Palladium-catalyzed *Z*-alkenylative cross-coupling via β-alkenyl elimination of *Z*-allylic alcohols

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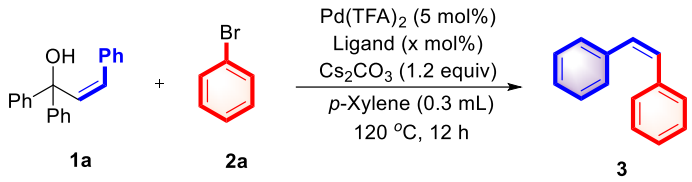
I. General Information

1H NMR and **13C NMR** spectra were recorded on a Bruker Avance 600 MHz and 400 MHz instruments. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26), carbon (chloroform δ 77.16) or tetramethylsilane (TMS δ 0.00) was used as a reference. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), dt (doublet of triplet). Coupling constants were reported in Hertz (Hz). High resolution mass spectra (HRMS) were recorded on quadrupole time-of-flight (QTOF) mass spectrometer (Bruker IMPACT II, Bremen, Germany) with Electron Spray Ionization (ESI) resource. For thin layer chromatography (**TLC**), Qingdao Haiyang Chemical was used, and compounds were visualized with a UV light at 254 nm. Further visualization was achieved by staining with phosphomolybdic acid solution or potassium permanganate solution followed by heating using a heat gun. Flash chromatography separations were performed on Qingdao Haiyang Chemical 200-300 mesh silica gel. All reactions were carried out under a nitrogen atmosphere. All commercially available reagents were used as received for the reactions without any purification. All solvents were dried on alumina columns using a solvent dispensing system.

Materials: $Pd(TFA)_2$, phosphine ligands, and Cs_2CO_3 were obtained from commercial suppliers and used without further purification. All Solvents were purified by standard procedure before use. Allylic alcohols[1-2] and bromobenzene[3] are synthesis via the known procedures.

II. Reaction Optimization

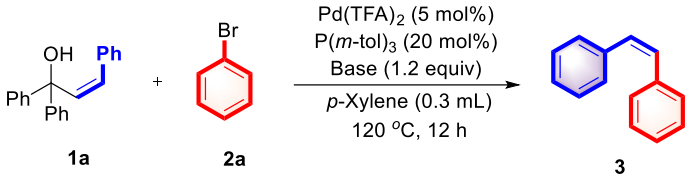
Table S1 Ligand screening of the reaction 1a and 2a



Entry	Ligand	Yield (%)
1	P(*m*-tol)$_3$ (20)	57
2	PPh$_3$ (20)	54
3[c]	P(*o*-tol)$_3$ (20)	45
4	P(*p*-tol)$_3$ (20)	47
5	P(1-nap)$_3$ (20)	30
6	SPhos (20)	trace
7	PCy$_3$ (10)	43
8	PAr$^F_3$ (10)	trace
9	DPPP (10)	NR
10	DPPPE (10)	10
11	DPPF (10)	22
12	DCyPF (10)	trace
13	Xantphos (10)	12

Reaction conditions: **1a** (0.1 mmol), **2a** (0.15 mmol), Pd(TFA)$_2$ (5 mol %), ligand (x mol %), Cs_2CO_3 (1.2 equiv.), and *p*-Xylene (0.3 mL) at 120 °C for 12 h. The yields are isolated yields. Ar^F = 3,5-(CF$_3$)$_2$C$_6$H$_3$.

Table S2 Base screening of the reaction 1a and 2a

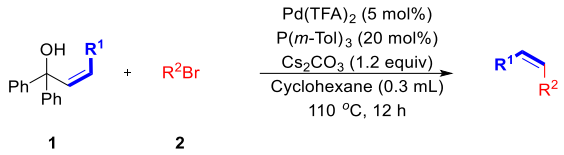


1a 2a 3

Entry	Base	Yield (%)
1	Cs_2CO_3	57
2	Na_2CO_3	NR
3[c]	K_2CO_3	NR
4	K_3PO_4	trace
5	NaOH	33
6	KOH	23
7	NaO^{t}Bu	42
8	KO^{t}Bu	39
9	TMG	NR
10	DBU	NR

Reaction conditions: **1a** (0.1 mmol), **2a** (0.15 mmol), $Pd(TFA)_2$ (5 mol %), P(*m*-tol)$_3$ (20 mol %), base (1.2 equiv.), and *p*-Xylene (0.3 mL) at 120 °C for 12 h. The yields are isolated yields.

III. General procedure

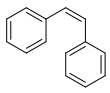


1 2

To a vial equipped with a dried stir bar was added cis-allyl alcohol 1 (0.1 mmol), aryl bromide 2 (0.15 mmol), Pd(TFA)2 (5 mol%), P(m-Tol)3 (20 mol%) and cyclohexane (0.3 mL) in a nitrogen box. The reaction mixture was sealed with a screw cap and stirred at 110 ^{o}C (oil bath) for 12 h. After cooling to room temperature, the residue was purified by column chromatography with silica gel to give the products.

IV. The analytical and spectral characterization data

(*Z*)-1,2-Diphenylethene (3)[4]



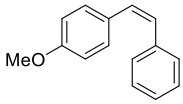
3

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 77% yield (13.9 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25-7.16 (m, 10H), 6.59 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.4, 130.4, 129.0, 128.3, 127.2.

(*Z*)-1-Methoxy-4-styrylbenzene (4)[4]



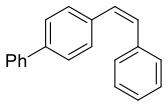
4

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 81% yield (17.1mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (d, *J* = 7.2 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 2H), 7.20-7.15 (m, 3H), 6.75 (d, *J* = 8.4 Hz, 2H), 6.54-6.48 (m, 2H), 3.77 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.8, 137.8, 130.3, 129.9, 129.8, 129.0, 128.9, 128.4, 127.0, 113.8, 55.2.

(*Z*)-1-Methoxy-4-styrylbenzene (5)[5]



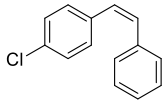
5

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 87% yield (22.3 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.35-7.28 (m, 5H), 7.26-7.19 (m, 3H), 6.65-6.58 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 140.8, 139.9, 137.5, 136.4, 130.6, 129.9, 129.5, 129.0, 128.9, 128.4, 127.4, 127.3, 127.0, 127.0.

(*Z*)-1-Chloro-4-styrylbenzene (6)[4]



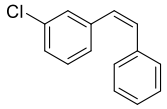
6

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 60% yield (12.9 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29-7.23 (m, 5H), 7.22-7.18 (m, 4H), 6.65 (d, *J* = 12.0 Hz, 1H), 6.56 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, CDCl3) δ 137.0, 135.8, 132.9, 131.1, 130.4, 129.1, 129.0, 128.6, 128.5, 127.5.

(*Z*)-1-Chloro-3-styrylbenzene (7)[4]



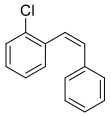
7

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 58% yield (12.4 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28-7.23 (m, 6H), 7.20-7.13 (m, 3H), 6.68 (d, *J* = 12.0 Hz, 1H), 6.55 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 139.3, 136.8, 134.2, 131.7, 129.6, 129.0, 129.0, 128.9, 128.5, 127.6, 127.3, 127.2.

(*Z*)-1-Chloro-2-styrylbenzene (8)[6]



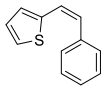
8

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 58% yield (12.5 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.8 Hz, 1H), 7.23-7.13 (m, 7H), 7.03 (t, *J* = 7.8 Hz, 1H), 6.71 (d, *J* = 12.0 Hz, 1H), 6.67 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 136.6, 136.2, 133.8, 131.9, 130.9, 129.7, 129.1, 128.6, 128.3, 127.5, 127.4, 126.5.

(*Z*)-2-Styrylthiophene (9)[7]



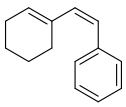
9

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 39% yield (7.3 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.33 (m, 4H), 7.30-7.28 (m, 1H), 7.08 (d, *J* = 4.2 Hz, 1H), 6.96 (s, 1H), 6.89 (t, *J* = 4.2 Hz, 1H), 6.70 (d, *J* = 12.0 Hz, 1H), 6.58 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 140.0, 137.5, 129.0, 129.0, 128.7, 128.3, 127.7, 126.6, 125.7, 123.5.

(*Z*)-(2-(Cyclohex-1-en-1-yl)vinyl)benzene (10)[8]



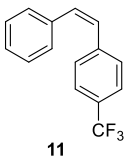
10

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 46% yield (8.4 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.2 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 1H), 6.34 (d, *J* = 12.0 Hz, 1H), 6.11 (d, *J* = 12.0 Hz, 1H), 5.78-5.74 (m, 1H), 2.13-2.07 (m, 2H), 1.96-1.90 (m, 2H), 1.61-1.57 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.8, 135.8, 133.9, 129.2, 129.0, 127.9, 127.4, 126.6, 28.3, 25.9, 23.0, 22.3.

(*Z*)-1-Styryl-4-(trifluoromethyl)benzene (11)[4]



11

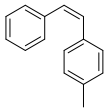
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 91% yield (22.6 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.24-7.18 (m, 4H), 6.72 (d, *J* = 12.6 Hz, 1H), 6.59 (d, *J* = 12.6 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 141.1, 136.7, 132.5, 129.3, 129.1 (q, *J* = 32.6 Hz), 129.0, 128.9, 128.6, 127.7, 125.3 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 272.1 Hz).

^{19}F NMR (565 MHz, $CDCl_3$) δ -62.53.

(*Z*)-1-Methyl-4-styrylbenzene (12)[4]



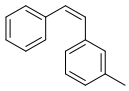
12

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 66% yield (12.8 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26-7.17 (m, 5H), 7.14 (d, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 6.58-6.52 (m, 2H), 2.31 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.7, 137.0, 134.4, 130.4, 129.7, 129.0, 129.0, 129.0, 128.3, 127.1.

(*Z*)-1-Methyl-3-styrylbenzene (13)[7]



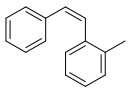
13

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 79% yield (15.3 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25-7.15 (m, 5H), 7.11-7.03 (m, 3H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.57 (s, 2H), 2.25 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.9, 137.5, 137.3, 130.5, 130.2, 129.7, 129.0, 128.3, 128.2, 128.0, 127.2, 126.0, 21.5.

(*Z*)-1-Methyl-2-styrylbenzene (14)[9]



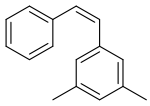
14

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 42% yield (8.1 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.19 (d, *J* = 7.2 Hz, 1H), 7.17-7.13 (m, 5H), 7.10 (d, *J* = 7.2 Hz, 2H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 12.0 Hz, 1H), 6.61 (d, *J* = 12.0 Hz, 1H), 2.27 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.3, 137.2, 136.2, 130.7, 130.2, 129.7, 129.0, 129.0, 128.2, 127.4, 127.2, 125.8, 12.0.

(*Z*)-1,3-Dimethyl-5-styrylbenzene (15)[4]



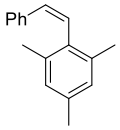
15

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 63% yield (13.1 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (d, *J* = 4.8 Hz, 2H), 7.22-7.16 (m, 3H), 6.87 (s, 2H), 6.83 (s, 1H), 6.55 (d, *J* = 12.0 Hz, 1H), 6.53 (d, *J* = 12.0 Hz, 1H), 2.21 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.8, 137.5, 137.3, 130.6, 130.0, 129.0, 128.9, 128.2, 127.1, 126.7, 21.3.

(*Z*)-1,3,5-Trimethyl-2-styrylbenzene (16)[10]



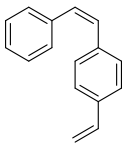
16

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 43% yield (9.5 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.15-7.10 (m, 3H), 7.01 (d, *J* = 7.8 Hz, 2H), 6.86 (s, 2H), 6.62 (d, *J* = 12.0 Hz, 1H), 6.51 (d, *J* = 12.0 Hz, 1H), 2.30 (s, 3H), 2.11 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.8, 136.5, 135.6, 134.2, 131.2, 129.1, 128.5, 128.3, 128.2, 127.2, 29.9, 21.2, 20.3.

(*Z*)-1-Styryl-4-vinylbenzene (17)[11]



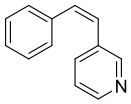
17

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 55% yield (11.4 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29-7.17 (m, 9H), 6.66 (dd, *J* = 18.0 Hz, 11.4 Hz, 1H), 6.60 (d, *J* = 12.0 Hz, 1H), 6.56 (d, *J* = 12.0 Hz, 1H), 5.71 (d, *J* = 18.0 Hz, 1H), 5.21 (d, *J* = 11.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.5, 137.0, 136.7, 136.5, 130.5, 130.0, 129.2, 129.0, 128.4, 127.3, 126.2, 113.8.

(*Z*)-3-Styrylpyridine (18)[4]



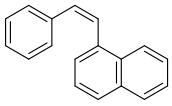
18

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 88% yield (15.9 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 1.2 Hz, 1H), 8.41 (dd, *J* = 4.8 Hz, 1.2 Hz, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.25-7.20 (m, 5H), 7.11 (dd, *J* = 7.8 Hz, 4.8 Hz, 1H), 6.75 (d, *J* = 12.0 Hz, 1H), 6.54 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 150.3, 148.2, 136.7, 135.9, 133.1, 132.8, 128.8, 128.6, 127.7, 126.6, 123.1.

(*Z*)-1-Styrylnaphthalene (19)[4]



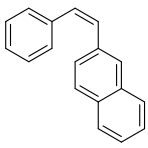
19

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 50% yield (11.6 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.53-7.46 (m, 2H), 7.37-7.31 (m, 2H), 7.08 (s, 5H), 7.05 (d, *J* = 12.0 Hz, 1H), 6.83 (d, *J* = 12.6 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 136.9, 135.4, 133.8, 132.2, 131.7, 129.2, 128.6, 128.6, 128.2, 127.7, 127.2, 126.6, 126.2, 126.1, 125.7, 125.1.

(*Z*)-2-Styrylnaphthalene (20)[12]



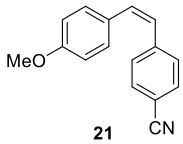
20

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 74% yield (17.0 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 6.0 Hz, 3.6 Hz, 1H), 7.74-7.69 (m, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.44-7.41 (m, 2H), 7.34 (dd, *J* = 9.0 Hz, 1.8 Hz, 1H), 7.28 (d, *J* = 6.6 Hz, 2H), 7.23-7.18 (m, 3H), 6.76 (d, *J* = 12.0 Hz, 1H), 6.68 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.4, 135.0, 133.6, 132.7, 130.8, 130.3, 129.1, 128.4, 128.1, 128.1, 127.8, 127.6, 127.4, 127.1, 126.1, 126.0.

(*Z*)-4-(4-Methoxystyryl)benzonitrile (21)[6]



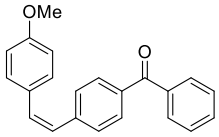
21

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 78% yield (18.4 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 6.68 (d, *J* = 12.0 Hz, 1H), 6.47 (d, *J* = 12.0 Hz, 1H), 3.79 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 159.4, 142.7, 133.0, 132.2, 130.3, 129.6, 128.7, 127.0, 119.1, 114.0, 110.4, 55.4.

(*Z*)-(4-(4-Methoxystyryl)phenyl)(phenyl)methanone (22)[13]



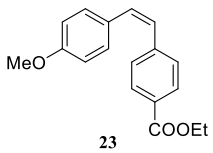
22

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 64% yield (20.1 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.2 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 6.66 (d, *J* = 12.0 Hz, 1H), 6.53 (d, *J* = 12.0 Hz, 1H), 3.79 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 196.4, 159.2, 142.3, 137.9, 135.9, 132.4, 132.1, 130.4, 130.4, 130.1, 129.2, 128.9, 128.4, 127.8, 113.9, 55.4.

Ethyl (*Z*)-4-(4-methoxystyryl)benzoate (23)[14]



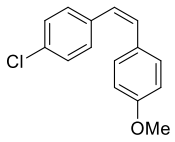
23

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 63% yield (17.8 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* = 9.0 Hz, 2H), 6.75 (d, *J* = 9.0 Hz, 2H), 6.63 (d, *J* = 12.0 Hz, 1H), 6.51 (d, *J* = 12.0 Hz, 1H), 4.36 (q, *J* = 7.2 Hz, 2H), 3.79 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.6, 159.2, 142.6, 131.8, 130.4, 129.7, 129.2, 128.9, 127.9, 113.9, 61.0, 55.3, 14.5.

(*Z*)-1-Chloro-4-(4-methoxystyryl)benzene (24)[6]



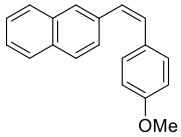
24

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 55% yield (13.4 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.19 (s, 4H), 7.15 (d, *J* = 9.0 Hz, 2H), 6.76 (d, *J* = 9.0 Hz, 2H), 6.55 (d, *J* = 12.0 Hz, 1H), 6.43 (d, *J* = 12.0 Hz, 1H), 3.79 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 159.0, 136.2, 132.6, 130.6, 130.3, 130.3, 129.4, 128.6, 127.6, 113.9, 55.4.

(*Z*)-2-(4-Methoxystyryl)naphthalene (25)[15]



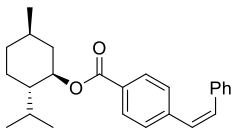
25

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 70% yield (18.3 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81-7.75 (m, 1H), 7.75-7.71 (m, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.44-7.41 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.67 (d, *J* = 12.0 Hz, 1H), 6.61 (d, *J* = 12.0 Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 135.4, 133.7, 132.3, 130.4, 130.3, 128.8, 128.1, 127.9, 127.8, 127.7, 127.2, 126.1, 125.9, 113.8, 55.4.

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl-4-((*Z*)-styryl)benzoate (26)



26

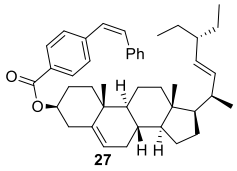
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 51% yield (18.5 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.25-7.20 (m, 5H), 6.70 (d, *J* = 12.0 Hz, 1H), 6.60 (d, *J* = 12.0 Hz, 1H), 4.91 (dt, *J* = 10.8, 4.2 Hz, 1H), 2.12 (d, *J* = 12.0 Hz, 1H), 1.99-1.92 (m, 1H), 1.72 (d, *J* = 11.4 Hz, 2H), 1.56-1.49 (m, 2H), 1.16-1.06 (m, 2H), 0.94-0.88 (m, 7H), 0.79 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.1, 142.0, 136.9, 132.3, 129.6, 129.5, 129.4, 129.0, 129.0, 128.5, 127.6, 74.9, 47.4, 41.2, 34.5, 31.6, 26.6, 23.8, 22.2, 20.9, 16.7.

HRMS(ESI): m/z Calcd. for $C_{25}H_{30}O_2Na$ $[M+Na]^+$: 385.2138; Found: 385.2138. Δ = 0.00 ppm.

(*3S,8S,9S,10R,13R,14S,17R*)-17-((*2R,5S,E*)-5-Ethyl-6-methylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-((*Z*)-styryl)benzoate (27)



27

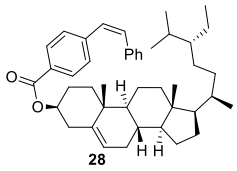
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 36% yield (22.0 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.22 (s, 5H), 6.70 (d, *J* = 12.0 Hz, 1H), 6.61 (d, *J* = 12.0 Hz, 1H), 5.41 (d, *J* = 4.2 Hz, 1H), 5.16 (dd, *J* = 15.6 Hz, 8.4 Hz, 1H), 5.02 (dd, *J* = 15.6 Hz, 8.4 Hz, 1H), 4.87-4.80 (m, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 2.07-1.97 (m, 5H), 1.91 (d, *J* = 13.2 Hz, 1H), 1.76-1.67 (m, 3H), 1.23-1.14 (m, 5H), 1.07-1.02 (m, 9H), 0.87-0.80 (m, 15H), 0.70 (d, *J* = 10.8 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.0, 142.0, 139.8, 138.5, 136.9, 132.3, 129.6, 129.5, 129.0, 128.9, 128.5, 127.6, 122.9, 74.7, 57.0, 56.1, 51.4, 50.3, 42.4, 40.6, 39.8, 38.4, 37.2, 36.8, 32.1, 29.1, 28.1, 25.6, 24.5, 21.4, 21.2, 21.2, 19.5, 19.2, 12.4, 12.2.

HRMS(ESI): m/z Calcd. for $C_{44}H_{58}O_2Na$ $[M+Na]^+$: 641.4329; Found: 641.4332. Δ = 0.47 ppm.

(*3S,8S,9S,10R,13R,14S,17R*)-17-((*2R,5R*)-5-Ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-((Z)-styryl)benzoate (28)



28

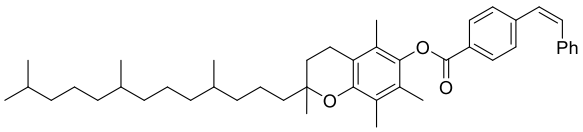
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 51% yield (31.7 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.22 (s, 5H), 6.70 (d, *J* = 12.0 Hz, 1H), 6.61 (d, *J* = 12.0 Hz, 1H), 5.41-5.37 (m, 1H), 4.87-4.80 (m, 1H), 2.45 (d, *J* = 7.8 Hz, 2H), 2.06-1.95 (m, 4H), 1.93-1.83 (m, 2H), 1.75-1.63 (m, 3H), 1.23-1.12 (m, 6H), 1.09-0.98 (m, 9H), 0.96-0.89 (m, 4H), 0.89-0.77 (m, 13H), 0.70 (d, *J* = 10.8 Hz, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.0, 142.1, 139.9, 136.9, 132.3, 129.6, 129.5, 129.0, 128.9, 128.5, 127.6, 122.9, 74.7, 56.9, 56.2, 51.4, 50.2, 46.0, 42.5, 39.9, 38.4, 37.2, 36.8, 36.3, 34.1, 32.1, 29.4, 28.1, 26.3, 24.5, 23.3, 21.2, 20.0, 19.5, 19.2, 19.2, 19.0, 12.1, 12.0.

