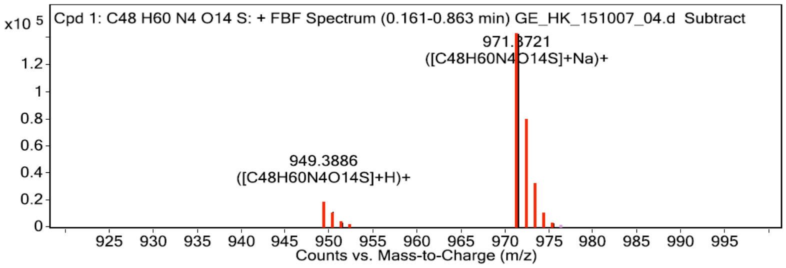
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C48 H60 N4 O14 S	0.379	948.3822	143198	C48 H60 N4 O14 S	948.3827	-0.48	C48 H60 N4 O14 S	C48 H60 N4 O14 S

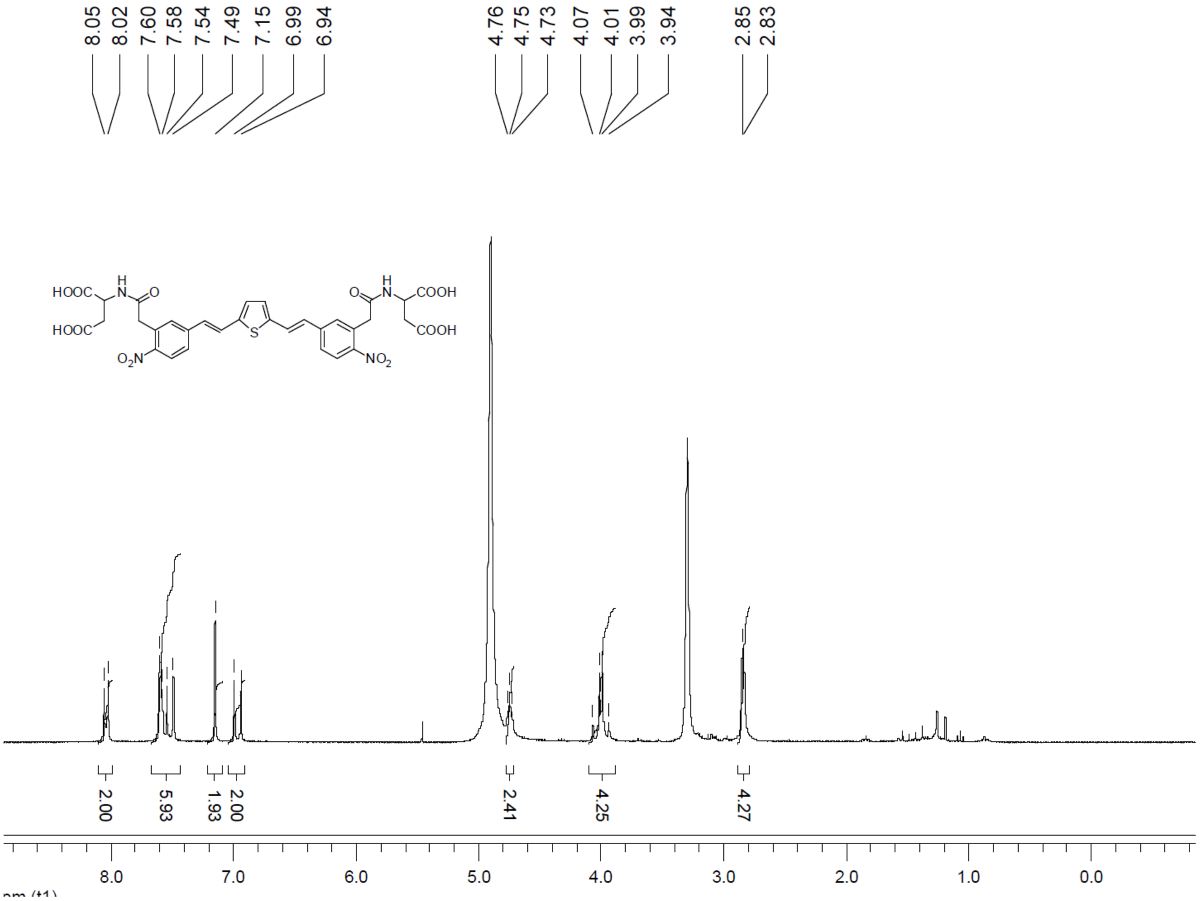
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C48 H60 N4 O14 S	971.3721	0.379	Find By Formula	948.3822

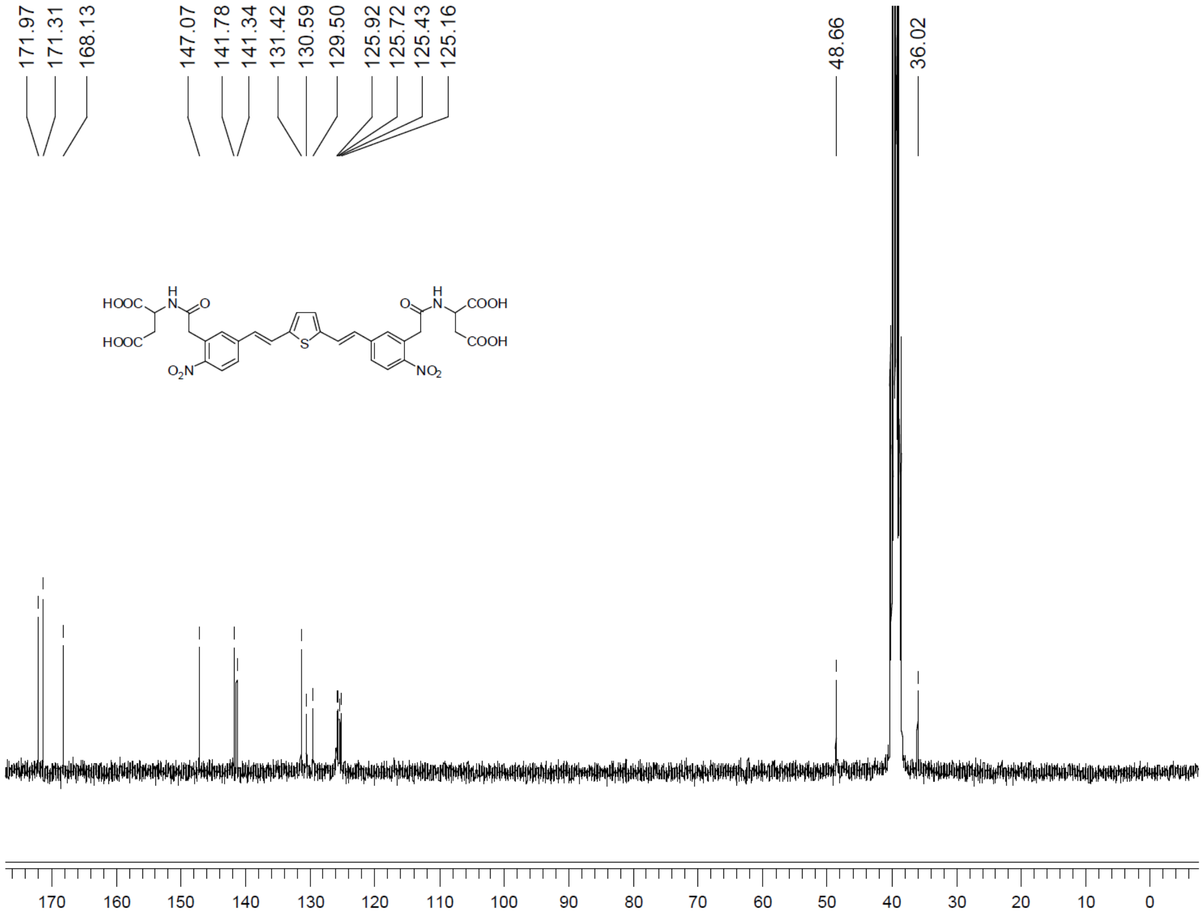
MS Spectrum



MS Zoomed Spectrum




8.05
8.02
7.60
7.58
7.54
7.49
7.15
6.99
6.94
4.76
4.75
4.73
4.07
4.01
3.99
3.94
2.85
2.83
HOOC
H
N
O
HOOC
O₂N
S
O
H
N
COOH
COOH
NO₂
2.00
5.93
1.93
2.00
2.41
4.25
4.27
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

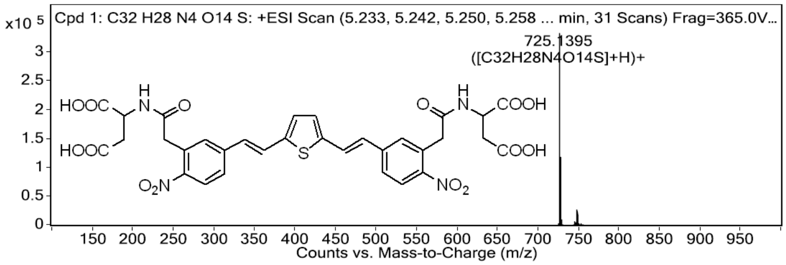

171.97
171.31
168.13
147.07
141.78
141.34
131.42
130.59
129.50
125.92
125.72
125.43
125.16
48.66
36.02
HOOC
H
N
O
HOOC
O_2N
S
O
H
N
COOH
COOH
NO_2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound Table

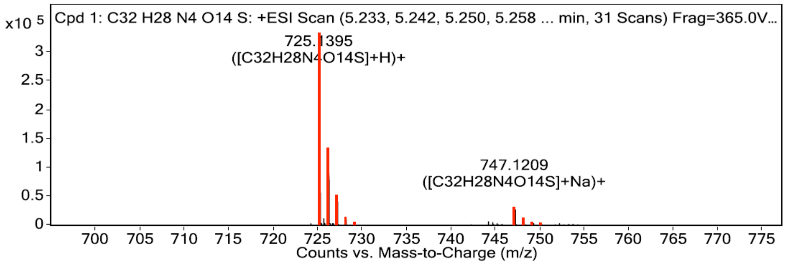
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C32 H28 N4 O14 S	5.317	724.1322	350154	C32 H28 N4 O14 S	724.1323	-0.05	C32 H28 N4 O14 S	C32 H28 N4 O14 S

