Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Highly Effective Copper-Catalyzed Decarboxylative Coupling of Aryl Halides with Alkynyl Carboxylic Acids

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Experimental Section

General

All reactions were carried out under an argon atmosphere condition. Solvents were dried and degassed by standard methods and all propiolic acids and aryl halides were purchased from Aldrich and Alfa. Flash column chromatography was performed using silica gel (300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 200-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). NMR spectra were measured in $CDCl_3$ on a Varian Inova-400 NMR spectrometer (400 MHz or 300 MHz) with TMS as an internal reference. Products were characterized by comparison of ^{1}H NMR, ^{13}C NMR and TOF-MS data in the literatures.

General procedure for copper-catalyzed decarboxylative coupling of various aryl halides and alkynoic acids in the presence of A: Aryl halide (0.5 mmol), alkynoic acid (0.6 mmol), CuI (2 mol%), **A** (4 mol%) and K_2CO_3 (1.0 mmol) were added to a screw-capped test tube. The tube was then evacuated and backfilled with argon (3 cycles). DMSO (2 mL) was added by syringe at room temperature. The tube was again evacuated and backfilled with argon (3 cycles). The mixture was heated to 90 ^{o}C and stirred for 24 h. After cooling to room temperature, the mixture was diluted with water, and the combined aqueous phases were extracted three times with ethyl acetate. The organic layers were combined, dried over Na_2SO_4, and concentrated to yield the crude product, which was further purified by silica gel chromatography, using petroleum ether and ethyl acetate as eluent to provide the desired product.

Copy of Certificate of Analysis of CuI from Aldrich:

Certificate of Analysis

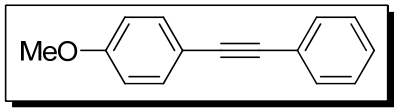
SIGMA-ALDRICH

Product Name	Copper(I) iodide, 99.999% trace metals basis
Product Number	215554
Product Brand	ALDRICH
CAS Number	7681-65-4
Molecular Formula	CuI
Molecular Weight	190.45

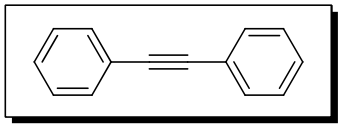
TEST	SPECIFICATION	LOT MKBB2521 RESULTS
Appearance (Color): Grey to Tan	Conforms to Requirements	Beige
Appearance (Form): Powder/Chunks	Conforms to Requirements	Powder
Complexometric EDTA: % Cu	31.0 - 34.0 %	33.7 %
ICP: Confirms Copper Component	Confirmed	Conforms
Trace Metal Analysis	≤20.0 ppm	3.7 ppm
Cesium (Cs)	ppm	0.4 ppm
Calcium (Ca)	ppm	2.1 ppm
Silver (Ag)	ppm	0.2 ppm
Zinc (Zn)	ppm	0.4 ppm
Lead (Pb)	ppm	0.3 ppm
Cobalt (Co)	ppm	0.2 ppm
Europium (Eu)	ppm	0.1 ppm
Purity	Meets Requirements 99.999% Based On Trace Metals Analysis	Meets Requirements
Specification Date:		MAR 2009
Date of QC Release:		SEP 2009
Print Date:		SEP 02 2009

Barbara Rajzer, Supervisor
Quality Control
Milwaukee, Wisconsin USA

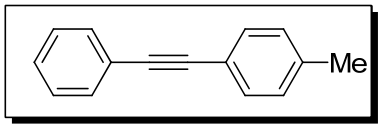
Characterization of the corresponding products:



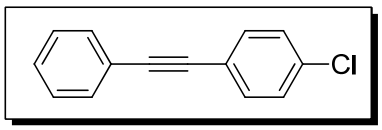
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50–7.52 (m, 2H), 7.47 (d, J = 8.8 Hz, 2H), 7.32–7.36 (m, 3H), 6.88 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.2 (C), 134.7 (CH), 133.1 (CH), 130.0 (CH), 129.6 (C), 125.2 (CH), 117.0 (C), 115.6 (CH), 91.0 (C), 89.7 (C), 56.9 (CH); HRMS (ESI$^+$): calcd. for $[C_{15}H_{12}O]^+$ requires m/z 208.0888, found 208.0896.



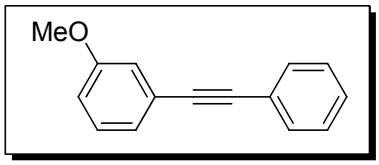
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48–7.59 (m, 4H), 7.29–7.39 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 133.3 (CH), 130.0 (CH), 129.9 (CH), 124.9 (C), 91.0 (C); HRMS (ESI$^+$): calcd. for $[C_{14}H_{10}]^+$ requires m/z 178.0783, found 178.0791.



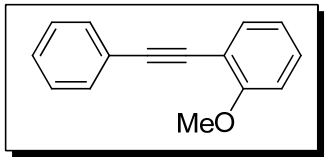
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52–7.54 (m, 2H), 7.43 (d, J = 8.0 Hz, 2H), 7.33–7.37 (m, 3H), 7.16 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.0 (C), 133.2 (CH), 133.1 (CH), 130.8 (CH), 130.0 (CH), 129.7 (CH), 125.1 (C), 121.8 (C), 91.2 (C), 90.4 (C), 23.2 (CH); HRMS (ESI$^+$): calcd. for $[C_{15}H_{12}]^+$ requires m/z 192.0939, found 192.0926.



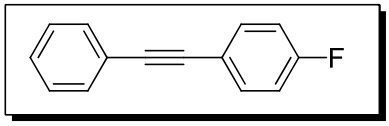
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.53 (t, J = 7.6 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.34–7.36 (m, 4H), 7.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.9 (C), 134.5 (CH), 133.3 (CH), 130.3 (CH), 130.1 (CH), 130.0 (CH), 124.6 (C), 123.4 (C), 91.9 (C), 89.9 (C); HRMS (ESI$^+$): calcd. for $[C_{14}H_9Cl]^+$ requires m/z 212.0393, found 212.0396.



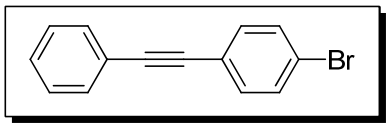
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52–7.55 (m, 2H), 7.34–7.37 (m, 3H), 7.23–7.27 (m, 1H), 7.13 (d, J = 7.6 Hz, 2H), 7.06 (s, 1H), 6.88–6.91(m, 1H), 2.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.0 (C), 133.3 (CH), 131.1 (CH), 130.0 (CH), 130.0 (CH), 125.9 (CH), 125.8 (C), 124.8 (CH), 117.9 (C)，116.6 (CH)，90.9 (C), 90.8 (C), 56.9 (CH); HRMS (ESI+): calcd. for $[C15H12O]^+$ requires m/z 208.0888, found 208.0884.



^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.64–7.67 (m, 2H), 7.59 (d, J = 7.6 Hz, 1H), 7.39–7.42 (m, 4H), 6.97–7.04 (m, 2H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.5 (C), 135.2 (CH), 133.3 (CH), 131.4 (CH), 129.9 (CH), 129.8(CH), 125.2 (CH), 122.1 (C), 114.0 (C), 112.3 (CH)，95.1 (C), 87.4 (C), 57.5 (CH); HRMS (ESI^+): calcd. for $[C_{15}H_{12}O]^+$ requires m/z 208.0888, found 208.1000.

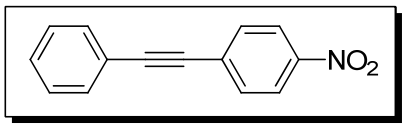


^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50–7.53 (m, 4H), 7.34–7.36 (m, 3H), 7.05 (t, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.4 (d, J = 249.5 Hz, C), 135.2 (d, J = 8.3 Hz, CH), 133.2 (CH), 130.0 (d, J = 3.7 Hz, CH), 124.7 (C), 121.0 (d, J = 3.4 Hz, CH), 117.4 (C), 117.2 (C), 90.7 (C), 89.2 (C); HRMS (ESI^+): calcd. for $[C_{14}H_9F]^+$ requires m/z 196.0688, found 196.0690.

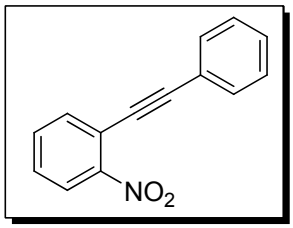


^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.47–7.52 (m, 4H), 7.35–7.40 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.7 (C), 134.6 (CH), 133.2 (CH), 130.1 (CH), 130.0 (CH), 124.5 (CH), 124.1 (C),

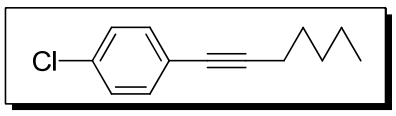
123.8 (C), 92.1 (C), 89.9 (C); HRMS (ESI$^+$): calcd. for $[C_{14}H_9Br]^+$ requires m/z 255.9888, found 255.9886.



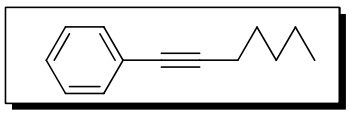
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.24 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.57–7.60 (m, 2H), 7.41–7.42 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.6(C), 133.9(CH), 133.5(CH), 131.9(CH), 130.9 (CH), 130.2(CH), 125.3 (C), 123.7(C), 96.3(C), 89.2(C); HRMS (ESI$^+$): calcd. for $[C_{14}H_9NO_2]^+$ requires m/z 223.0633, found 223.0635.



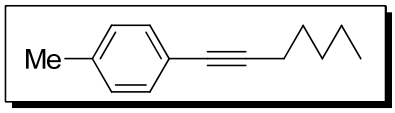
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.08 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 7.6 Hz, 1H), 7.59–7.61 (m, 3H), 7.46 (t, J = 8.0 Hz, 1H), 7.38–7.39 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.68(C), 136.22(C), 134.54(C), 133.65(CH), 130.89(CH), 130.21(CH), 130.10(CH), 126.39 (CH), 123.96(CH), 120.34(CH), 123.7(CH), 98.73(C), 86.43(C); HRMS (ESI$^+$): calcd. for $[C_{14}H_9NO_2]^+$ requires m/z 223.0633, found 223.0637.



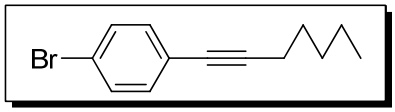
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.31 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 2.38 (t, J = 7.2 Hz, 2H), 1.56–1.63 (m, 2H), 1.34–1.44 (m, 4H), 0.92 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 134.4 (CH), 131.5 (CH), 130.1 (CH), 121.7 (CH), 93.2 (C), 81.1 (C), 32.8 (CH_2), 30.0 (CH_2), 23.9 (CH_2), 21.0 (CH_2), 15.6 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{13}H_{15}Cl]^+$ requires m/z 206.0862, found 206.0864.



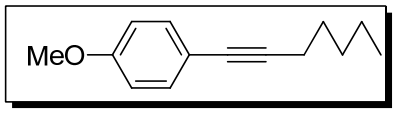
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41–7.43 (m, 2H), 7.29–7.30 (m, 3H), 2.43 (t, J = 7.2 Hz, 2H), 1.60–1.67 (m, 2H), 1.37–1.48 (m, 4H), 0.95 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 133.17 (CH), 129.83 (CH), 129.11 (CH), 125.68 (CH), 92.13 (C), 82.15 (C), 32.79 (CH_2), 30.13 (CH_2), 23.94 (CH_2), 21.04 (CH_2), 15.72 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{13}H_{16}]^+$ requires m/z 172.1252, found 172.1250.



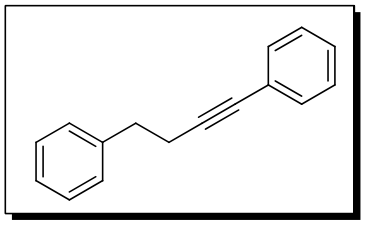
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 2.38 (t, J = 7.2 Hz, 2H), 2.32 (s, 3H), 1.56–1.63 (m, 2H), 1.32–1.46 (m, 4H), 0.92 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.63 (C), 131.64 (C), 129.17 (CH), 121.23 (CH), 89.89 (C), 80.78 (C), 31.40 (CH_2), 28.80 (CH_2), 22.52 (CH_2), 21.65 (CH_2), 19.66 (CH_3), 14.29 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{14}H_{18}]^+$ requires m/z 186.1409, found 186.1409.



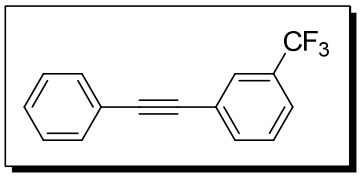
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 7.6 Hz, 2H), 2.39 (t, J = 7.2 Hz, 2H), 1.58–1.65 (m, 2H), 1.33–1.47 (m, 4H), 0.94 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 133.25 (C), 131.62 (CH), 123.30 (CH), 121.75 (C), 92.03 (C), 79.79 (C), 31.37 (CH_2), 28.58 (CH_2), 22.49 (CH_2), 19.66 (CH_2), 14.27 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{13}H_{15}Br]^+$ requires m/z 250.0357, found 250.0357.



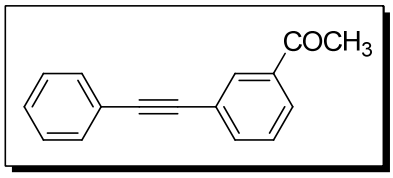
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33–7.35 (m, 2H), 6.81–6.83 (m, 2H), 3.80 (s, 3H), 2.39 (t, J = 7.2 Hz, 2H), 1.57–1.64 (m, 2H), 1.43–1.46 (m, 2H), 1.34–1.40 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.7 (CH), 134.4 (CH), 117.9 (CH), 115.4 (CH), 90.4 (C), 81.8 (C), 56.8 (CH_3), 32.8 (CH_2), 30.2 (CH_2), 23.9 (CH_2), 21.0 (CH_2), 15.7 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{14}H_{18}O]^+$ requires m/z 202.1358, found 202.1360.



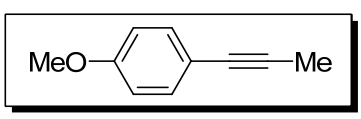
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58 (d, J = 7.2 Hz, 2H), 7.44 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.2 Hz, 2H), 7.31(d, J = 7.2 Hz, 2H), 7.25–7.26 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.63 (C),138.82 (C), 134.64 (CH), 132.31 (CH), 130.56 (CH), 130.21 (CH), 128.39 (CH), 121.18 (CH), 88.05 (C), 82.21 (C), 68.06 (CH_2), 36.54 (CH_2); HRMS (ESI$^+$): calcd. for $[C_{16}H_{14}]^+$ requires m/z 206.1096, found 206.1095.



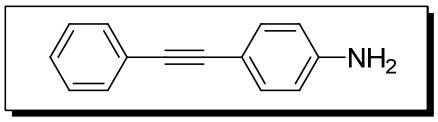
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.80 (s, 1H), 7.70 (d, J = 7.6 Hz, 2H), 7.54–7.59 (m, 3H), 7.48 (t, J = 8.0 Hz, 1H), 7.35 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 136.2 (C), 134.1 (CH), 133.3 (CH), 130.4 (q, J = 186 Hz)， 130.1 (C), 130.0(C), 129.9 (CH), 126.7 (CH), 126.4 (q, J = 44 Hz), 125.9 (CH), 124.2 (CH), 92.5 (C), 89.4 (C); HRMS (ESI$^+$): calcd. for $[C_{15}H_9F]^+$ requires m/z 246.0656, found 246.0653.



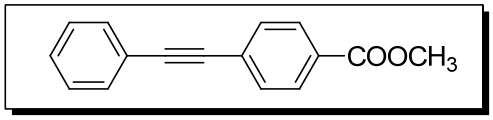
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.17 (s, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.61–7.63 (m, 2H), 7.51–7.53 (m, 1H), 7.41–7.43 (m, 3H), 2.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.0 (C),138.8 (C), 137.4 (CH), 133.3 (CH), 133.2 (CH), 130.4 (CH), 130.3 (CH), 130.1 (CH)，129.5 (C)，125.5 (C), 124.4 (CH)，92.0 (C), 90.0 (C), 28.3 (CH); HRMS (ESI$^+$): calcd. for $[C_{16}H_{12}O]^+$ requires m/z 220.0888, found 220.0887.



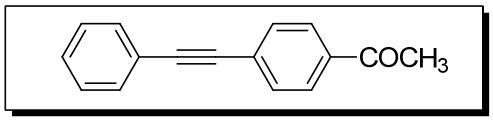
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39 (d, J = 7.6 Hz, 2H), 6.88 (d, J = 7.6 Hz, 2H), 3.86 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.2 (C), 133.0 (C), 116.4 (CH), 114.0 (CH)，84.4 (C), 79.7 (C), 55.5 (CH_3), 31.2 (CH_3); HRMS (ESI^+): calcd. for $[C_{10}H_{10}O]^+$ requires m/z 146.0732, found 146.0734.



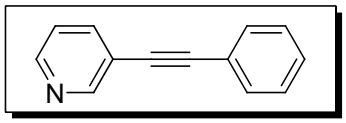
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.54 (d, J = 6.4 Hz, 2H, ArH), 7.38–7.32 (m, 5H, ArH), 7.64 (d, J = 6.4 Hz, 2H, ArH), 3.77 (s, 2H, NH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 139.5 (C), 134.6 (CH), 133.0 (CH), 130.0 (CH), 129.4 (CH), 119.0 (CH), 116.4 (C), 114.1 (C), 91.9 (C), 89.0 (C); HRMS (ESI^+): calcd. for $[C_{14}H_{11}N]^+$ requires m/z 193.0891, found 193.0892.



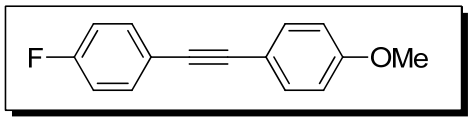
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.03 (d, J = 8.0 Hz, 2H, ArH), 7.59 (d, J = 8.0 Hz, 2H, ArH), 7.57–7.54 (m, 2H, ArH), 7.38–7.36 (m, 3H, ArH), 3.92 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.2 (C), 133.4 (CH), 133.1 (CH), 131.1 (CH), 130.4 (CH), 130.1 (CH), 129.9 (CH), 129.6 (C), 124.3 (C), 94.0 (C), 90.3 (C), 53.9 (CH_3); HRMS (ESI^+): calcd. for $[C_{16}H_{12}O_2]^+$ requires m/z 236.0837, found 236.0837.



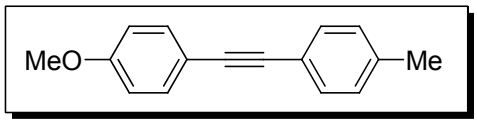
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.95 (d, J = 8.0 Hz, 2H, ArH), 7.62 (d, J = 8.0 Hz, 2H, ArH), 7.57–7.56 (m, 2H, ArH), 7.38 (s, 3H, ArH), 2.62 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.0 (C), 137.7 (C), 133.4 (CH), 133.3 (CH), 130.5 (CH), 130.1 (CH), 129.9 (CH), 129.8 (C), 124.2 (C), 94.3 (C), 90.2 (C), 28.3 (CH_3); HRMS (ESI^+): calcd. for $[C_{16}H_{12}O]^+$ requires m/z 220.0888, found 220.0887.



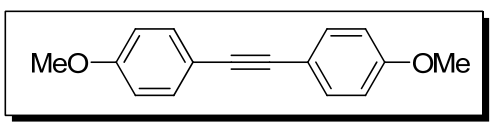
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.78 (s, 1H), 8.55 (d, J = 4.0 Hz, 1H, ArH), 7.83–7.80 (m, 1H, ArH), 7.57–7.55 (m, 2H, ArH), 7.38–7.37 (m, 3H, ArH), 7.30–7.28 (m, 1H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.4 (CH), 148.7 (C), 138.7 (CH), 132.0 (CH), 129.0 (CH), 128.7 (CH), 123.3 (CH), 122.7 (CH), 120.7 (C), 92.9 (C), 86.1 (C); HRMS (ESI$^+$): calcd. for $[C_{13}H_9N]^+$ requires m/z 179.0735, found 179.0735.



^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.89 (d, J = 8.8 Hz, 2H, ArH), 7.02–7.06 (m, 2H, ArH), 7.46–7.51 (m, 4H, ArH), 3.84 (s, OCH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 164.2 (d, J = 247.5 Hz, C), 159.9 (CH), 133.5 (d, J = 7.5 Hz, CH), 133.2 (CH), 119.9 (C), 115.9 (d, J = 22.5 Hz, CH), 115.4 (C), 114.2 (C), 89.2 (C), 87.2 (C), 55.5 (OCH_3); HRMS (ESI$^+$): calcd. for $[C_{15}H_{11}FO]^+$ requires m/z 226.0794, found 226.0794.

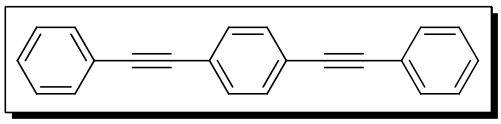


1H NMR (300 MHz, $CDCl_3$) δ: 7.47–7.39 (m, 4H, ArH), 7.14 (d, J = 6.0 Hz, 2H, ArH), 6.87 (d, J = 6.0 Hz, 2H, ArH), 3.83 (s, 3H, OCH_3), 2.36 (s, 3H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 159.7 (C), 138.2 (C), 133.2 (CH), 131.2 (CH), 129.5 (CH), 120.7 (CH), 115.8 (C), 114.2 (C), 88.9 (C), 88.4 (C), 55.5 (OCH_3), 21.7(CH_3); HRMS (ESI$^+$): calcd. for $[C_{16}H_{14}O]^+$ requires m/z 222.1045, found 222.1042.

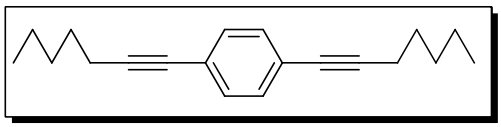


1H NMR (300 MHz, $CDCl_3$) δ: 7.15 (d, J = 9.0 Hz, 4H, ArH), 6.85 (d, J = 9.0 Hz, 4H, ArH), 3.81 (s, 6H, OCH3); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 159.6 (C), 133.1 (C), 115.9 (CH), 114.2 (CH),

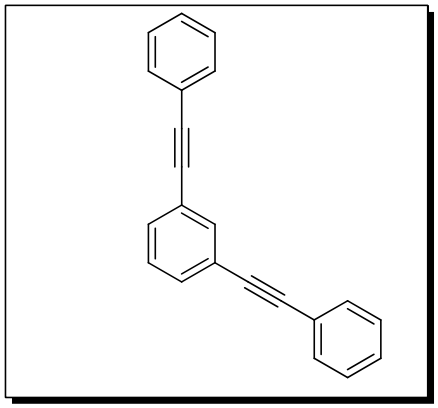
88.2 (C), 55.5 (OCH_3); HRMS (ESI^+): calcd. for $[C_{16}H_{14}O_2]^+$ requires m/z 238.0994, found 238.0990.