HRMS(ESI): m/z Calcd. for $C_{44}H_{60}O_2Na$ $[M+Na]^+$: 641.4486; Found: 643.4495. Δ = 1.40 ppm.

2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl (*Z*)-4-styrylbenzoate (29)



29

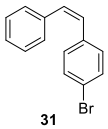
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 54% yield (34.3 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.8 Hz, 2H), 7.38 (d, *J* = 7.8 Hz, 2H), 7.27-7.23 (m, 5H), 6.75 (d, *J* = 12.0 Hz, 1H), 6.64 (d, *J* = 12.0 Hz, 1H), 2.61 (t, *J* = 6.6 Hz, 2H), 2.11 (s, 3H), 2.05 (s, 3H), 2.01 (s, 3H), 1.86-1.74 (m, 2H), 1.53-1.50 (m, 1H), 1.43-1.33 (m, 5H), 1.29-1.22 (m, 11H), 1.16-1.03 (m, 7H), 0.87-0.74 (m, 12H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 165.1, 149.6, 142.7, 136.8, 132.6, 130.2, 129.3, 129.2, 129.0, 128.6, 128.2, 127.7, 127.1, 125.3, 123.3, 75.2, 39.5, 37.6, 33.0, 28.1, 25.0, 24.6, 22.9, 22.8, 21.2, 20.8, 19.9, 19.9, 13.2, 12.4, 12.0.

HRMS(ESI): m/z Calcd. for $C_{44}H_{66}O_3Na$ $[M+Na]^+$: 659.4435; Found: 659.4430. Δ = 0.76 ppm.

(*Z*)-1-Bromo-4-styrylbenzene (31)[11]



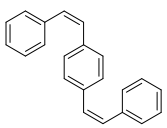
31

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 78% yield (20.2 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.4 Hz, 2H), 7.24-7.18 (m, 5H), 7.10 (d, *J* = 8.4 Hz, 2H), 6.63 (d, *J* = 12.0 Hz, 1H), 6.50 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.0, 136.3, 131.5, 131.2, 130.7, 129.1, 129.0, 128.5, 127.5, 121.1.

1,4-Di((*Z*)-styryl)benzene (32)[4]



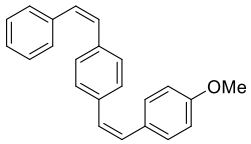
32

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 81% yield (22.8 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (t, *J* = 7.2 Hz, 4H), 7.21 (t, *J* = 7.2 Hz, 4H), 7.17 (t, *J* = 7.2 Hz, 2H), 7.10 (s, 4H), 6.57 (d, *J* = 12.0 Hz, 2H), 6.53 (d, *J* = 12.0 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.5, 136.2, 130.4, 130.1, 129.0, 128.9, 128.3, 127.3.

1-Methoxy-4-((*Z*)-4-((*Z*)-styryl)styryl)benzenel (34)



34

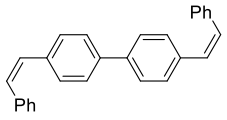
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 52% yield (16.2 mg) as a colorless oil.

1H NMR (600 MHz, CDCl3) δ 7.27 (d, J = 7.2 Hz, 2H), 7.23-7.19 (m, 5H), 7.12 (dd, J = 10.2 Hz, 8.4 Hz, 4H), 6.75 (d, J = 8.4 Hz, 2H), 6.57 (d, J = 12.6 Hz, 1H), 6.54 (d, J = 12.6 Hz, 1H), 6.50 (d, J = 12.6 Hz, 1H), 6.44 (d, J = 12.6 Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9, 137.5, 136.6, 136.0, 130.3, 130.3, 130.2, 130.0, 129.9, 129.0, 128.9, 128.8, 128.6, 128.3, 127.2, 113.7, 55.3.

HRMS(ESI): m/z Calcd. for $C_{23}H_{20}ONa$ $[M+Na]^+$: 335.1406; Found: 335.1405. Δ = 0.29 ppm.

4,4'-Di((*Z*)-styryl)-1,1'-biphenyl (36)[16]



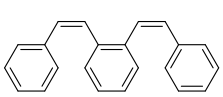
36

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 82% yield (29.4 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz, 4H), 7.31-7.27 (m, 8H), 7.23 (t, *J* = 7.8 Hz, 4H), 7.19 (t, *J* = 7.2 Hz, 2H), 6.63-6.57 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 139.3, 137.5, 136.4, 130.6, 129.9, 129.5, 129.0, 128.4, 127.3, 126.7.

1,2-Di((*Z*)-styryl)benzene (38)[17]



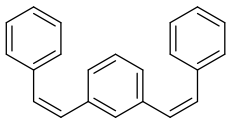
38

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 75% yield (21.1 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24-7.20 (m, 2H), 7.18-7.10 (m, 10H), 7.08-7.03 (m, 2H), 6.63 (d, *J* = 12.0 Hz, 2H), 6.59 (d, *J* = 12.0 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.6, 137.4, 130.5, 130.2, 129.6, 129.0, 128.3, 128.2, 127.7, 127.2.

1,3-Di((*Z*)-styryl)benzene (40)



40

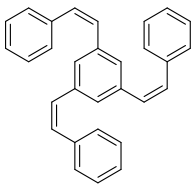
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 81% yield (22.9 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24-7.14 (m, 11H), 7.07-7.03 (m, 3H), 6.55 (d, *J* = 12.0 Hz, 2H), 6.49 (d, *J* = 12.0 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.2, 136.7, 130.9, 129.5, 129.3, 129.1, 128.2, 127.2, 127.2.

HRMS(ESI): m/z Calcd. for $C_{22}H_{19}$ $[M+H]^+$: 283.1481; Found: 283.1476. Δ = 1.77 ppm.

1,3,5-Tri((*Z*)-styryl)benzene (42)



42

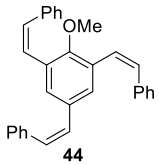
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 62% yield (23.8 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 (s, 15H), 6.98 (s, 3H), 6.48 (d, *J* = 12.6 Hz, 3H), 6.39 (d, *J* = 12.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 137.7, 137.2, 130.6, 130.0, 129.0, 128.3, 128.1, 127.2.

HRMS(ESI): m/z Calcd. for $C_{30}H_{24}Na$ $[M+Na]^+$: 407.1770; Found: 407.1772. Δ = 0.49 ppm.

((1*Z*,1'*Z*,1''*Z*)-(2-methoxybenzene-1,3,5-triyl)tris(ethene-2,1-diyl))tribenzene (44)



44

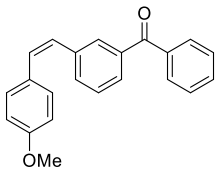
The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 62% yield (17.6 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23-7.12 (m, 10H), 7.08 (m, 1H), 7.03 (m, 4H), 6.99 (s, 2H), 6.64 (d, *J* = 12.0 Hz, 2H), 6.58 (d, *J* = 12.0 Hz, 2H), 6.34 (d, *J* = 12.0 Hz, 1H), 6.21 (d, *J* = 12.0 Hz, 1H), 3.77 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 155.5, 137.1, 137.0, 132.9, 131.3, 131.1, 130.0, 129.9, 129.4, 129.0, 128.8, 128.3, 128.2, 127.3, 127.0, 125.9, 61.2.

HRMS(ESI): m/z Calcd. for $C_{31}H_{26}ONa$ $[M+Na]^+$: 437.1876; Found: 437.1876. Δ = 0 ppm.

(*Z*)-(3-(4-Methoxystyryl)phenyl)(phenyl)methanone (47)



47

The title compound was prepared according to the general procedure as described. Silica gel flash column chromatography was performed using hexanes resulting in 65% yield (20.5 mg) as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69-7.66 (m, 3H), 7.64 (s, 1H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.41-7.35 (m, 3H), 7.15 (d, *J* = 9.0 Hz, 2H), 6.77 (d, *J* = 9.0 Hz, 2H), 6.61 (d, *J* = 12.0 Hz, 1H), 6.54 (d, *J* = 12.0 Hz, 1H), 3.79 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 196.6, 159.0, 137.9, 137.8, 137.6, 132.9, 132.4, 131.2, 130.9, 130.4, 130.1, 129.4, 128.6, 128.5, 128.3, 128.0, 113.9, 55.4.

HRMS(ESI): m/z Calcd. for $C_{22}H_{18}O_2Na$ $[M+Na]^+$: 337.1199; Found: 337.1198. Δ = 0.30 ppm.

V Reference

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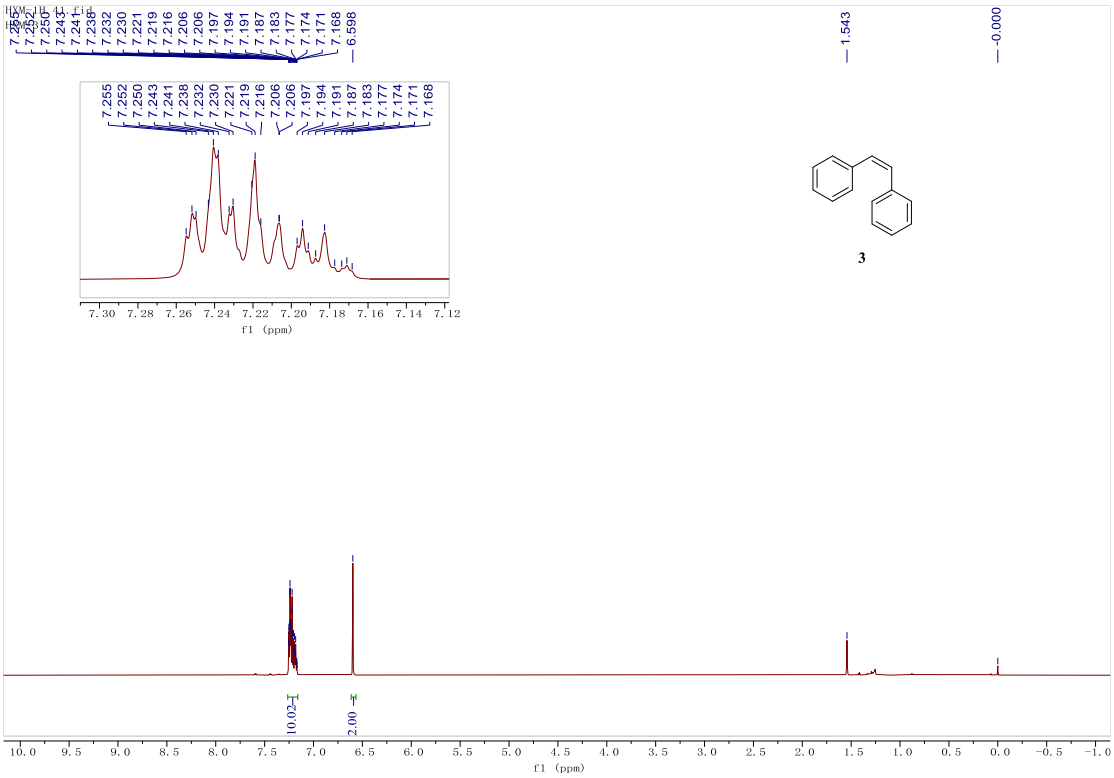
VI. NMR spectra of the products



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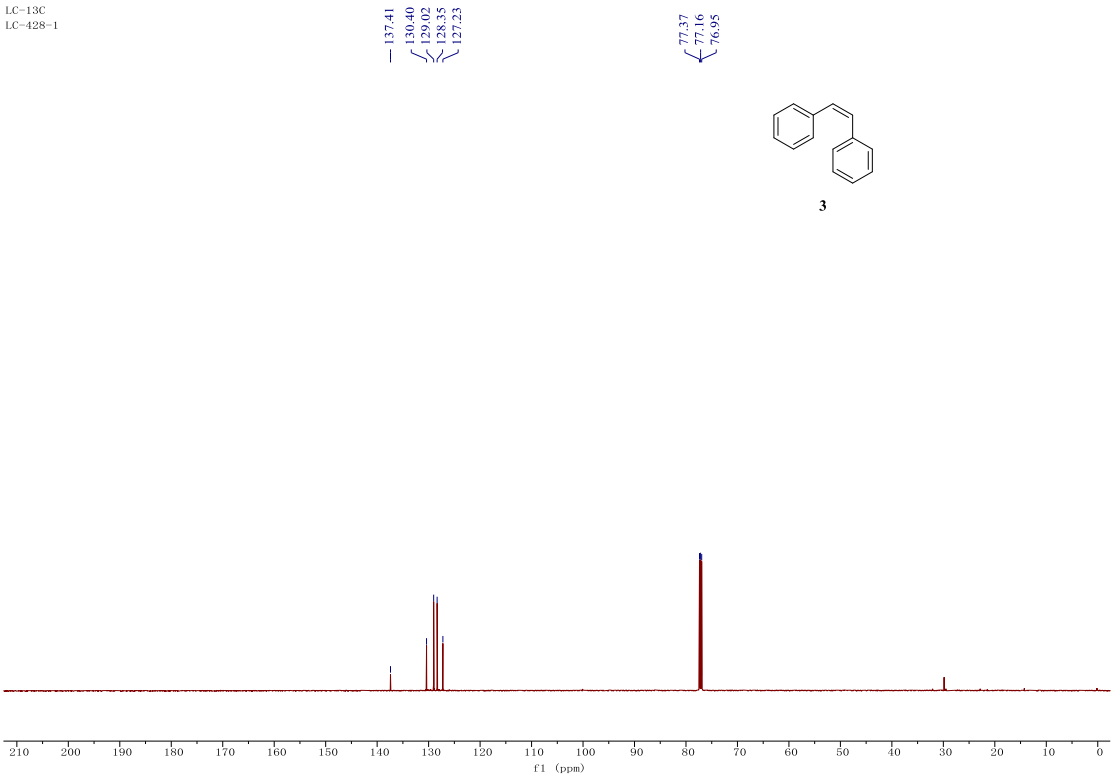

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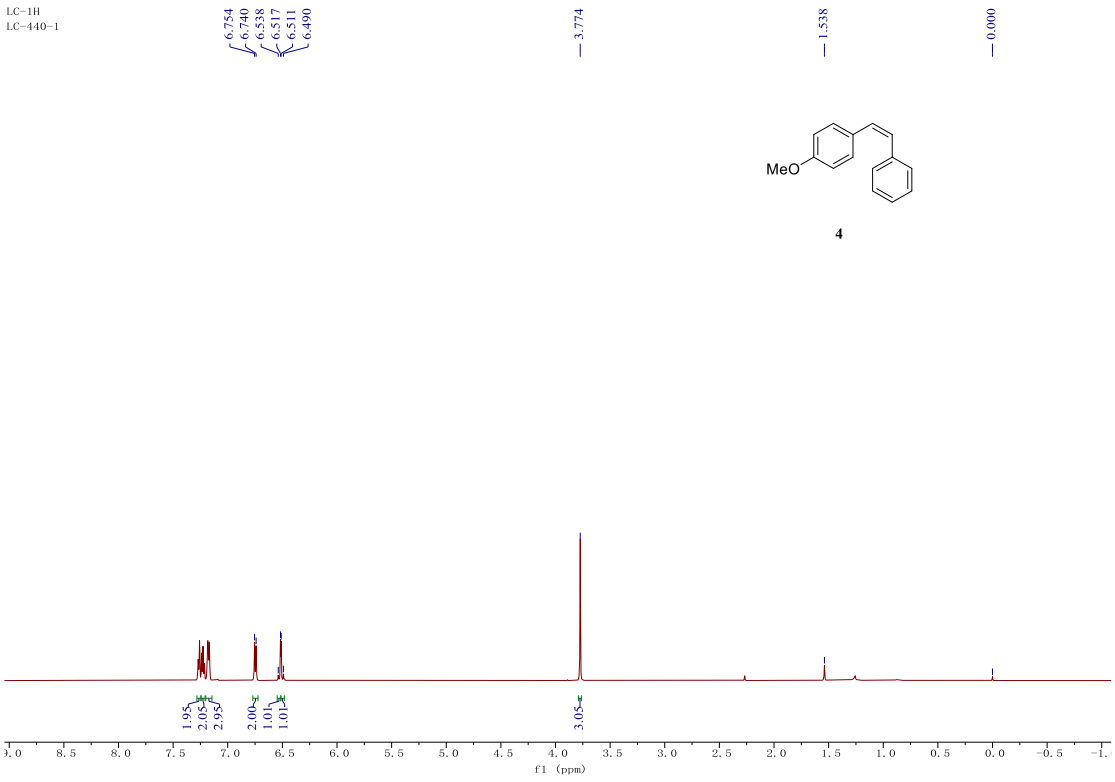
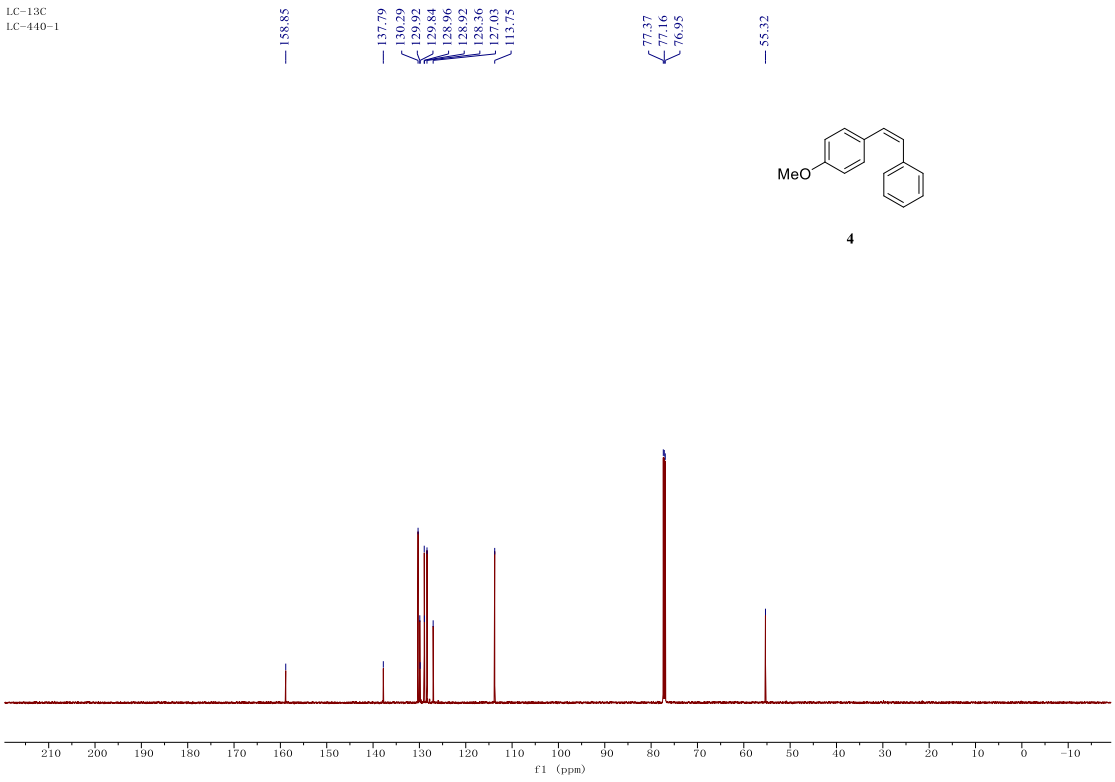
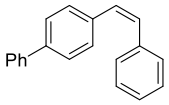
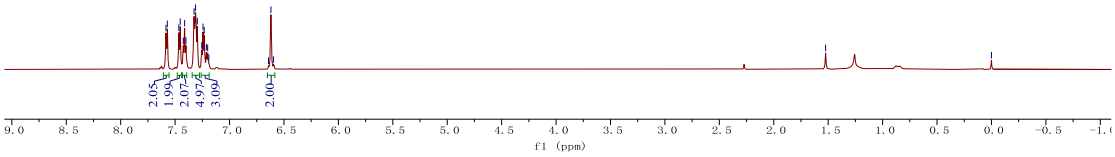

LC-1H
LC-440-1
6.754
6.740
6.538
6.517
6.511
6.490
3.774
1.538
0.000
MeO
4
1.95
2.05
2.95
2.00
1.01
1.01
3.05
f1 (ppm)


LC-13C
LC-440-1
158.85
137.79
130.29
129.92
129.84
128.96
128.92
128.36
127.03
113.75
77.37
77.16
76.95
55.32
MeO
4
f1 (ppm)

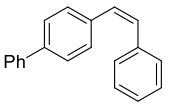

LC-1H
LC-455-1
7.584
7.581
7.466
7.453
7.425
7.413
7.400
7.326
7.312
7.296
7.255
7.244
7.232
7.213
6.642
6.620
6.597
1.524
-0.000


Ph

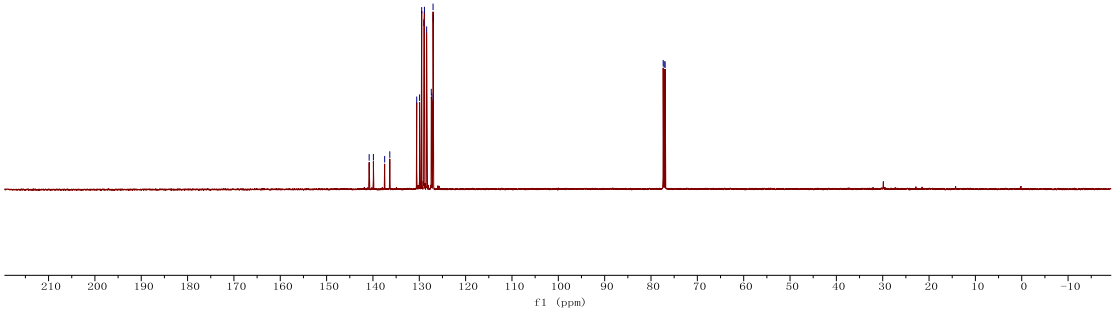
5


2.05
1.99
2.07
4.97
3.09
2.00
f1 (ppm)