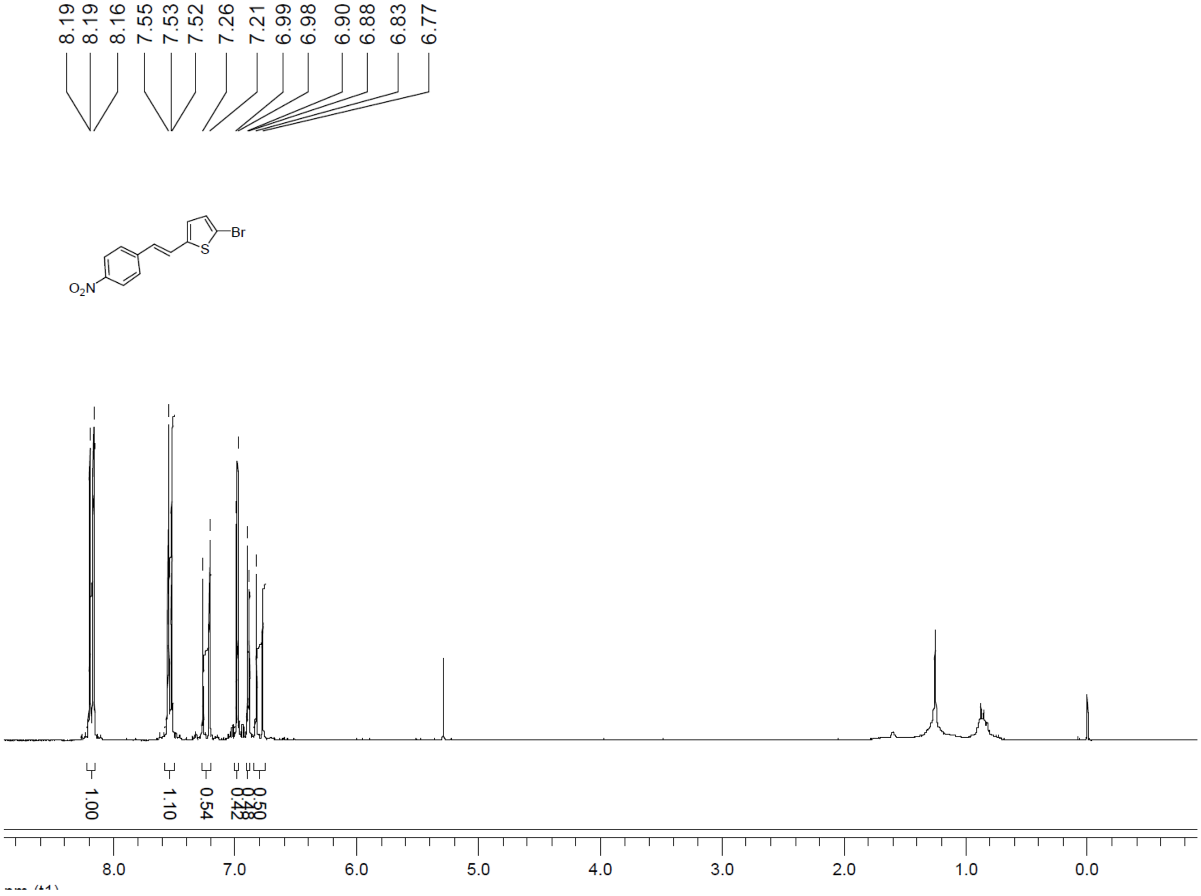
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C32 H28 N4 O14 S	725.1395	5.317	Find By Formula	724.1322

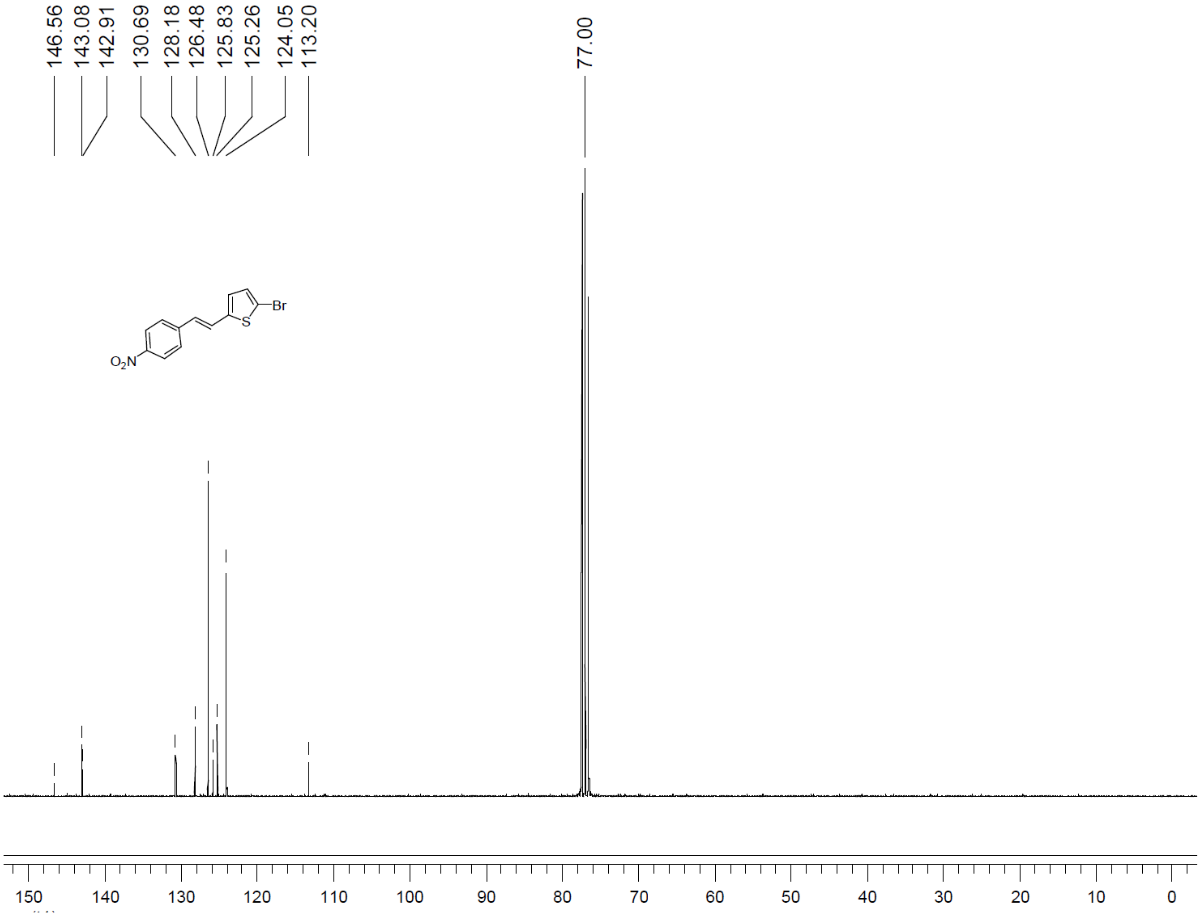
MS Spectrum



MS Zoomed Spectrum




8.19
8.19
8.16
7.55
7.53
7.52
7.26
7.21
6.99
6.98
6.90
6.88
6.83
6.77
Br
S
O2N
1.00
1.10
0.54
0.42
0.48
0.50
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

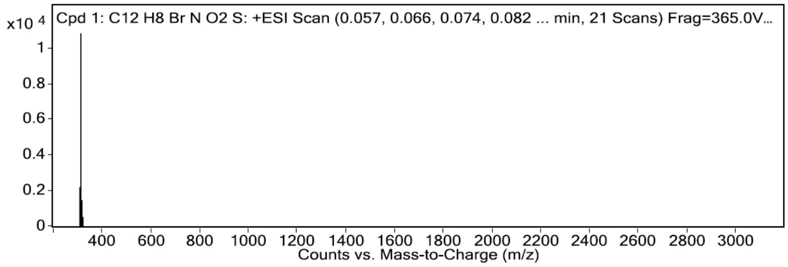

146.56
143.08
142.91
130.69
128.18
126.48
125.83
125.26
124.05
113.20
77.00
Br
S
O_2N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound Table

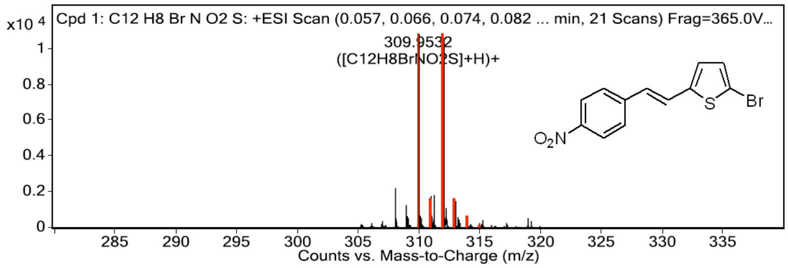
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C12 H8 Br N O2 S	0.091	308.9457	11036	C12 H8 Br N O2 S	308.9459	-0.77	C12 H8 Br N O2 S	C12 H8 Br N O2 S

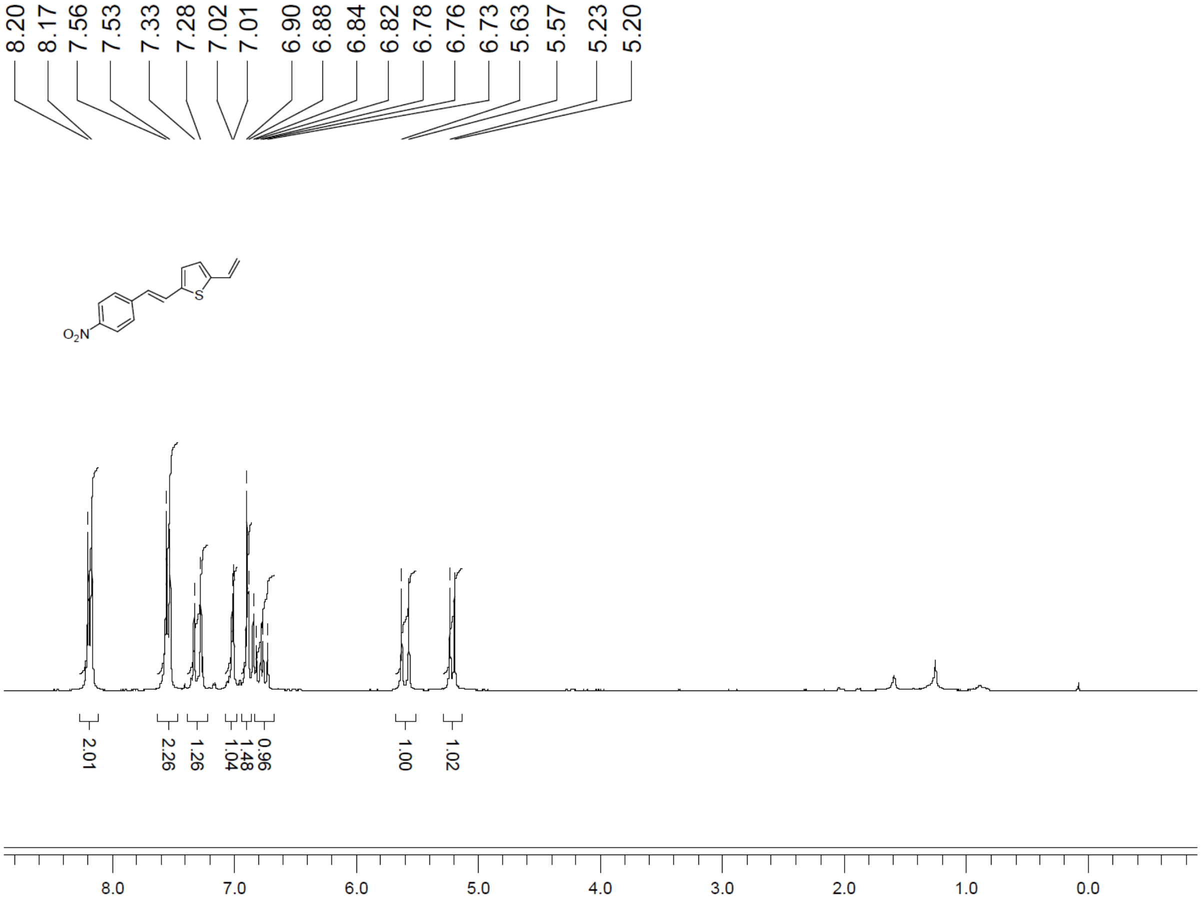
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C12 H8 Br N O2 S	309.9532	0.091	Find By Formula	308.9457