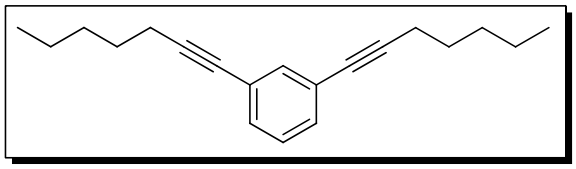
^1H NMR (400 MHz, $CDCl_3$) δ: 7.53–7.56 (m, 8H), 7.38 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 133.3 (C), 133.2 (C), 130.1 (CH), 130.0 (CH), 124.7 (CH), 124.6 (CH), 92.9 (C), 90.7 (C); HRMS (ESI^+): calcd. for $[C_{22}H_{14}]^+$ requires m/z 278.1096, found 278.1091.



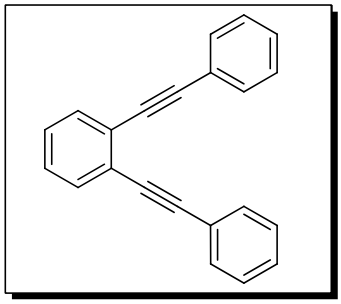
^1H NMR (400 MHz, $CDCl_3$) δ: 7.31 (s, 4H), 2.40 (t, J = 7.2 Hz, 4H), 1.57–1.64 (m, 4H), 1.33–1.47 (m, 8H), 0.93 (t, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 131.6 (C), 123.4 (CH), 92.2 (C), 80.6 (C), 31.4 (CH_2), 28.7 (CH_2), 22.5 (CH_2), 19.7 (CH_2), 14.3 (CH_3); HRMS (ESI^+): calcd. for $[C_{20}H_{26}]^+$ requires m/z 266.2035, found 266.2032.



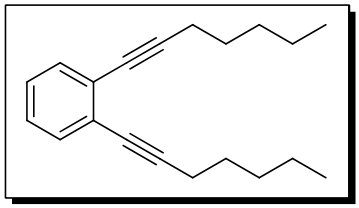
^1H NMR (400 MHz, $CDCl_3$) δ: 7.32–7.39 (m, 7H), 7.49 (d, J = 7.6 Hz, 2H), 7.54 (t, J = 7.6 Hz, 4H), 7.72 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 136.2 (CH), 133.3 (CH), 132.9 (CH), 130.1 (CH), 130.1 (CH), 130.1(CH), 125.2 (C), 124.6 (C), 91.6 (C), 90.2 (C); HRMS (ESI^+): calcd. for $[C_{22}H_{14}]^+$ requires m/z 278.1096, found 278.1096.



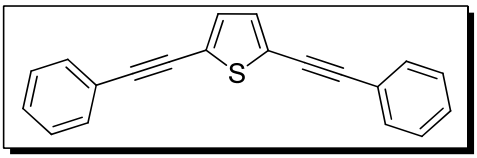
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (s, 1H), 7.28 (d, J = 7.6 Hz, 2H), 7.19 (t, J = 7.6 Hz, 1H), 2.38 (t, J = 7.2 Hz, 4H), 1.58–1.61 (m, 4H), 1.33–1.46 (m, 8H), 0.92 (t, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 134.8 (C), 130.8 (CH), 128.3 (CH), 124.4 (CH), 91.1 (C), 80.2 (C), 31.4 (CH_2), 28.6 (CH_2), 22.5 (CH_2), 19.6 (CH_2), 14.3 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{20}H_{26}]^+$ requires m/z 266.2035, found 266.2037.



^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59–7.63 (m, 6H), 7.37–7.38 (m, 6H), 7.33–7.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 133.4 (C), 133.3 (C), 130.1 (CH), 130.0 (CH), 129.6 (CH), 127.5 (CH), 124.9 (CH), 95.3 (C), 90.0 (C); HRMS (ESI$^+$): calcd. for $[C_{22}H_{14}]^+$ requires m/z 278.1096, found 278.1093.

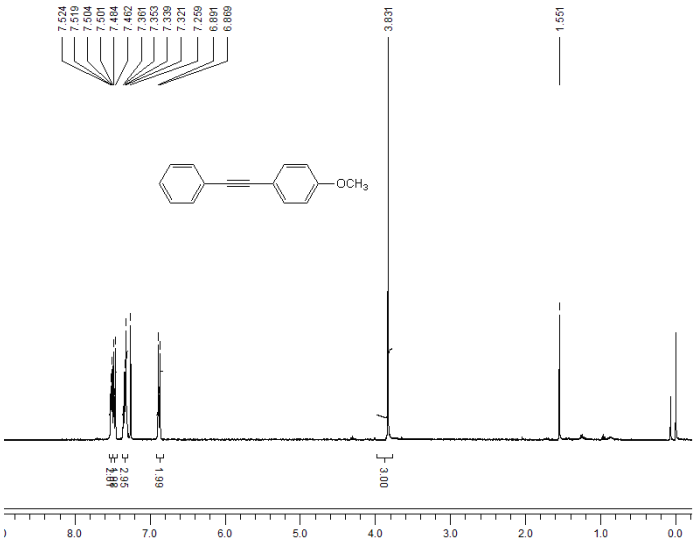


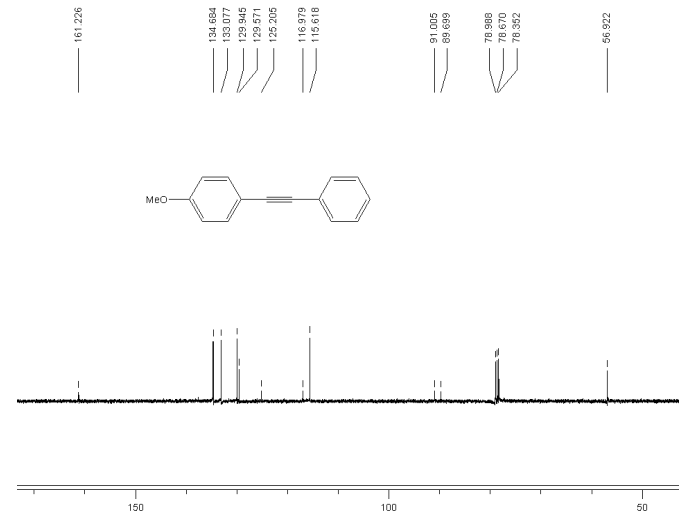
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37–7.40 (m, 2H), 7.17–7.19 (m, 2H), 2.47 (t, J = 7.2 Hz, 4H), 1.61–1.69 (m, 4H), 1.33–1.52 (m, 8H), 0.94 (t, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 133.4 (C), 128.7 (CH), 127.9 (CH), 95.8 (C), 81.2 (C), 32.7 (CH_2), 30.2 (CH_2), 23.9 (CH_2), 21.3 (CH_2), 15.7 (CH_3); HRMS (ESI$^+$): calcd. for $[C_{20}H_{26}]^+$ requires m/z 266.2035, found 266.2036.

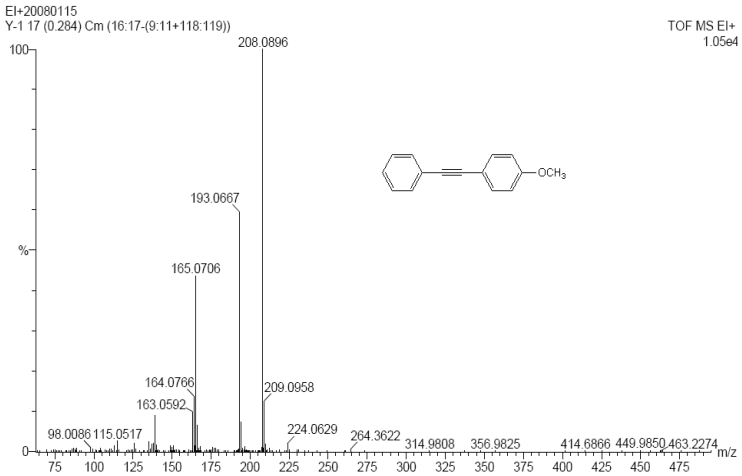


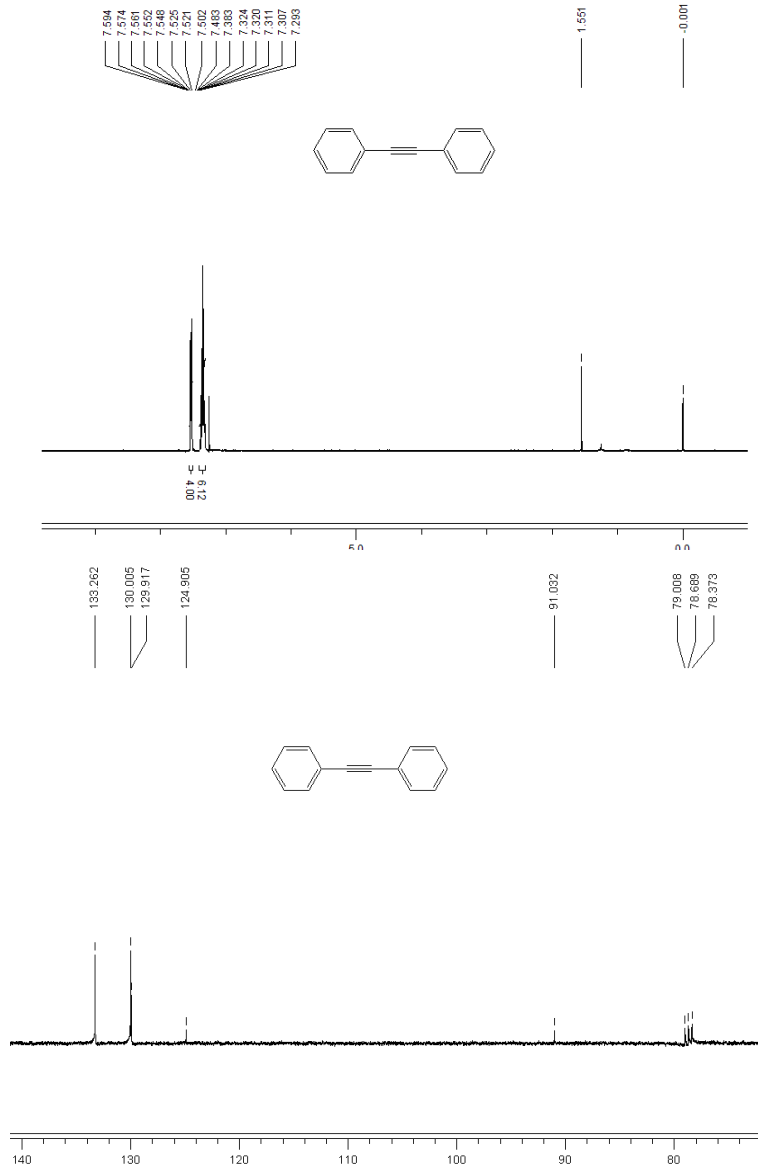
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.51–7.53 (m, 4H), 7.35–7.37 (m, 6H), 7.16 (s, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 133.5 (C), 133.1 (C), 130.3 (CH), 130.1 (CH), 126.24 (CH), 124.2 (CH), 95.7 (C), 83.9 (C); HRMS (ESI^+): calcd. for $[C_{20}H_{12}S]^+$ requires m/z 284.0660, found 284.0660.

Copy of HRMS and NMR Spectra for desired products:





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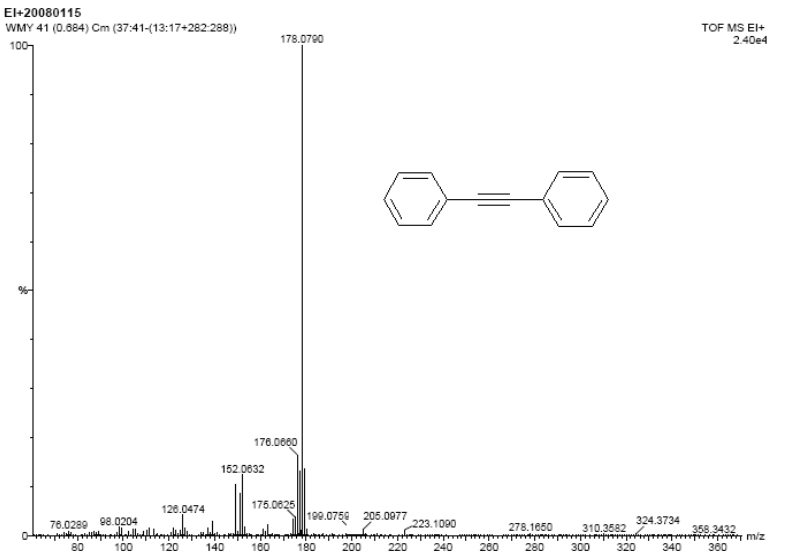
7.561
7.552
7.548
7.525
7.521
7.502
7.483
7.383
7.324
7.320
7.311
7.307
7.293
1.551
0.001
4.00
6.12
133.262
130.005
129.917
124.905
91.032
79.008
78.689
78.373
140
130
120
110
100
90
80


EI+20080115
WMY 41 (0.684) Cm (37:41-(13:17+282:288))
TOF MS EI+
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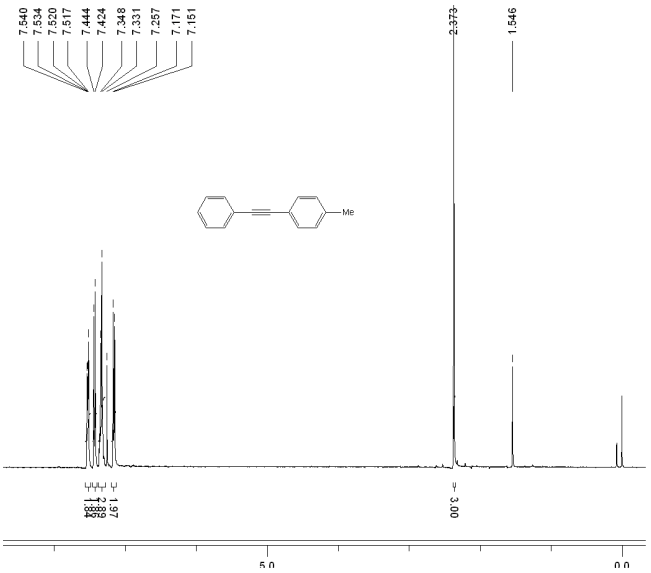
176.0660
152.0632
175.0625
126.0474
76.0289
98.0204
199.0756
205.0977
223.1090
278.1650
310.3582
324.3734
358.3432
m/z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7.520
7.517
7.444
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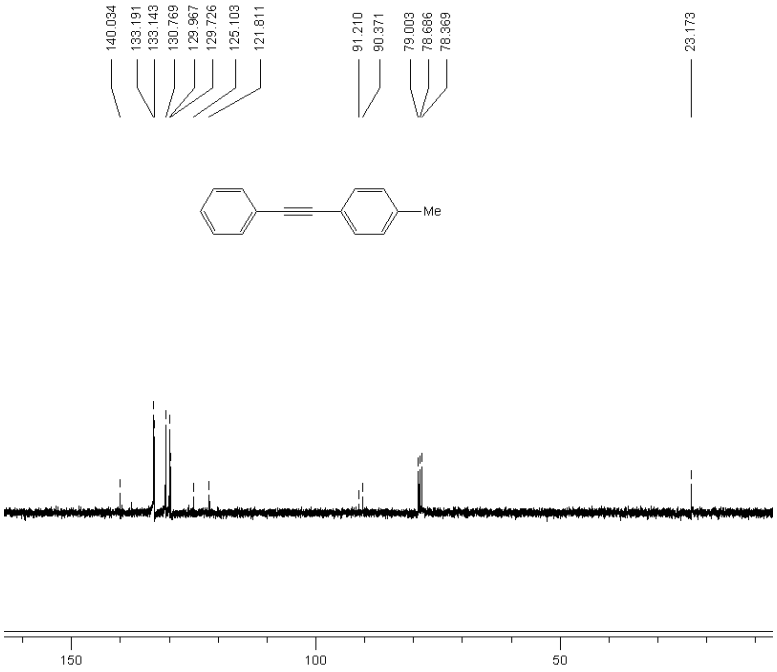
7.257
7.171
7.151
2.373
1.546
Me
1.97
3.00
5.0
0.0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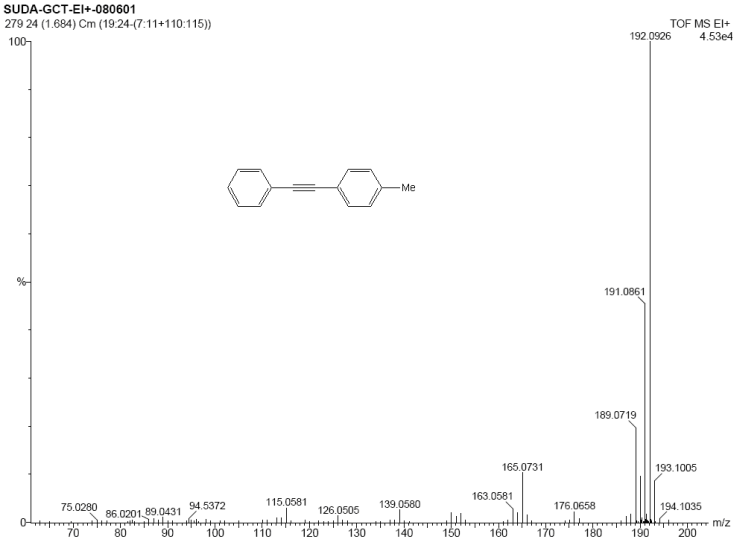
133.191
133.143
130.769
129.967
129.726
125.103
121.811
91.210
90.371
79.003
78.686
78.369
23.173
Me
150
100
50


SUDA-GCT-EI+-080601
279 24 (1.684) Cm (19:24-(7:11+110:115))
TOF MS EI+
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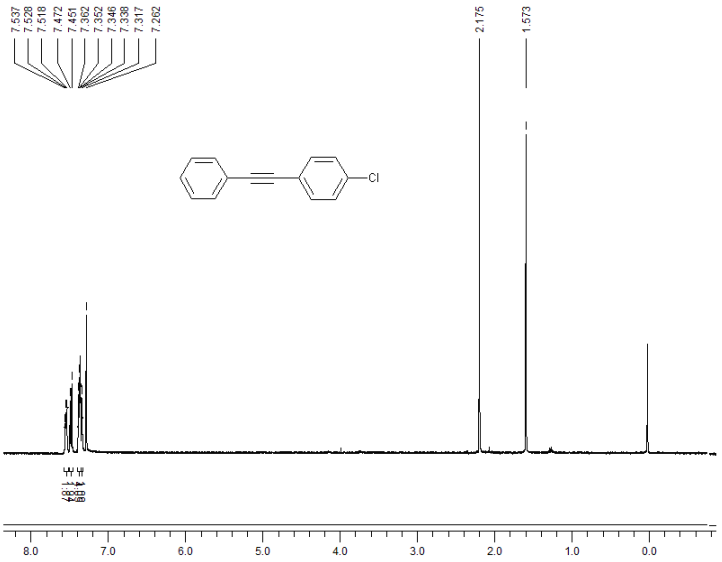
4.53e4
100
%
Me
191.0861
189.0719
193.1005
165.0731
163.0581
194.1035
176.0658
139.0580
126.0505
115.0581
94.5372
89.0431
86.0201
75.0280
0
70
80
90
100
110
120
130
140
150
160
170
180
190
200
m/z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7.362
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7.346
7.338
7.317
7.262
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Cl
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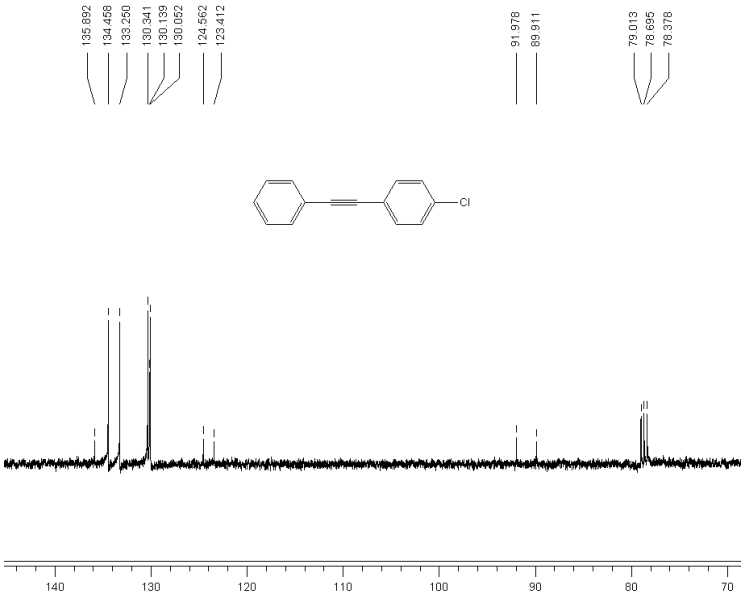
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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130.139
130.052
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123.412
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89.911
79.013
78.695
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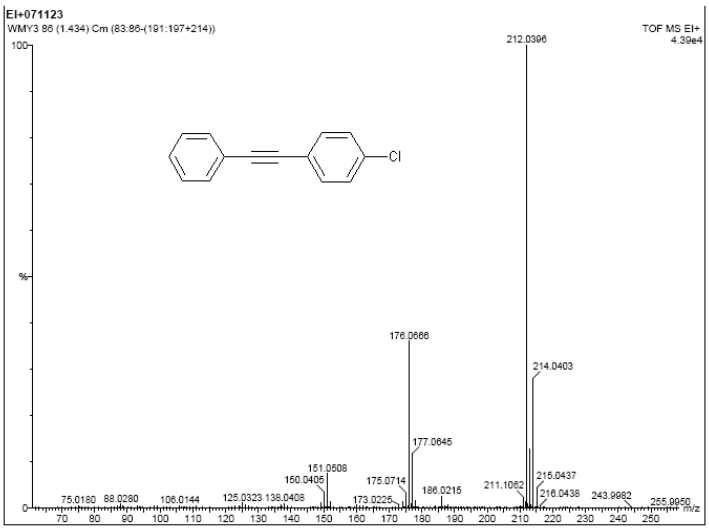
Cl
140
130
120
110
100
90
80
70