LC-13C
LC-455-1
140.82
139.91
137.47
136.37
130.56
129.94
129.49
129.02
128.89
128.42
127.41
127.30
127.03
126.96
77.37
77.16
76.95

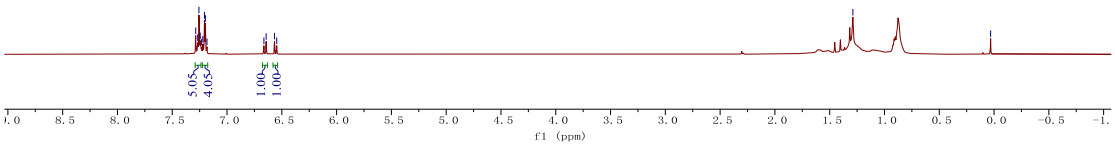

Ph

5


f1 (ppm)

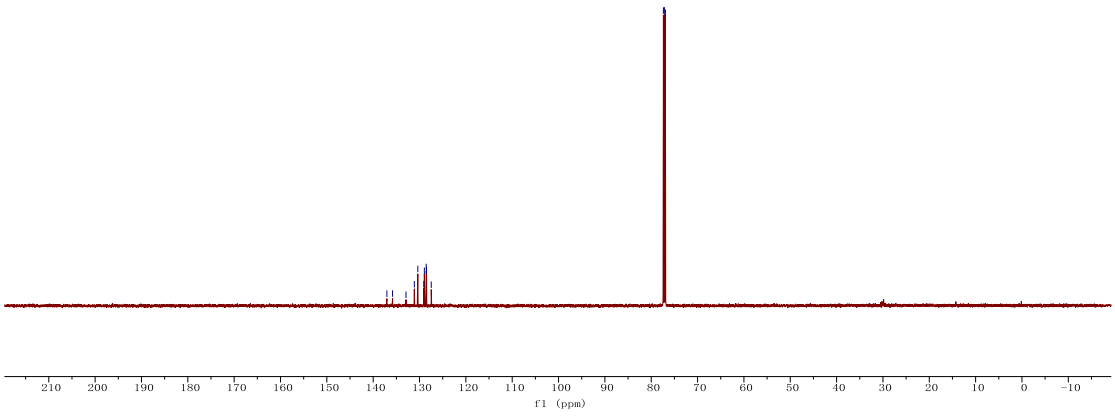

3ca. LC-452-1-XL
Lc-452-1
7.288
7.260
7.257
7.245
7.235
7.221
7.211
7.206
7.197
7.183
6.664
6.643
6.567
6.547
1.288
0.031
Cl

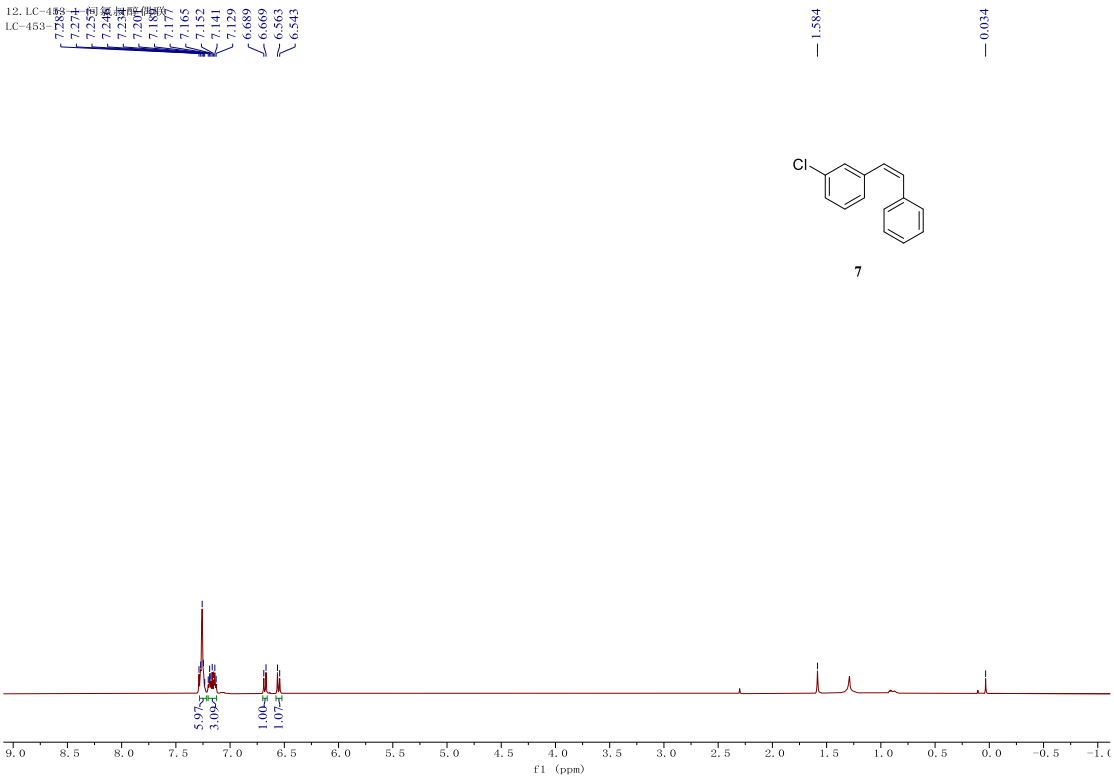
6

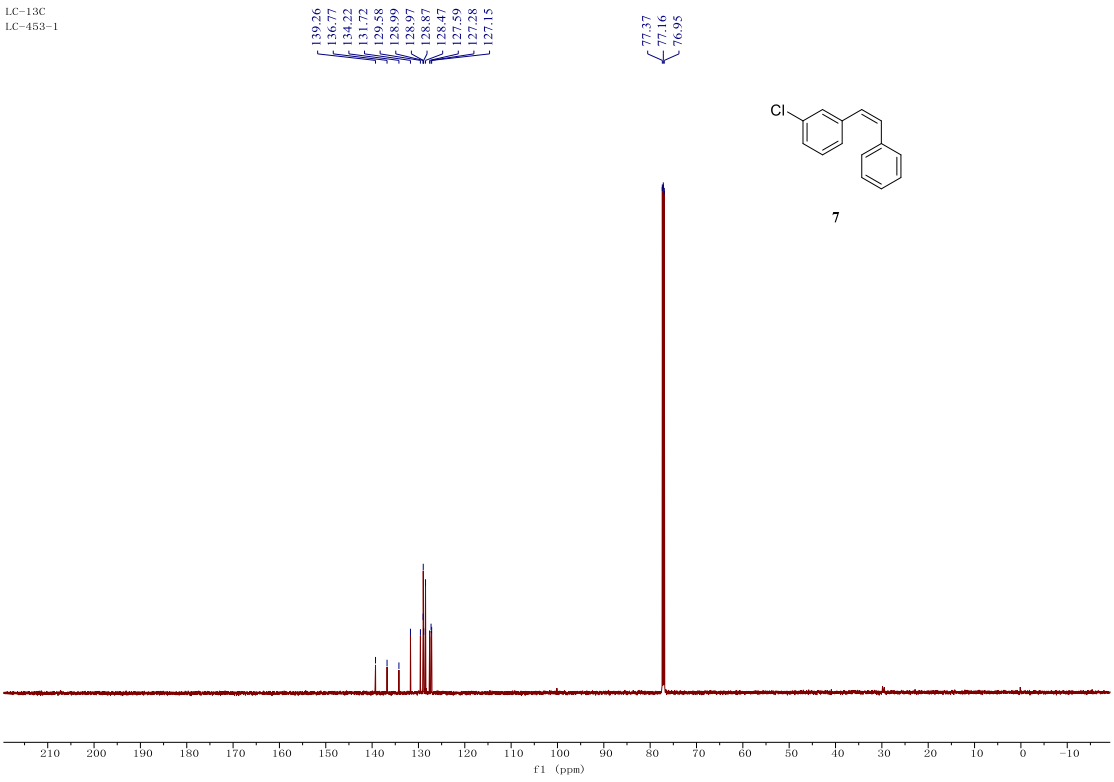

5.05
4.05
1.00
1.00
f1 (ppm)


LC-13C. 40. fid
LC-452-1
137.04
135.82
132.92
131.12
130.37
129.08
128.96
128.56
128.49
127.47
77.37
77.16
76.95
Cl

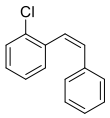
6


f1 (ppm)


12. LC-453
LC-453-1
7.283
7.274
7.252
7.248
7.234
7.201
7.185
7.177
7.165
7.152
7.141
7.129
6.689
6.669
6.563
6.543
1.584
0.034
Cl
7
5.97
3.09
1.00
1.07
f1 (ppm)


LC-13C
LC-453-1
139.26
136.77
134.22
131.72
129.58
128.99
128.97
128.87
128.47
127.59
127.28
127.15
77.37
77.16
76.95
Cl
7
f1 (ppm)

13. LC-453-2-氢氧核酸偶联
LC-453-2



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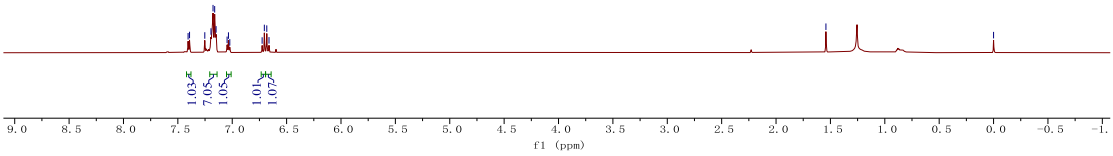
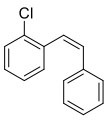


LC-13C
LC-453-2



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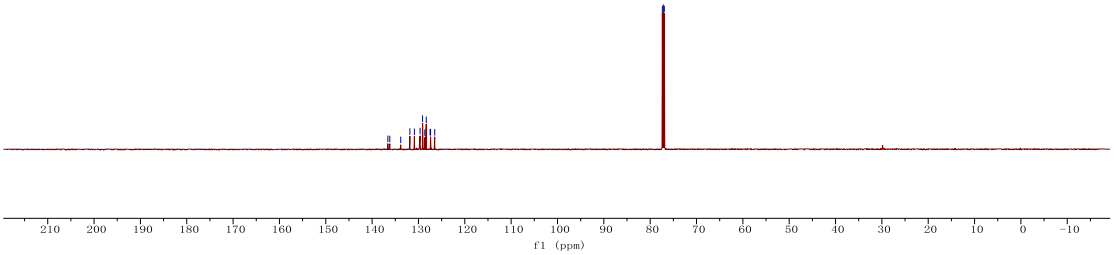
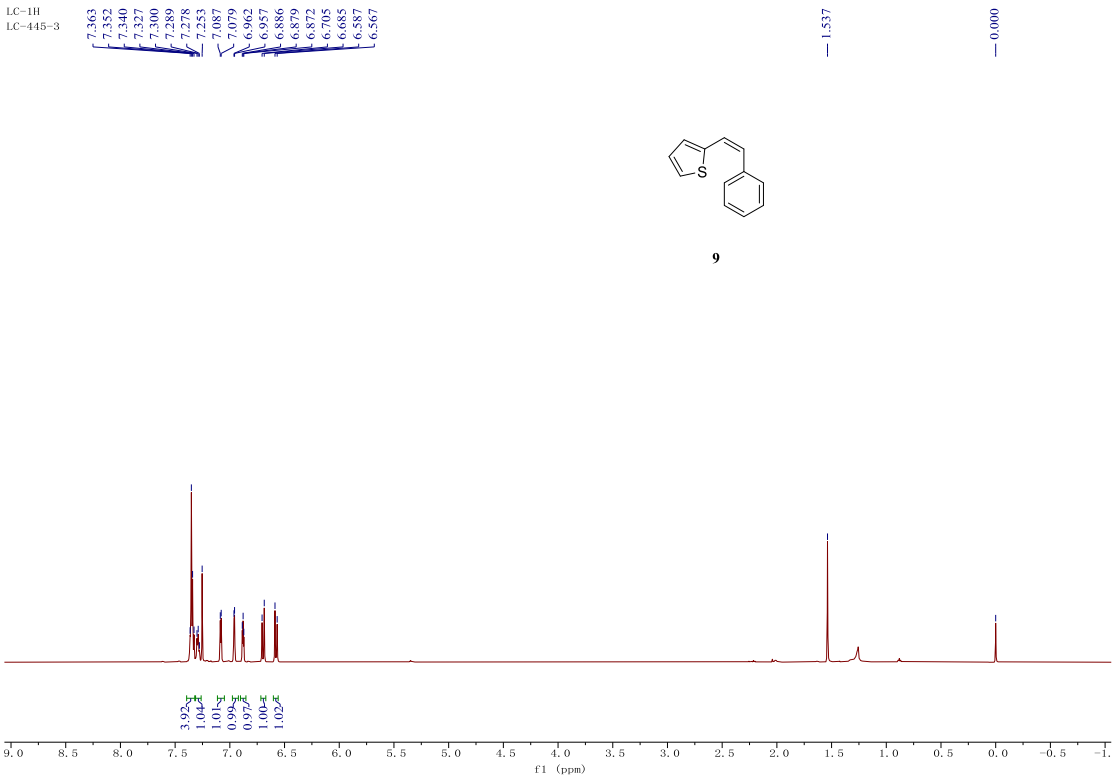
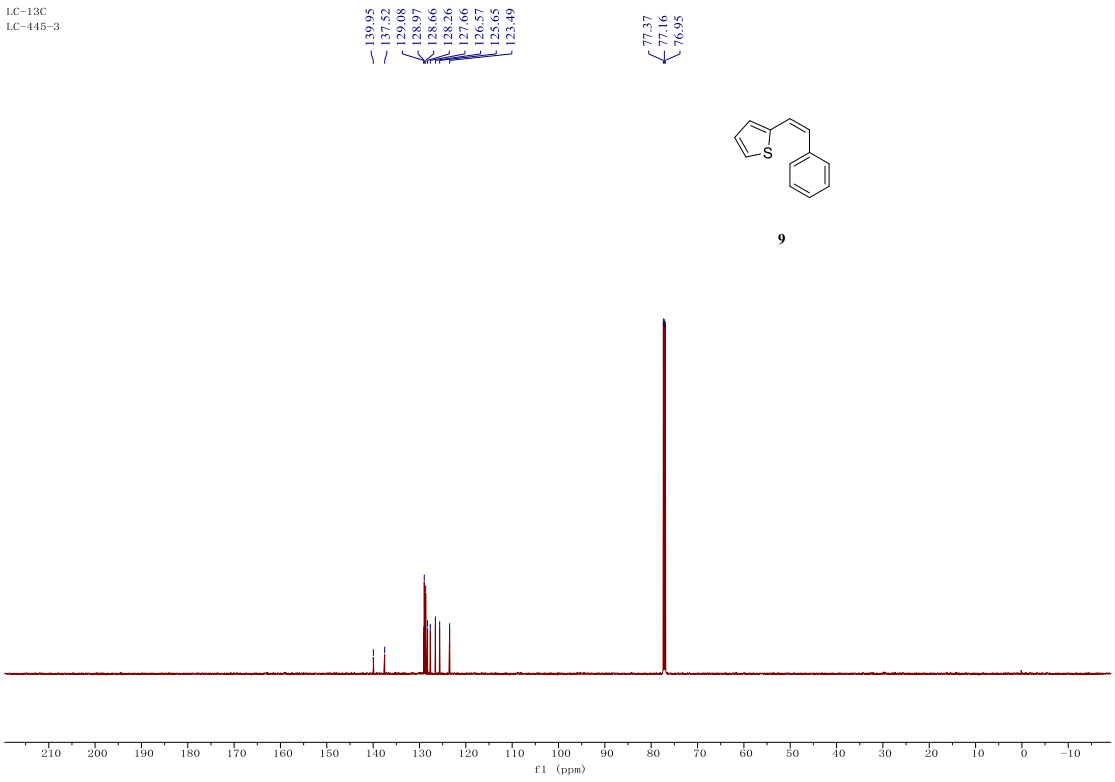
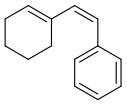



LC-1H
LC-445-3
7.363
7.352
7.340
7.327
7.300
7.289
7.278
7.253
7.087
7.079
6.962
6.957
6.886
6.879
6.872
6.705
6.685
6.587
6.567
1.537
0.000
S
9
3.92
1.04
1.01
0.99
0.97
1.00
1.02
f1 (ppm)

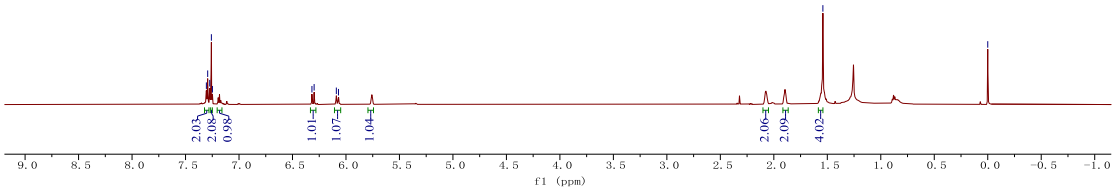

LC-13C
LC-445-3
139.95
137.52
129.08
128.97
128.66
128.26
127.66
126.57
125.65
123.49
77.37
77.16
76.95
S
9
f1 (ppm)

5. 第五批
Lc-518-2

7.305
7.293
7.274
7.258
7.249
6.318
6.298
6.090
6.070
1.541
-0.000

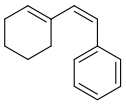


10

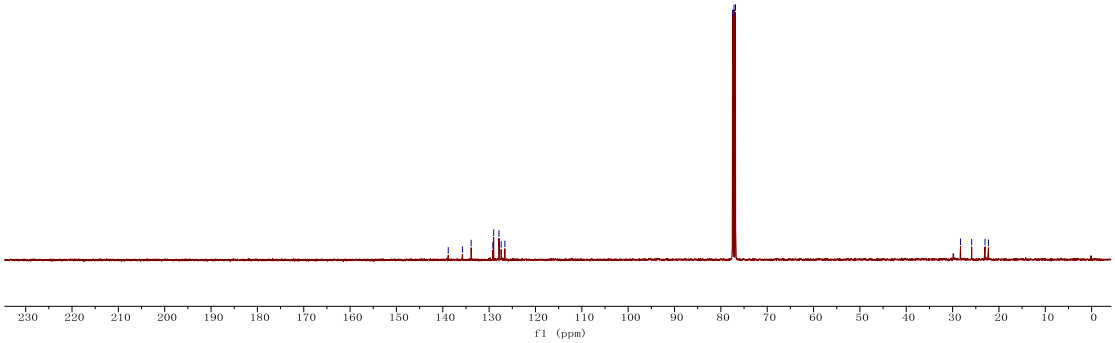


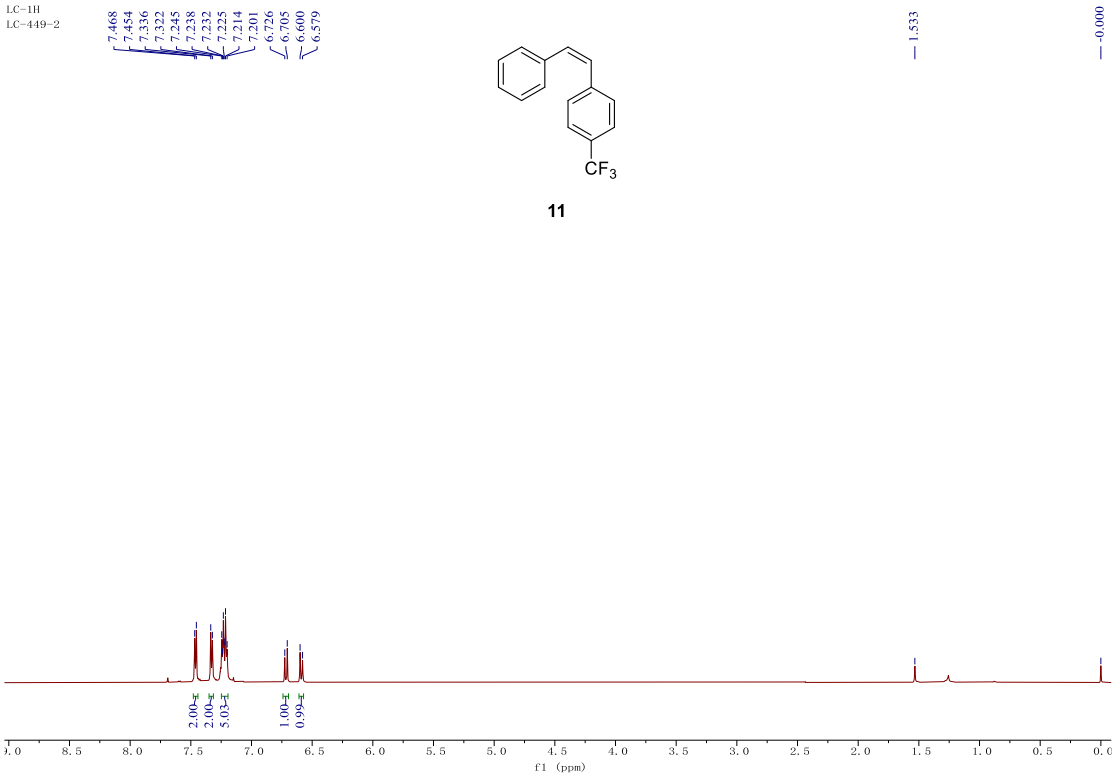
LC-58-2.1.fid

138.83
135.77
133.88
129.20
129.02
127.88
127.40
126.60
77.48
77.16
76.84
28.30
25.89
23.00
22.27