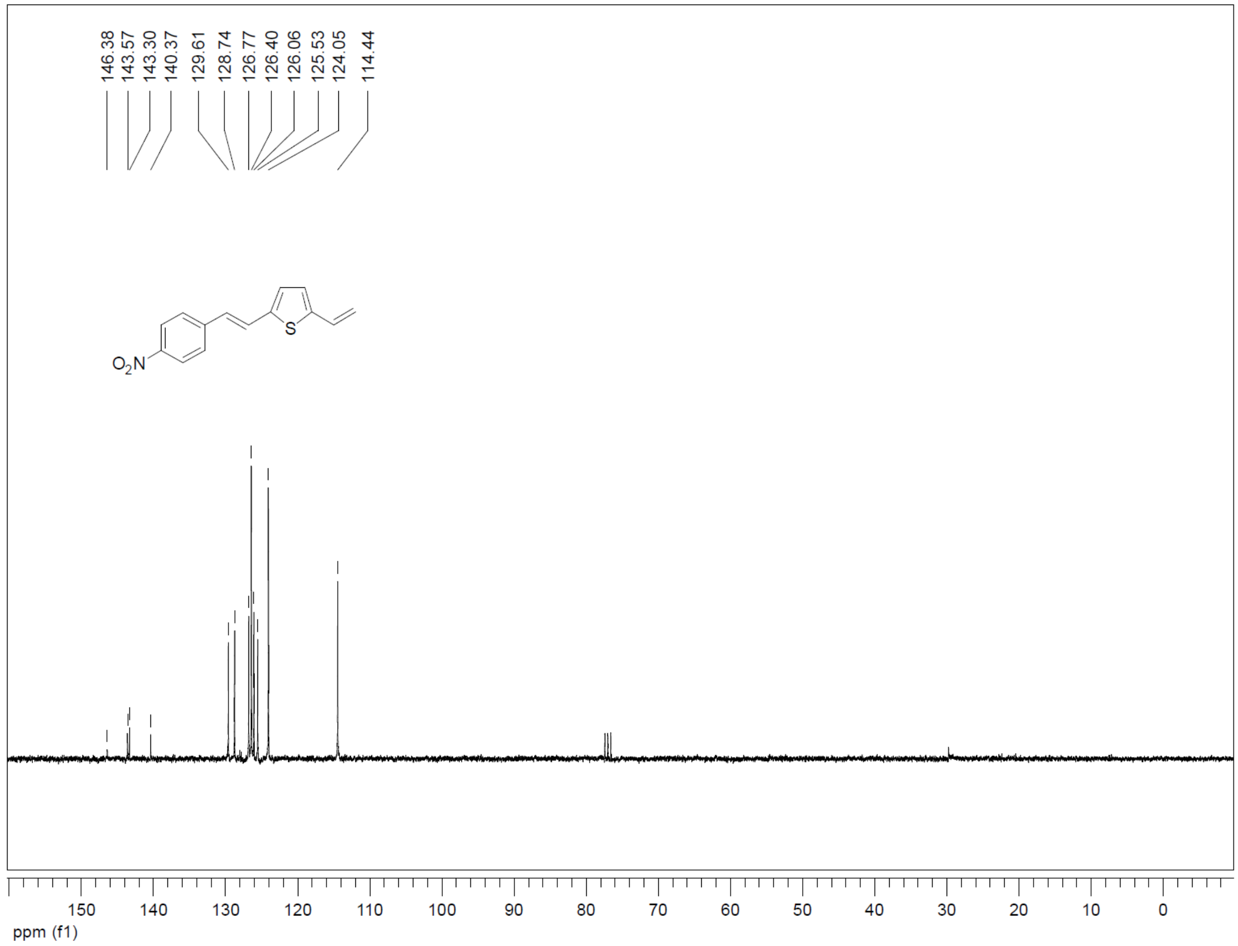
MS Spectrum



MS Zoomed Spectrum




8.20
8.17
7.56
7.53
7.33
7.28
7.02
7.01
6.90
6.88
6.84
6.82
6.78
6.76
6.73
5.63
5.57
5.23
5.20
O_2N
S
2.01
2.26
1.26
1.04
1.48
0.96
1.00
1.02
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

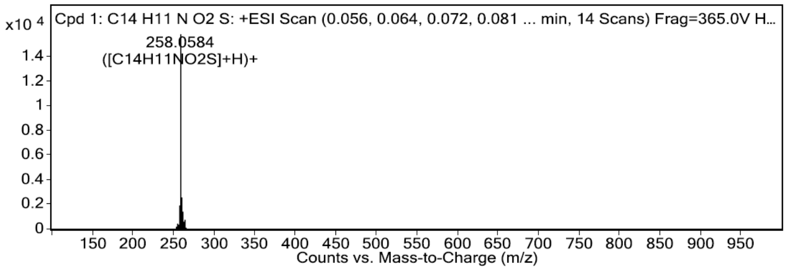

146.38
143.57
143.30
140.37
129.61
128.74
126.77
126.40
126.06
125.53
124.05
114.44
O$_2$N
S
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)

Compound Table

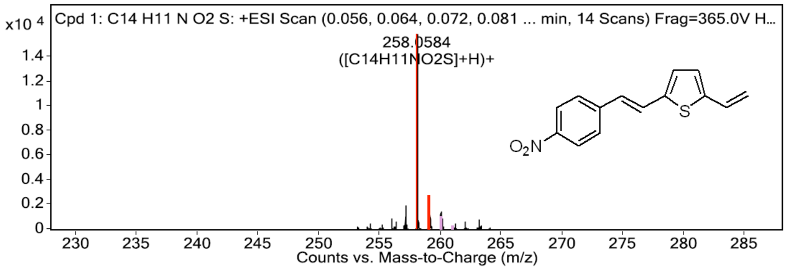
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H11 N O2 S	0.097	257.0512	16448	C14 H11 N O2 S	257.051	0.42	C14 H11 N O2 S	C14 H11 N O2 S

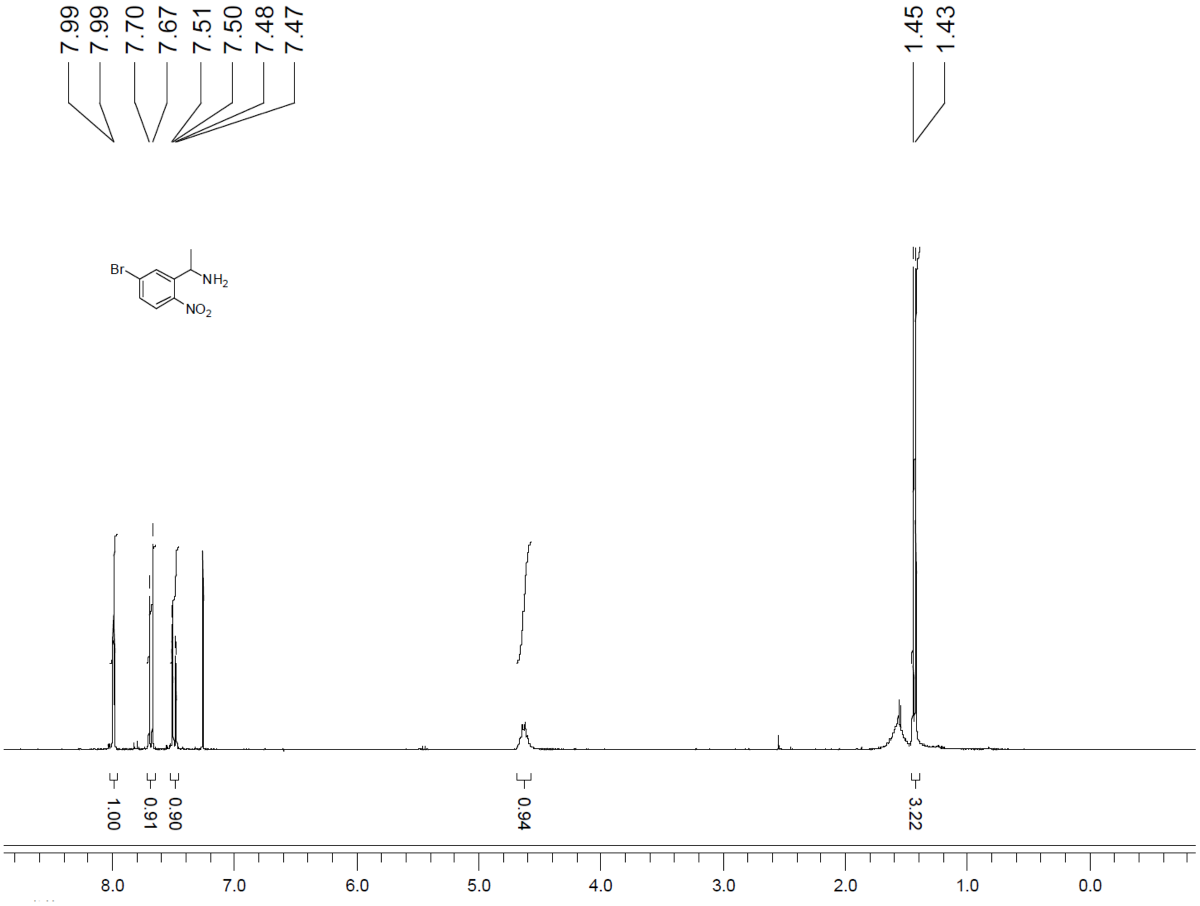
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H11 N O2 S	258.0584	0.097	Find By Formula	257.0512