EI+071123
WMY3 86 (1.434) Cm (83:86-(191:197+214))
TOF MS EI+
4.39e4
100
%
212.0396
Cl
176.0666
214.0403
177.0645
151.0508
150.0405
175.0714
215.0437
211.1062
216.0438
186.0215
243.9982
75.0180
88.0280
106.0144
125.0323
138.0408
173.0225
255.9950
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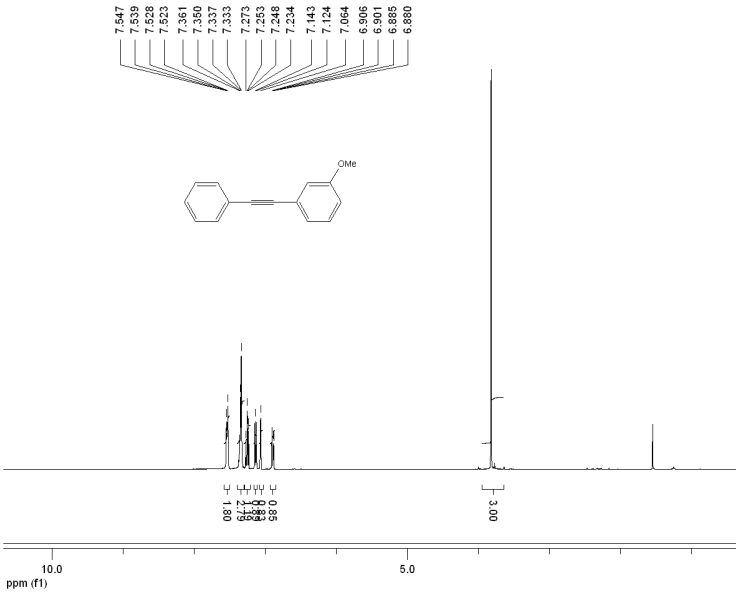
160
170
180
190
200
210
220
230
240
250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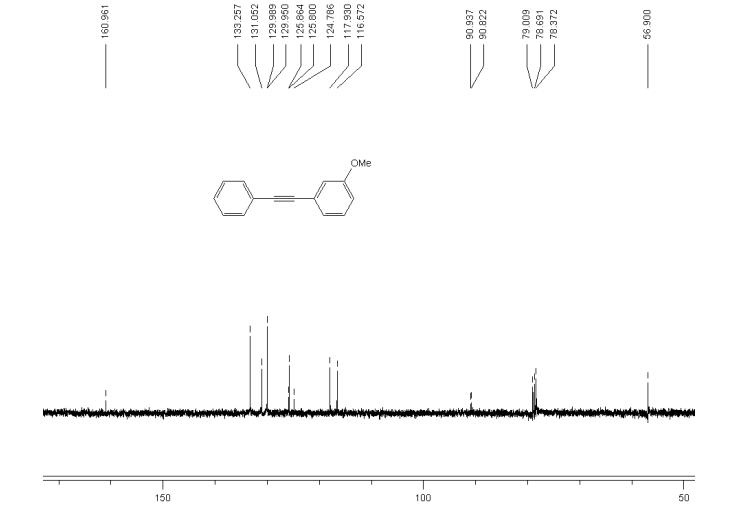
7.523
7.361
7.350
7.337
7.333
7.273
7.253
7.248
7.234
7.143
7.124
7.064
6.906
6.901
6.885
6.880
OMe
1.180
2.179
0.885
3.00
10.0
5.0
ppm (f1)


160.961
133.257
131.052
129.989
129.950
125.864
125.800
124.786
117.990
116.572
90.937
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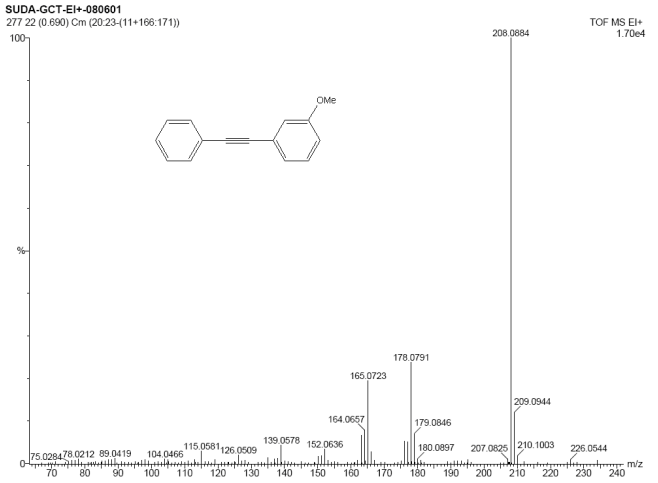
78.691
78.372
56.900
OMe
150
100
50


SUDA-GCT-EI+-080601
277 22 (0.690) Cm (20:23-(11+166:171))
TOF MS EI+
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OMe
178.0791
165.0723
209.0944
164.0657
179.0846
139.0578
152.0636
180.0897
207.0825
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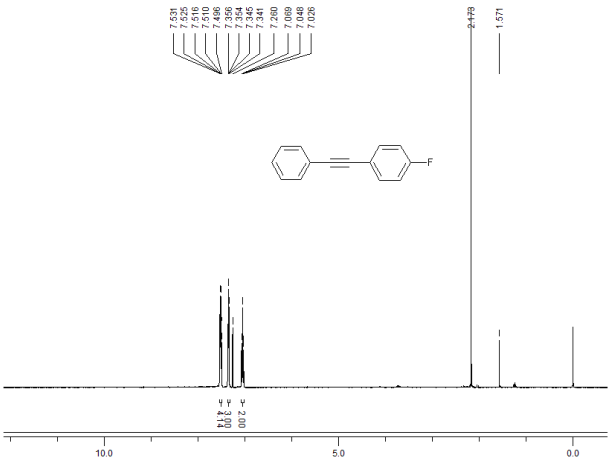
226.0544
115.0581
126.0509
104.0466
89.0419
78.0212
75.0284
m/z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7.496
7.366
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7.048
7.028
2.179
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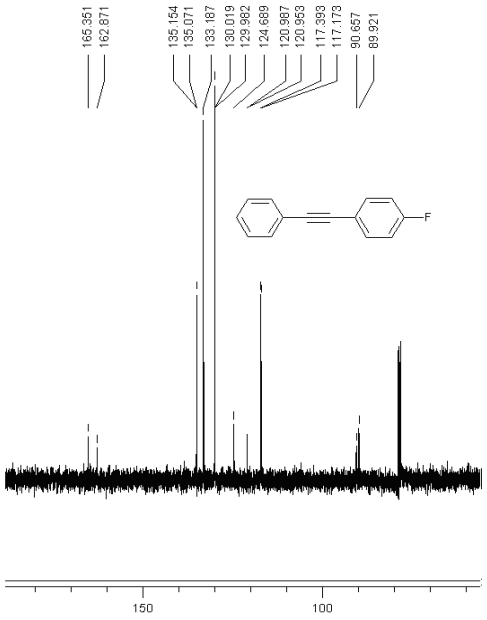
F
2.114
2.200
10.0
5.0
0.0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130.019
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124.689
120.987
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117.393
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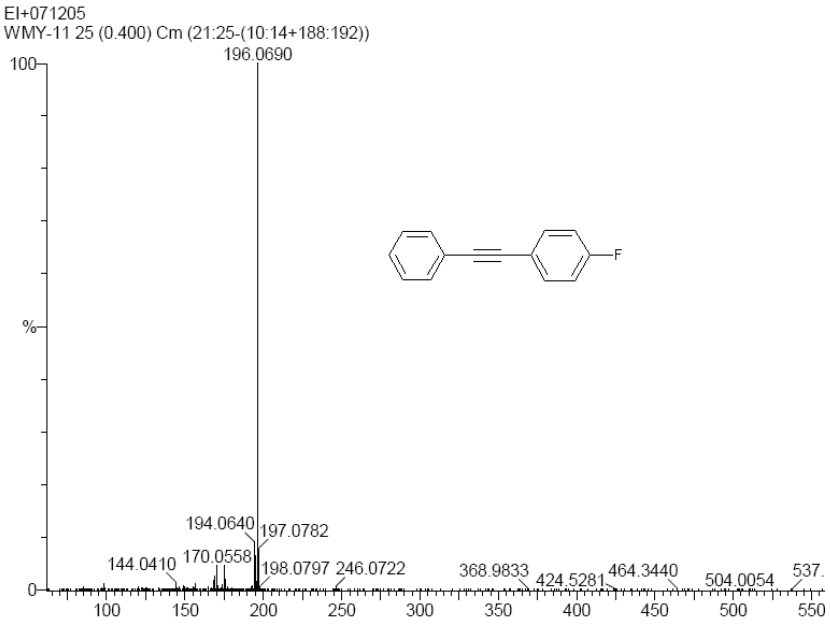
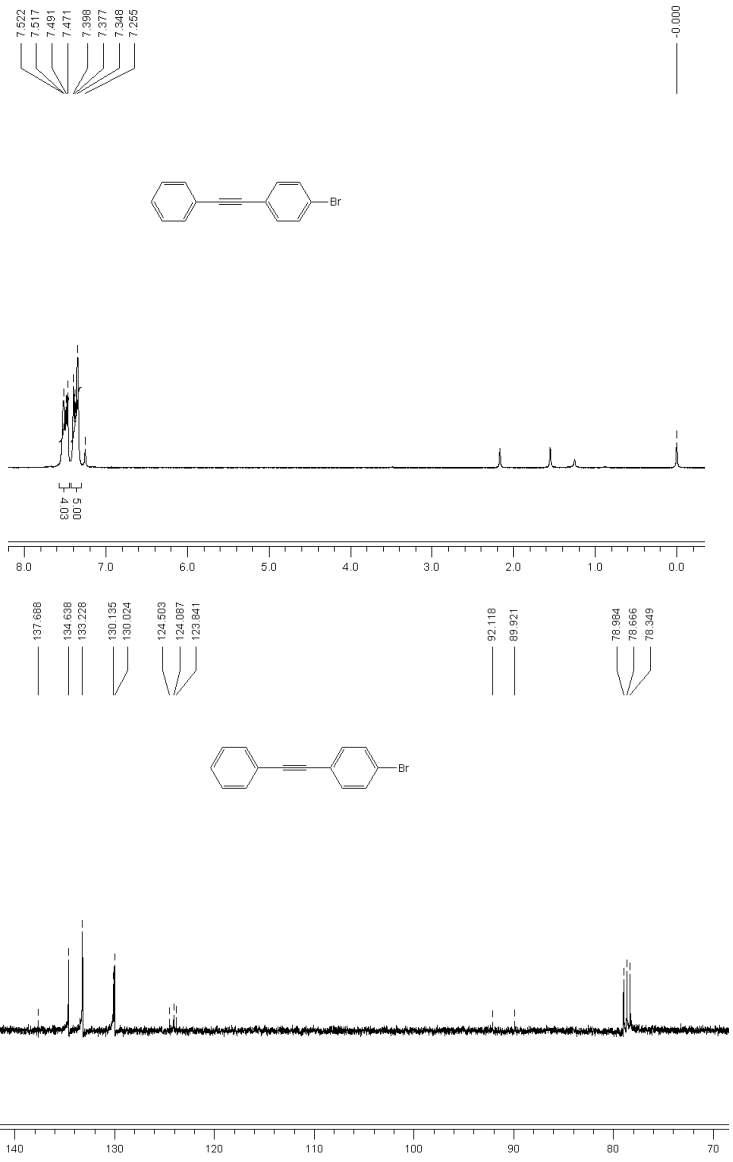
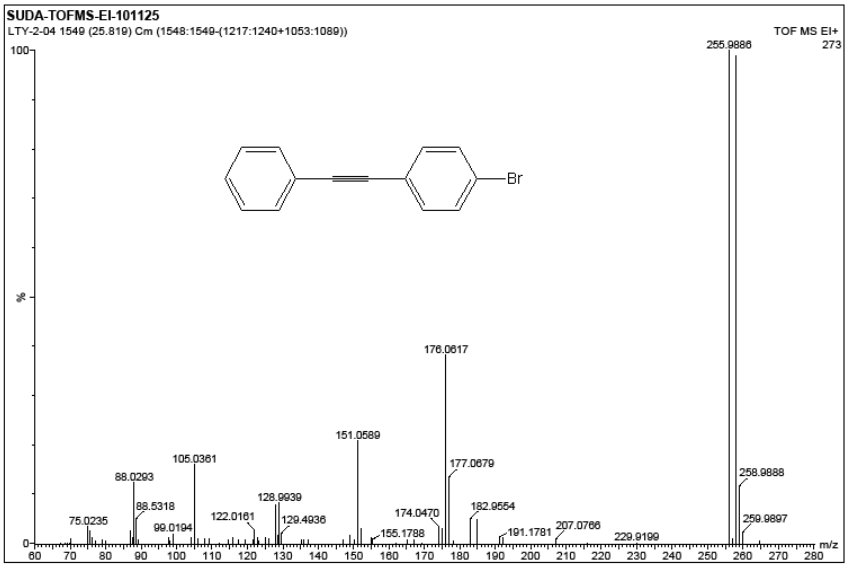
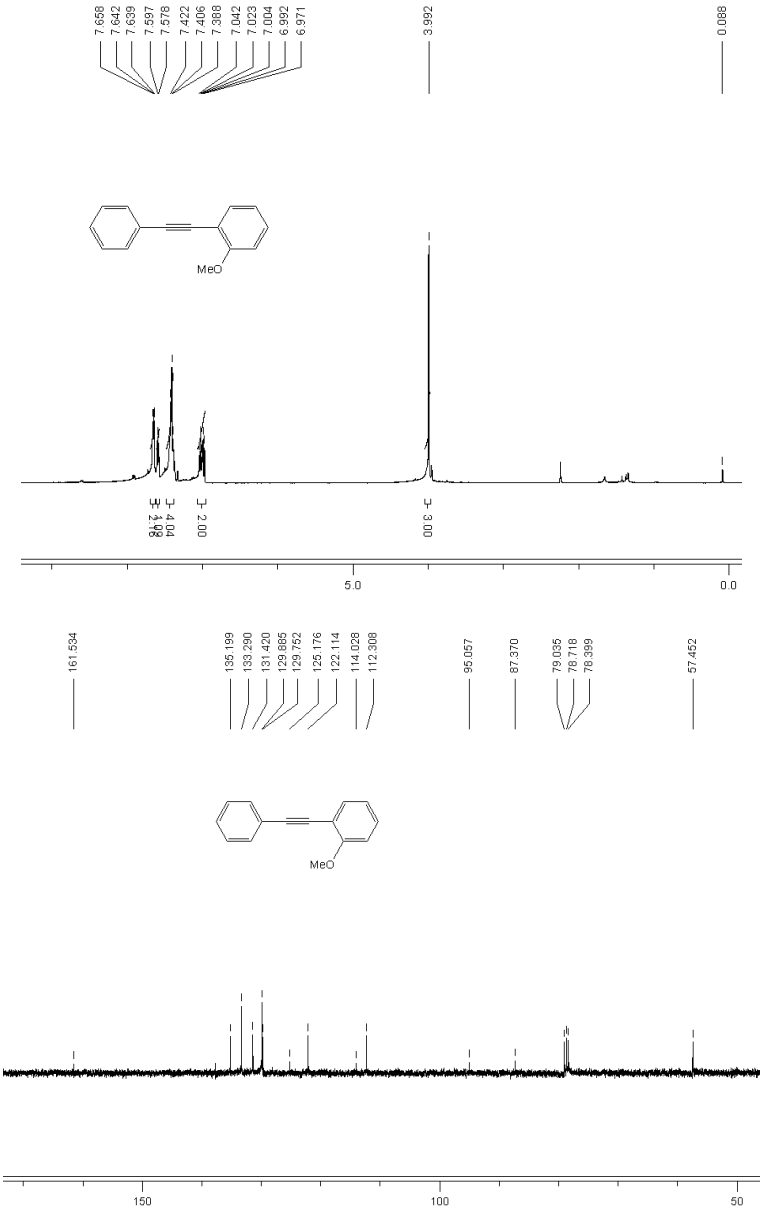
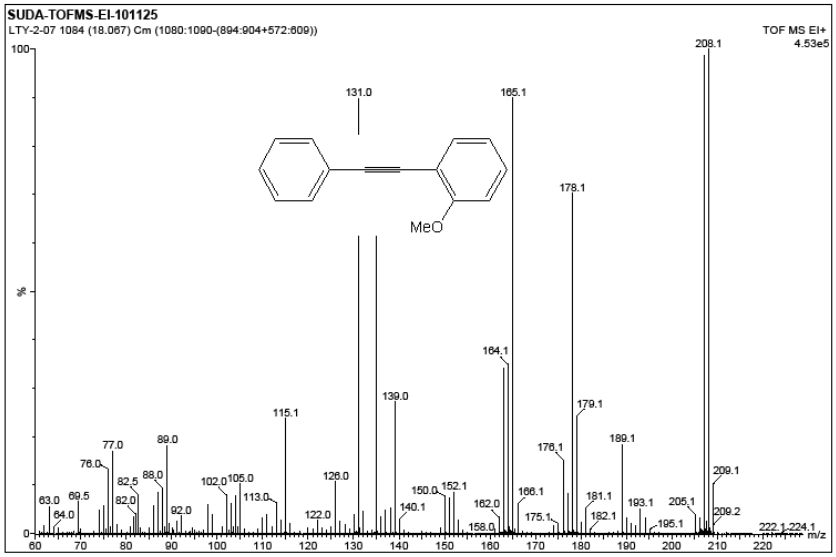
90.657
89.921
F
150
100

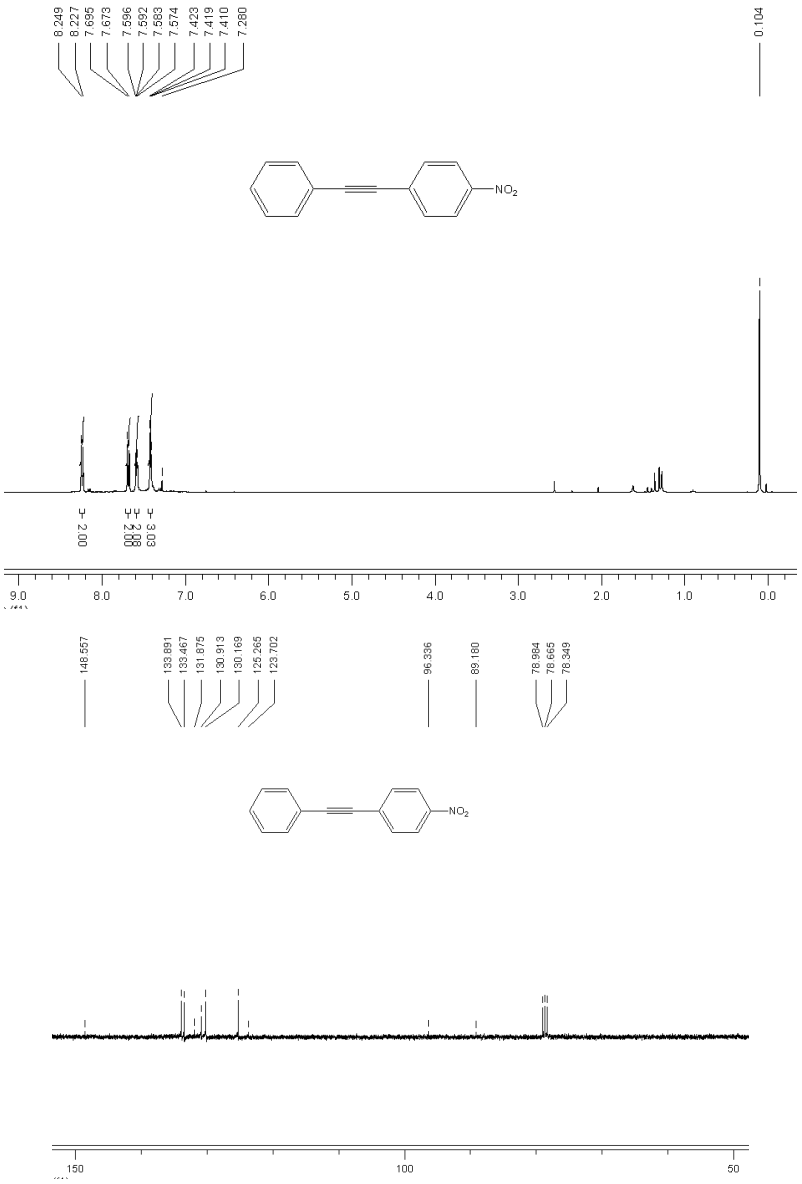

EI+071205
WMY-11 25 (0.400) Cm (21:25-(10:14+188:192))
196.0690
100
%
0
F
194.0640
197.0782
144.0410
170.0558
198.0797
246.0722
368.9833
424.5281
464.3440
504.0054
537.
100
150
200
250
300
350
400
450
500
550