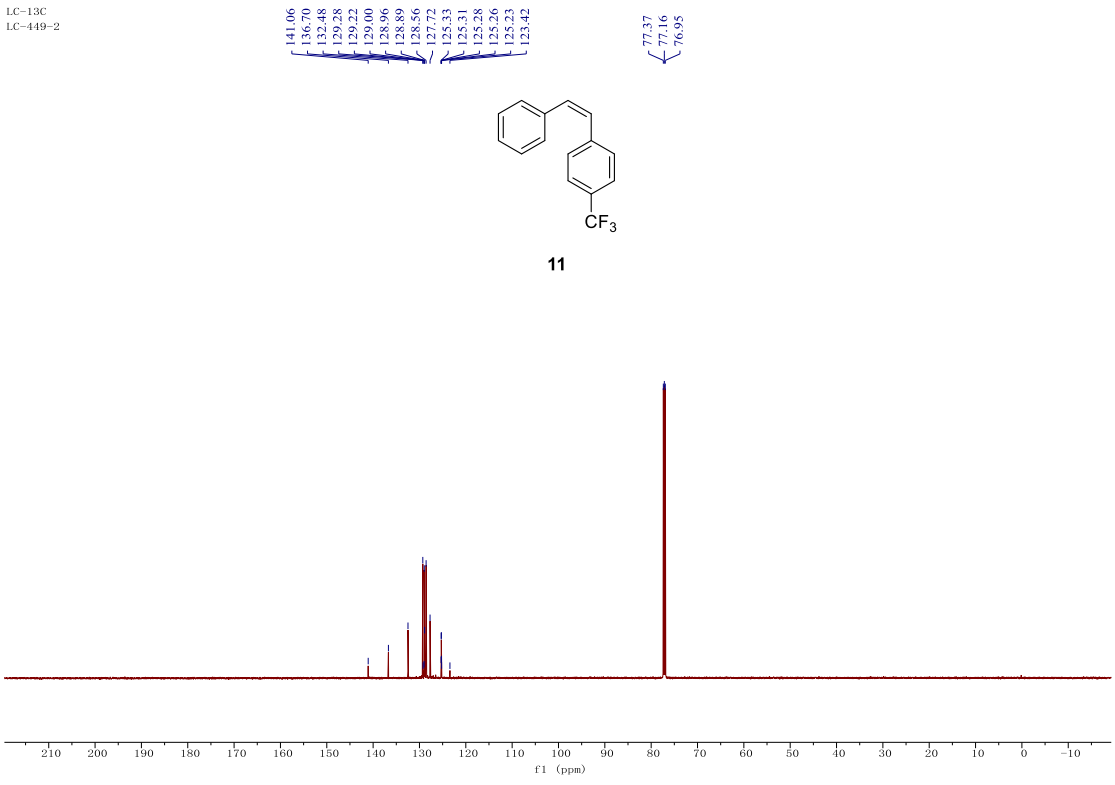


10



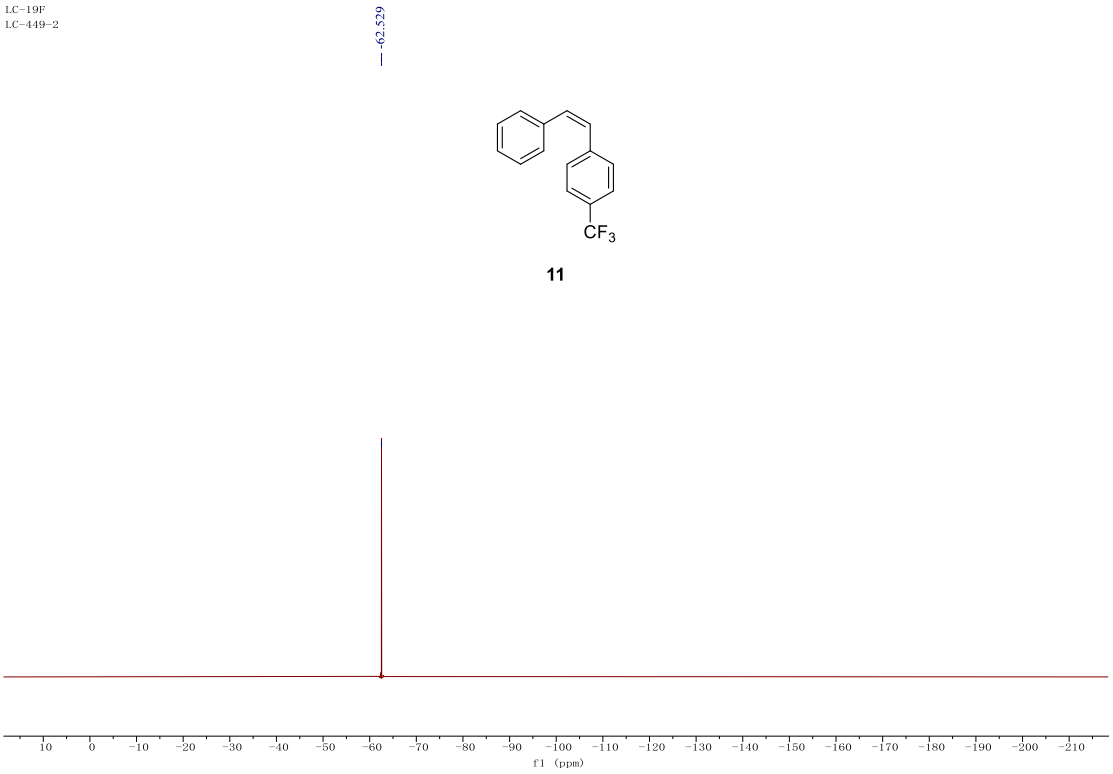

LC-1H
LC-449-2
7.468
7.454
7.336
7.322
7.245
7.238
7.232
7.225
7.214
7.201
6.726
6.705
6.600
6.579
1.533
-0.000
CF3
2.00
2.00
5.03
1.00
0.99
f1 (ppm)

11

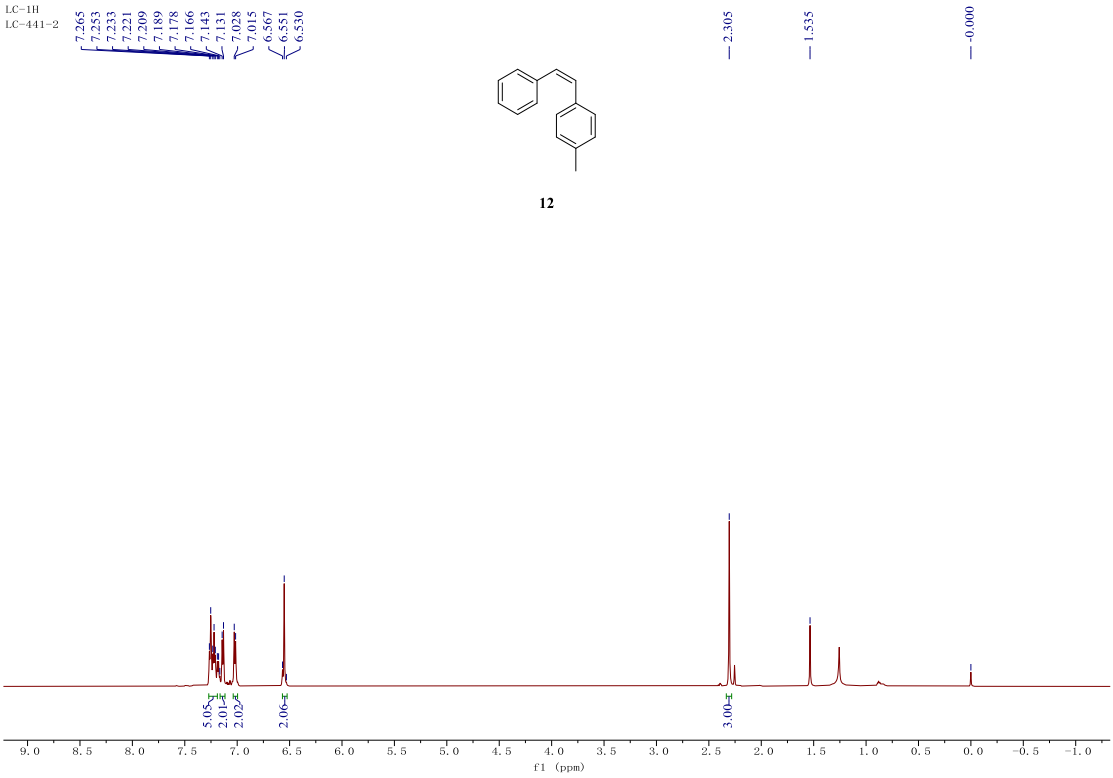

LC-13C
LC-449-2
141.06
136.70
132.48
129.28
129.22
129.00
128.96
128.89
128.56
127.72
125.33
125.31
125.28
125.26
125.23
123.42
77.37
77.16
76.95
CF3
f1 (ppm)

11

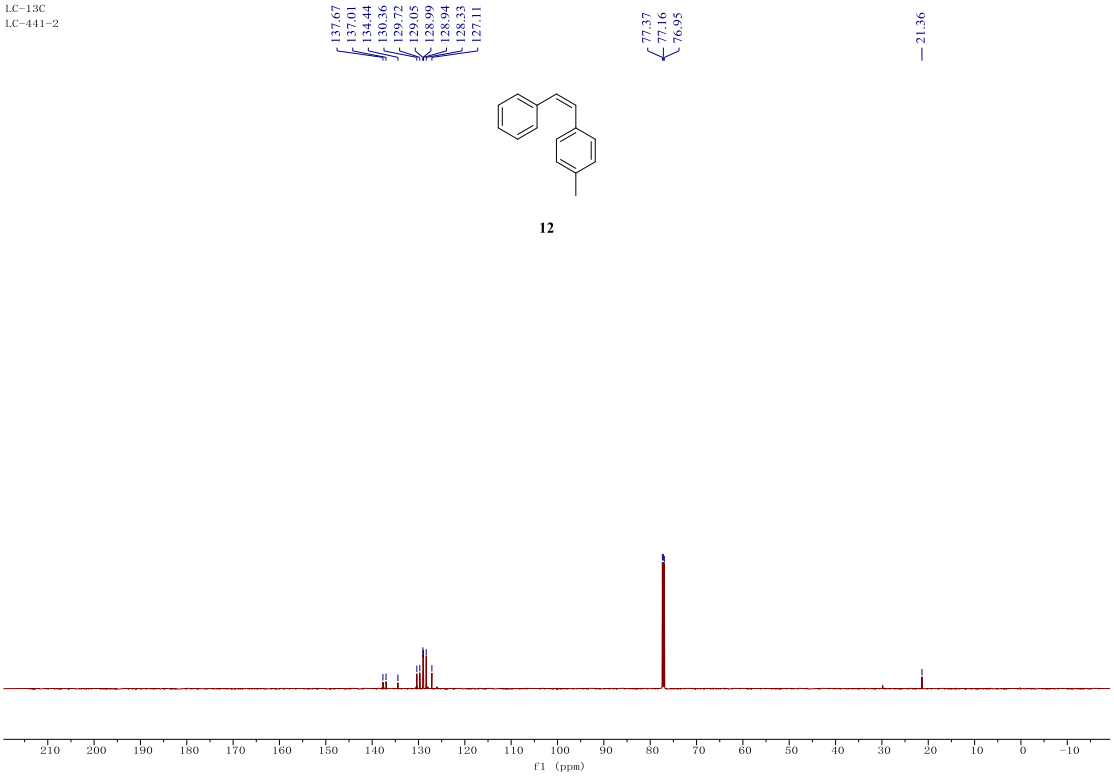
LC-19F
LC-449-2



11


LC-1H
LC-441-2
7.265
7.253
7.233
7.221
7.209
7.189
7.178
7.166
7.143
7.131
7.028
7.015
6.567
6.551
6.530
2.305
1.535
-0.000
5.05
2.01
2.02
2.06
3.00
f1 (ppm)

12


LC-13C
LC-441-2
137.67
137.01
134.44
130.36
129.72
129.05
128.99
128.94
128.33
127.11
77.37
77.16
76.95
21.36
f1 (ppm)

12


LC-1H
LC-445-1
7.255
7.241
7.223
7.212
7.199
7.186
7.174
7.162
7.109
7.096
7.084
7.067
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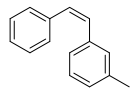
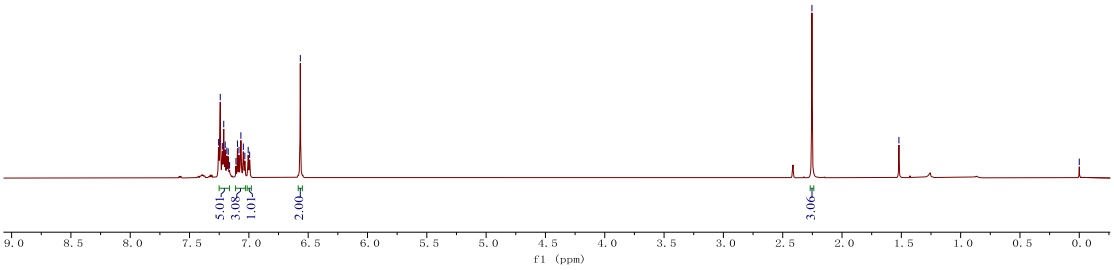
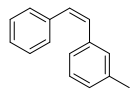
7.006
6.993
6.566
2.254
1.520
0.000



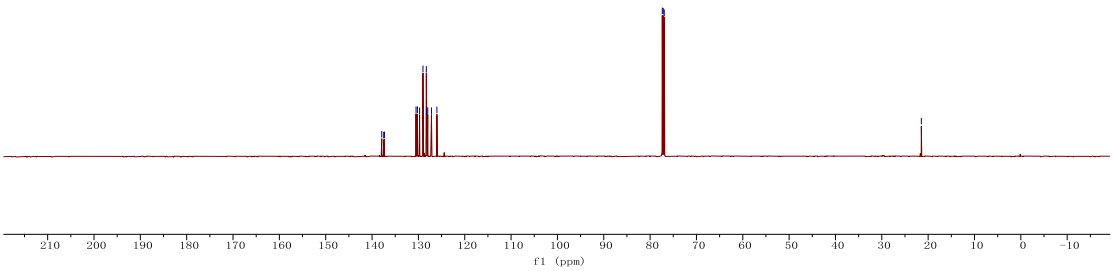
13

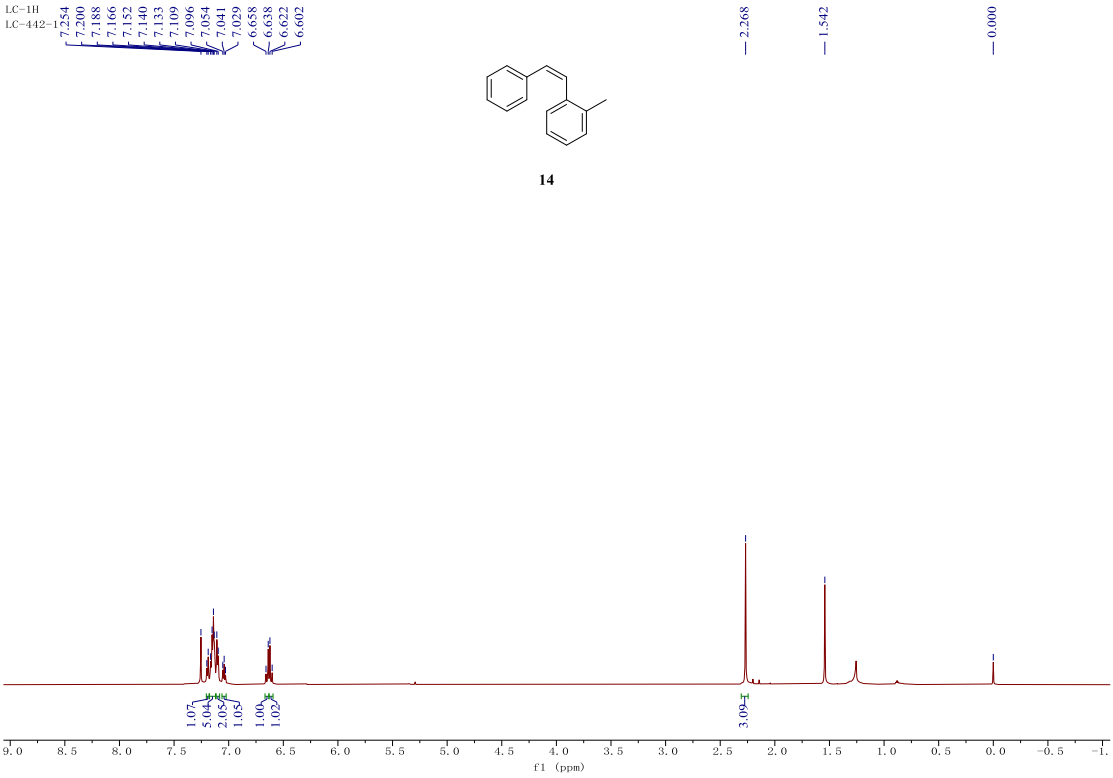

5.01
3.08
1.01
2.00
3.06
f1 (ppm)


LC-13C
LC-445-1
137.90
137.48
137.33
130.51
130.21
129.74
129.02
128.29
128.21
127.98
127.18
126.00
77.37
77.16
76.95
21.47

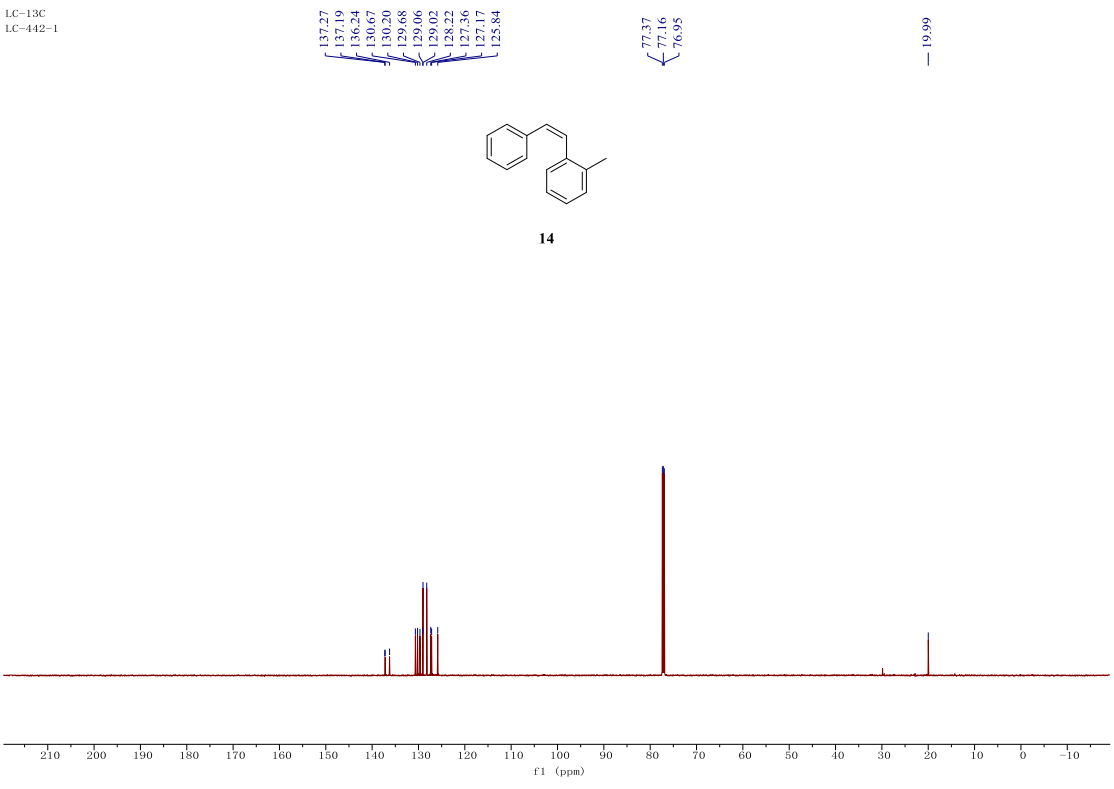


13

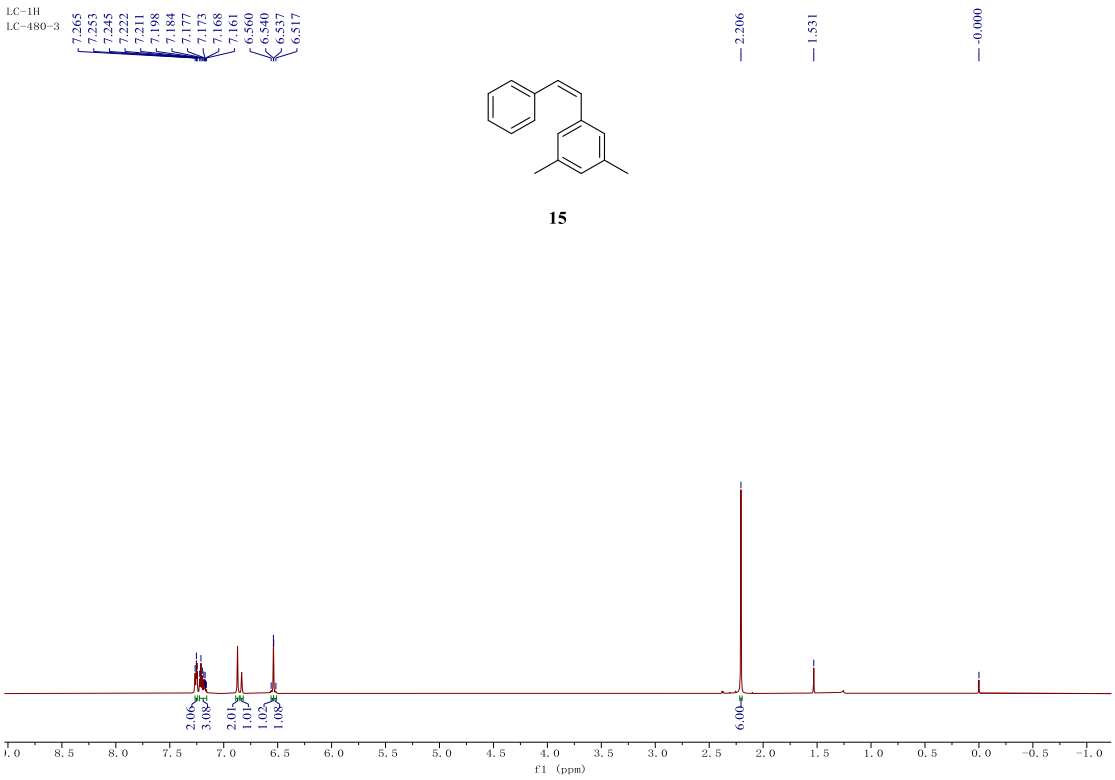

f1 (ppm)