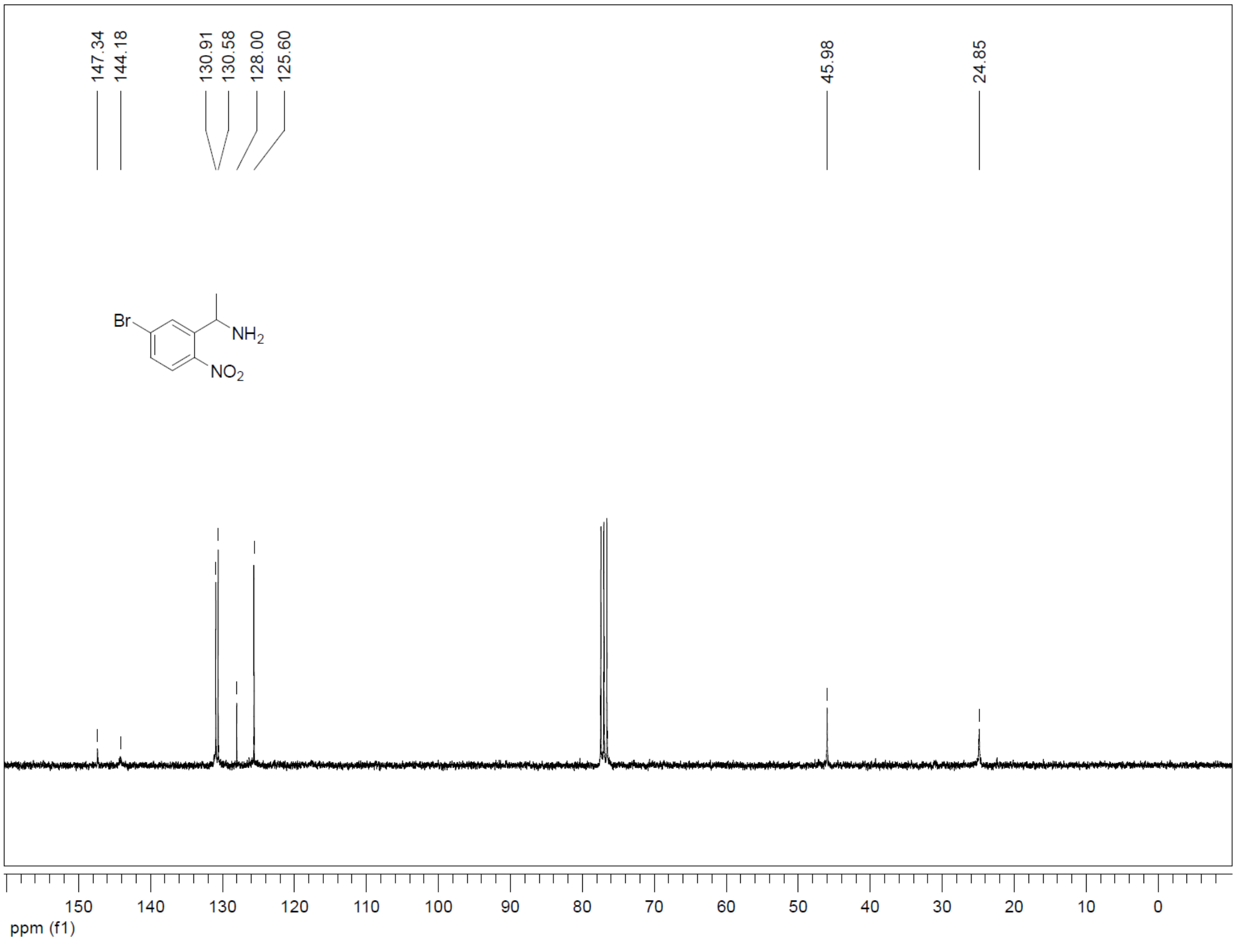
MS Spectrum

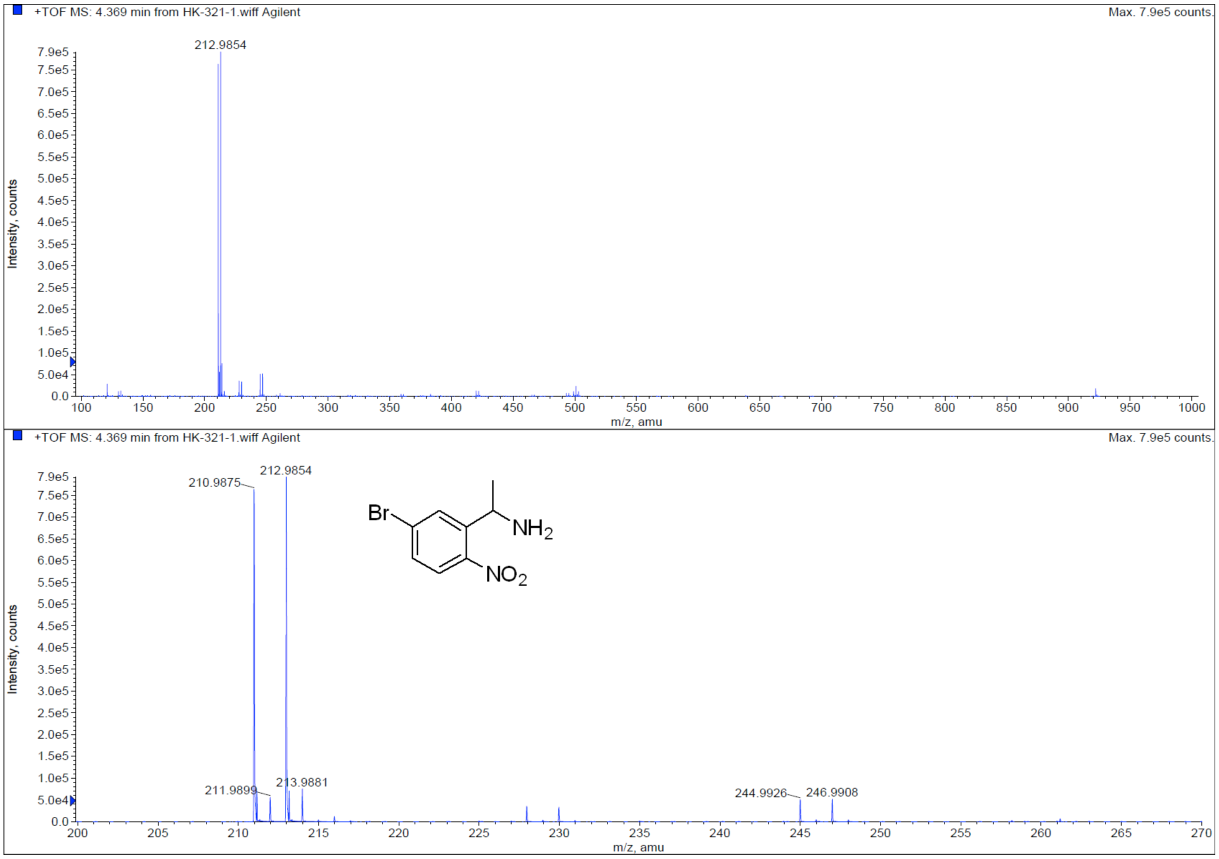


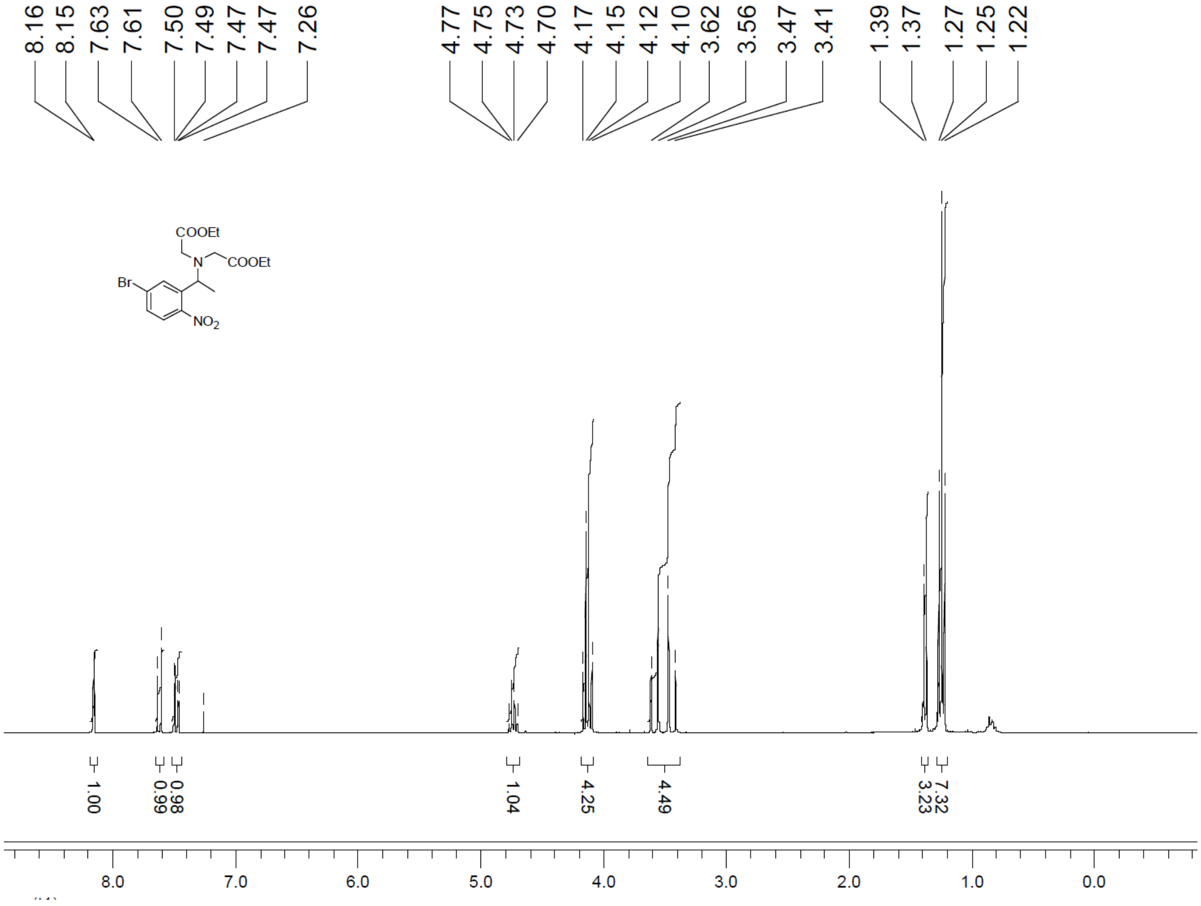
MS Zoomed Spectrum

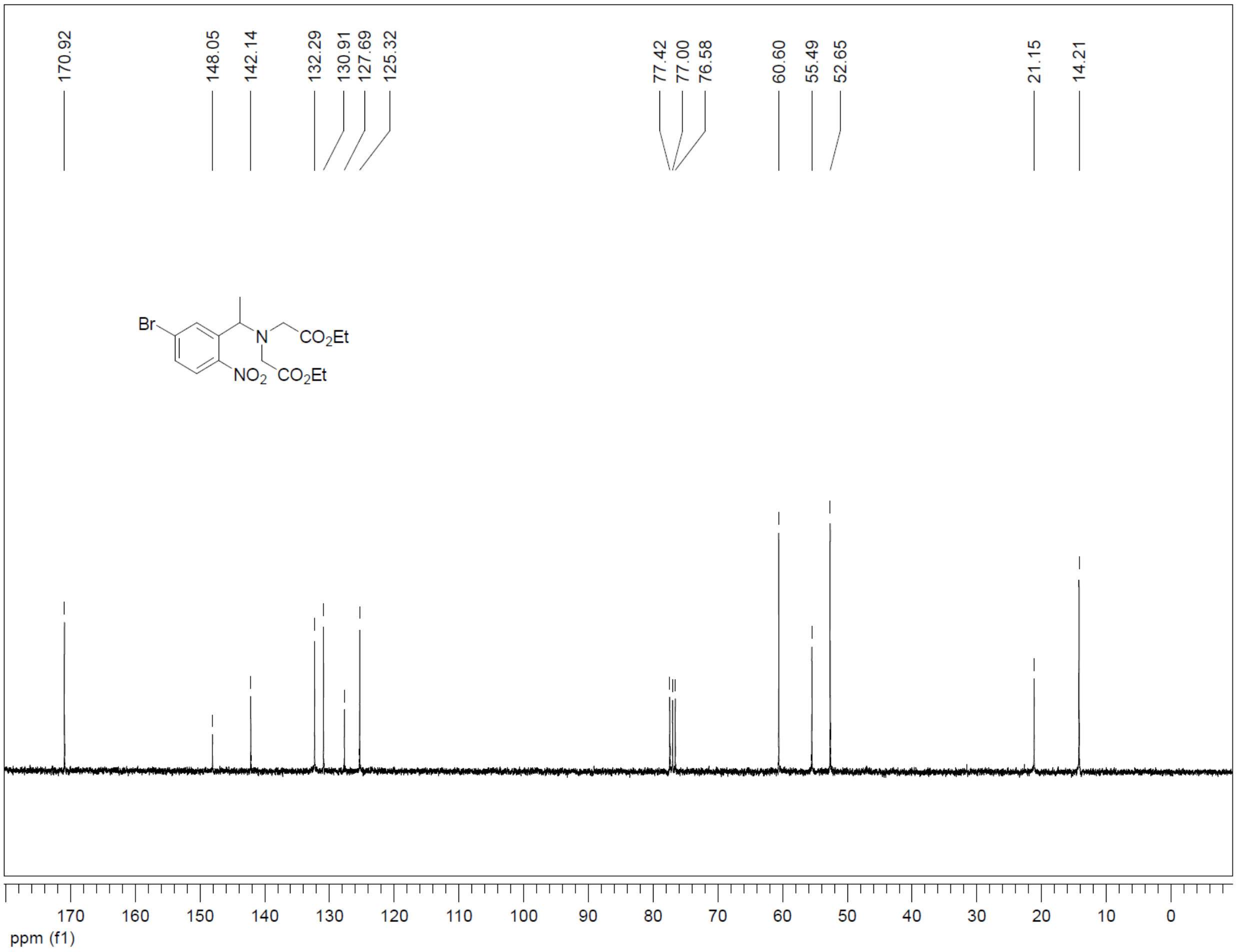


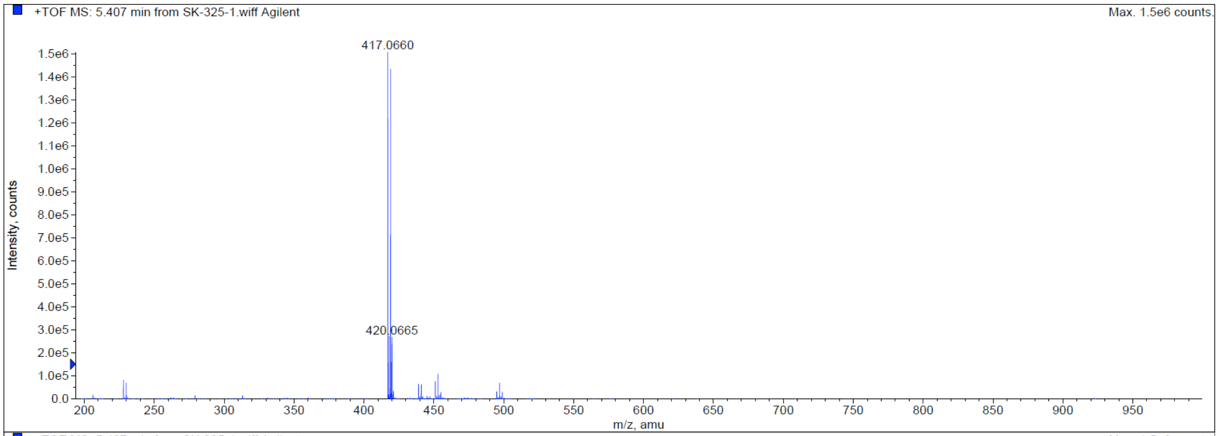

7.99
7.99
7.70
7.67
7.51
7.50
7.48
7.47
1.45
1.43
Br
NH2
NO2
1.00
0.91
0.90
0.94
3.22
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

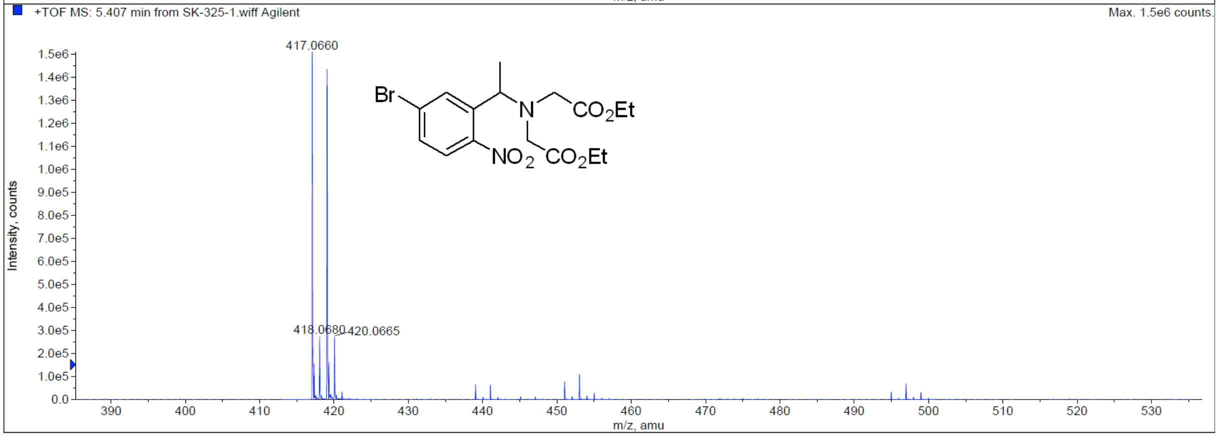