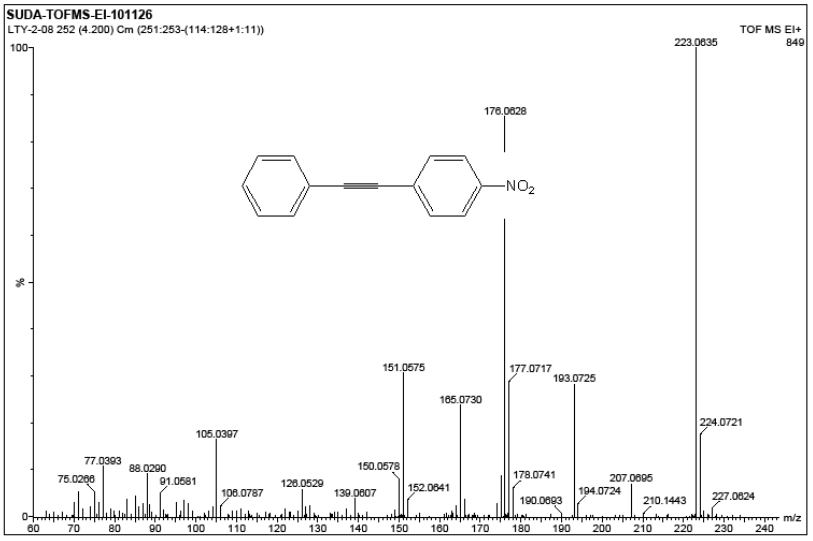


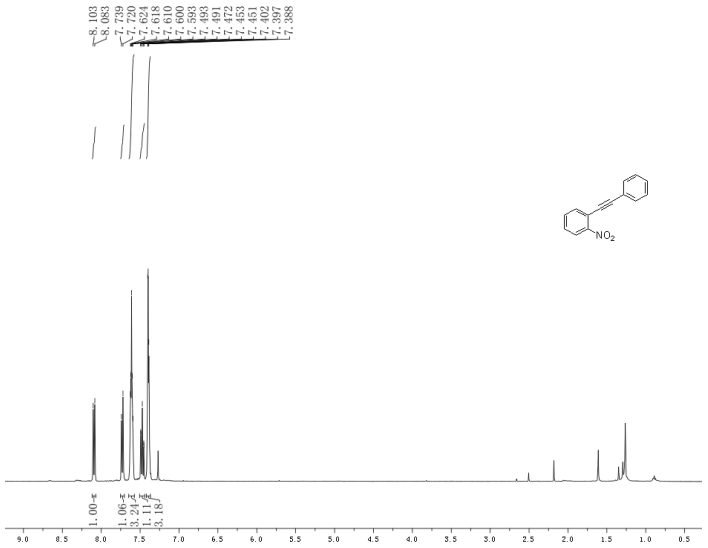


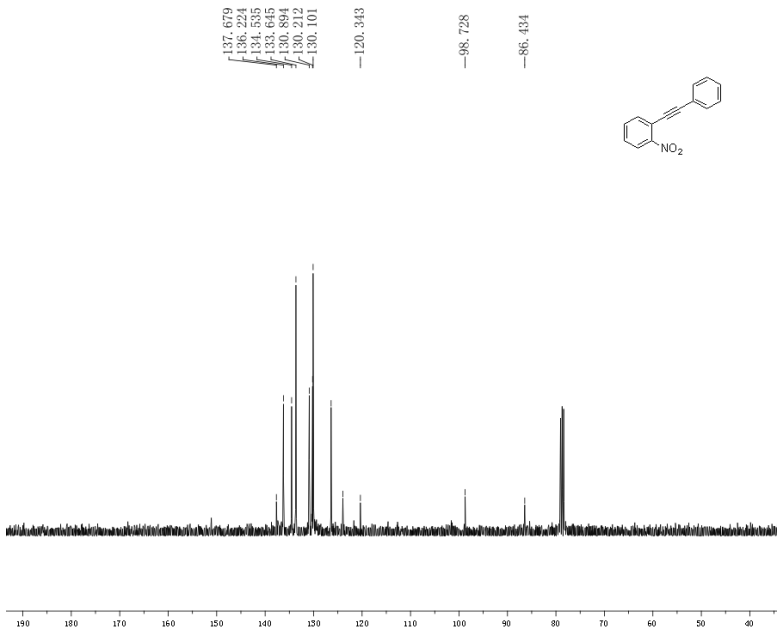




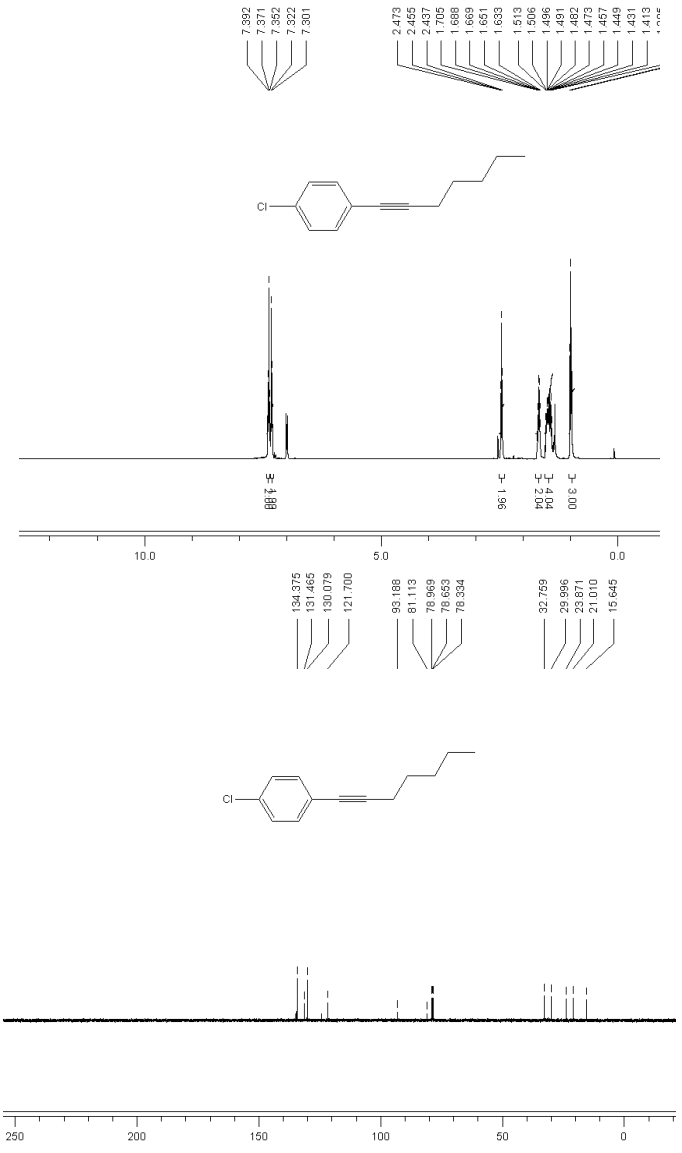

8.249
8.227
7.695
7.673
7.596
7.592
7.583
7.574
7.423
7.419
7.410
7.260
0.104
NO2
2.00
3.88
3.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
146.557
133.891
133.467
131.875
130.913
130.169
125.265
123.702
96.336
89.180
78.984
78.665
78.349
NO2
150
100
50

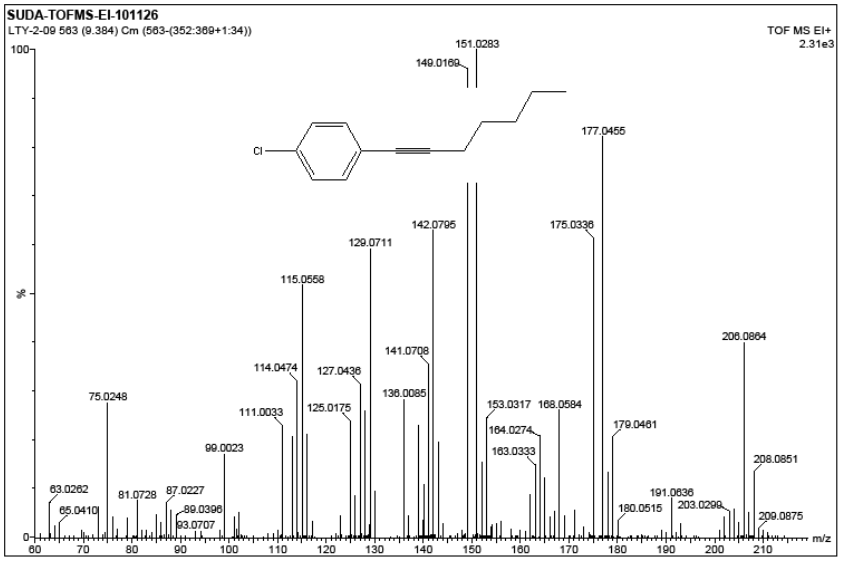

SUDA-TOFMS-EI-101126
LTY-2-08 252 (4.200) Cm (251:253-(114:128+1:11))
TOF MS EI+
849
100
%
0
223.0635
176.0628
NO2
151.0575
177.0717
193.0725
165.0730
224.0721
105.0397
77.0393
88.0290
75.0266
91.0581
150.0578
178.0741
207.0695
106.0787
126.0529
139.0607
152.0641
194.0724
190.0693
210.1443
227.0624
m/z
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240

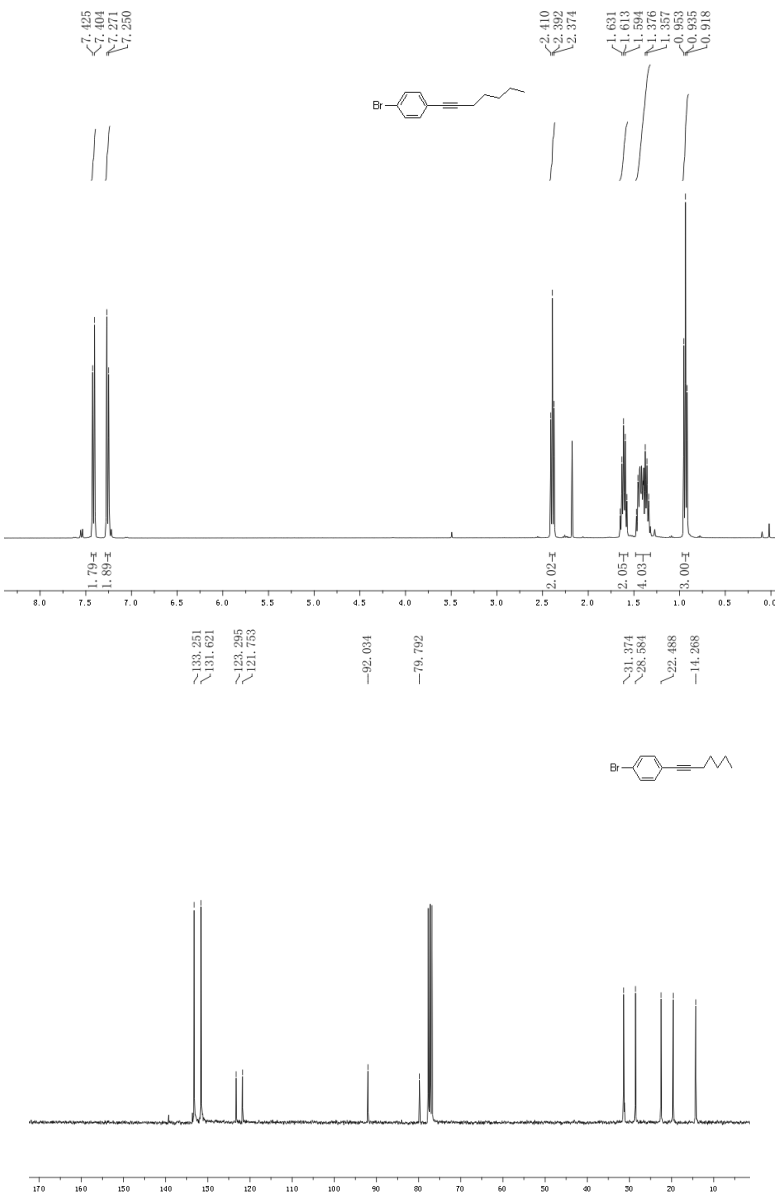

8.103
8.083
7.739
7.720
7.624
7.618
7.610
7.600
7.593
7.493
7.491
7.472
7.453
7.451
7.402
7.397
7.388
NO2
1.00
1.06
2.24
1.11
3.18

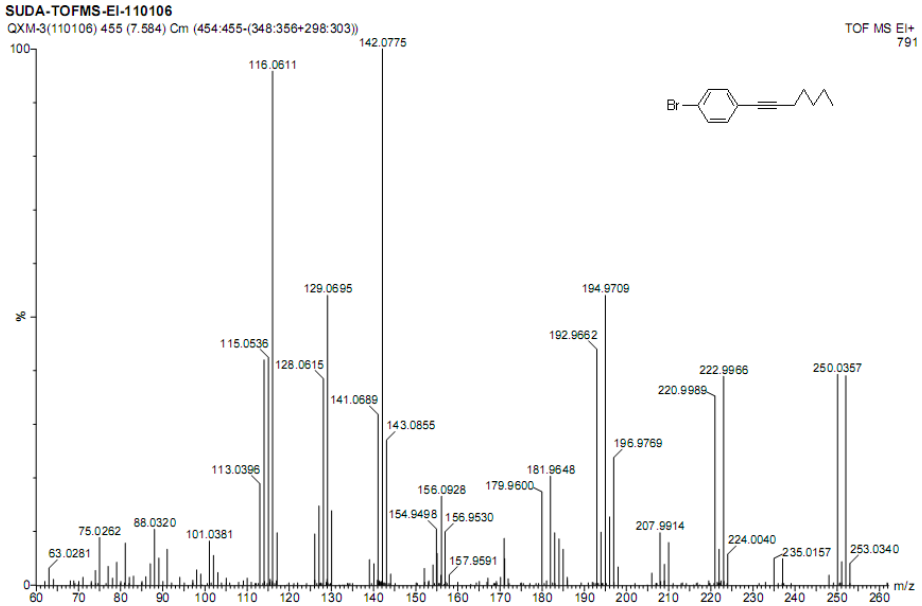

137.679
136.224
134.535
133.645
130.894
130.212
130.101
120.343
98.728
86.434
NO2

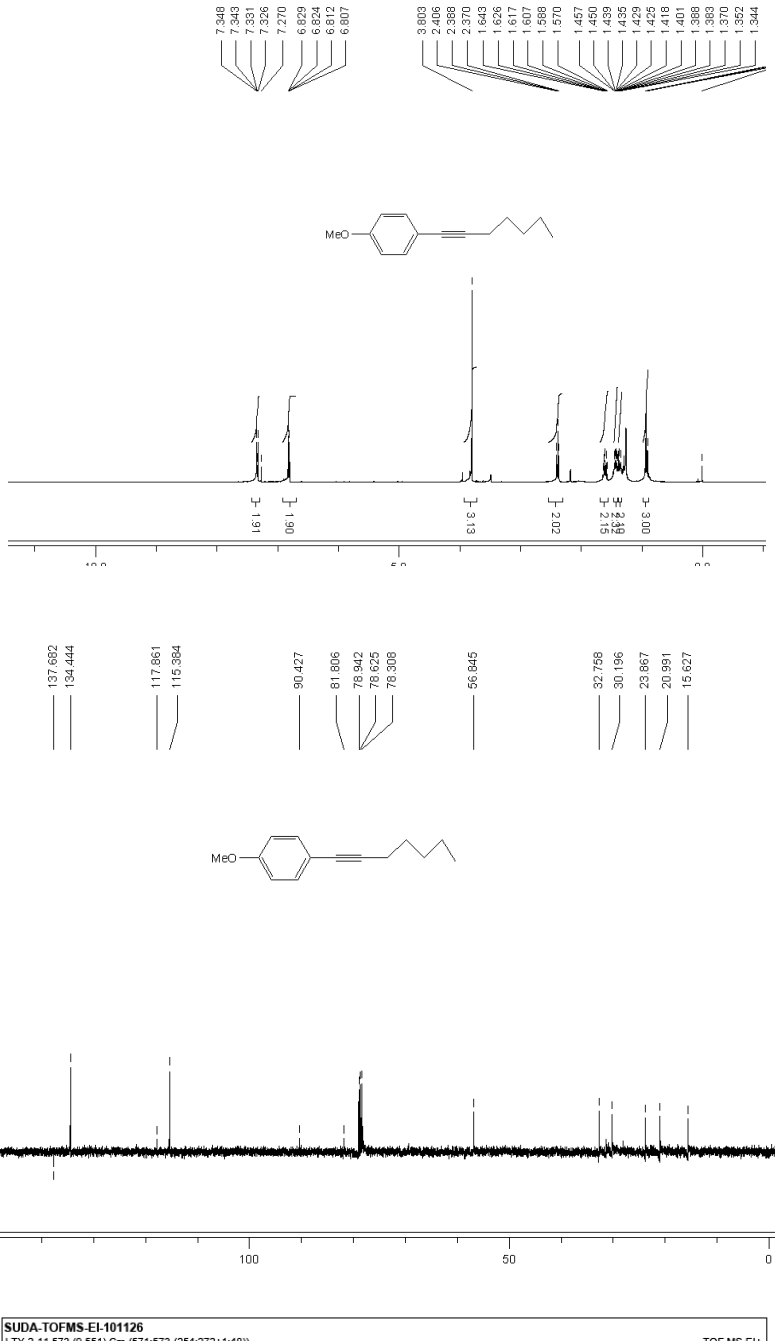
SUDA-TOFMS-EI-110106
QXM-1(110106) 199 (3.316) Cm (199-(77:84+2:26))
TOF MS EI+
158
105.0359
NO2
77.0427
223.0637
179.0737
206.0655
176.0658
207.0756
71.0915
83.0864
98.0098
85.0988
119.0924
111.1192
151.0510
163.0659
224.0516
128.0564
139.0557
152.0592
195.0812
191.1737
208.0051
%
m/z

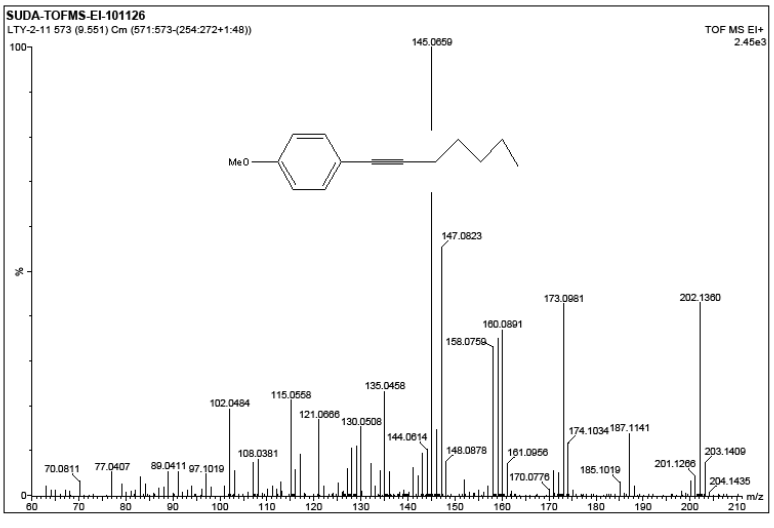

7.392
7.371
7.352
7.322
7.301
2.473
2.455
2.437
1.705
1.688
1.669
1.651
1.633
1.513
1.506
1.496
1.491
1.482
1.473
1.457
1.449
1.431
1.413
Cl
4.88
1.96
2.04
3.00
10.0
5.0
0.0
134.375
131.465
130.079
121.700
93.188
81.113
78.969
78.653
78.334
32.759
29.996
23.871
21.010
15.645
Cl
250
200
150
100
50
0

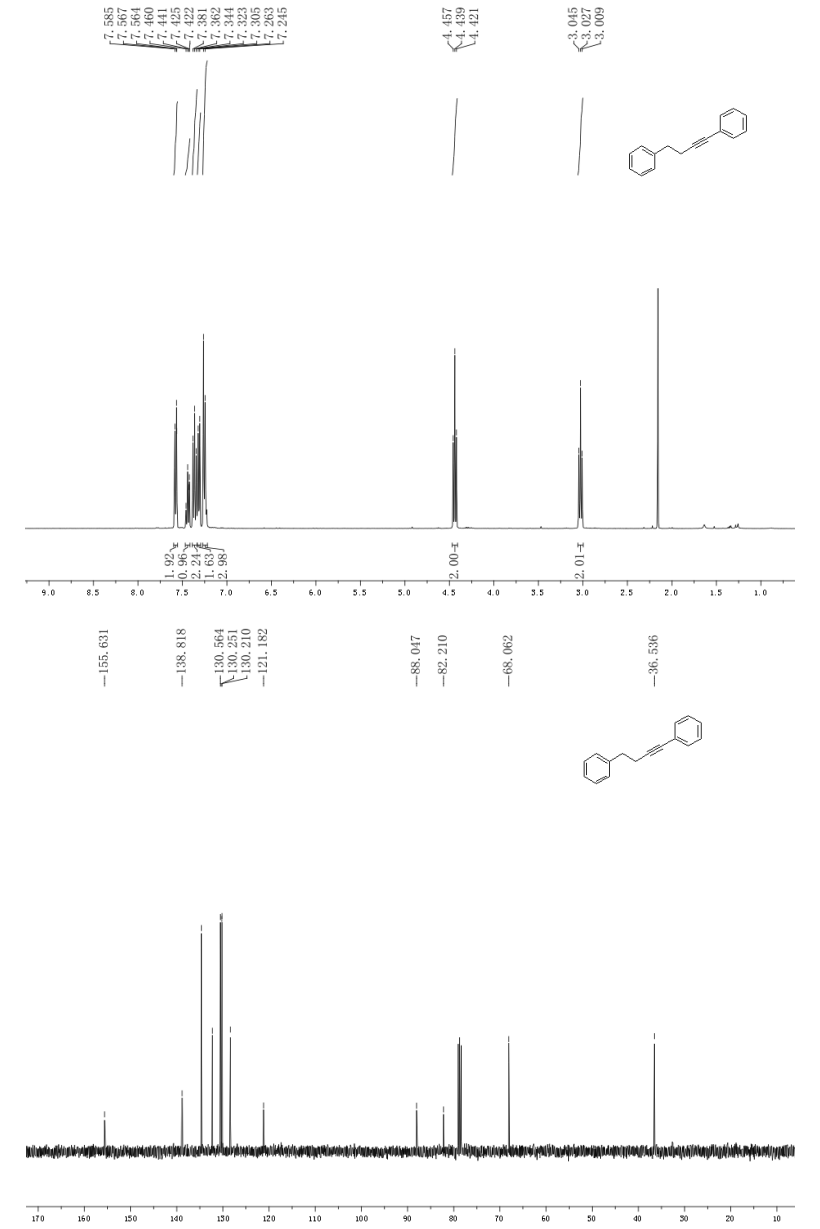

SUDA-TOFMS-EI-101126
LTY-2-09 563 (9.384) Cm (563-(352:369+1:34))
TOF MS EI+
2.31e3
100
%
0
151.0283
149.0169
Cl
177.0455
142.0795
175.0338
129.0711
115.0558
206.0864
141.0708
114.0474
127.0436
136.0085
75.0248
111.0033
125.0175
153.0317
168.0584
164.0274
179.0461
99.0023
163.0333
208.0851
63.0262
81.0728
87.0227
191.0636
65.0410
89.0396
180.0515
203.0299
93.0707
209.0875
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
m/z

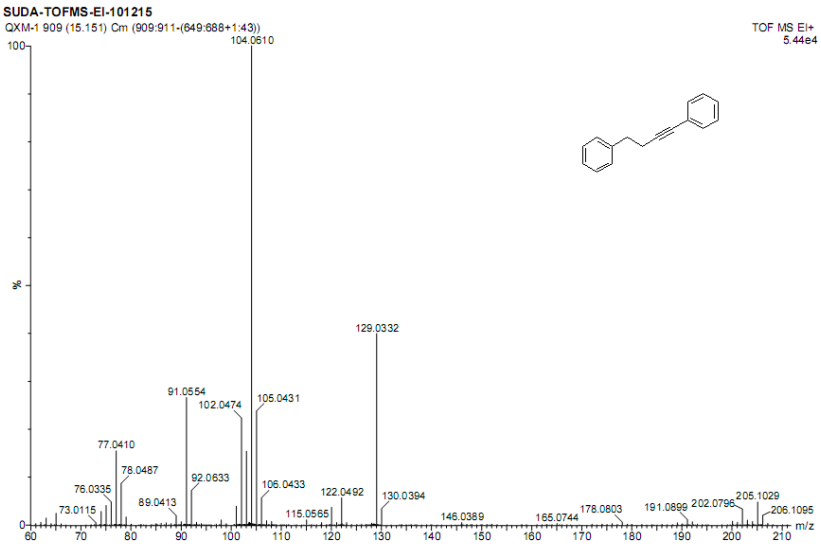

7.425
7.404
7.271
7.250
2.410
2.392
2.374
1.631
1.613
1.594
1.376
1.357
0.953
0.935
0.918
Br
1.79
1.89
2.02
2.05
4.03
3.00
133.251
131.621
123.295
121.753
92.034
79.792
31.374
28.584
22.488
14.268
Br