LC-1H
LC-442-1
7.254
7.200
7.188
7.166
7.152
7.140
7.133
7.109
7.096
7.054
7.041
7.029
6.658
6.638
6.622
6.602
2.268
1.542
0.000
1.07
5.04
2.05
1.05
1.00
1.02
3.09
f1 (ppm)

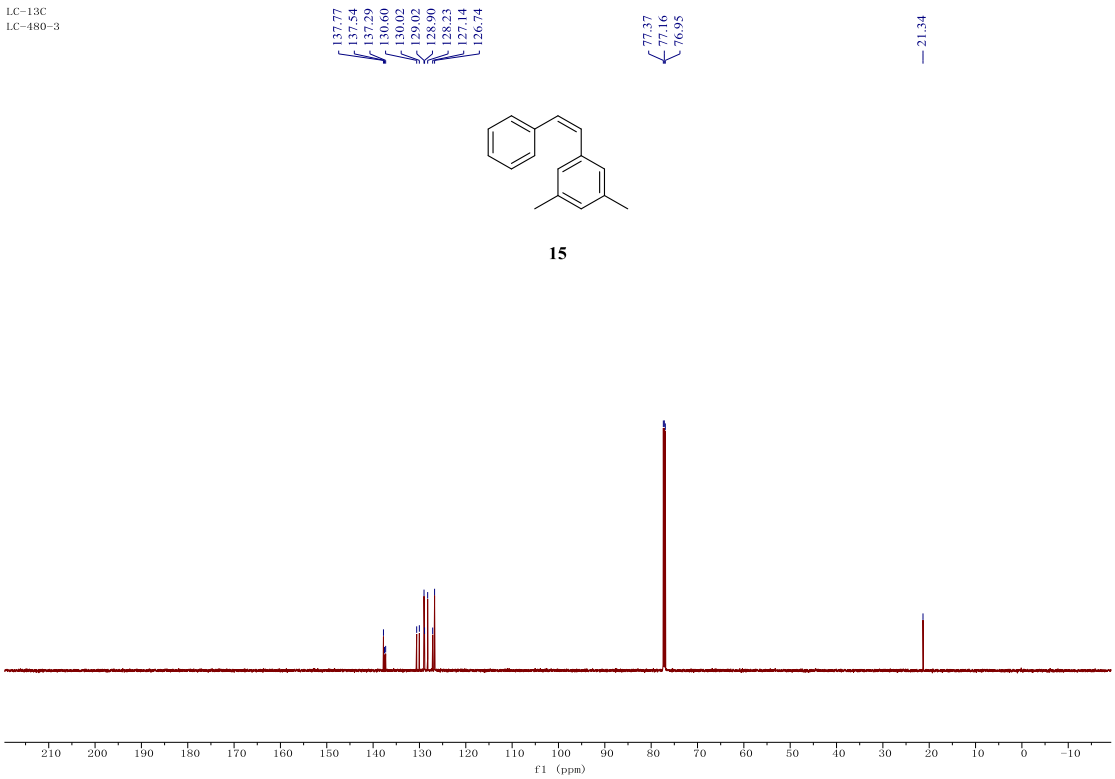
14


LC-13C
LC-442-1
137.27
137.19
136.24
130.67
130.20
129.68
129.06
129.02
128.22
127.36
127.17
125.84
77.37
77.16
76.95
19.99
f1 (ppm)

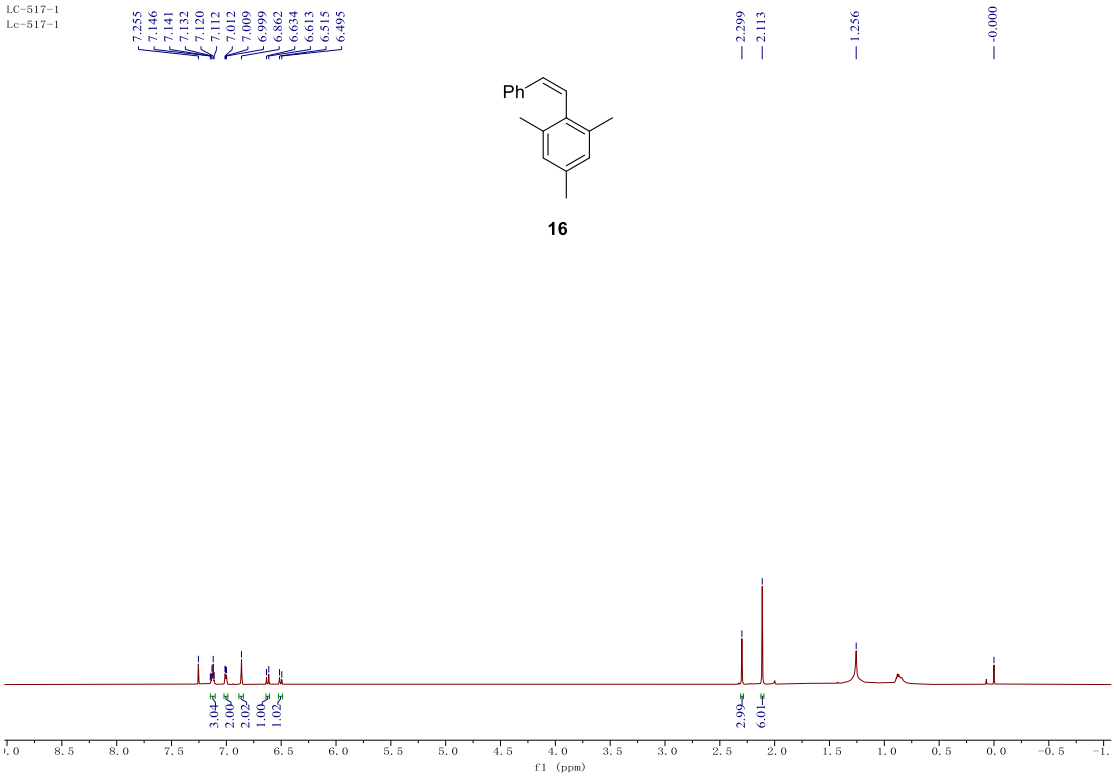
14


LC-1H
LC-480-3
7.265
7.253
7.245
7.222
7.211
7.198
7.184
7.177
7.173
7.168
7.161
6.560
6.540
6.537
6.517
2.206
1.531
-0.000
2.06
3.08
2.01
1.01
1.02
1.08
6.00
f1 (ppm)

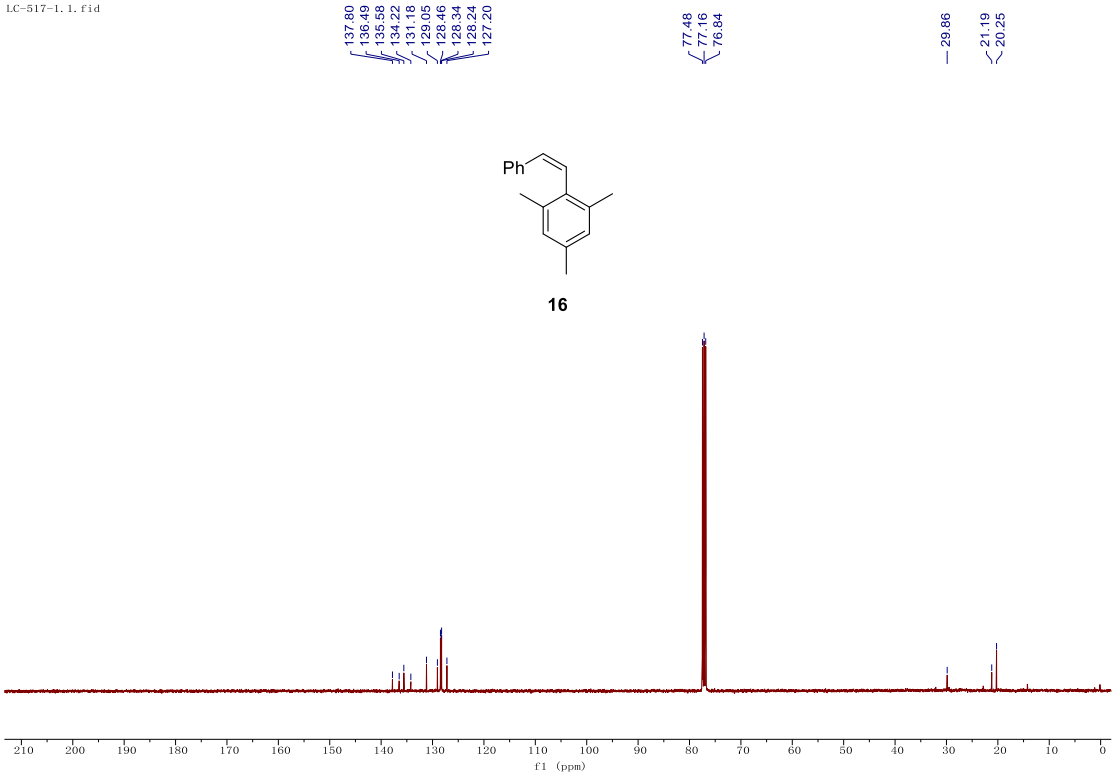
15


LC-13C
LC-480-3
137.77
137.54
137.29
130.60
130.02
129.02
128.90
128.23
127.14
126.74
77.37
77.16
76.95
21.34
f1 (ppm)

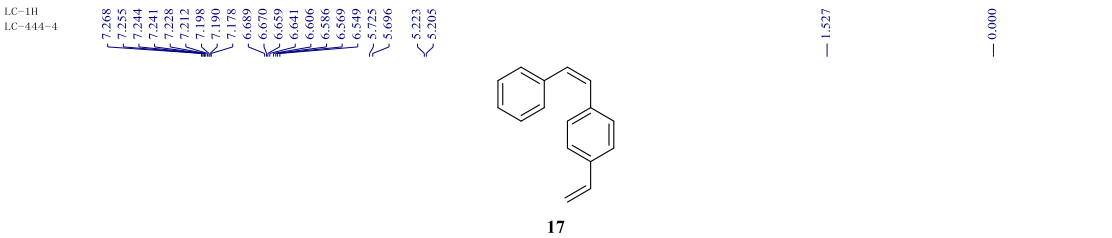
15


LC-517-1
Lc-517-1
7.255
7.146
7.141
7.132
7.120
7.112
7.012
7.009
6.999
6.862
6.634
6.613
6.515
6.495
2.299
2.113
1.256
-0.000
Ph
3.04
2.00
2.02
1.00
1.02
2.99
6.01
f1 (ppm)

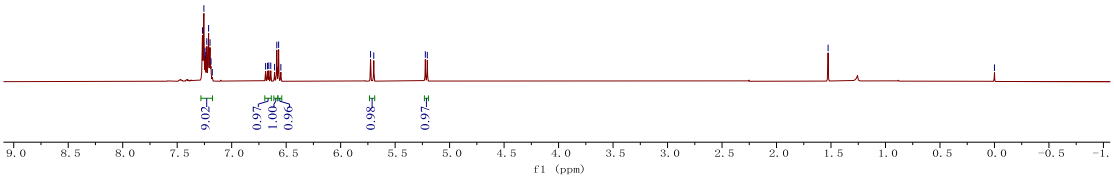
16

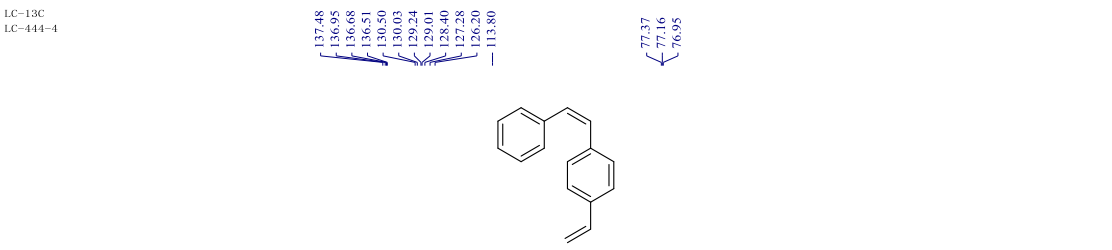

LC-517-1.1.fid
137.80
136.49
135.58
134.22
131.18
129.05
128.46
128.34
128.24
127.20
77.48
77.16
76.84
29.86
21.19
20.25
Ph
f1 (ppm)

16

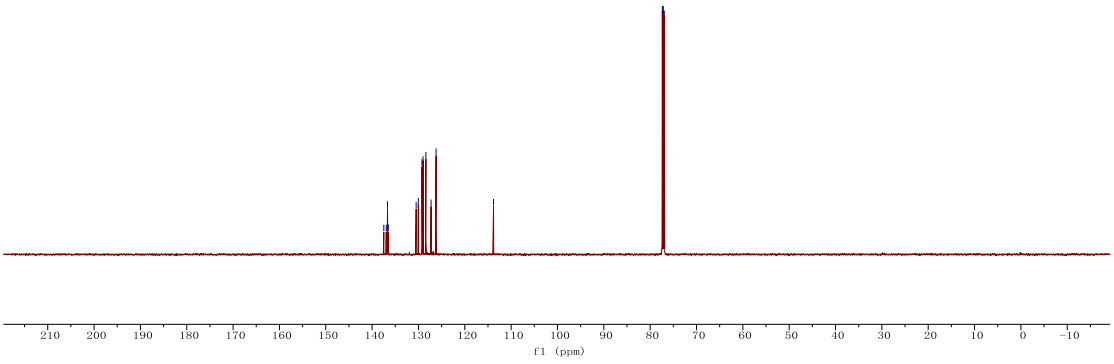

LC-1H
LC-444-4
7.268
7.255
7.244
7.241
7.228
7.212
7.198
7.190
7.178
6.689
6.670
6.659
6.641
6.606
6.586
6.569
6.549
5.725
5.696
5.223
5.205
1.527
0.000

17

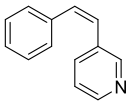

9.02
0.97
1.00
0.96
0.98
0.97
f1 (ppm)


LC-13C
LC-444-4
137.48
136.95
136.68
136.51
130.50
130.03
129.24
129.01
128.40
127.28
126.20
113.80
77.37
77.16
76.95

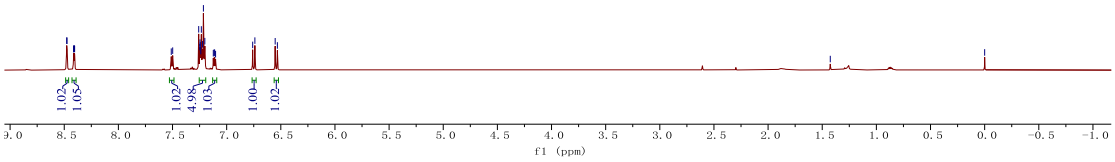
17


f1 (ppm)

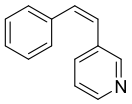

LC-1H
LC-469-1
8.415
8.414
8.412
8.406
8.404
7.512
7.499
7.258
7.249
7.246
7.243
7.239
7.234
7.222
7.215
7.202
7.123
7.115
7.110
7.102
6.760
6.739
6.552
6.532
1.426
-0.000



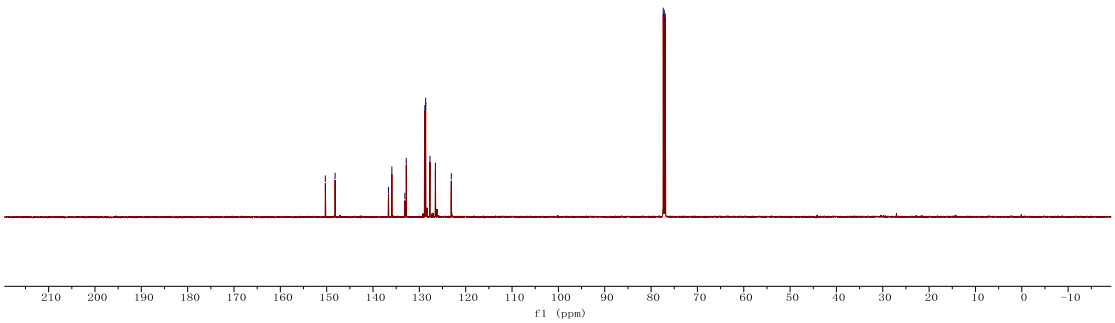
18

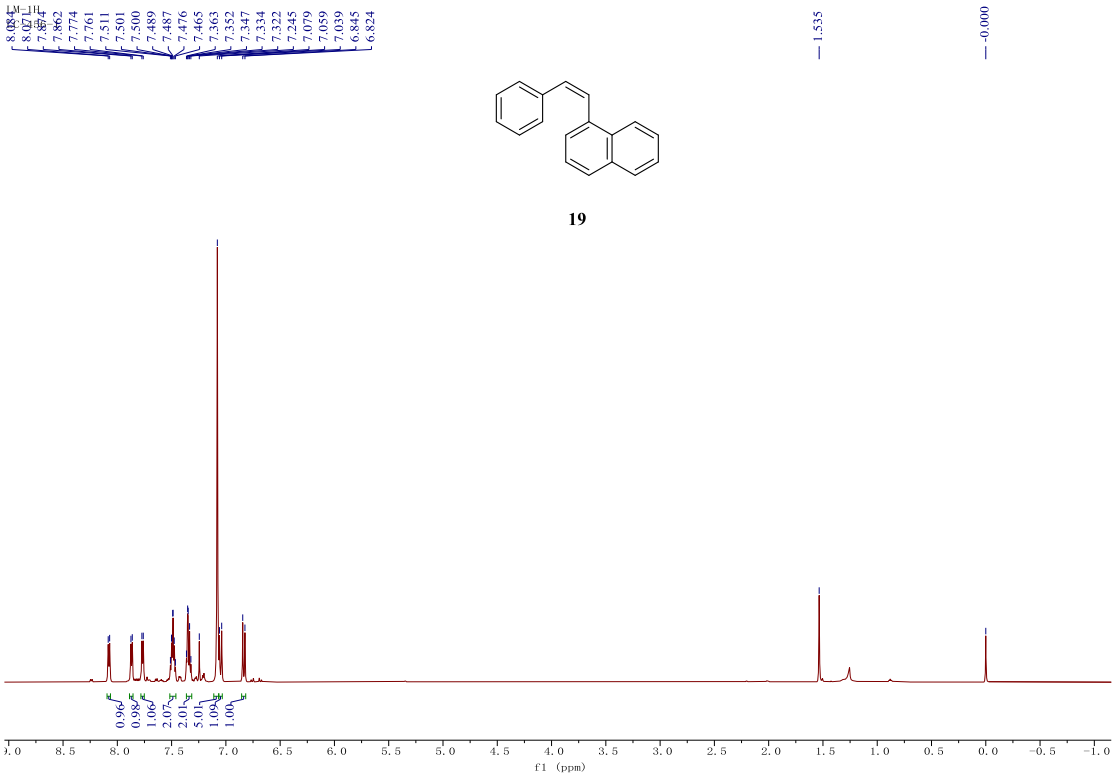

1.02
1.05
1.02
4.98
1.03
1.00
1.02
f1 (ppm)