147.34
144.18
130.91
130.58
128.00
125.60
45.98
24.85
Br
NH2
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)

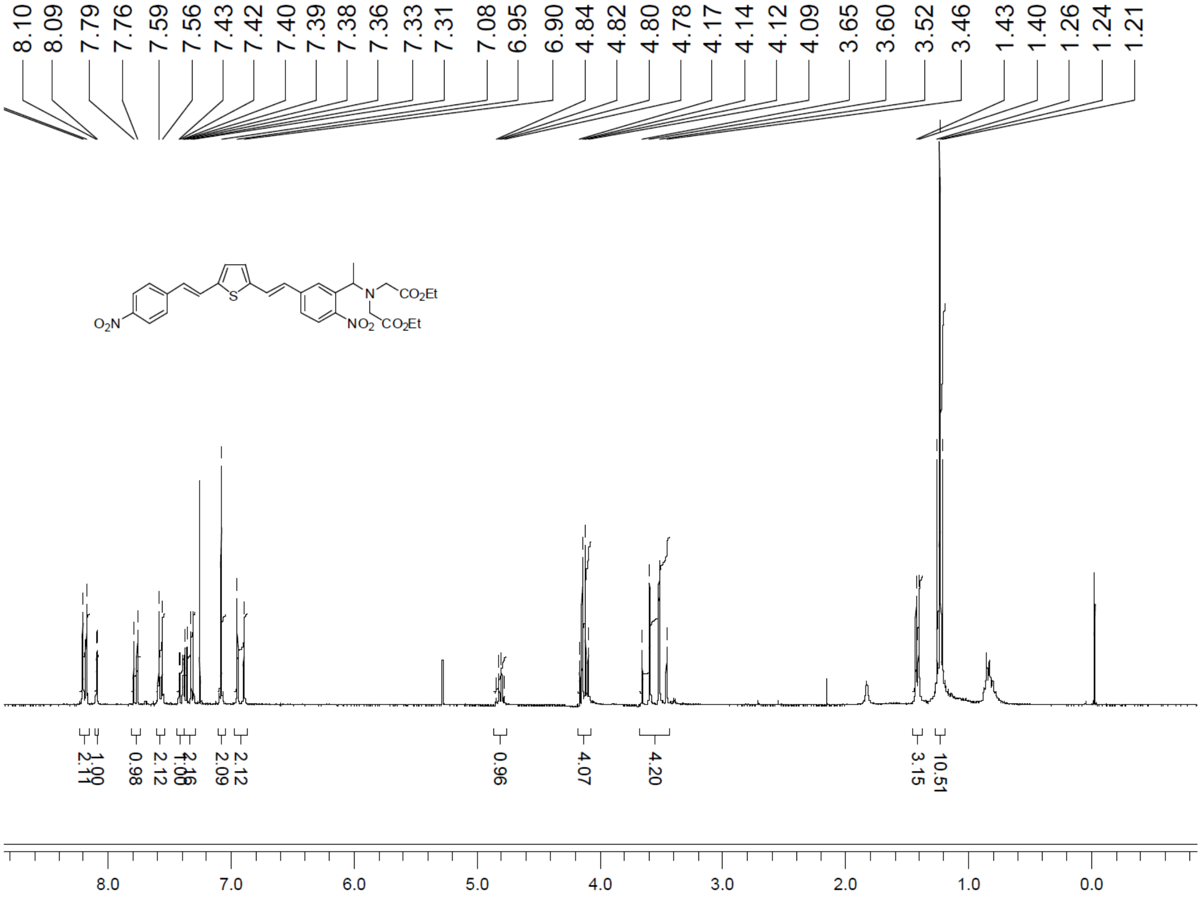

+TOF MS: 4.369 min from HK-321-1.wiff Agilent
Max. 7.9e5 counts.
212.9854
Intensity, counts
m/z, amu
+TOF MS: 4.369 min from HK-321-1.wiff Agilent
Max. 7.9e5 counts.
210.9875
212.9854
211.9899
213.9881
244.9926
246.9908
Br
NH2
NO2
Intensity, counts
m/z, amu