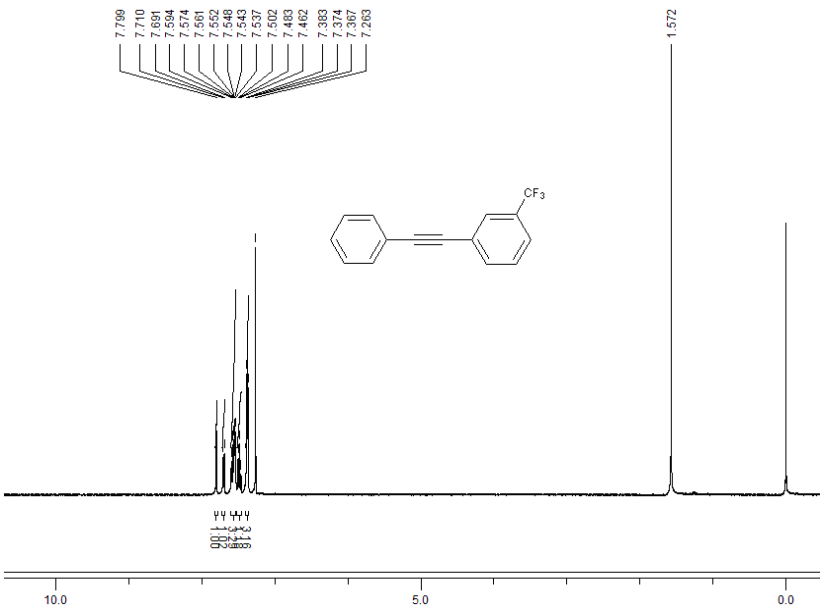

SUDA-TOFMS-EI-110106
QXM-3(110106) 455 (7.584) Cm (454:455-(348:356+298:303))
TOF MS EI+
791
Br
%
m/z
142.0775
116.0611
129.0695
194.9709
192.9662
115.0536
128.0615
222.9966
250.0357
220.9989
141.0689
143.0855
196.9769
113.0396
181.9648
179.9600
156.0928
154.9498
156.9530
207.9914
75.0262
88.0320
101.0381
224.0040
235.0157
253.0340
63.0281
157.9591

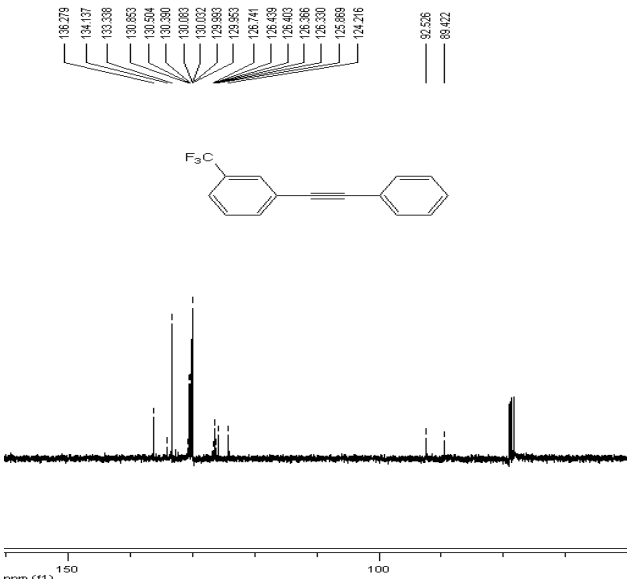

7.348
7.343
7.331
7.326
7.270
6.829
6.824
6.812
6.807
3.803
2.406
2.388
2.370
1.643
1.626
1.617
1.607
1.588
1.570
1.457
1.450
1.439
1.435
1.429
1.425
1.418
1.401
1.388
1.383
1.370
1.352
1.344
MeO
1.91
1.90
3.13
2.02
3.00
137.682
134.444
117.861
115.384
90.427
81.806
78.942
78.625
78.308
56.845
32.758
30.196
23.867
20.991
15.627
MeO
150
100
50
0

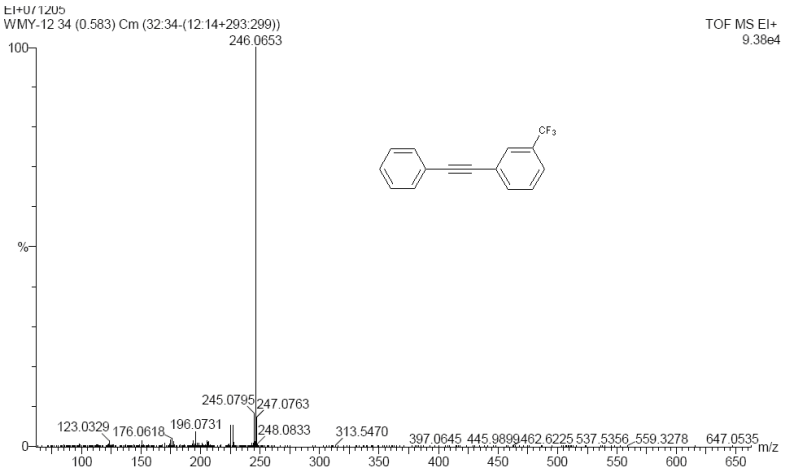

SUDA-TOFMS-EI-101126
LTY-2-11 573 (9.551) Cm (571:573-(254:272+1:48))
TOF MS EI+
2.45e3
100
%
0
MeO
145.0659
147.0823
173.0981
202.1360
160.0891
158.0759
135.0458
115.0558
102.0484
121.0666
130.0508
144.0614
174.1034
187.1141
148.0878
161.0956
203.1409
108.0381
70.0811
77.0407
89.0411
97.1019
170.0776
185.1019
201.1266
204.1435
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
m/z

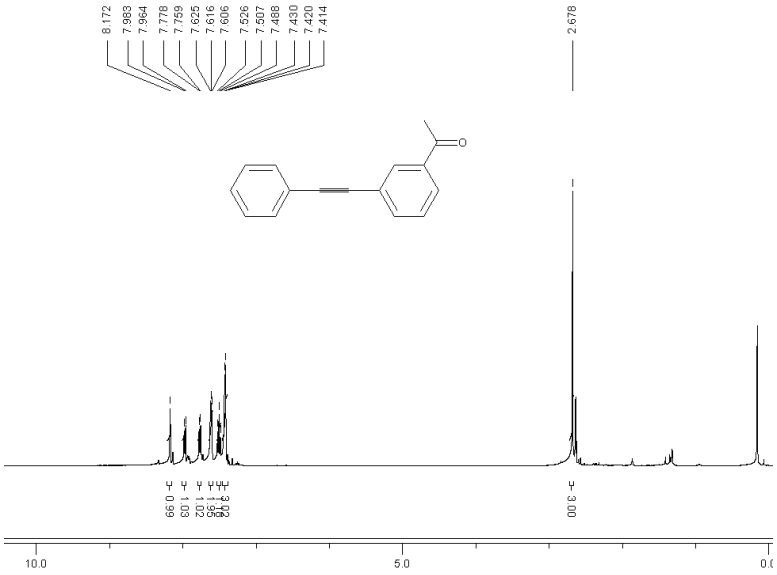

7.585
7.567
7.564
7.460
7.441
7.425
7.422
7.381
7.362
7.344
7.323
7.305
7.263
7.245
4.457
4.439
4.421
3.045
3.027
3.009
1.92
0.96
2.24
1.63
2.98
2.00
2.01
155.631
138.818
130.564
130.251
130.210
121.182
88.047
82.210
68.062
36.536

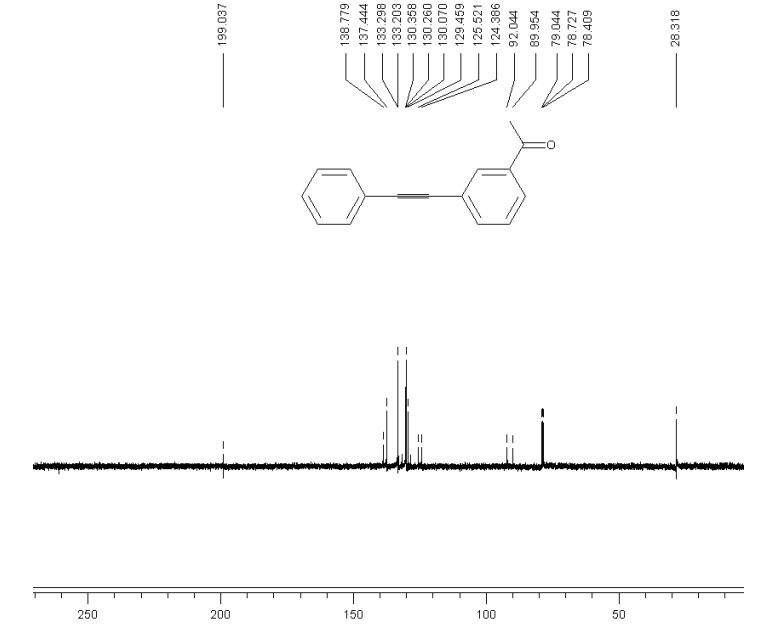

SUDA-TOFMS-EI-101215
QXM-1 909 (15.151) Cm (909:911-(649:688+1:43))
TOF MS EI+
5.44e4
104.0610
129.0332
91.0554
102.0474
105.0431
77.0410
78.0487
92.0633
106.0433
122.0492
130.0394
76.0335
73.0115
89.0413
115.0565
146.0389
165.0744
178.0803
191.0899
202.0796
205.1029
206.1095
m/z

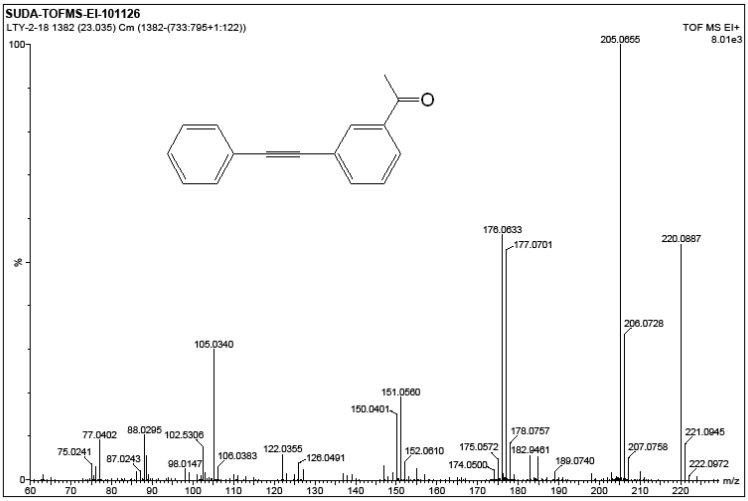

7.799
7.710
7.691
7.594
7.574
7.561
7.552
7.548
7.543
7.537
7.502
7.483
7.462
7.383
7.374
7.367
7.263
1.572
CF3
10.0
5.0
0.0

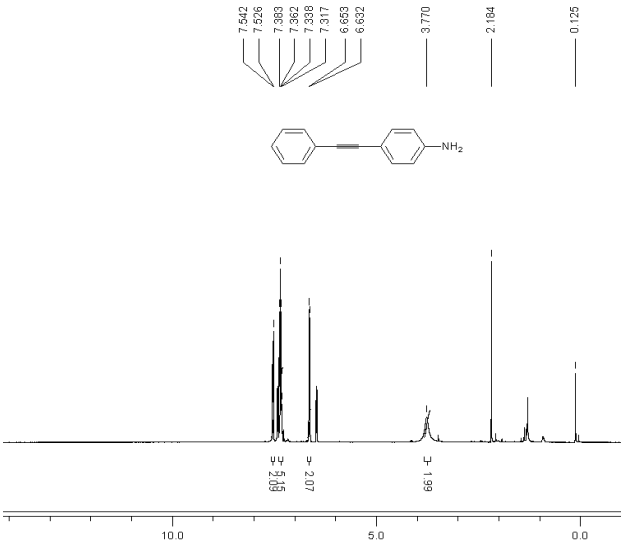

136.279
134.137
133.338
130.853
130.594
130.390
130.083
130.032
129.993
129.953
126.741
126.439
126.403
126.366
126.330
125.869
124.216
92.526
89.422
F3C
150
100

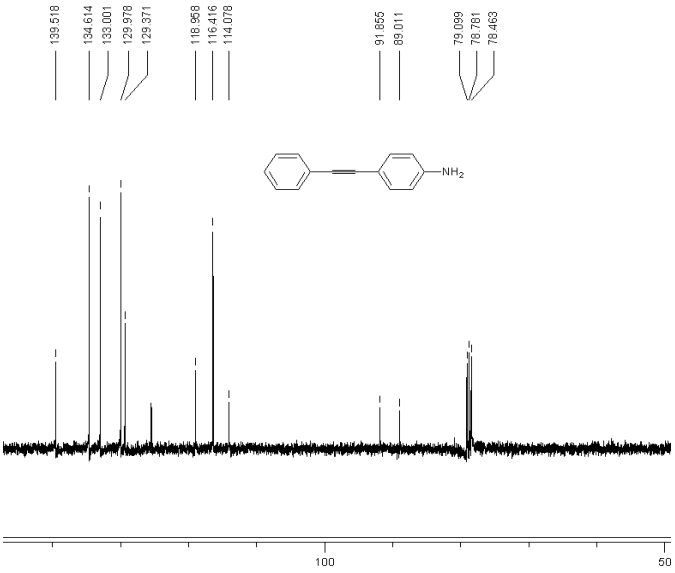

EI+071205
WMY-12 34 (0.583) Cm (32:34-(12:14+293:299))
TOF MS EI+
9.38e4
246.0653
100
%
CF3
245.0795
247.0763
123.0329
176.0618
196.0731
248.0833
313.5470
397.0645
445.9899
462.6225
537.5356
559.3278
647.0535
0
100
150
200
250
300
350
400
450
500
550
600
650
m/z

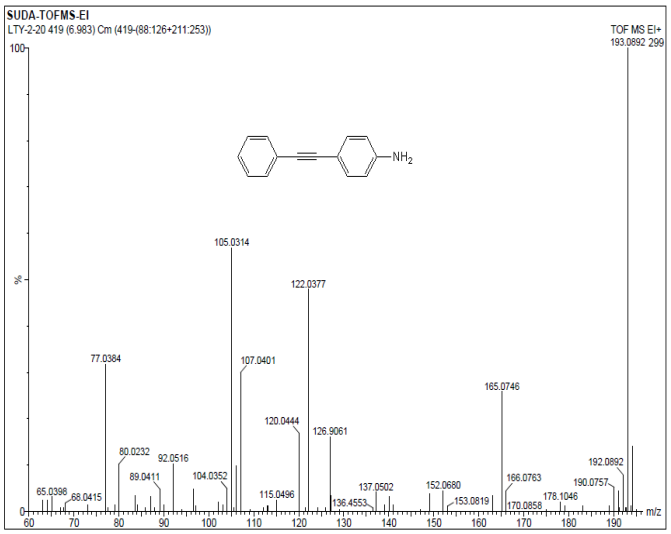

8.172
7.983
7.964
7.778
7.759
7.625
7.616
7.606
7.526
7.507
7.488
7.430
7.420
7.414
2.678
O
3.100
10.0
5.0

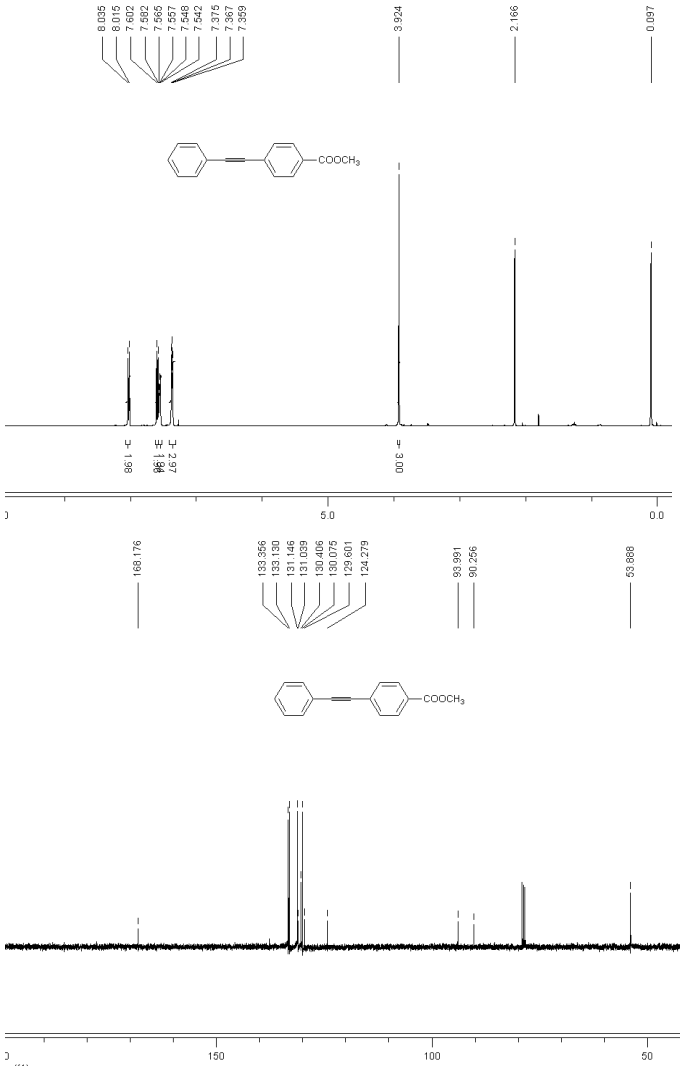

199.037
138.779
137.444
133.298
133.203
130.358
130.260
130.070
129.459
125.521
124.386
92.044
89.954
79.044
78.727
78.409
28.318
O
250
200
150
100
50

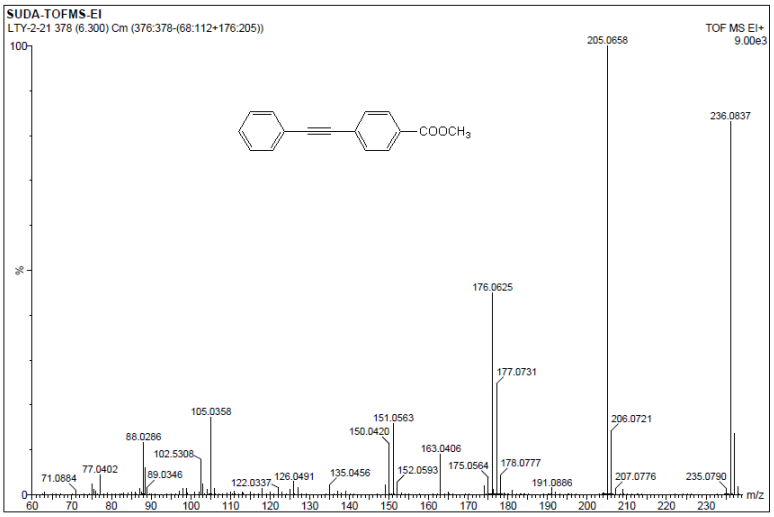

SUDA-TOFMS-EI-101126
LTY-2-18 1382 (23.035) Cm (1382-(733:795+1:122))
TOF MS EI+
8.01e3
100
%
205.0655
176.0633
177.0701
220.0887
206.0728
105.0340
151.0560
150.0401
178.0757
221.0945
77.0402
88.0295
102.5306
75.0241
87.0243
98.0147
106.0383
122.0355
126.0491
152.0610
175.0572
182.9461
189.0740
207.0758
174.0500
222.0972
0
m/z
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220

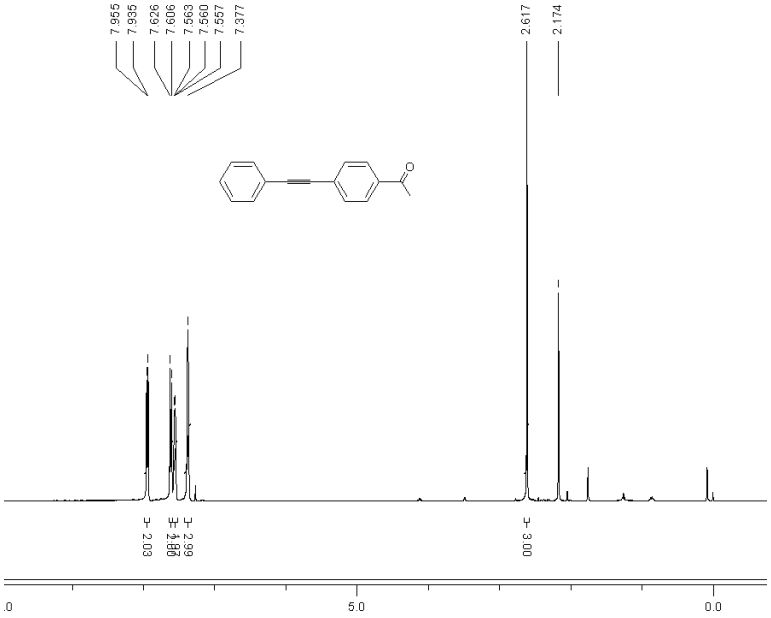

7.542
7.526
7.383
7.362
7.338
7.317
6.653
6.632
3.770
2.184
0.125
NH2
3.15
2.09
2.07
1.99
10.0
5.0
0.0

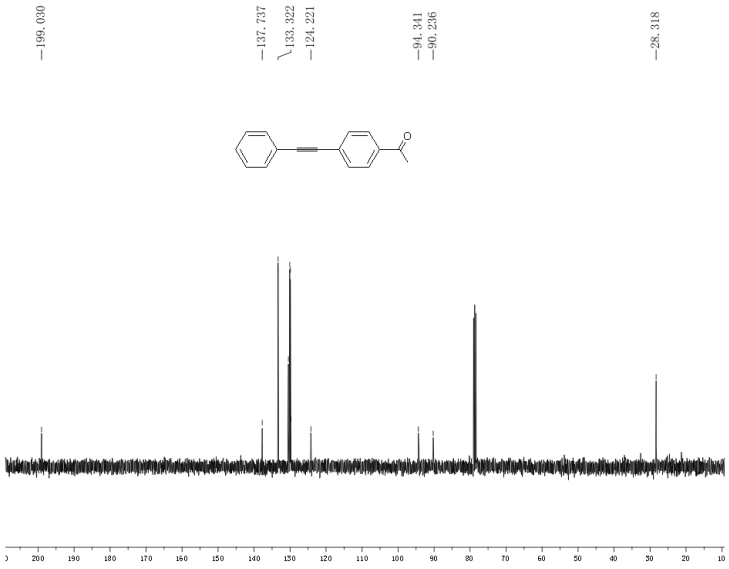

139.518
134.614
133.001
129.978
129.371
118.958
116.416
114.078
91.655
89.011
79.099
78.781
78.463
NH2
100
50

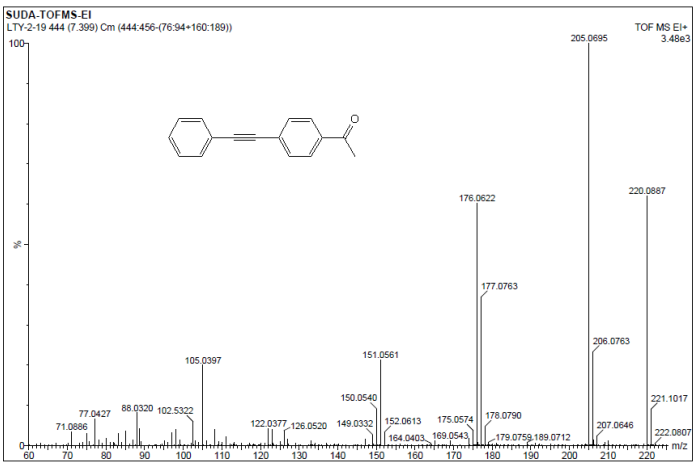

SUDA-TOFMS-EI
LTY-2-20 419 (6.983) Cm (419-(88:126+211:253))
TOF MS EI+
193.0892 299
100
%
NH2
105.0314
122.0377
77.0384
107.0401
165.0746
120.0444
126.9061
80.0232
92.0516
89.0411
104.0352
192.0892
65.0398
68.0415
115.0496
137.0502
152.0680
166.0763
190.0757
136.4553
153.0819
170.0858
178.1046
0
60
70
80
90
100
110
120
130
140
150
160
170
180
190
m/z