LC-13C
LC-469-1
150.29
148.19
136.66
135.93
133.13
132.83
128.82
128.64
127.71
126.55
123.11
77.37
77.16
76.95

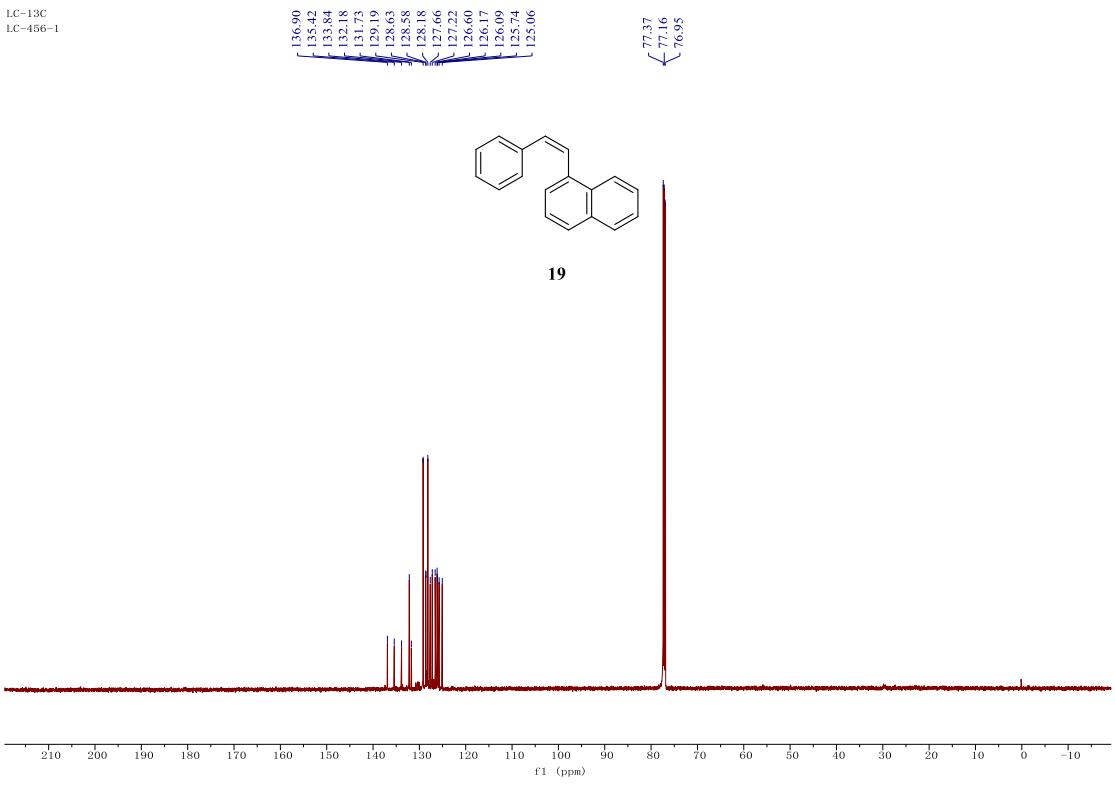


18

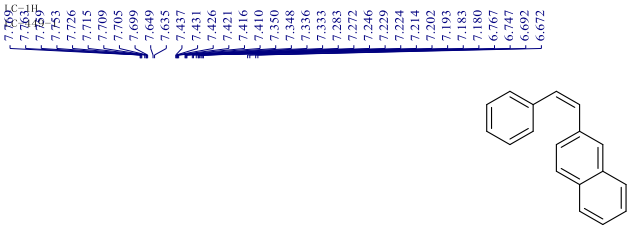

f1 (ppm)


8.084
8.067
7.865
7.862
7.774
7.761
7.511
7.501
7.500
7.489
7.487
7.476
7.465
7.363
7.352
7.347
7.334
7.322
7.245
7.079
7.059
7.039
6.845
6.824
1.535
0.000
0.96
0.98
1.06
2.07
2.01
5.01
1.09
1.00
f1 (ppm)

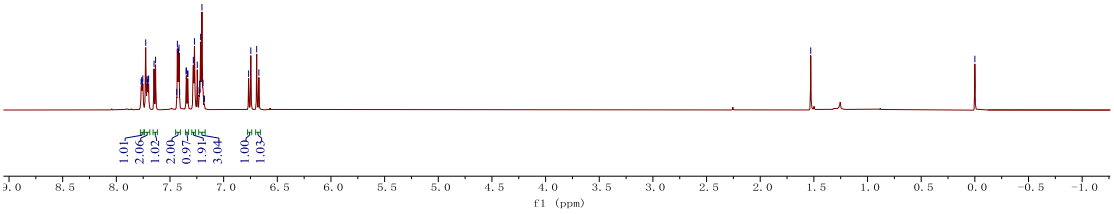
19


LC-13C
LC-456-1
136.90
135.42
133.84
132.18
131.73
129.19
128.63
128.58
128.18
127.66
127.22
126.60
126.17
126.09
125.74
125.06
77.37
77.16
76.95
f1 (ppm)

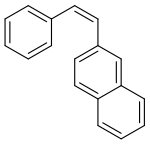
19



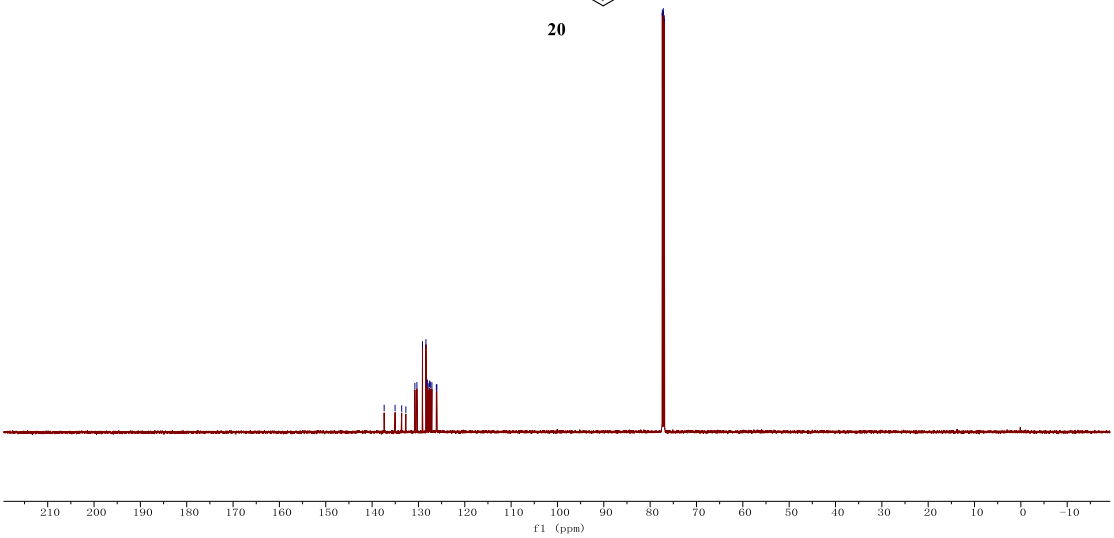
20

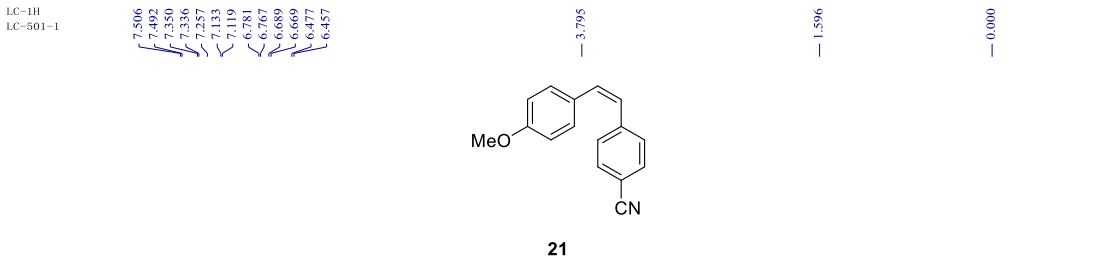


LC-13C
LC-449-1

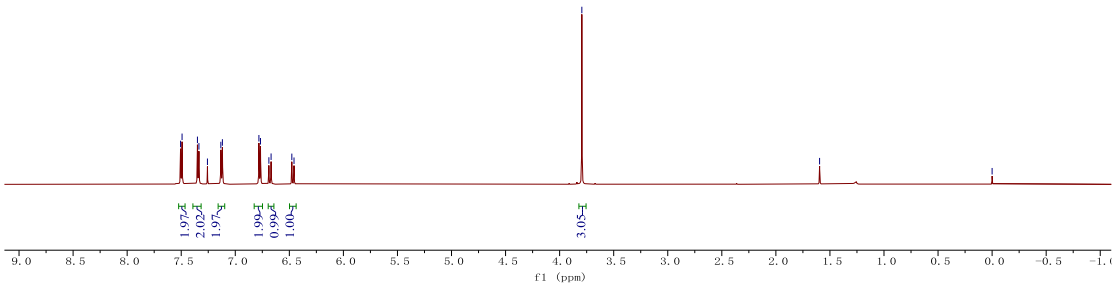


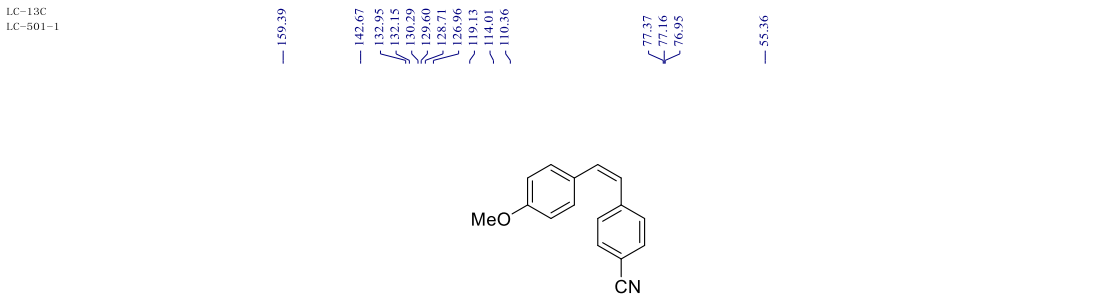
20



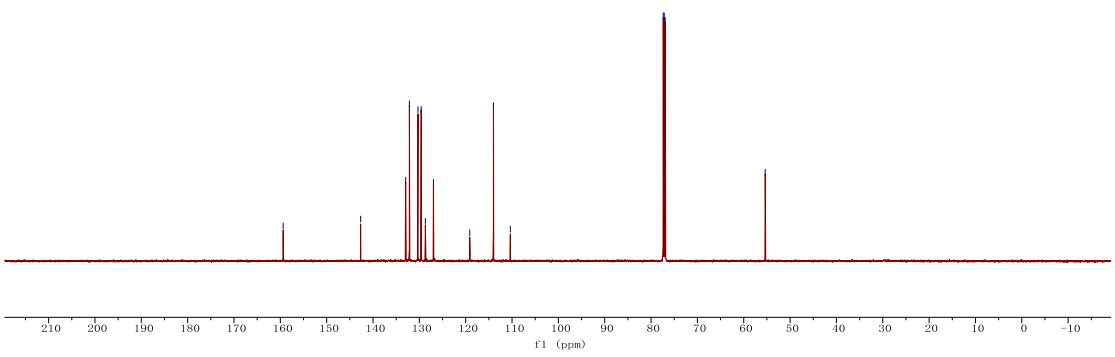

LC-1H
LC-501-1
7.506
7.492
7.350
7.336
7.257
7.133
7.119
6.781
6.767
6.689
6.669
6.477
6.457
3.795
1.596
0.000
MeO
CN

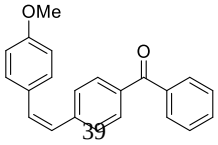
21


1.97
2.02
1.97
1.99
0.99
1.00
3.05
f1 (ppm)

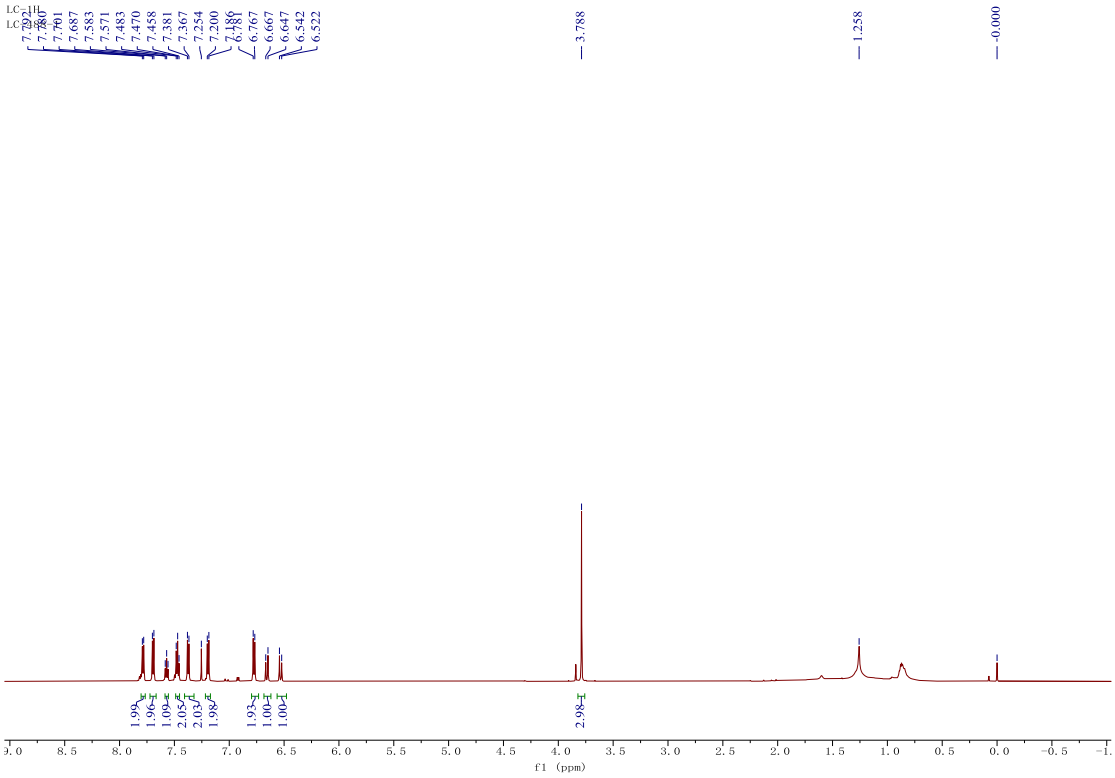

LC-13C
LC-501-1
159.39
142.67
132.95
132.15
130.29
129.60
128.71
126.96
119.13
114.01
110.36
77.37
77.16
76.95
55.36
MeO
CN

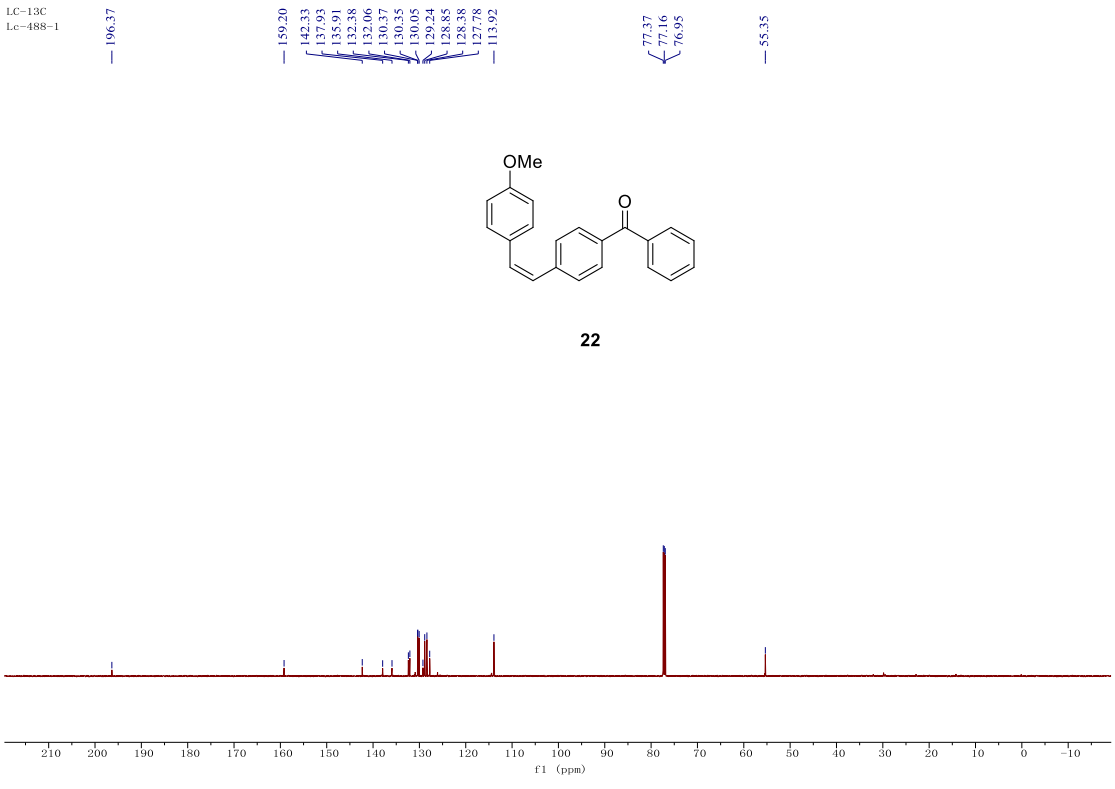
21


f1 (ppm)


OMe
O

22


LC-1H
Lc-488-1
7.792
7.786
7.780
7.691
7.687
7.583
7.571
7.483
7.470
7.458
7.381
7.367
7.254
7.200
6.767
6.667
6.647
6.542
6.522
3.788
1.258
0.000
1.99
1.96
1.09
2.05
2.03
1.98
1.93
1.00
1.00
2.98
f1 (ppm)

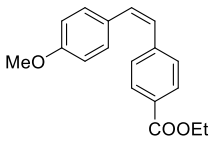

LC-13C
Lc-488-1
196.37
159.20
142.33
137.93
135.91
132.38
132.06
130.37
130.35
130.05
129.24
128.85
128.38
127.78
113.92
77.37
77.16
76.95
55.35
f1 (ppm)

OMe
O

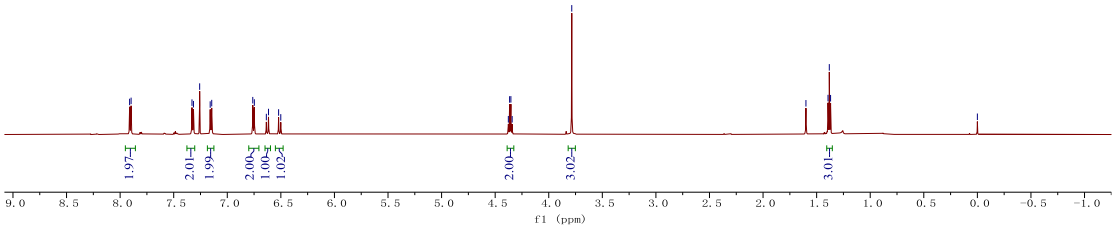
22

LC-1H
LC-473-1

7.911
7.898
7.329
7.316
7.258
7.160
7.145
6.762
6.747
6.635
6.615
6.521
6.501
4.377
4.365
4.353
4.341
3.785
1.600
1.394
1.382
1.370
0.000

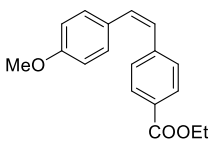


23

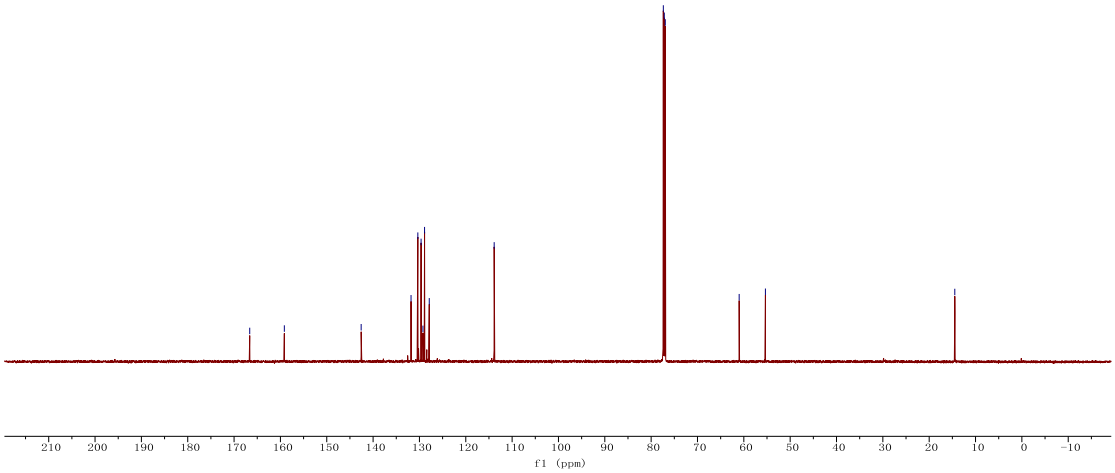


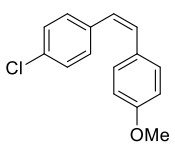
LC-13C
LC-473-2

166.62
159.15
142.58
131.81
130.35
129.65
129.24
128.89
127.88
113.87
77.37
77.16
76.95
61.01
55.34
14.48