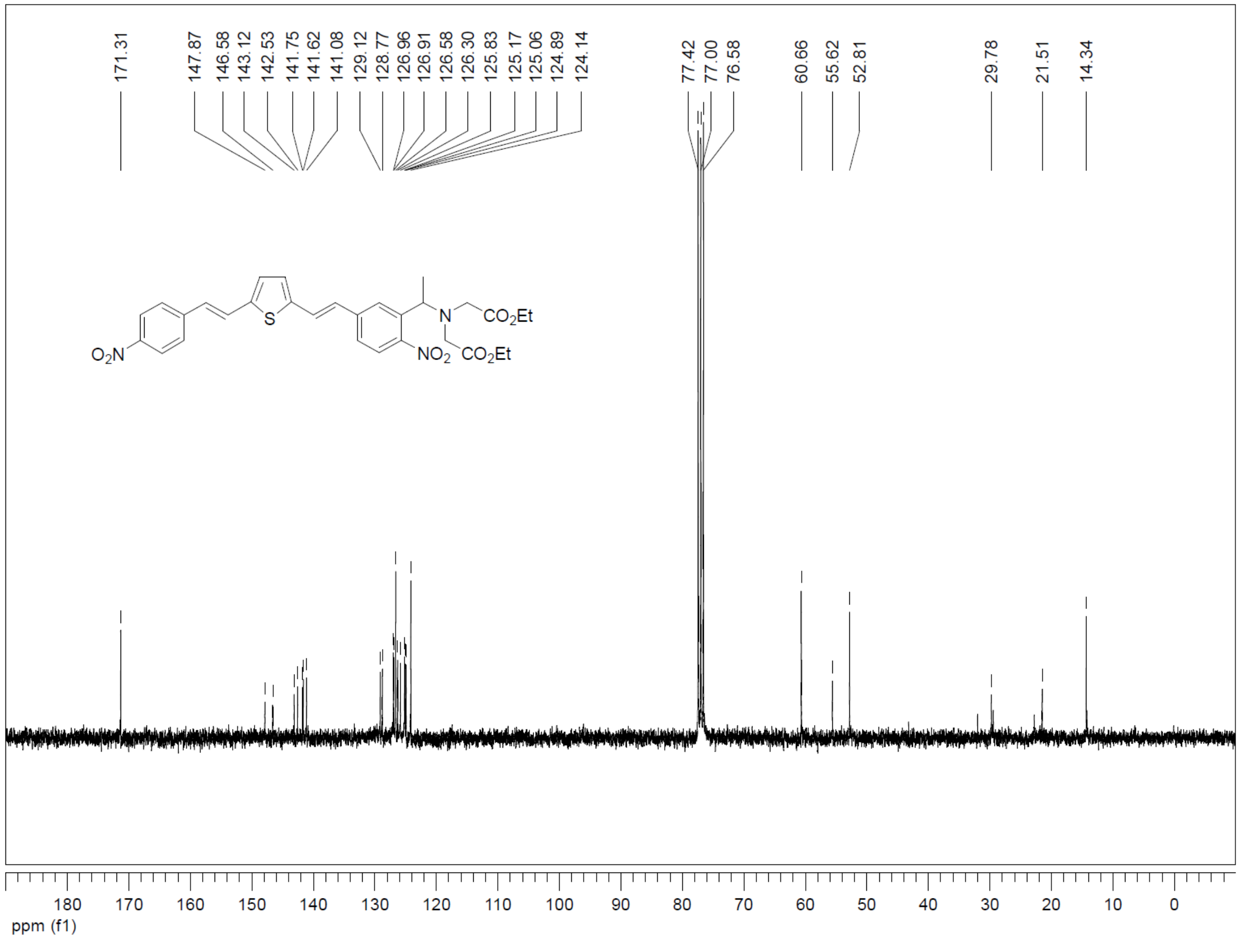

8.16
8.15
7.63
7.61
7.50
7.49
7.47
7.47
7.26
4.77
4.75
4.73
4.70
4.17
4.15
4.12
4.10
3.62
3.56
3.47
3.41
1.39
1.37
1.27
1.25
1.22
COOEt
N
COOEt
Br
NO2
1.00
0.99
0.98
1.04
4.25
4.49
3.23
7.32
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

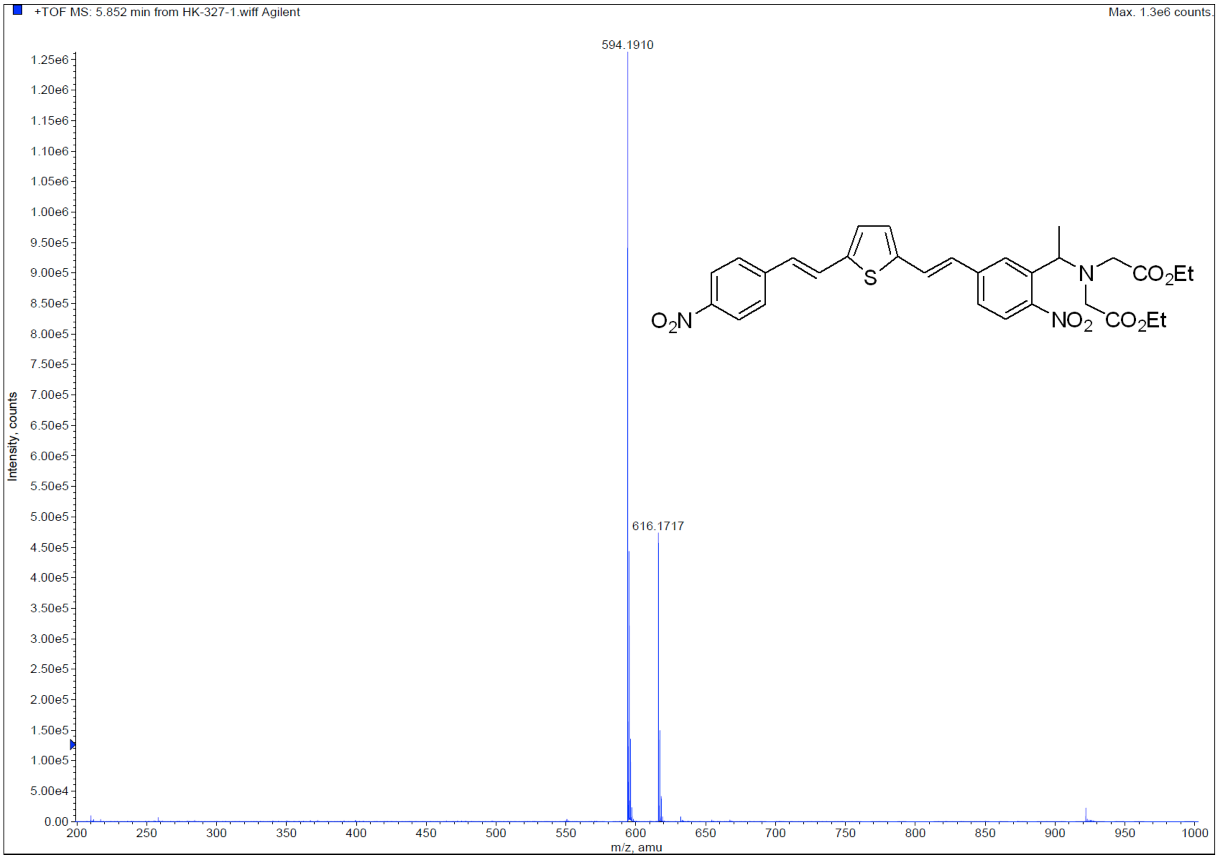

170.92
148.05
142.14
132.29
130.91
127.69
125.32
77.42
77.00
76.58
60.60
55.49
52.65
21.15
14.21
Br
N
CO_2Et
NO_2
CO_2Et
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)

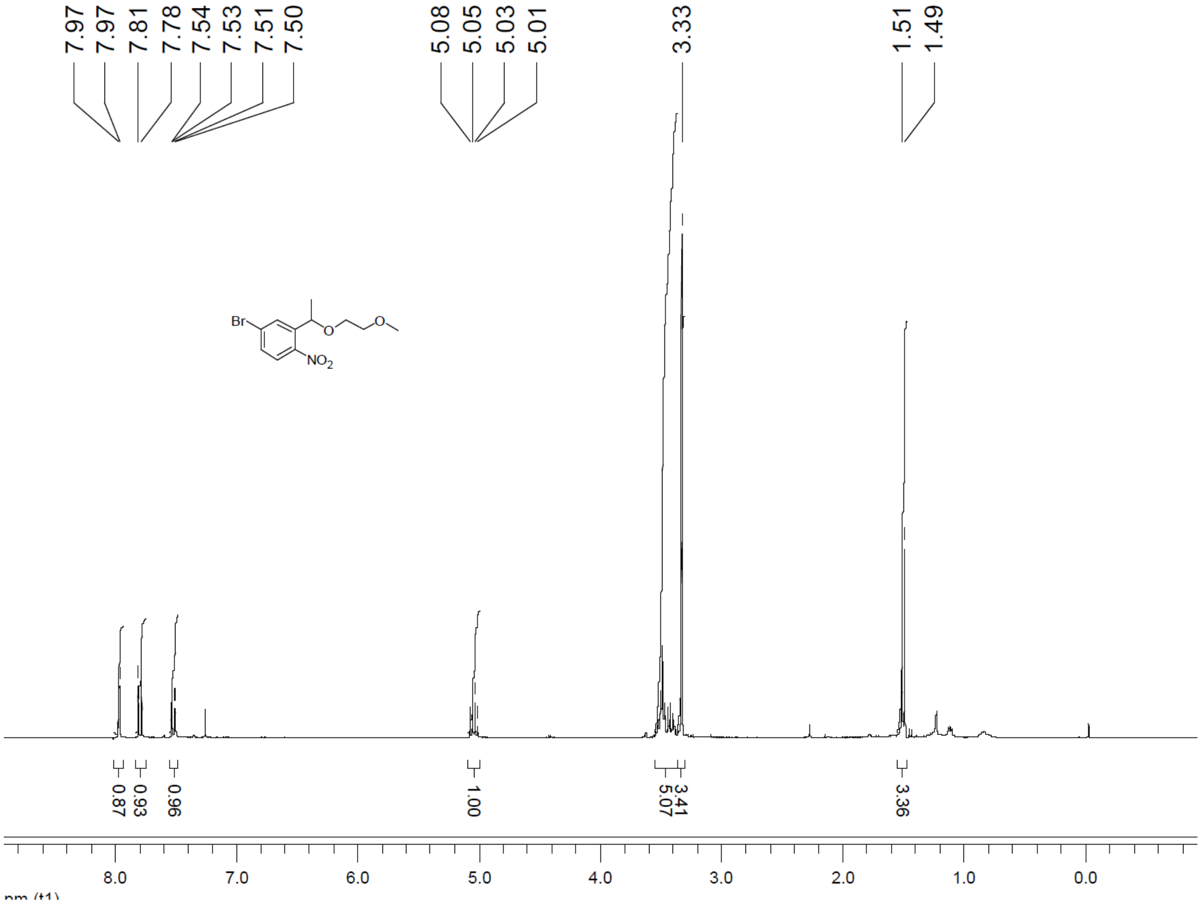

+TOF MS: 5.407 min from SK-325-1.wiff Agilent
Max. 1.5e6 counts.
417.0660
420.0665
Intensity, counts
1.5e6
1.4e6
1.3e6
1.2e6
1.1e6
1.0e6
9.0e5
8.0e5
7.0e5
6.0e5
5.0e5
4.0e5
3.0e5
2.0e5
1.0e5
0.0
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
m/z, amu