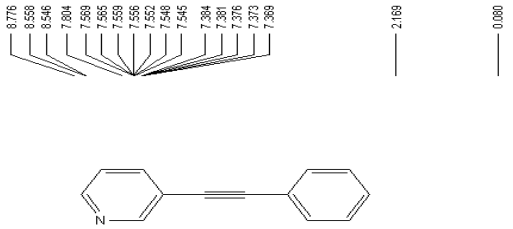

8.035
8.015
7.602
7.582
7.565
7.557
7.548
7.542
7.375
7.367
7.359
3.924
2.166
0.097
COOCH3
3.00
5.0
0.0
168.176
133.356
133.130
131.146
131.039
130.406
130.075
129.601
124.279
93.991
90.256
53.888
150
100
50

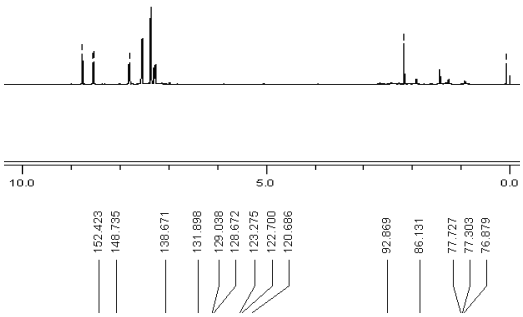

SUDA-TOFMS-EI
LTY-2-21 378 (6.300) Cm (376:378-(68:112+176:205))
TOF MS EI+
9.00e3
100
%
COOCH3
205.0658
236.0837
176.0625
177.0731
206.0721
105.0358
151.0563
150.0420
88.0286
102.5308
163.0406
175.0564
178.0777
77.0402
71.0884
89.0346
122.0337
126.0491
135.0456
152.0593
191.0886
207.0776
235.0790
m/z
60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230

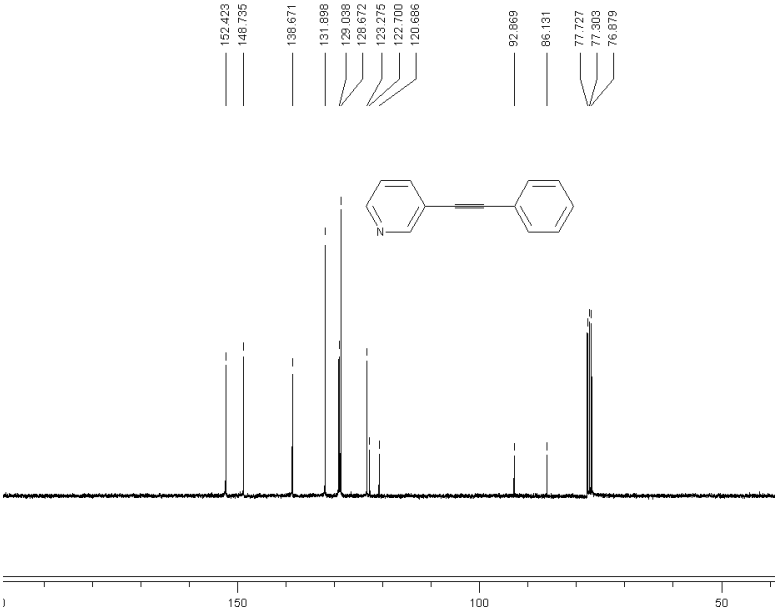

7.955
7.935
7.626
7.606
7.563
7.560
7.557
7.377
2.617
2.174
2.03
3.48
2.99
3.00
5.0
0.0

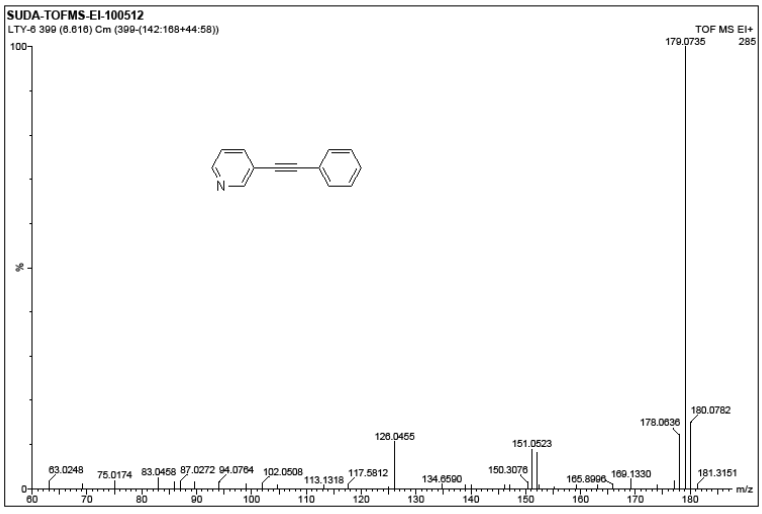

199.030
137.737
133.322
124.221
94.341
90.236
28.318

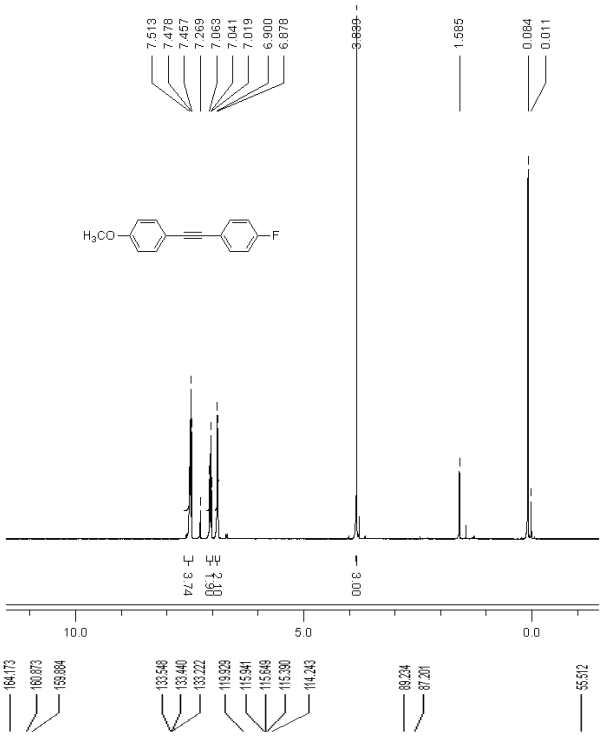

SUDA-TOFMS-EI
LTY-2-19 444 (7.399) Cm (444:456-(76:94+160:189))
TOF MS EI+
3.48e3
205.0695
220.0887
176.0622
177.0763
206.0763
151.0561
105.0397
150.0540
221.1017
77.0427
88.0320
102.5322
71.0886
122.0377
126.0520
149.0332
152.0613
175.0574
178.0790
164.0403
169.0543
179.0759
189.0712
207.0646
222.0807
m/z

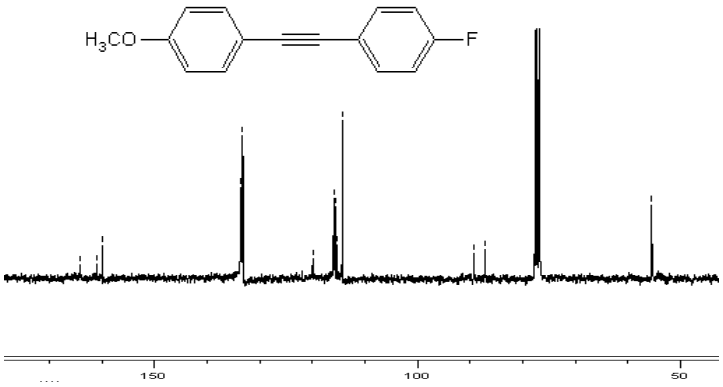

8.776
8.558
8.546
7.804
7.569
7.565
7.559
7.555
7.552
7.548
7.545
7.384
7.381
7.376
7.373
7.369
2.169
0.000
N

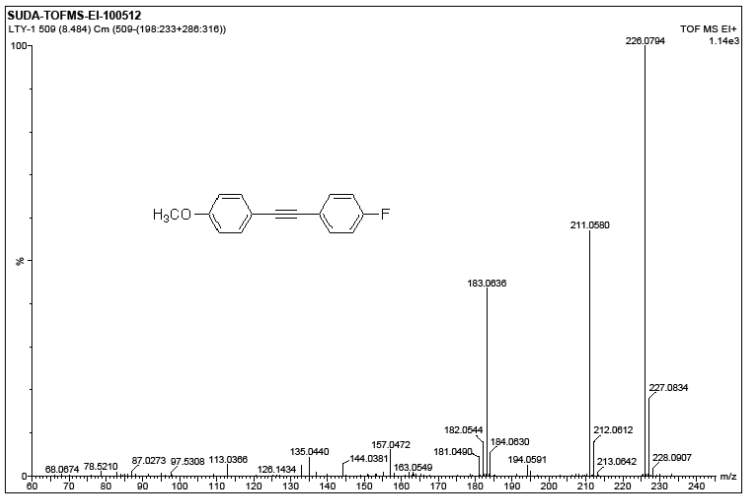

10.0
5.0
0.0

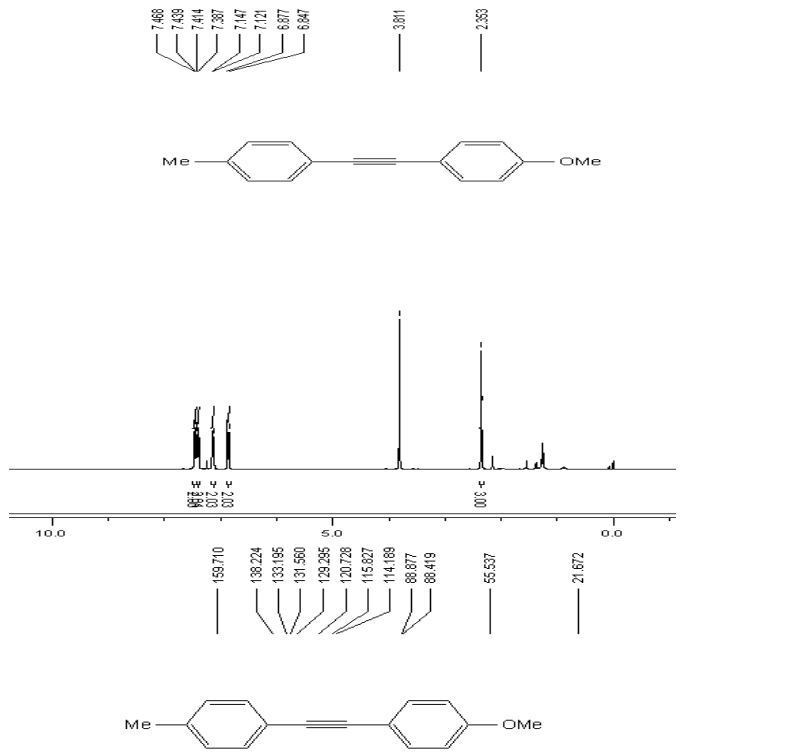

152.423
148.735
138.671
131.898
129.038
128.672
123.275
122.700
120.686
92.869
86.131
77.727
77.303
76.879
N
150
100
50

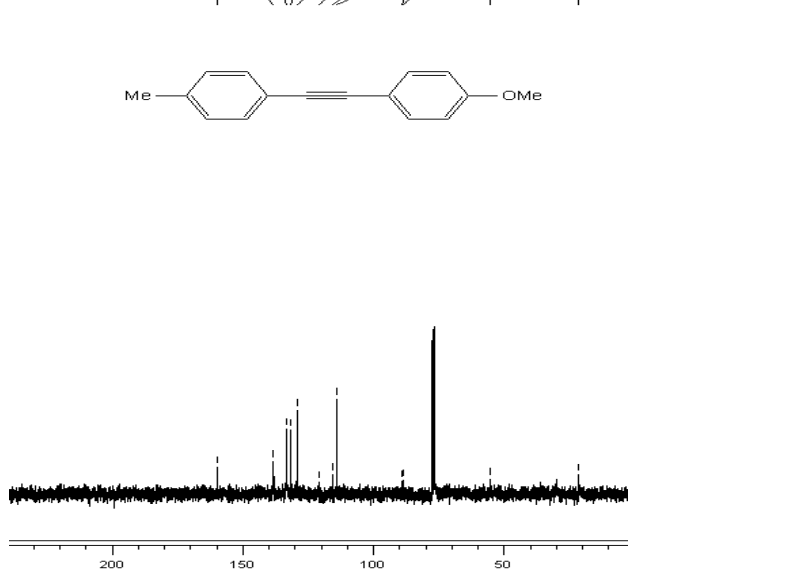

SUDA-TOFMS-EI-100512
LTY-6 399 (6.616) Cm (399-(142:168+44:58))
TOF MS EI+
179.0735
285
100
%
0
N
178.0636
180.0782
126.0455
151.0523
63.0248
75.0174
83.0458
87.0272
94.0764
102.0508
113.1318
117.5812
134.6590
150.3076
165.8996
169.1330
181.3151
m/z
60
70
80
90
100
110
120
130
140
150
160
170
180


7.513
7.478
7.457
7.269
7.063
7.041
7.019
6.900
6.878
3.889
1.585
0.084
0.011
H3CO
F
3.24
2.10
3.00
10.0
5.0
0.0
164.173
160.873
159.884
133.548
133.440
133.222
119.929
115.941
115.849
115.380
114.243
89.234
87.201
55.512

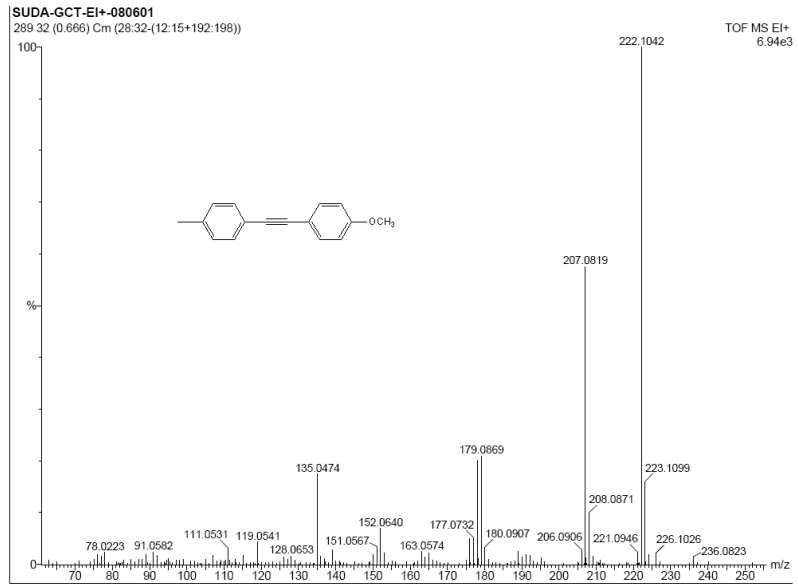

H3CO
F
150
100
50

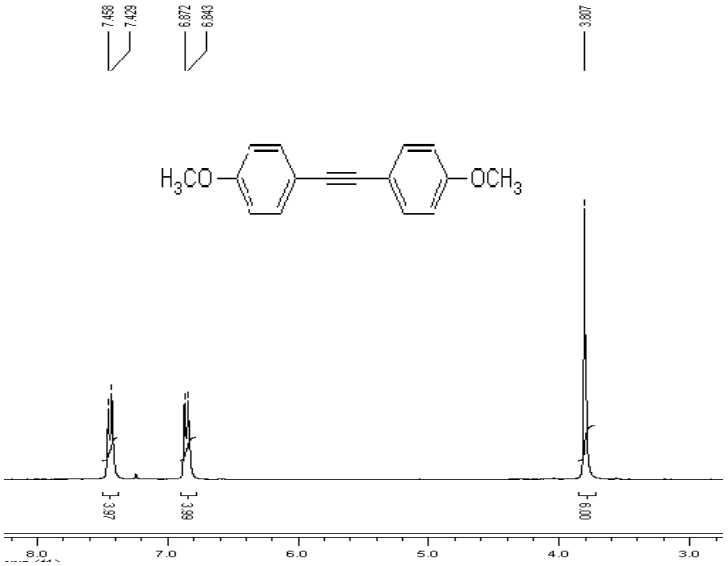

SUDA-TOFMS-EI-100512
LTY-1 509 (8.484) Cm (509-(198:233+286:316))
TOF MS EI+
1.14e3
100
%
H3CO
F
226.0794
211.0580
183.0636
227.0834
212.0612
182.0544
184.0630
181.0490
194.0591
213.0642
228.0907
157.0472
135.0440
144.0381
163.0549
68.0674
78.5210
87.0273
97.5308
113.0366
126.1434
m/z

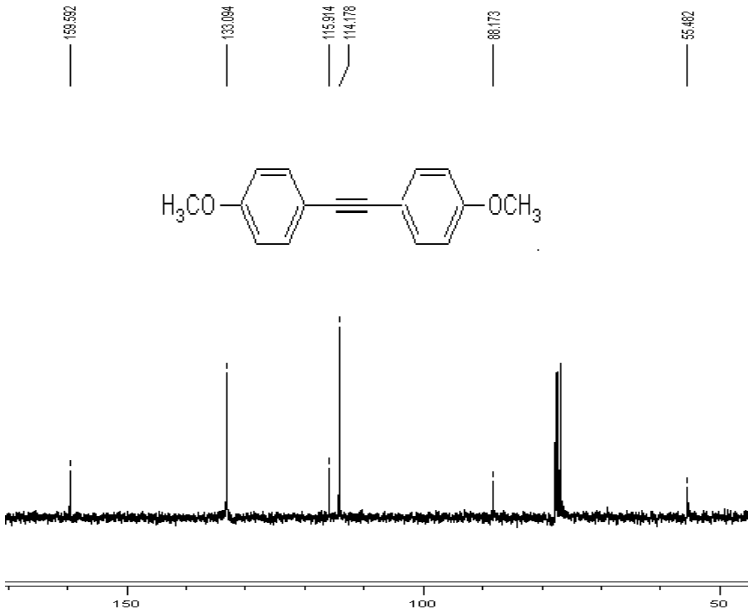

7.468
7.439
7.414
7.387
7.147
7.121
6.877
6.847
3.811
2.353
Me
OMe
10.0
5.0
0.0

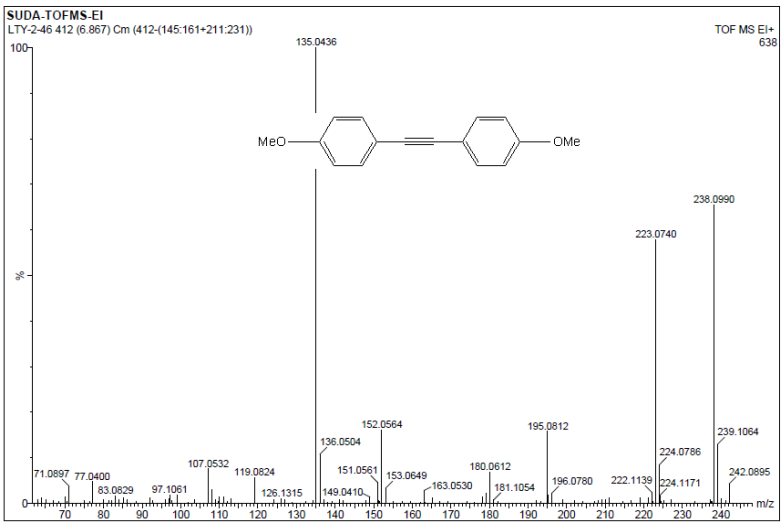

159.710
138.224
133.195
131.560
129.395
120.728
115.627
114.169
88.877
88.419
55.537
21.672
Me
OMe

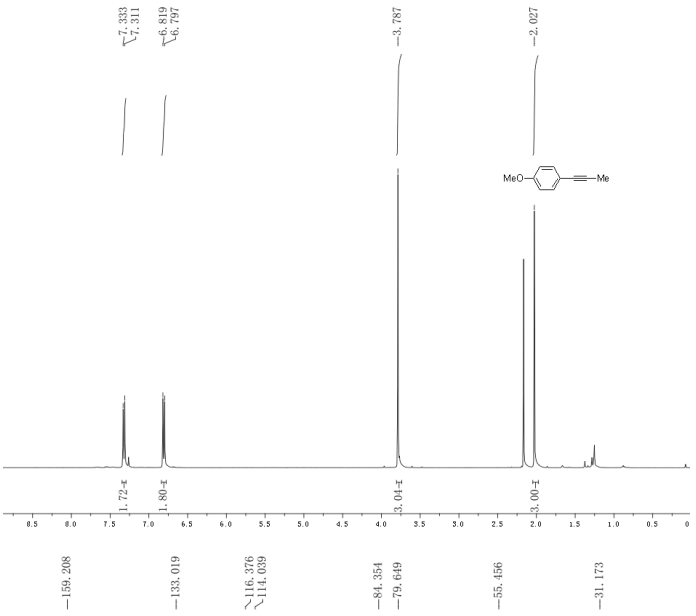
200
150
100
50

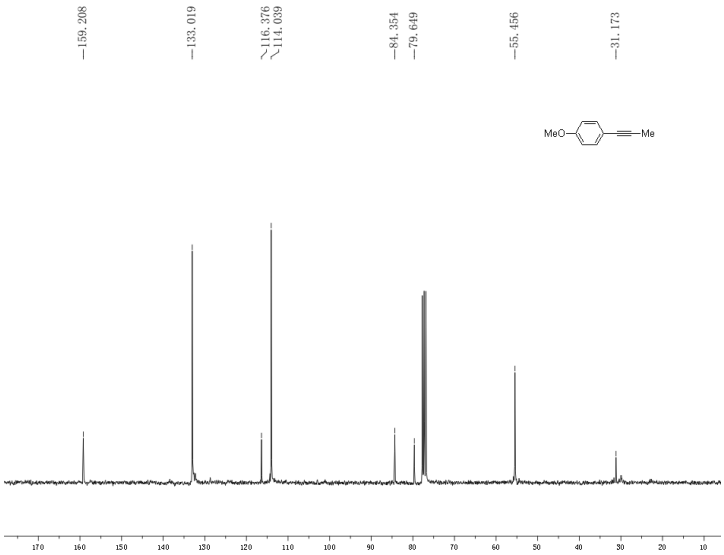

SUDA-GCT-EI+-080601
289 32 (0.666) Cm (28:32-(12:15+192:198))
TOF MS EI+
6.94e3
222.1042
207.0819
179.0869
135.0474
223.1099
208.0871
152.0640
177.0732
180.0907
206.0906
221.0946
226.1026
111.0531
119.0541
128.0653
151.0567
163.0574
78.0223
91.0582
236.0823
m/z