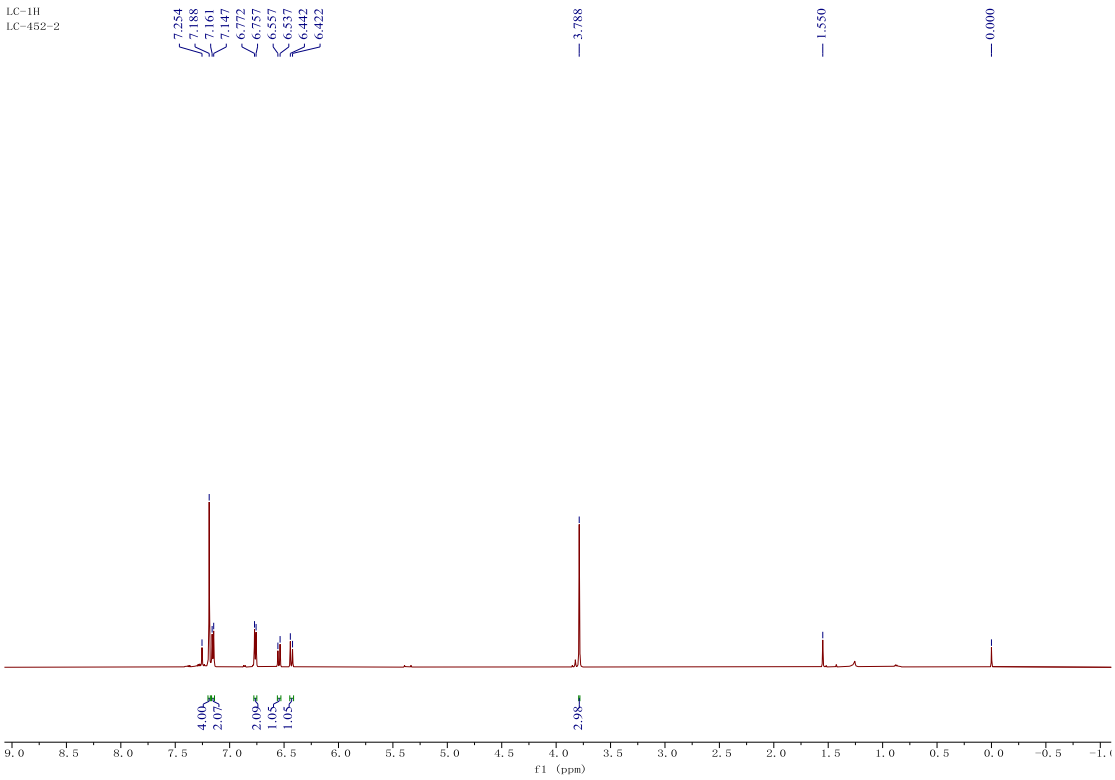


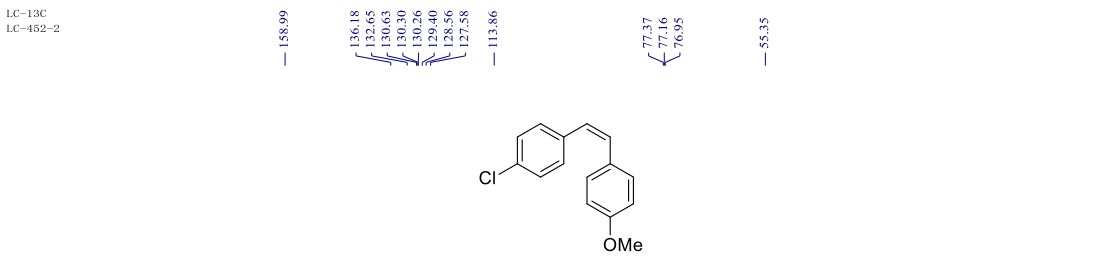
23





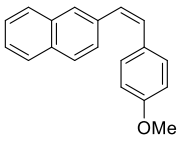
24


LC-1H
LC-452-2
7.254
7.188
7.161
7.147
6.772
6.757
6.557
6.537
6.442
6.422
3.788
1.550
0.000
4.00
2.07
2.09
1.05
1.05
2.98
f1 (ppm)

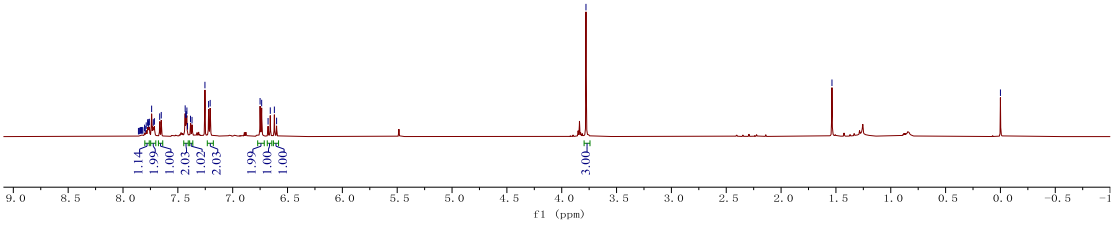

LC-13C
LC-452-2
158.99
136.18
132.65
130.63
130.30
130.26
129.40
128.56
127.58
113.86
77.37
77.16
76.95
55.35
f1 (ppm)

Cl
OMe

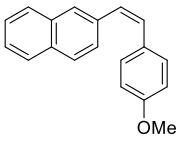
24



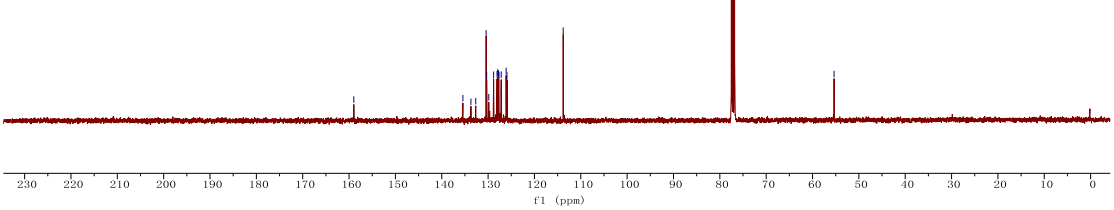
25



LC-515-1.1.fid



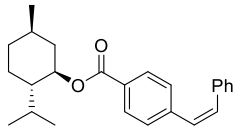
25



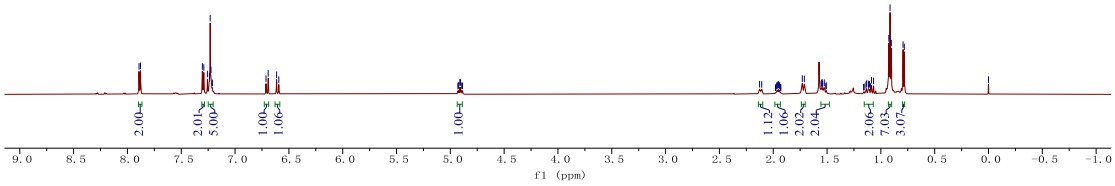
LC-1H
LC-493-1

7.892
7.879
7.304
7.290
7.257
7.238
7.231
7.224
7.210
6.713
6.692
6.614
6.594

4.930
4.923
4.912
4.905
4.894
4.887
2.127
2.107
1.979
1.975
1.968
1.963
1.956
1.952
1.945
1.940
1.933
1.929
1.730
1.711
1.555
1.550
1.545
1.541
1.525
1.511
1.507
1.160
1.155
1.138
1.134
1.117
1.112
1.107
1.096
1.087
1.068
0.926
0.915
0.903
0.794
0.782
-0.000



26



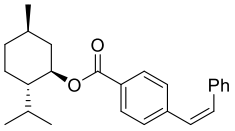
LC-13C
LC-493-1

166.08

141.99
136.91
132.26
129.64
129.47
129.44
129.00
128.95
128.51
127.63

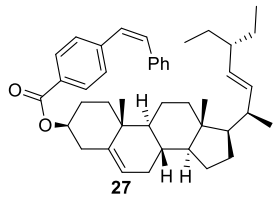
77.37
77.16
76.95
74.93

47.43
41.15
34.49
31.60
26.62
23.79
22.19
20.93
16.66

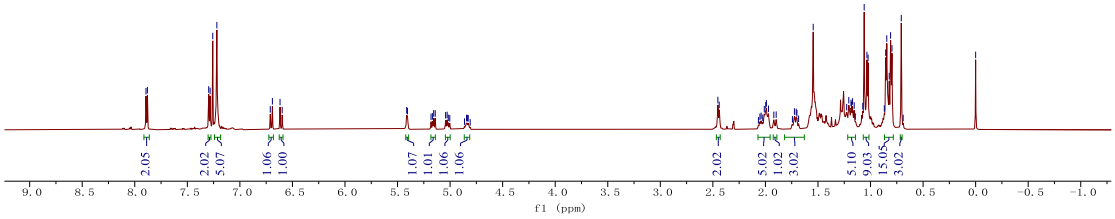


26

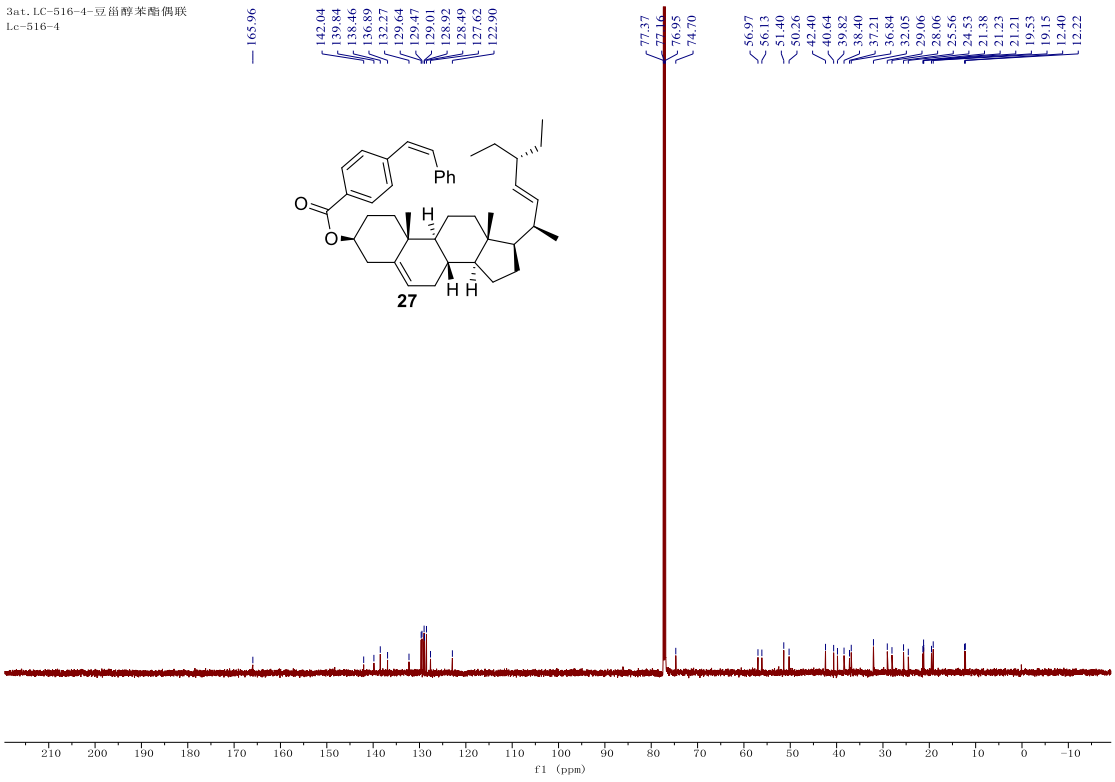
LC-1H
LC-516-4



27

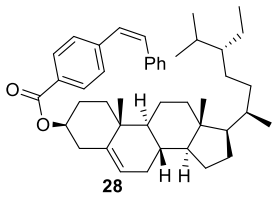


3at.LC-516-4-豆甾醇苯酯偶联
Lc-516-4

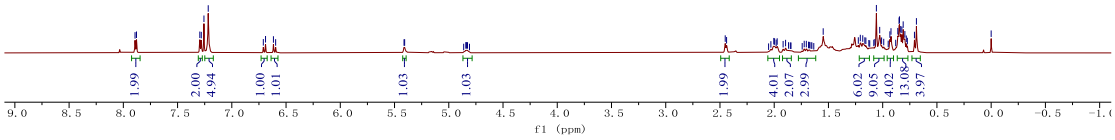


27

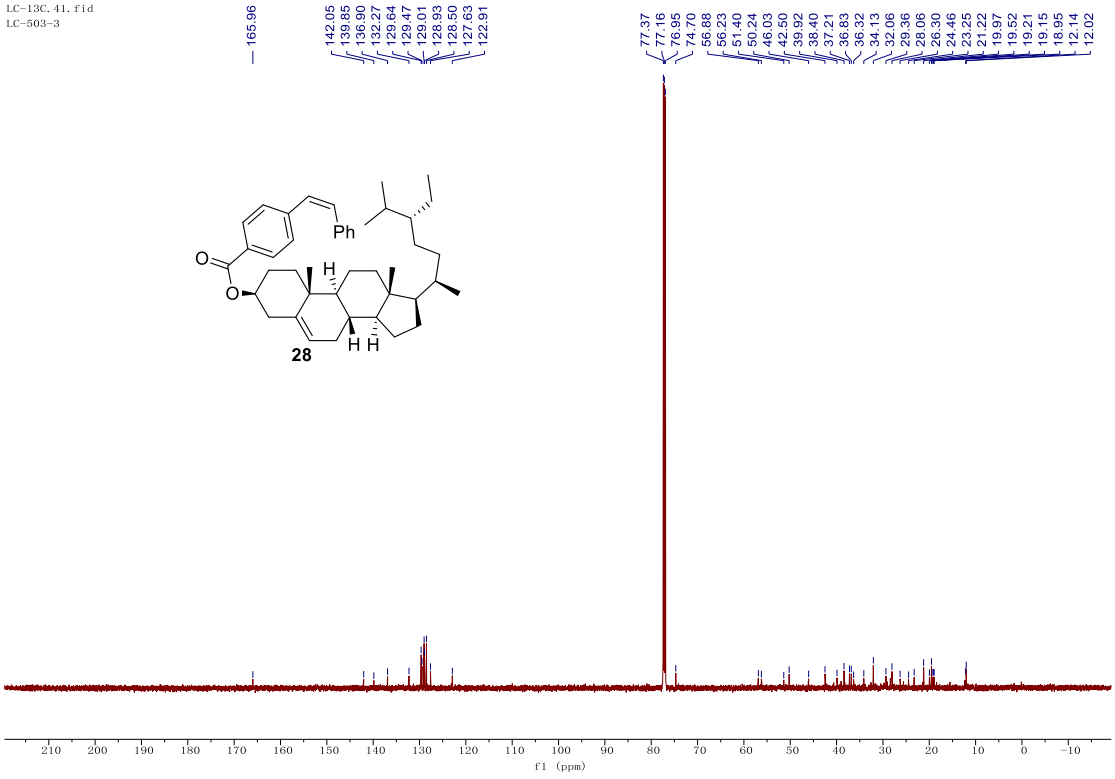
LC-1H
LC-503-3



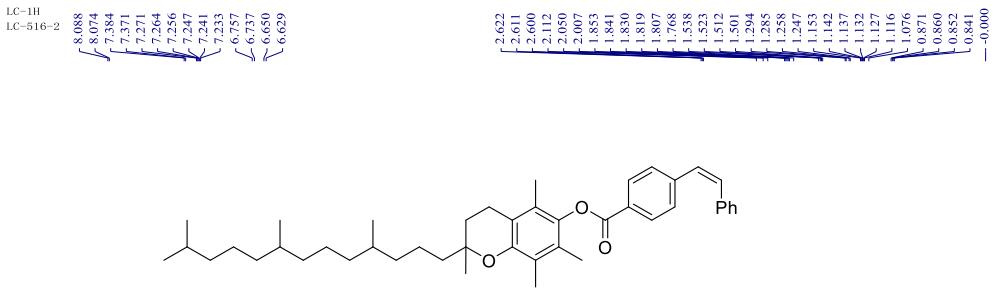
28



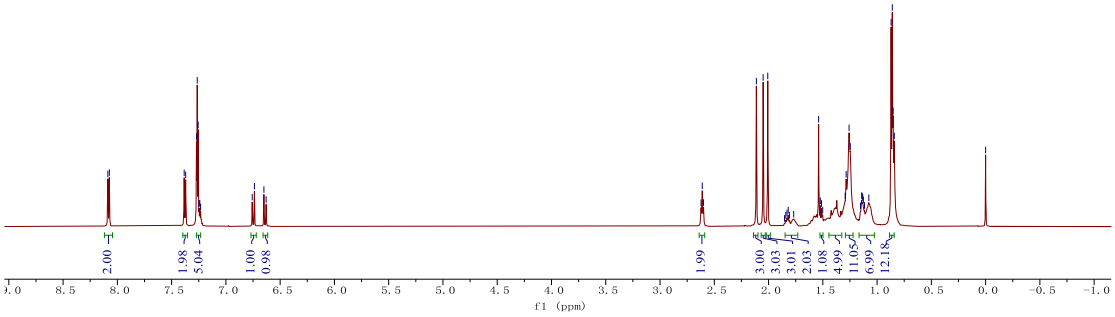
LC-13C.41.fid
LC-503-3

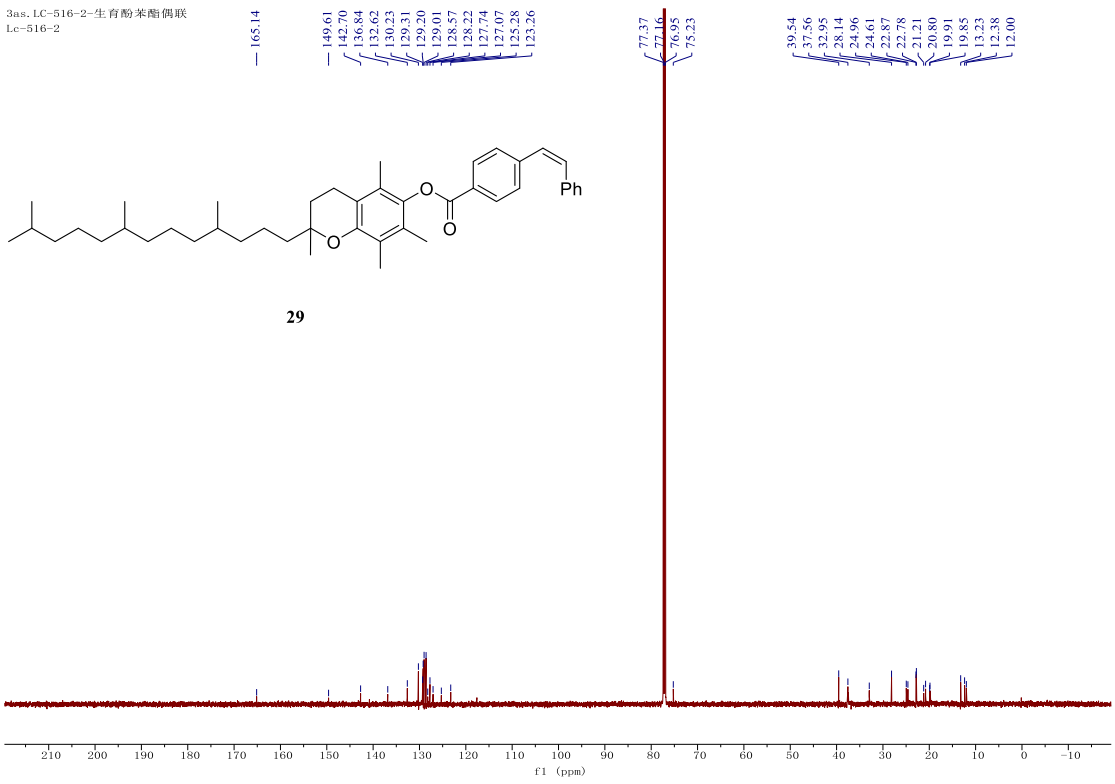


28

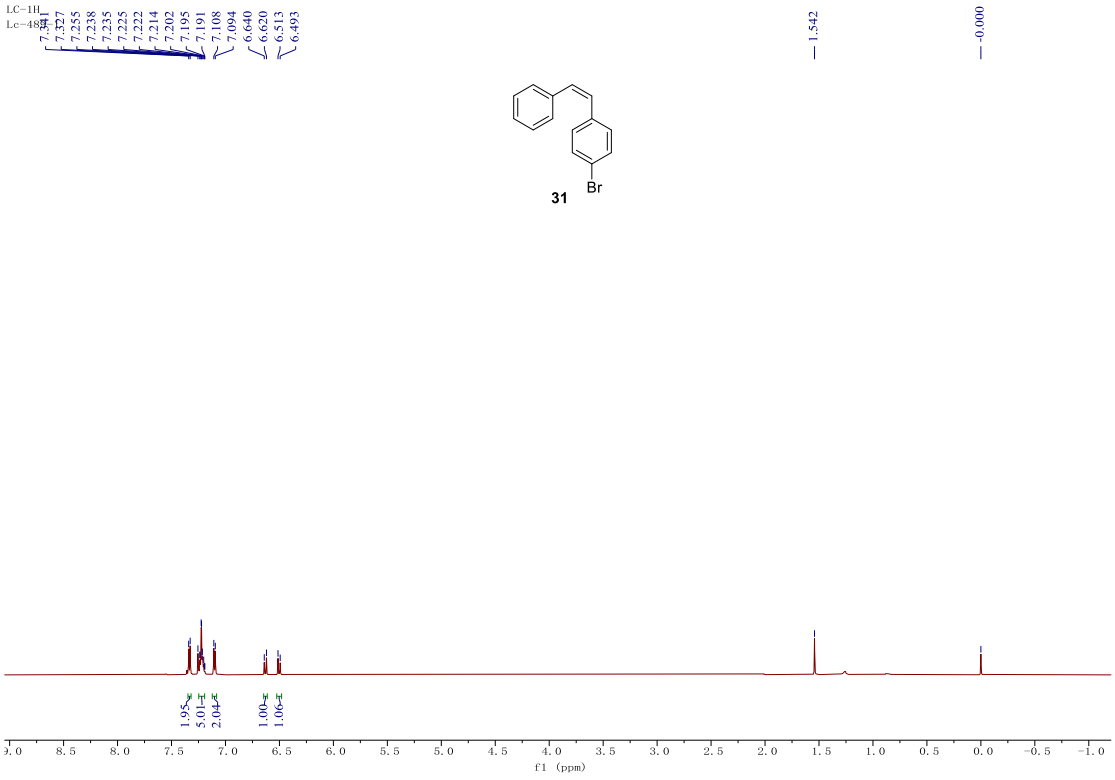

LC-1H
LC-516-2
8.088
8.074
7.384
7.371
7.271
7.264
7.256
7.247
7.241
7.233
6.757
6.737
6.650
6.629
2.622
2.611
2.600
2.112
2.050
2.007
1.853
1.841
1.830
1.819
1.807
1.768
1.538
1.523
1.512
1.501
1.294
1.285
1.258
1.247
1.153
1.142
1.137
1.132
1.127
1.116
1.076
0.871
0.860
0.852
0.841
-0.000
O
O
O
Ph