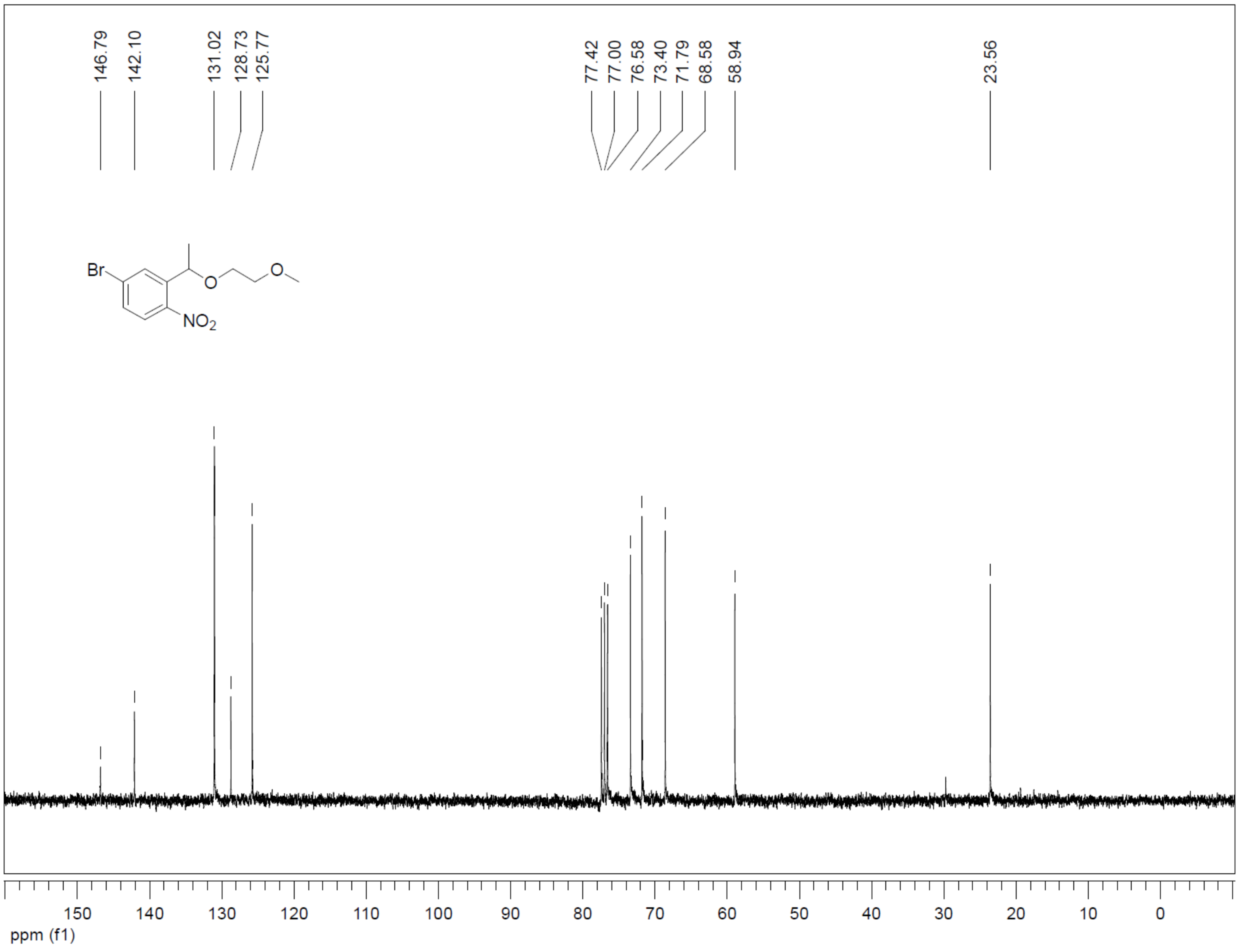

+TOF MS: 5.407 min from SK-325-1.wiff Agilent
Max. 1.5e6 counts.
417.0660
418.0680
420.0665
Br
N
CO2Et
NO2
CO2Et
Intensity, counts
1.5e6
1.4e6
1.3e6
1.2e6
1.1e6
1.0e6
9.0e5
8.0e5
7.0e5
6.0e5
5.0e5
4.0e5
3.0e5
2.0e5
1.0e5
0.0
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
m/z, amu

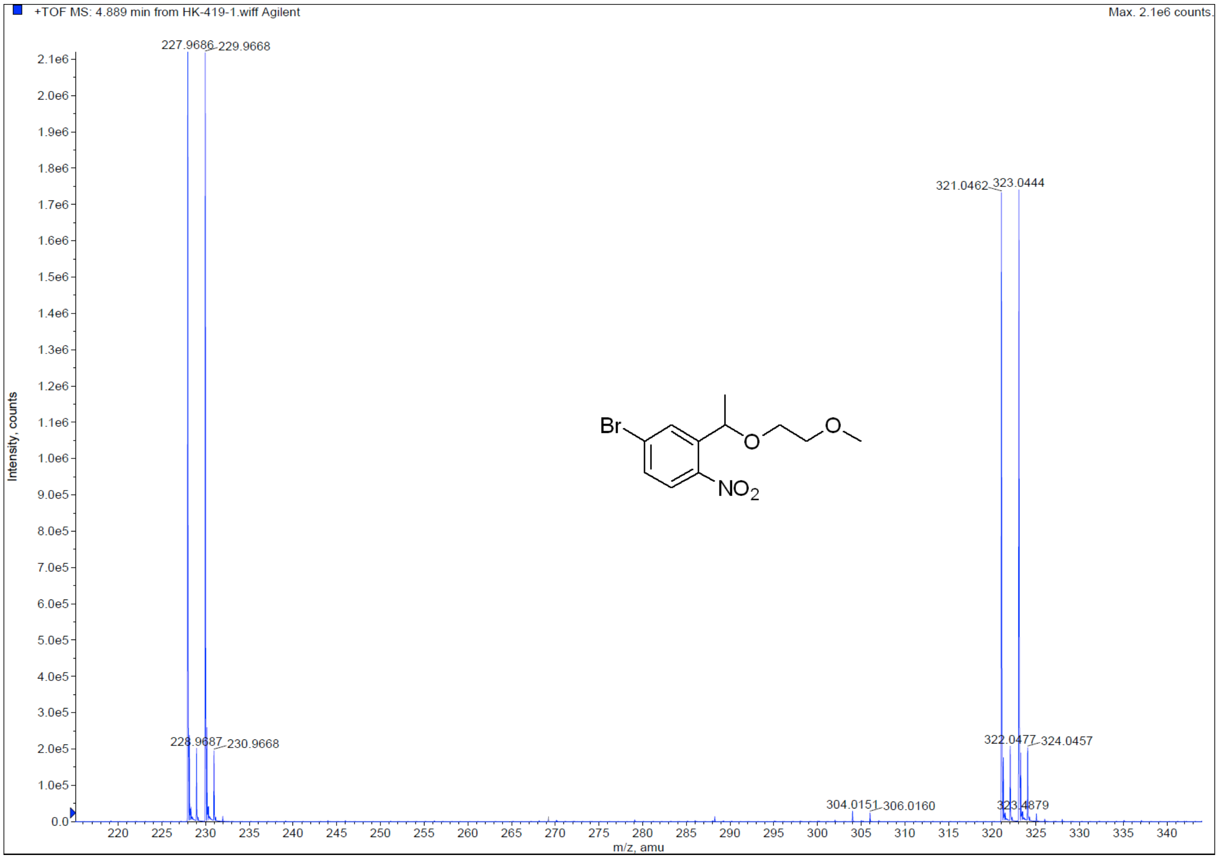

8.10
8.09
7.79
7.76
7.59
7.56
7.43
7.42
7.40
7.39
7.38
7.36
7.33
7.31
7.08
6.95
6.90
4.84
4.82
4.80
4.78
4.17
4.14
4.12
4.09
3.65
3.60
3.52
3.46
1.43
1.40
1.26
1.24
1.21
S
N
CO2Et
O2N
NO2
CO2Et
2.11
1.00
0.98
2.12
1.08
2.16
2.09
2.12
0.96
4.07
4.20
3.15
10.51
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

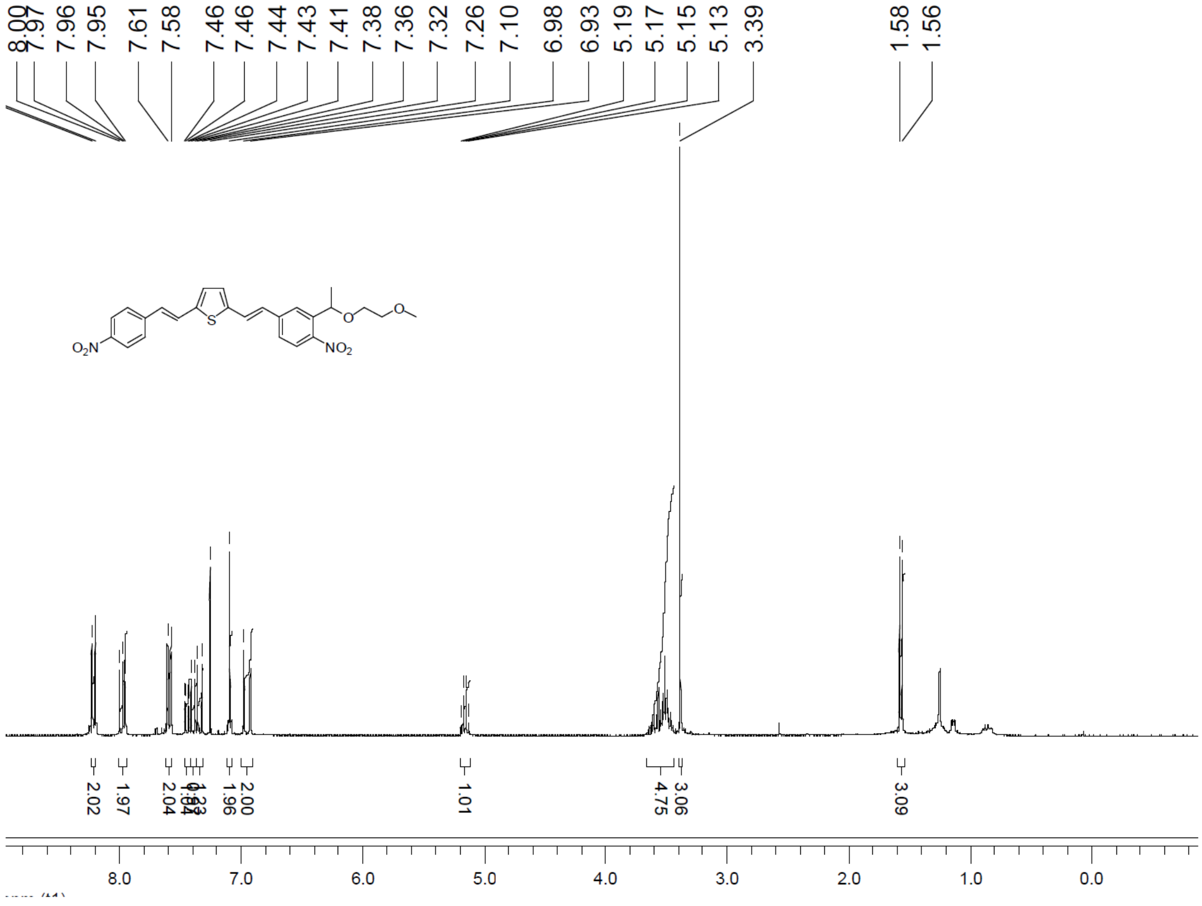

171.31
147.87
146.58
143.12
142.53
141.75
141.62
141.08
129.12
128.77
126.96
126.91
126.58
126.30
125.83
125.17
125.06
124.89
124.14
77.42
77.00
76.58
60.66
55.62
52.81
29.78
21.51
14.34
O2N
S
N
CO2Et
NO2
CO2Et
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)