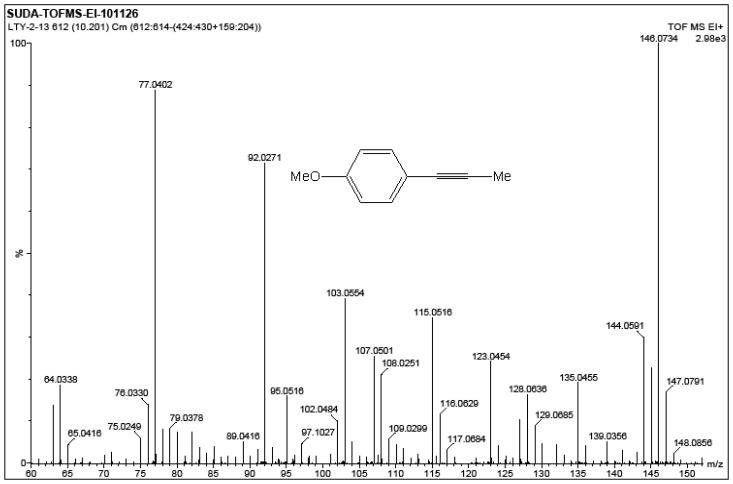

7.458
7.429
6.872
6.843
3.807
H_3CO
OCH_3
3.97
3.99
6.00
8.0
7.0
6.0
5.0
4.0
3.0

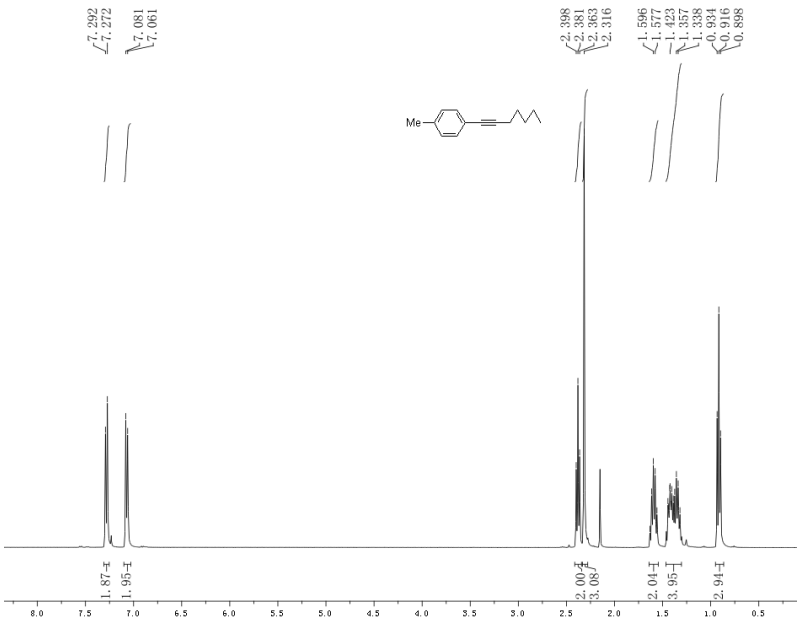

159.592
133.094
115.914
114.178
88.173
55.482
H_3CO
OCH_3
150
100
50

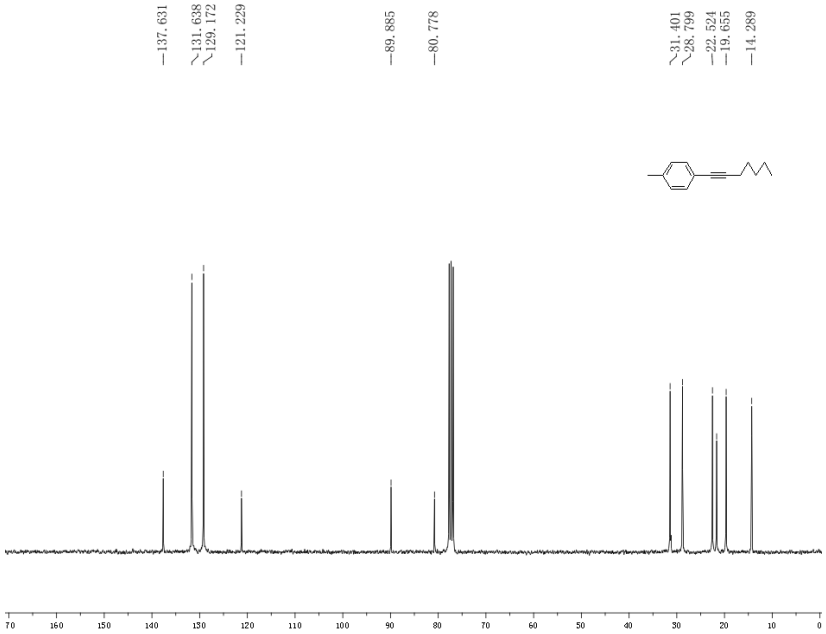

SUDA-TOFMS-EI
LTY-2-46 412 (6.867) Cm (412-(145:161+211:231))
TOF MS EI+
638
100
%
135.0436
MeO
OMe
238.0990
223.0740
239.1064
224.0786
242.0895
152.0564
136.0504
195.0812
180.0612
151.0561
153.0649
163.0530
181.1054
196.0780
222.1139
224.1171
107.0532
119.0824
126.1315
149.0410
71.0897
77.0400
83.0829
97.1061
0
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
m/z

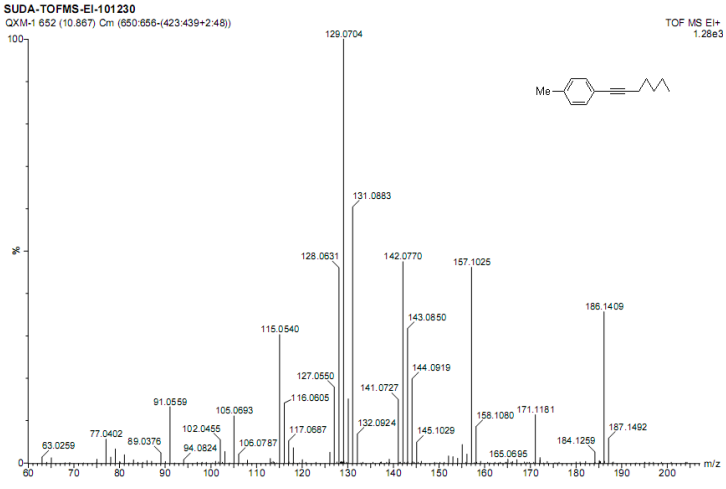

7.333
7.311
6.819
6.797
3.787
2.027
MeO
Me
1.72
1.80
3.04
3.00

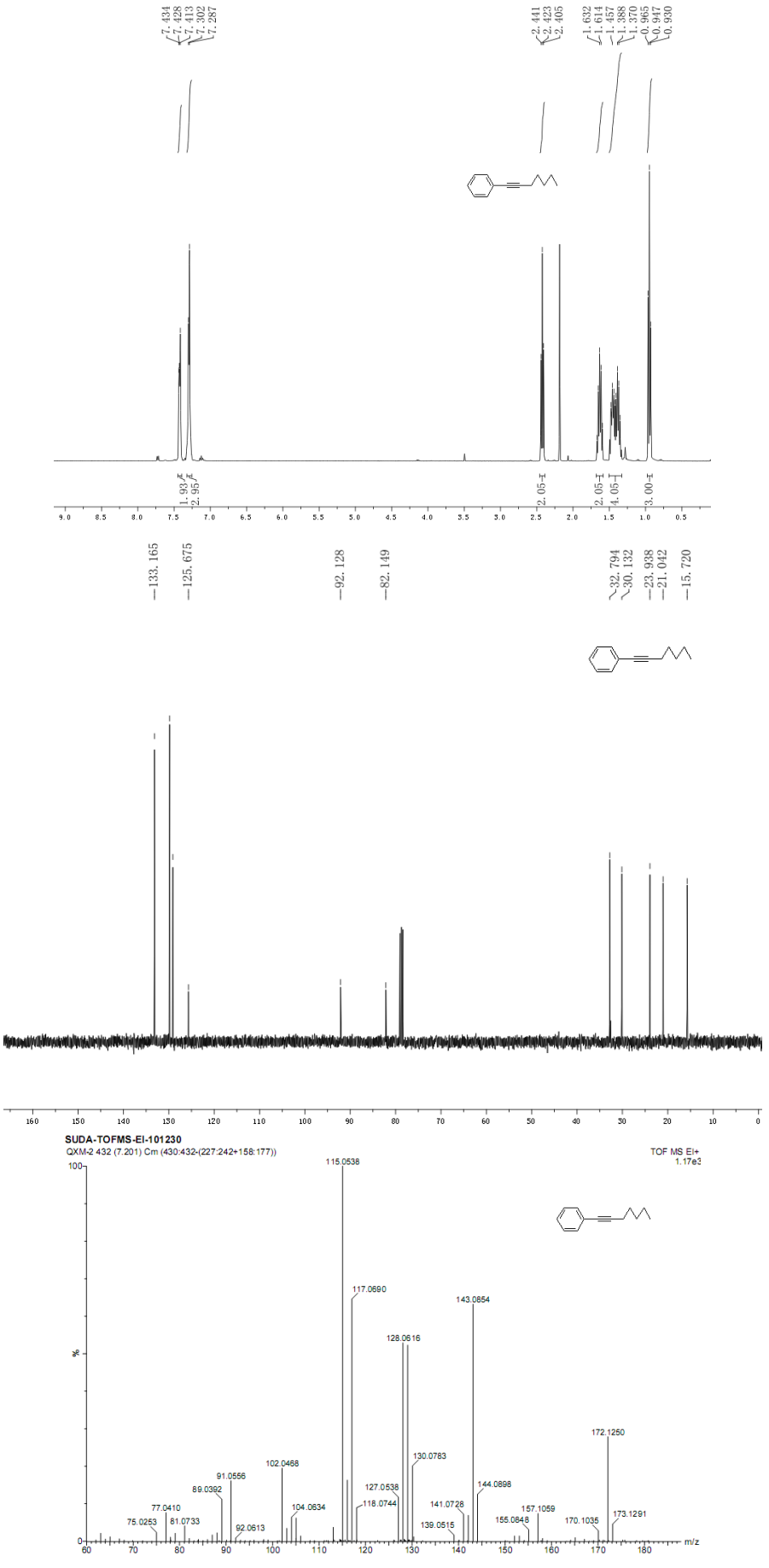

159.208
133.019
116.376
114.039
84.354
79.649
55.456
31.173
MeO
Me

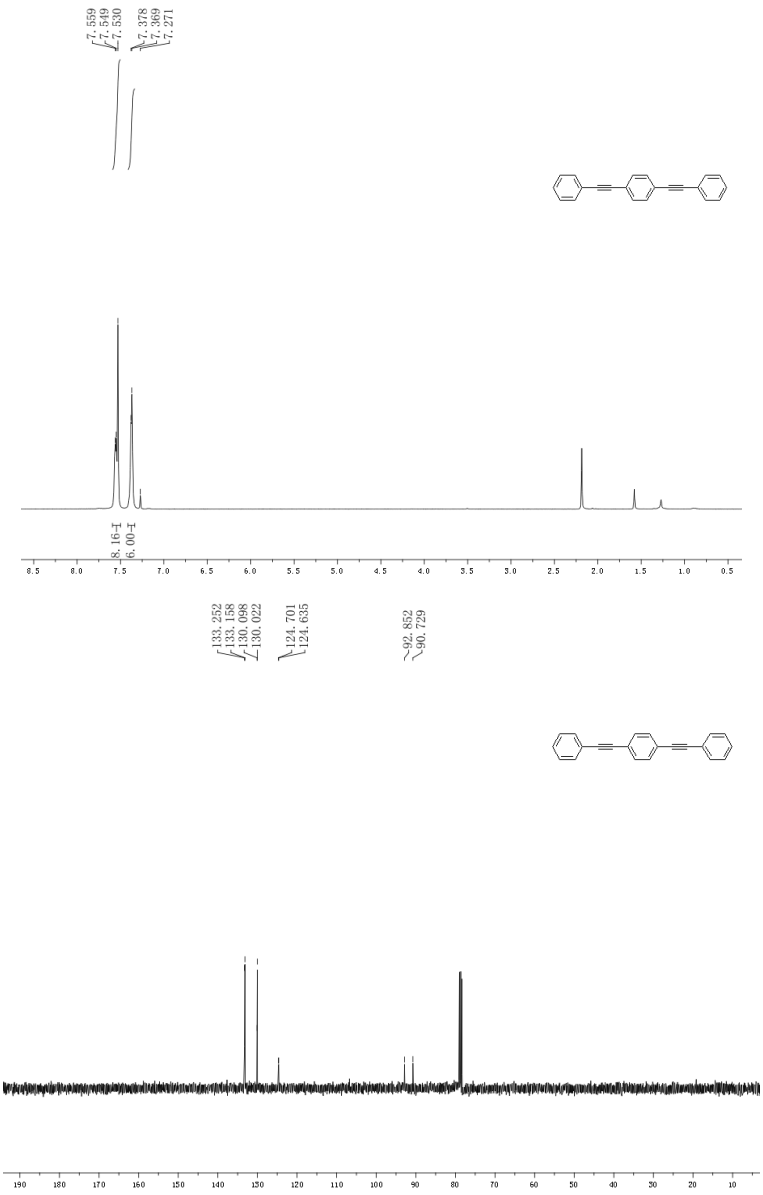

SUDA-TOFMS-EI-101126
LTY-2-13 612 (10.201) Cm (612:614-(424:430+159:204))
TOF MS EI+
146.0734 2.98e3
77.0402
92.0271
MeO
Me
103.0554
115.0516
144.0591
107.0501
108.0251
123.0454
64.0338
135.0455
147.0791
76.0330
95.0516
128.0636
102.0484
116.0629
129.0685
79.0378
75.0249
65.0416
89.0416
97.1027
109.0299
117.0684
139.0356
148.0856
%
m/z

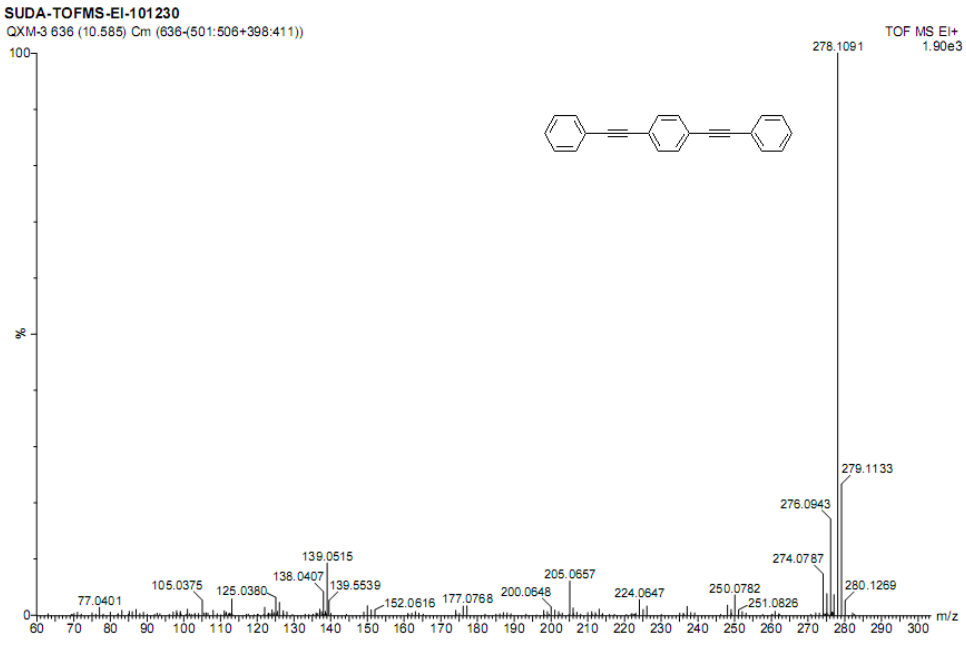


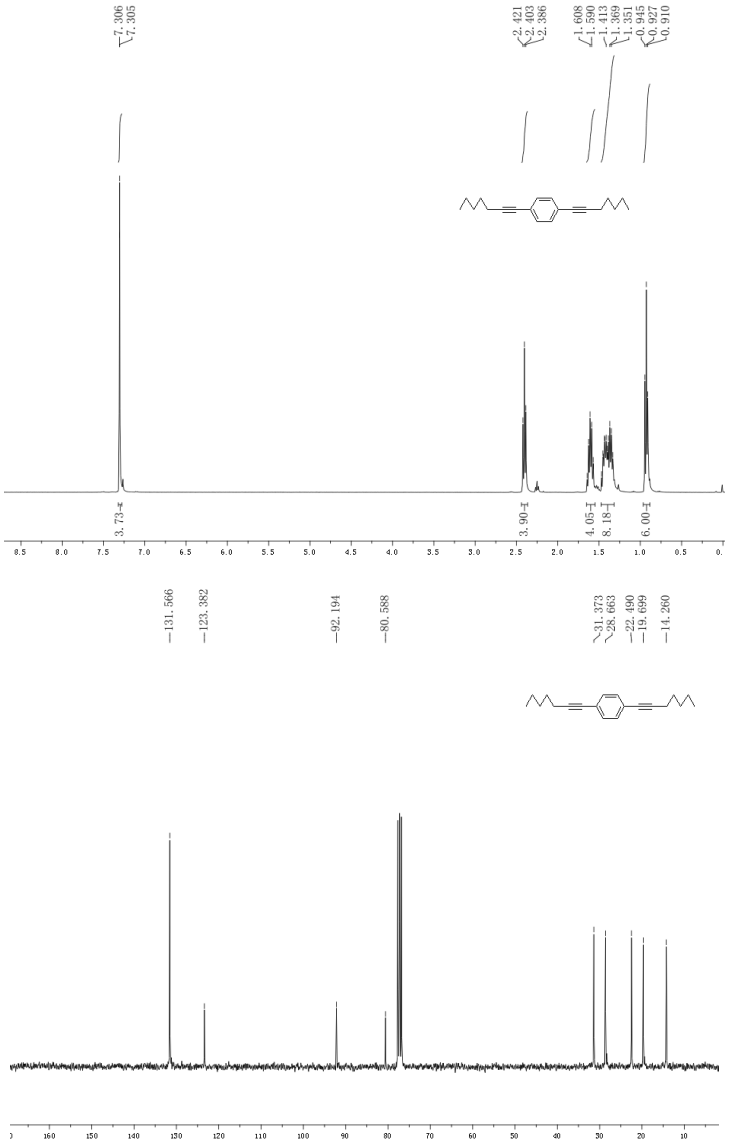


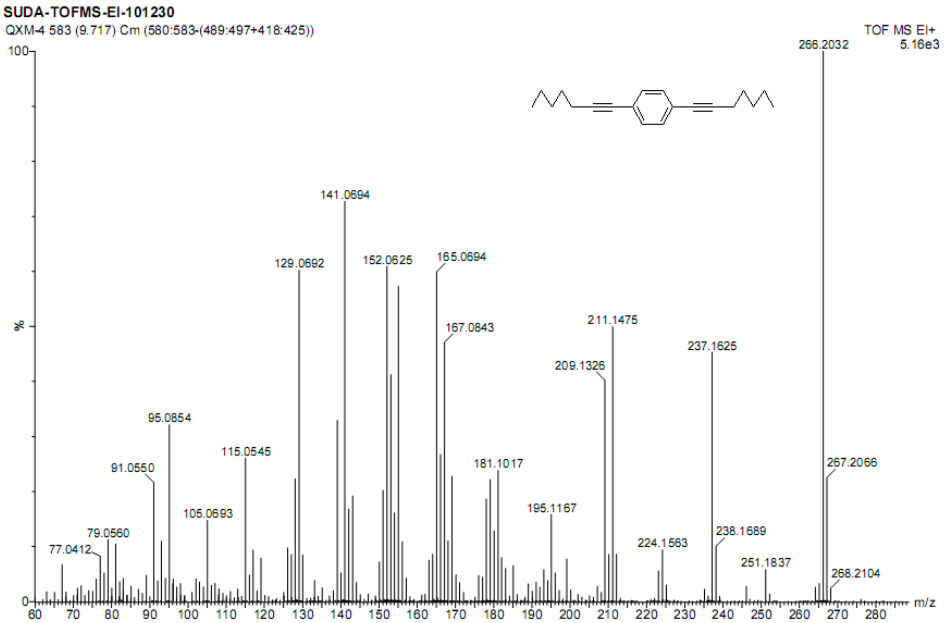


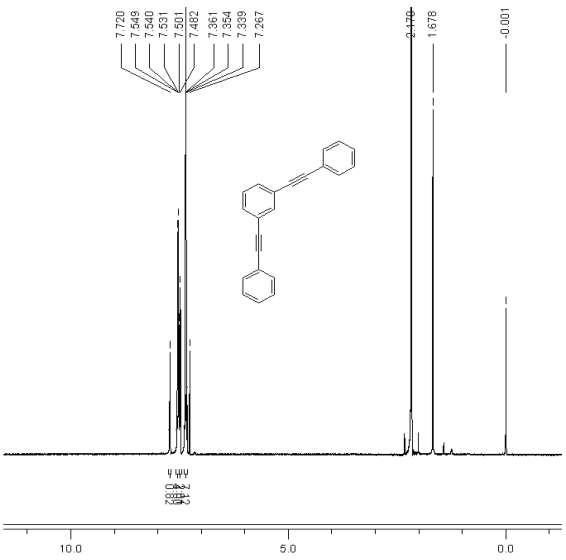


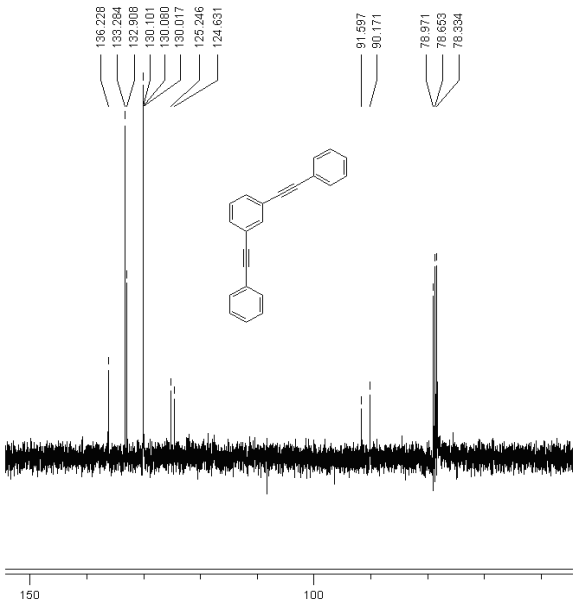

7.559
7.549
7.530
7.378
7.369
7.271
8.16
6.00
133.252
133.158
130.098
130.022
124.701
124.635
92.852
90.729