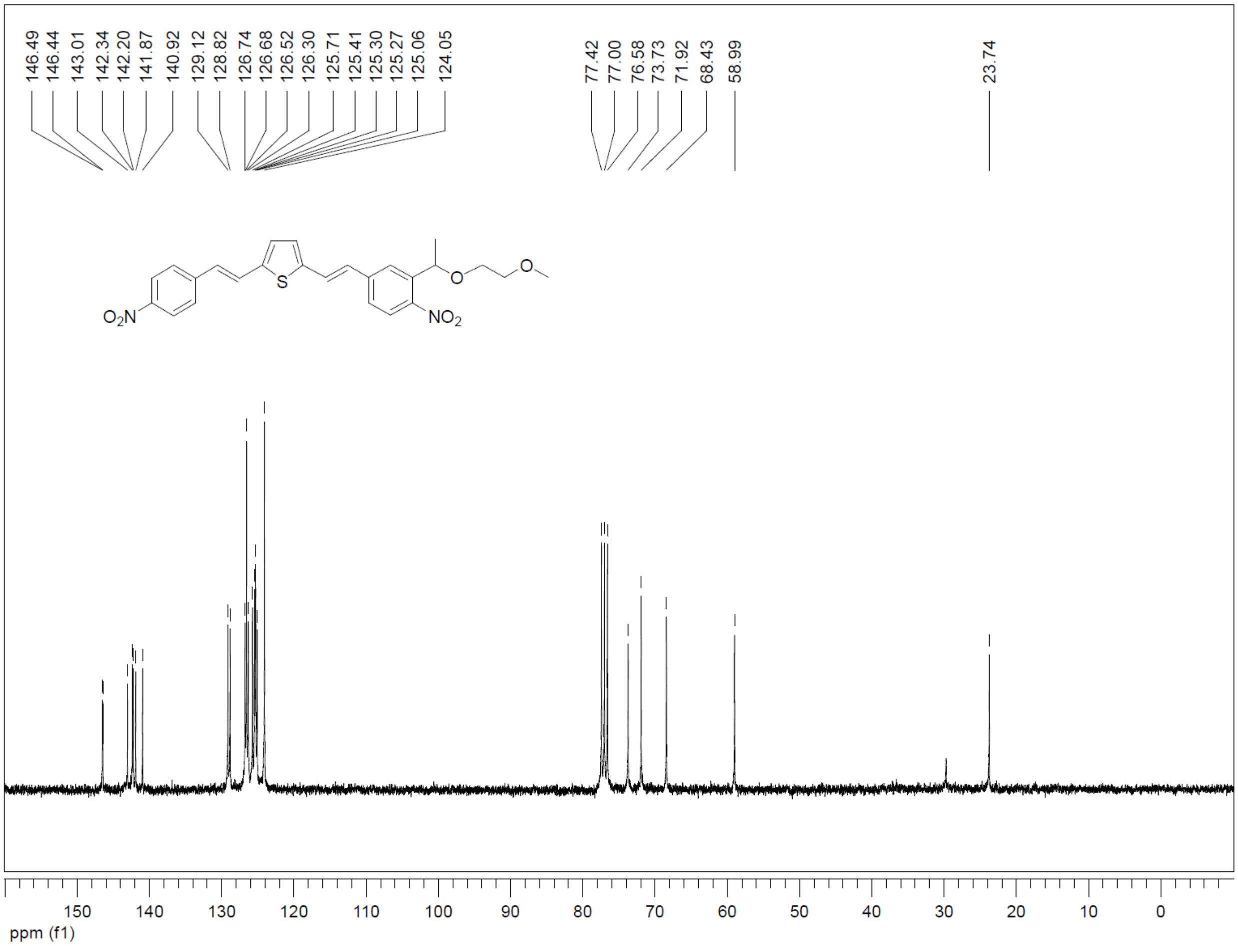

+TOF MS: 5.852 min from HK-327-1.wiff Agilent
Max. 1.3e6 counts.
594.1910
616.1717
Intensity, counts
m/z, amu
1.25e6
1.20e6
1.15e6
1.10e6
1.05e6
1.00e6
9.50e5
9.00e5
8.50e5
8.00e5
7.50e5
7.00e5
6.50e5
6.00e5
5.50e5
5.00e5
4.50e5
4.00e5
3.50e5
3.00e5
2.50e5
2.00e5
1.50e5
1.00e5
5.00e4
0.00
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
O2N
S
N
CO2Et
CO2Et
NO2

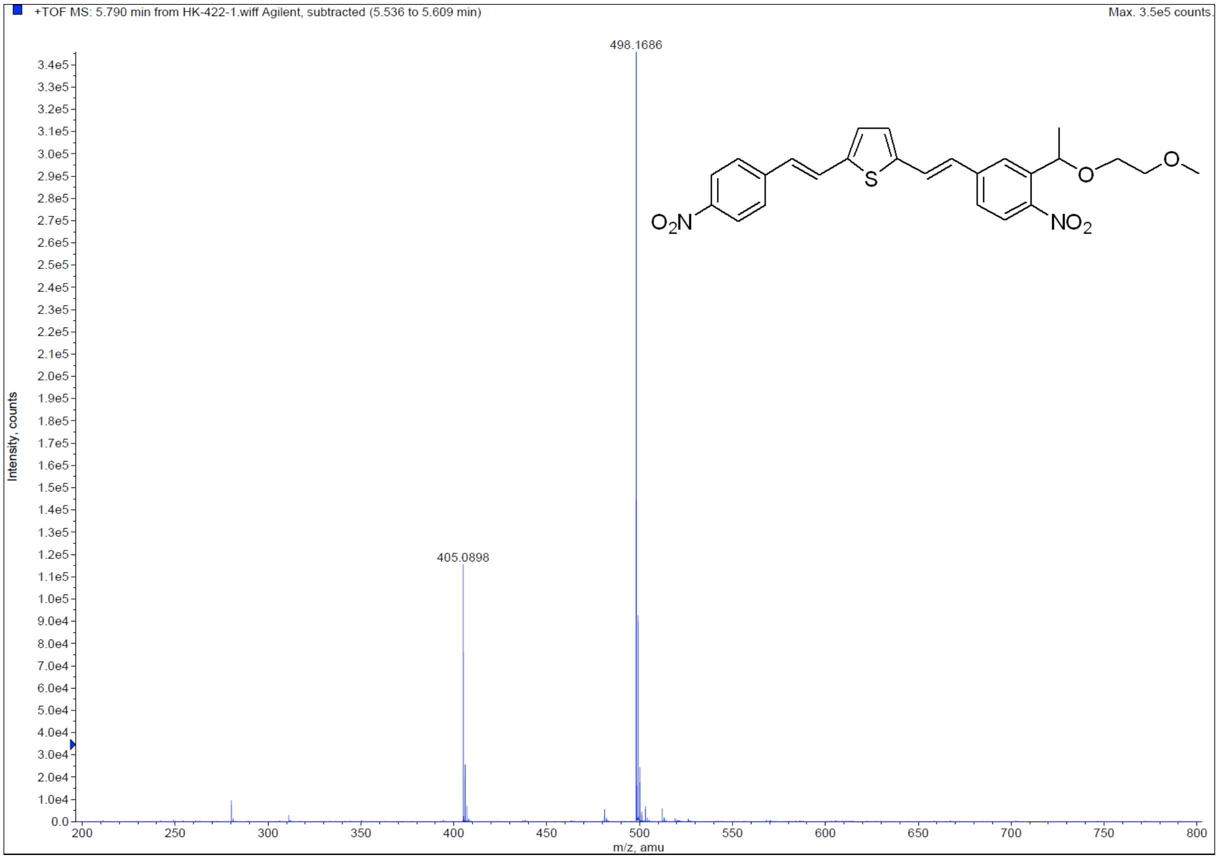

7.97
7.97
7.81
7.78
7.54
7.53
7.51
7.50
5.08
5.05
5.03
5.01
3.33
1.51
1.49
Br
O
O
NO2
0.87
0.93
0.96
1.00
5.07
3.41
3.36
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


146.79
142.10
131.02
128.73
125.77
77.42
77.00
76.58
73.40
71.79
68.58
58.94
23.56
Br
O
O
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)


+TOF MS: 4.889 min from HK-419-1.wiff Agilent
Max. 2.1e6 counts.
227.9686
229.9668
228.9687
230.9668
321.0462
323.0444
322.0477
324.0457
323.4879
304.0151
306.0160
Intensity, counts
m/z, amu
2.1e6
2.0e6
1.9e6
1.8e6
1.7e6
1.6e6
1.5e6
1.4e6
1.3e6
1.2e6
1.1e6
1.0e6
9.0e5
8.0e5
7.0e5
6.0e5
5.0e5
4.0e5
3.0e5
2.0e5
1.0e5
0.0
220
225
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
330
335
340
Br
O
O
NO2


8.00
7.97
7.96
7.95
7.61
7.58
7.46
7.46
7.44
7.43
7.41
7.38
7.36
7.32
7.26
7.10
6.98
6.93
5.19
5.17
5.15
5.13
3.39
1.58
1.56
O_2N
S
O
O
NO_2
2.02
1.97
2.04
1.96
2.00
1.01
4.75
3.06
3.09
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


146.49
146.44
143.01
142.34
142.20
141.87
140.92
129.12
128.82
126.74
126.68
126.52
126.30
125.71
125.41
125.30
125.27
125.06
124.05
77.42
77.00
76.58
73.73
71.92
68.43
58.99
23.74
O2N
S
O
O
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (f1)


+TOF MS: 5.790 min from HK-422-1.wiff Agilent, subtracted (5.536 to 5.609 min)
Max. 3.5e5 counts.
498.1686
405.0898
Intensity, counts
m/z, amu
0.0
1.0e4
2.0e4
3.0e4
4.0e4
5.0e4
6.0e4
7.0e4
8.0e4
9.0e4
1.0e5
1.1e5
1.2e5
1.3e5
1.4e5
1.5e5
1.6e5
1.7e5
1.8e5
1.9e5
2.0e5
2.1e5
2.2e5
2.3e5
2.4e5
2.5e5
2.6e5
2.7e5
2.8e5
2.9e5
3.0e5
3.1e5
3.2e5
3.3e5
3.4e5
200
250
300
350
400
450
500
550
600
650
700
750
800
S
O
O
O_2N
NO_2