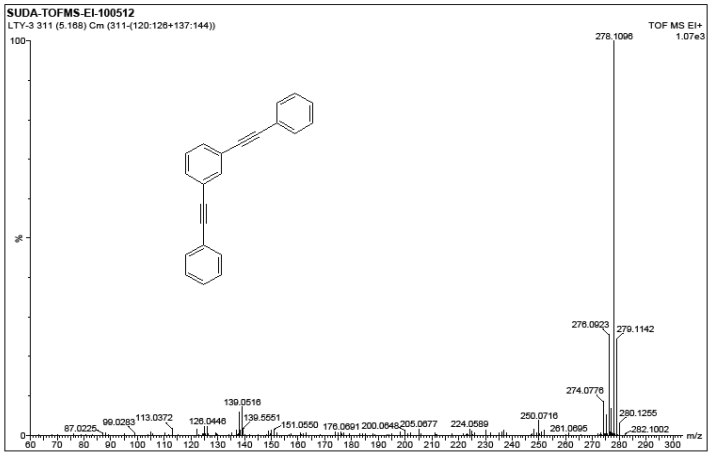

SUDA-TOFMS-EI-101230
QXM-3 636 (10.585) Cm (636-(501:506+398:411))
TOF MS EI+
1.90e3
100
%
0
278.1091
279.1133
276.0943
274.0787
280.1269
139.0515
138.0407
139.5539
105.0375
125.0380
77.0401
152.0616
177.0768
200.0648
205.0657
224.0647
250.0782
251.0826
m/z

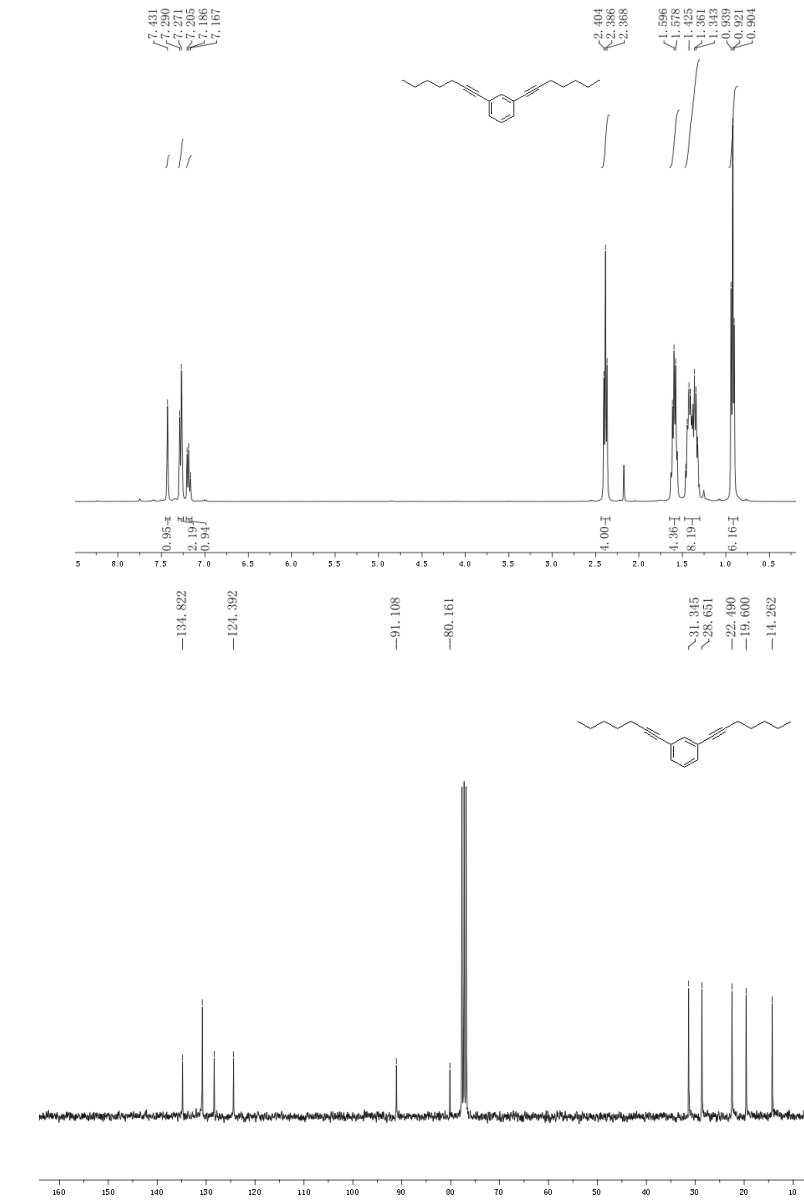

7.306
7.305
2.421
2.403
2.386
1.608
1.590
1.413
1.369
1.351
0.945
0.927
0.910
3.73
3.90
4.05
8.18
6.00
131.566
123.382
92.194
80.588
31.373
28.663
22.490
19.699
14.260

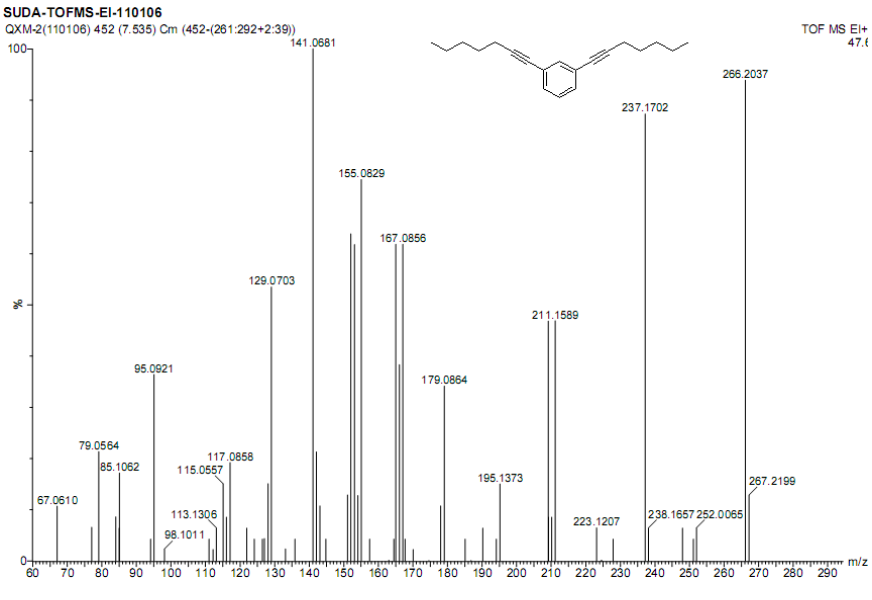

SUDA-TOFMS-EI-101230
QXM-4 583 (9.717) Cm (580:583-(489:497+418:425))
TOF MS EI+
5.16e3
266.2032
141.0694
129.0692
152.0625
165.0694
167.0843
211.1475
237.1625
209.1326
95.0854
115.0545
91.0550
181.1017
267.2066
105.0693
195.1167
79.0560
77.0412
224.1563
238.1689
251.1837
268.2104
%
m/z

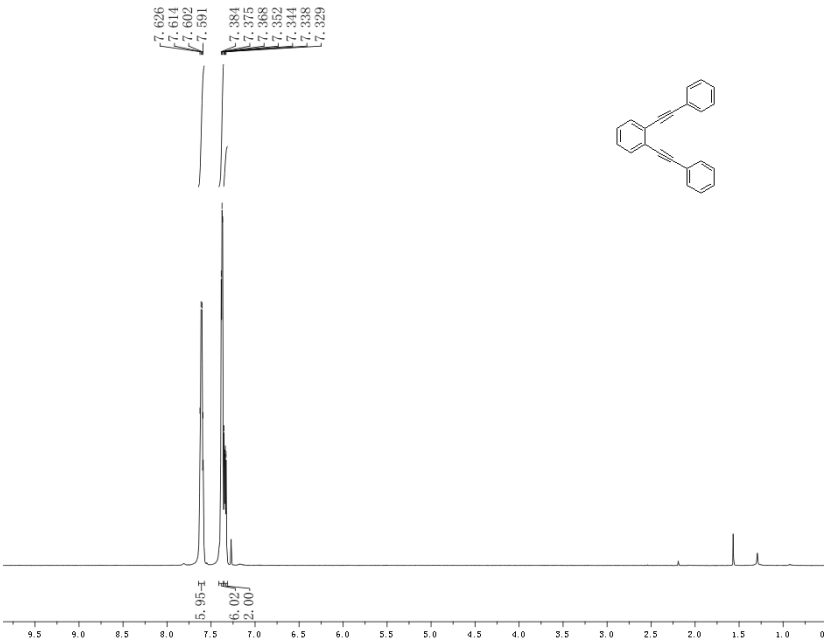

7.720
7.549
7.540
7.531
7.501
7.482
7.361
7.354
7.339
7.267
2.170
1.678
-0.001
10.0
5.0
0.0

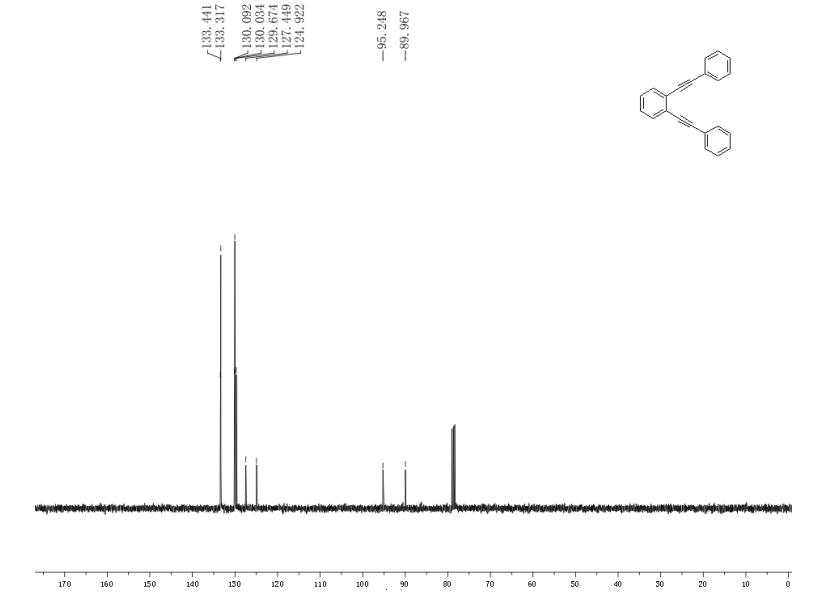

136.228
133.284
132.908
130.101
130.080
130.017
125.246
124.631
91.597
90.171
78.971
78.653
78.334
150
100

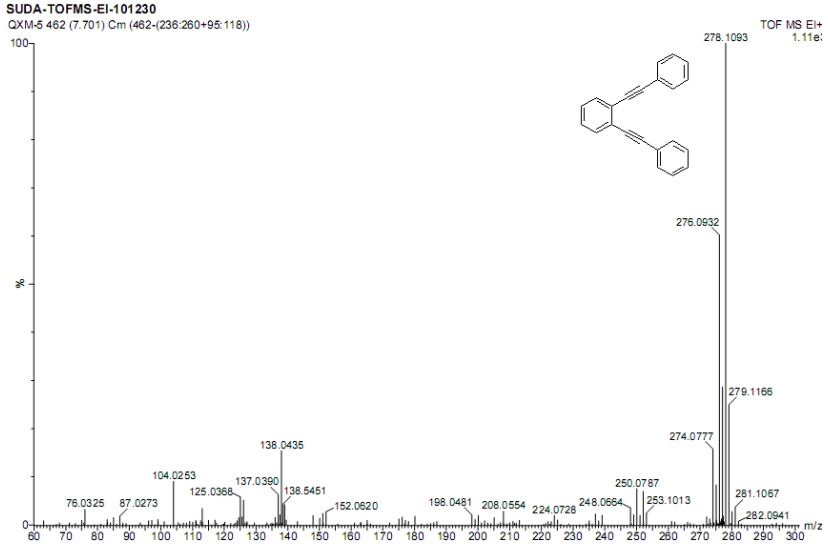

SUDA-TOFMS-EI-100512
LTY-3 311 (5.168) Cm (311-(120:126+137:144))
TOF MS EI+
1.07e3
278.1096
276.0923
279.1142
274.0776
280.1255
282.1002
261.0695
250.0716
224.0589
205.0677
200.0648
176.0691
151.0550
139.5551
130.0516
126.0446
113.0372
99.0283
87.0225
%
m/z

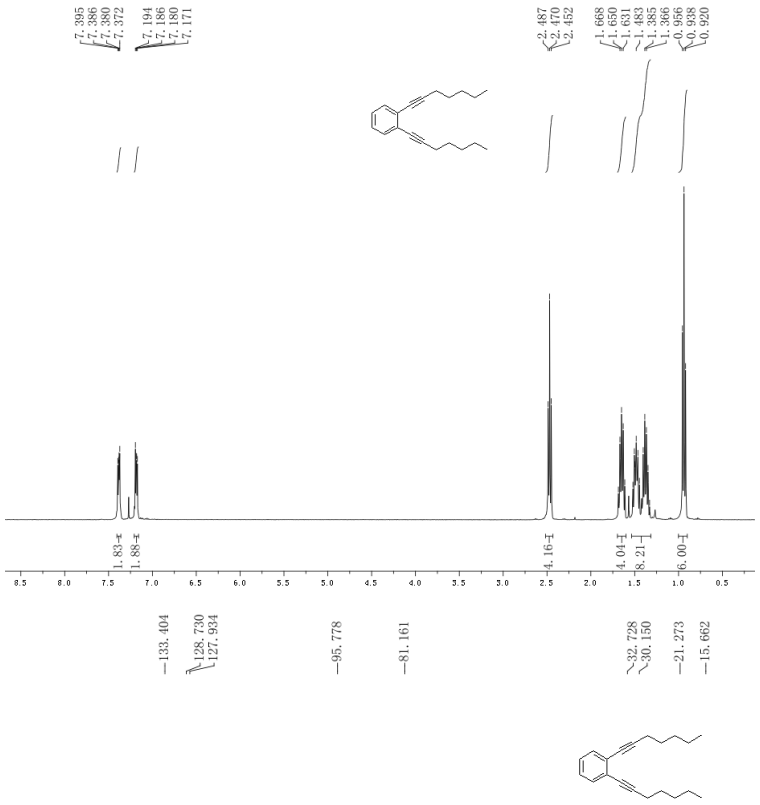

7.431
7.290
7.271
7.205
7.186
7.167
2.404
2.386
2.368
1.596
1.578
1.425
1.361
1.343
0.939
0.921
0.904
0.95
2.19
0.94
4.00
4.36
8.19
6.16
134.822
124.392
91.108
80.161
31.345
28.651
22.490
19.600
14.262

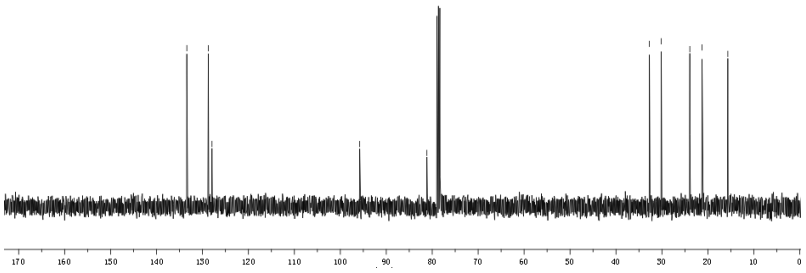

SUDA-TOFMS-EI-110106
QXM-2(110106) 452 (7.535) Cm (452-(261:292+2:39))
TOF MS EI+
141.0681
266.2037
237.1702
155.0829
167.0856
129.0703
211.1589
95.0921
179.0864
79.0564
85.1062
117.0858
115.0557
195.1373
67.0610
113.1306
98.1011
223.1207
238.1657
252.0065
267.2199
%
m/z

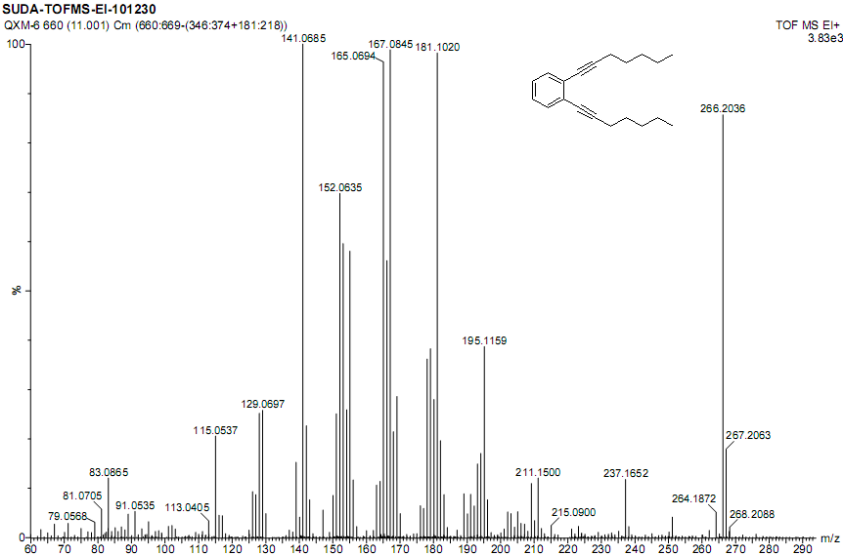

7.626
7.614
7.602
7.591
7.384
7.375
7.368
7.352
7.344
7.338
7.329
5.95
6.02
2.00

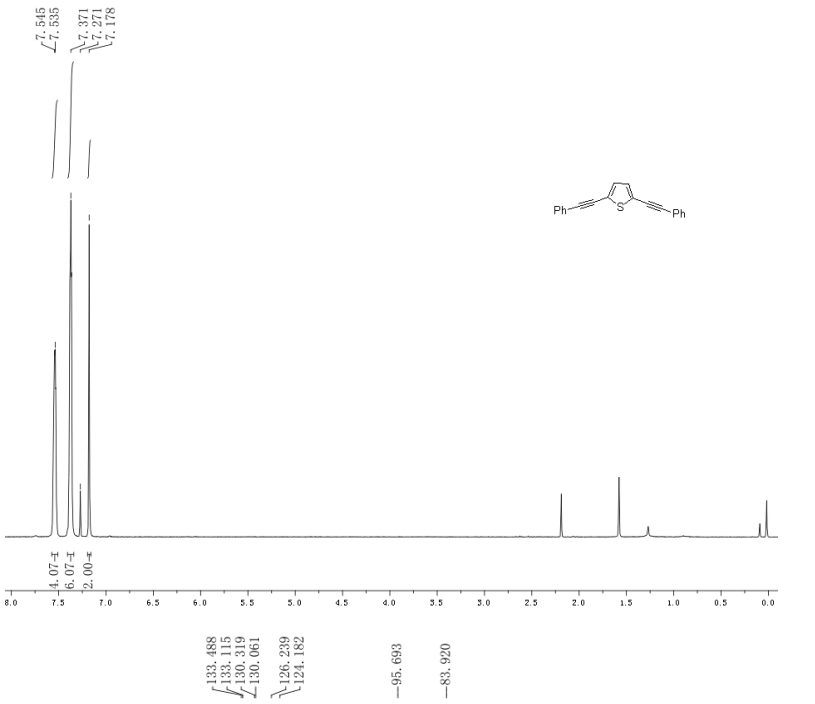

133.441
133.317
130.092
130.034
129.674
127.449
124.922
95.248
89.967

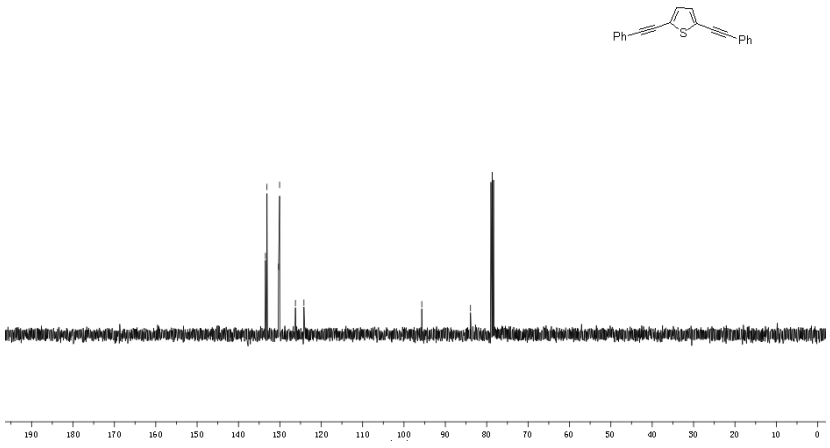

SUDA-TOFMS-EI-101230
QXM-5 462 (7.701) Cm (462-(236:260+95:118))
TOF MS EI+
278.1093
276.0932
279.1166
274.0777
138.0435
104.0253
137.0390
125.0368
138.5451
76.0325
87.0273
152.0620
198.0481
208.0554
224.0728
248.0664
250.0787
253.1013
281.1067
282.0941
%
m/z

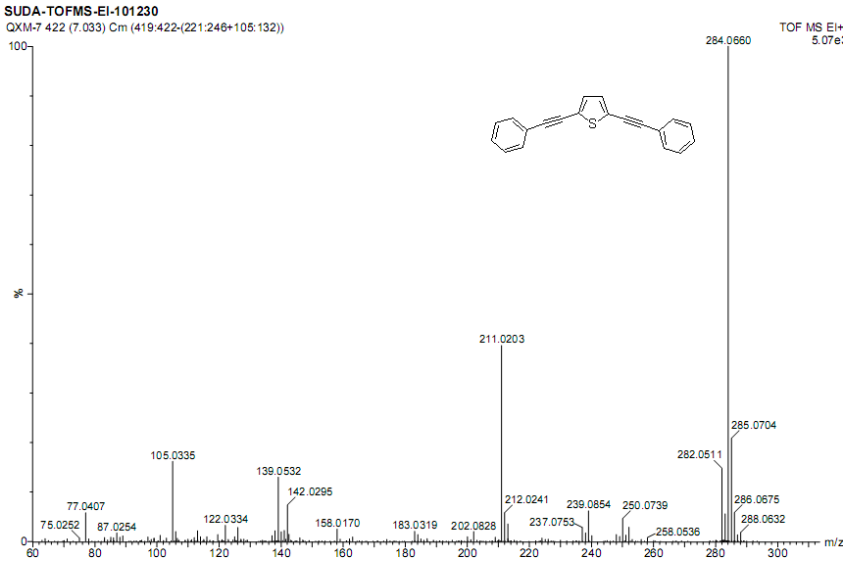







7.545
7.535
7.371
7.271
7.178
Ph
S
Ph
4.07
6.07
2.00
133.488
133.115
130.319
130.061
126.239
124.182
95.693
83.920


Ph
S
Ph


SUDA-TOFMS-EI-101230
QXM-7 422 (7.033) Cm (419:422-(221:246+105:132))
TOF MS EI+
5.07e
284.0660
211.0203
285.0704
282.0511
105.0335
139.0532
142.0295
286.0675
288.0632
77.0407
75.0252
87.0254
122.0334
158.0170
183.0319
202.0828
212.0241
237.0753
239.0854
250.0739
258.0536
%
m/z