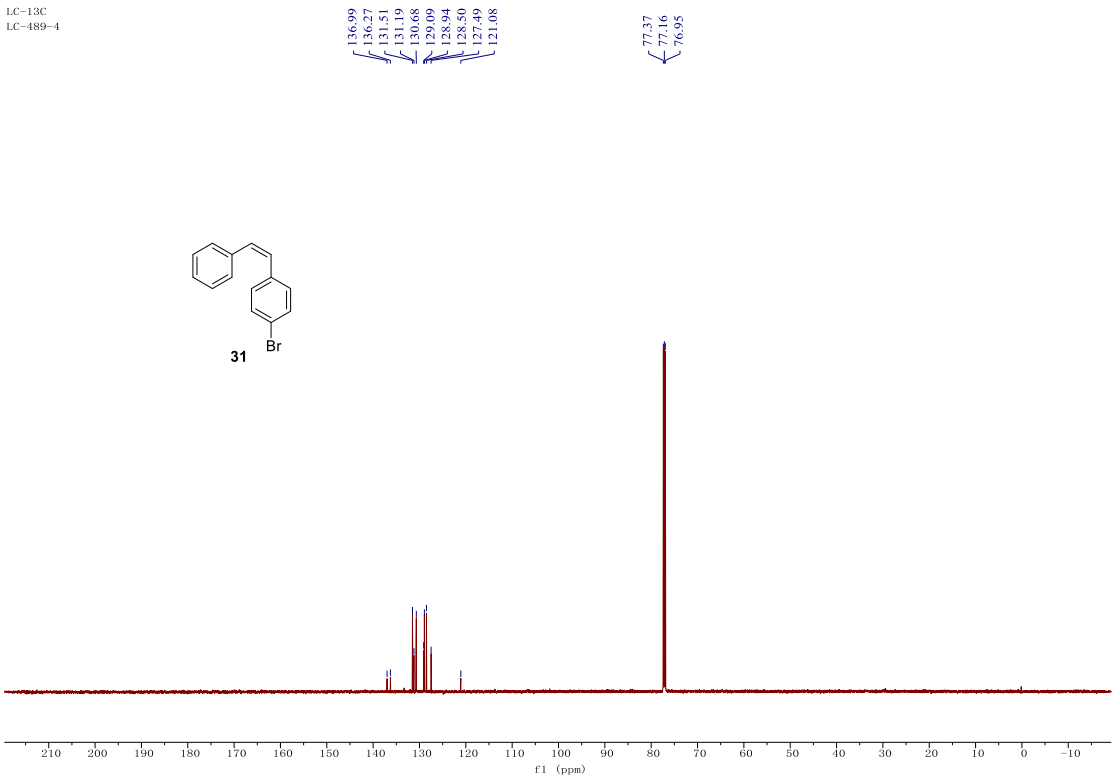
29


2.00
1.98
5.04
1.00
0.98
1.99
3.00
3.03
3.01
2.03
1.08
4.99
11.05
6.99
12.18
f1 (ppm)


3as.LC-516-2-生育酚苯酯偶联
Lc-516-2
165.14
149.61
142.70
136.84
132.62
130.23
129.31
129.20
129.01
128.57
128.22
127.74
127.07
125.28
123.26
77.37
77.16
76.95
75.23
39.54
37.56
32.95
28.14
24.96
24.61
22.87
22.78
21.21
20.80
19.91
19.85
13.23
12.38
12.00
O
O
O
Ph
f1 (ppm)

29


LC-1H
Lc-489-4
7.341
7.327
7.255
7.238
7.235
7.225
7.222
7.214
7.202
7.195
7.191
7.108
7.094
6.640
6.620
6.513
6.493
1.542
0.000
Br
31
1.95
5.01
2.04
1.00
1.06
f1 (ppm)

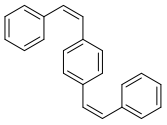

LC-13C
LC-489-4
136.99
136.27
131.51
131.19
130.68
129.09
128.94
128.50
127.49
121.08
77.37
77.16
76.95
Br
31
f1 (ppm)

LC-1H
LC-488-3

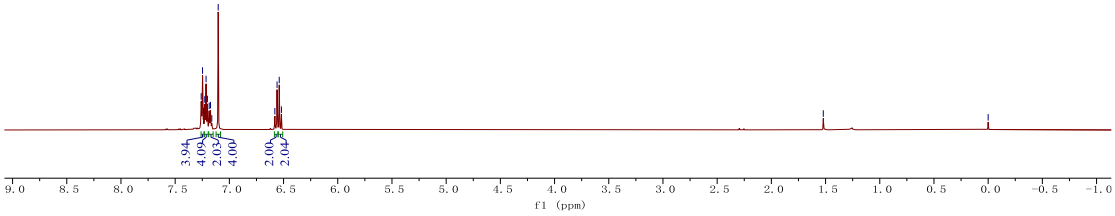
7.260
7.248
7.238
7.227
7.215
7.203
7.186
7.174
7.162
7.103
6.580
6.560
6.540
6.520

1.521

0.000



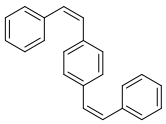
32



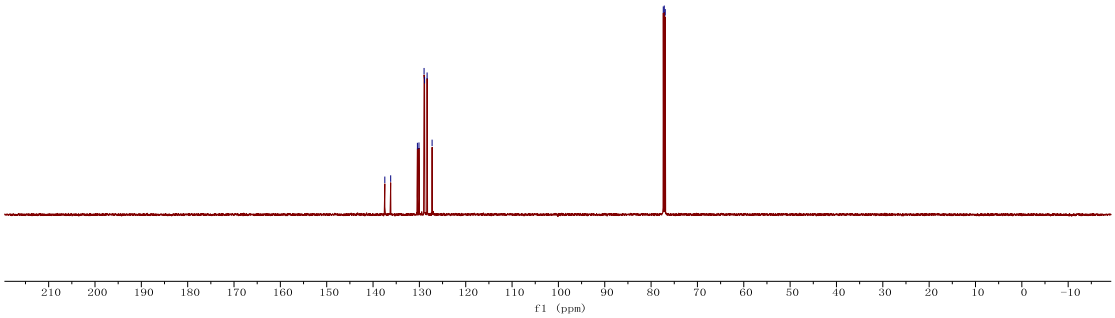
LC-13C
Lc-488-3

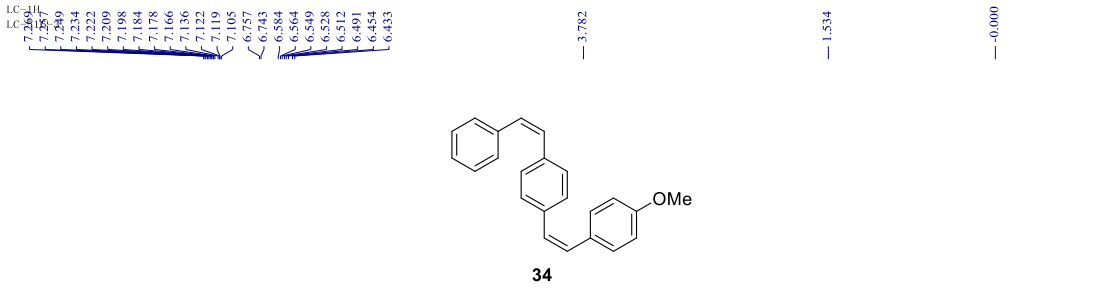
137.46
136.19
130.43
130.09
128.99
128.88
128.33
127.26

77.37
77.16
76.95



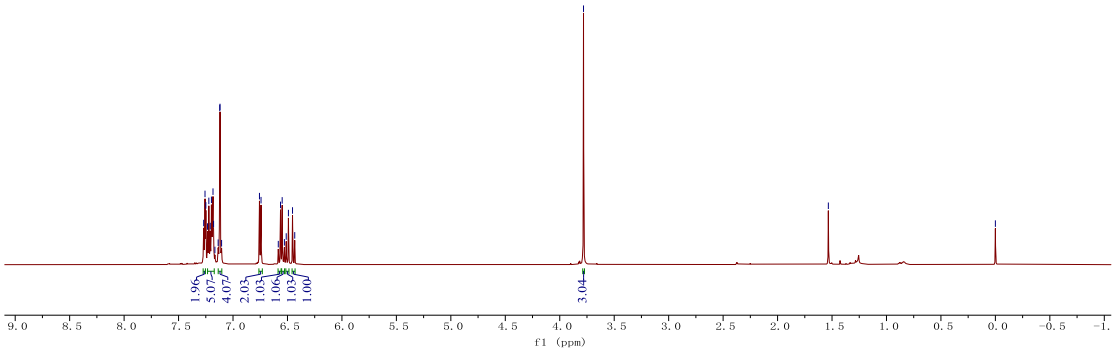
32

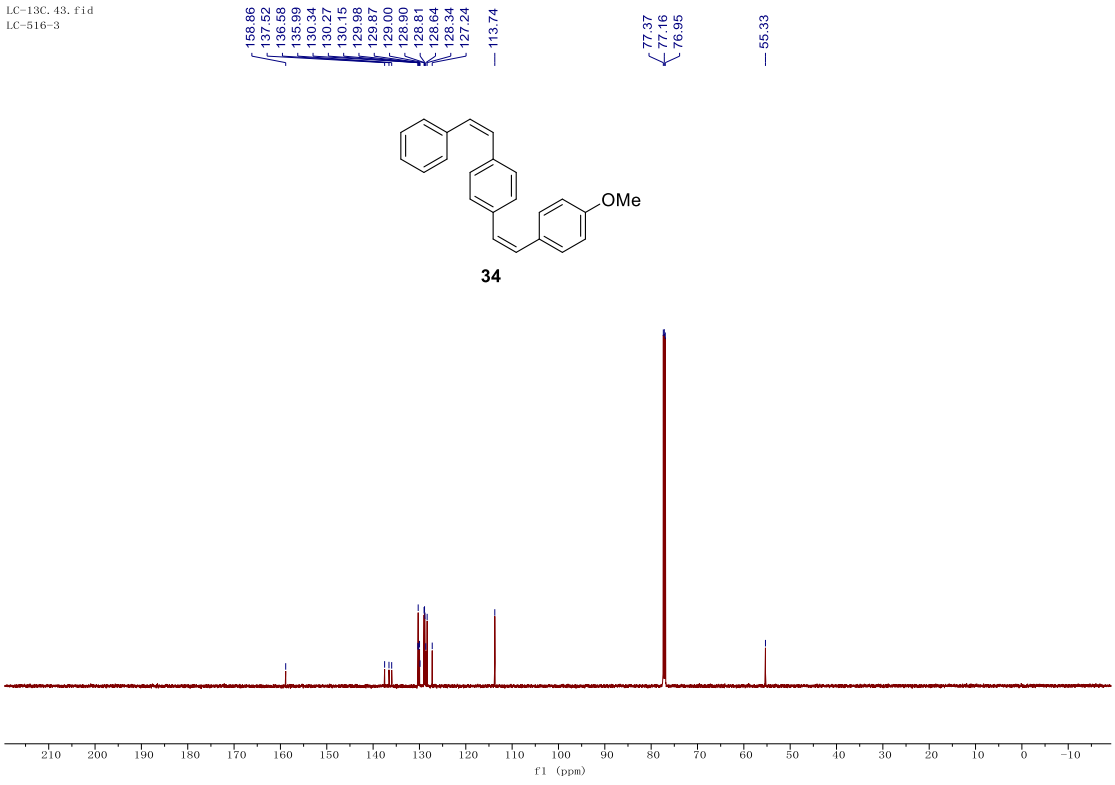



7.260
7.257
7.249
7.234
7.222
7.209
7.198
7.184
7.178
7.166
7.136
7.122
7.119
7.105
6.757
6.743
6.584
6.564
6.549
6.528
6.512
6.491
6.454
6.433
3.782
1.534
0.000

OMe

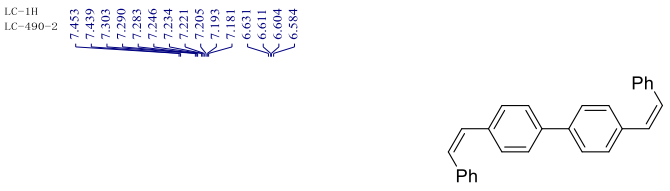
34


1.96
5.07
4.07
2.03
1.03
1.06
1.03
1.00
3.04
f1 (ppm)

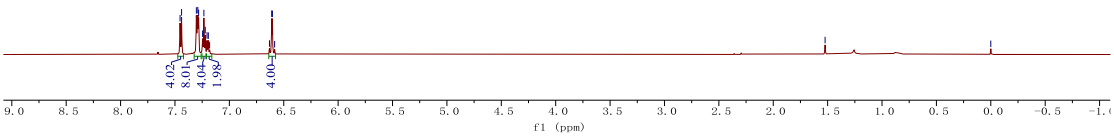

LC-13C.43.fid
LC-516-3
158.86
137.52
136.58
135.99
130.34
130.27
130.15
129.98
129.87
129.00
128.90
128.81
128.64
128.34
127.24
113.74
77.37
77.16
76.95
55.33
f1 (ppm)

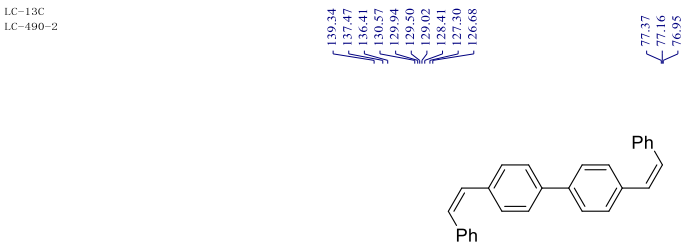
OMe

34

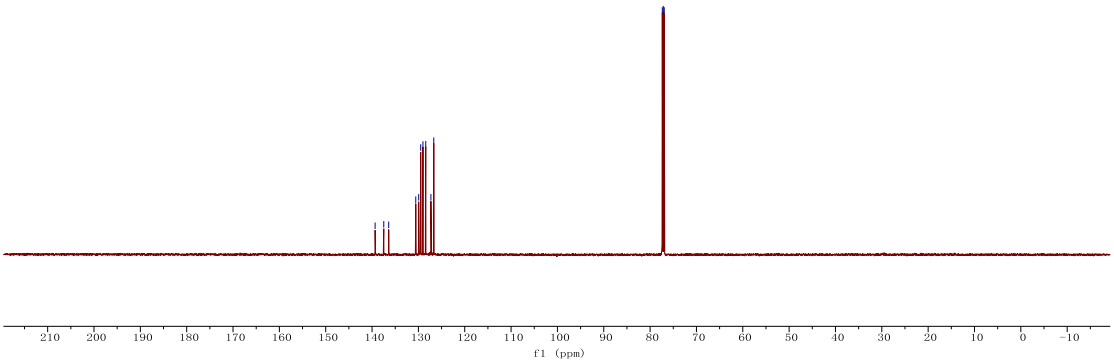

LC-1H
LC-490-2
7.453
7.439
7.303
7.290
7.283
7.246
7.234
7.221
7.205
7.193
7.181
6.631
6.611
6.604
6.584
1.523
0.000
Ph
Ph

36

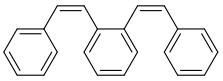

4.02
8.01
4.04
1.98
4.00
f1 (ppm)


LC-13C
LC-490-2
139.34
137.47
136.41
130.57
129.94
129.50
129.02
128.41
127.30
126.68
77.37
77.16
76.95
Ph
Ph

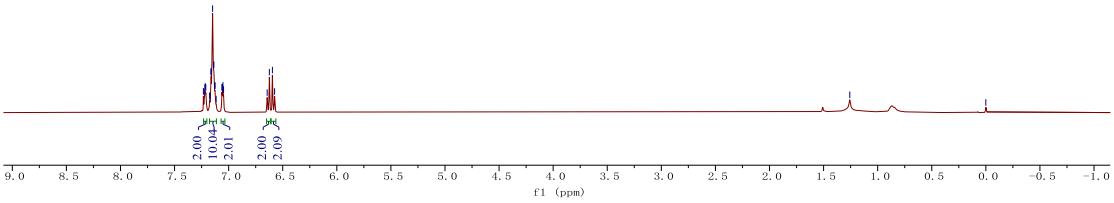
36


f1 (ppm)

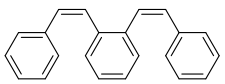

7.220
7.216
7.211
7.163
7.161
7.149
7.139
7.137
7.128
7.126
7.062
7.059
7.056
7.053
6.624
6.595
6.575
1.258
0.000



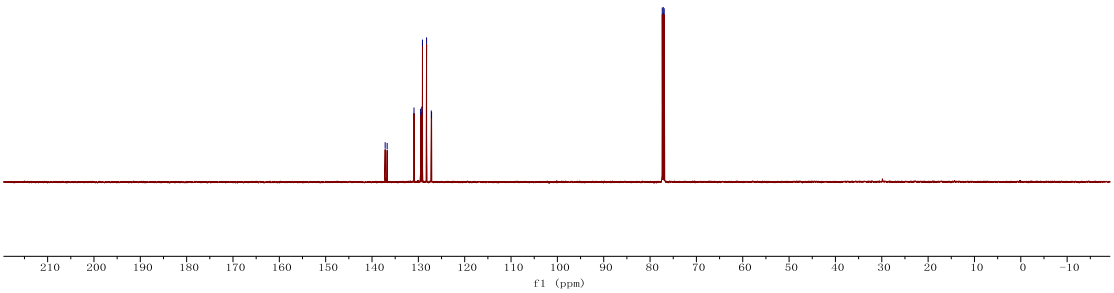
38


2.00
10.04
2.01
2.00
2.09
f1 (ppm)


LC-13C
LC-506-1
137.16
136.73
130.94
129.52
129.27
129.11
128.23
127.21
127.15
77.37
77.16
76.95



38

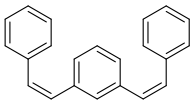

f1 (ppm)

LC-1H
LC-509-3

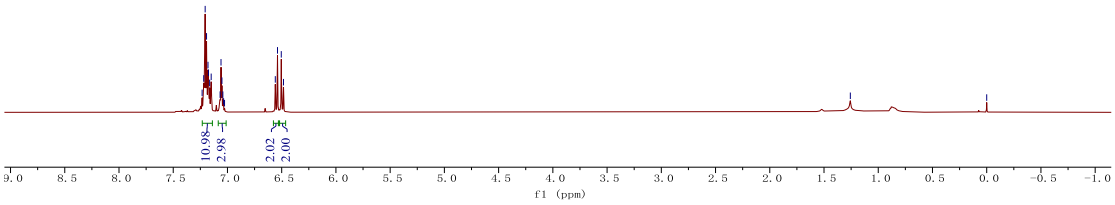
7.249
7.206
7.193
7.179
7.175
7.164
7.150
7.068
7.059
7.051
7.042
7.036
7.027
6.559
6.539
6.504
6.483

1.257

-0.000



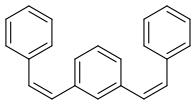
40



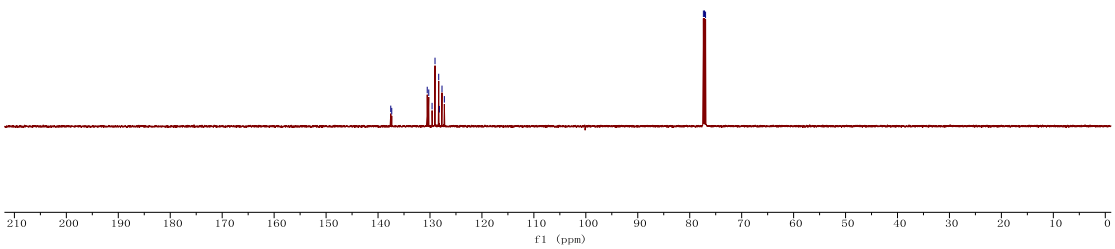
LC-13C
LC-509-3

137.55
137.36
130.53
130.24
129.60
129.03
128.32
128.20
127.69
127.23

77.37
77.16
76.95

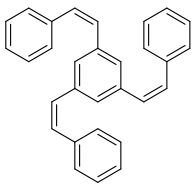


40

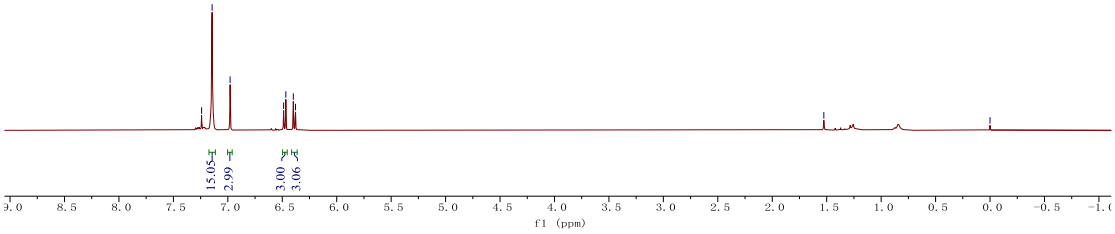


LC-1H
LC-491-1-1

7.241
7.144
6.979
6.488
6.467
6.399
6.378
1.526
0.000

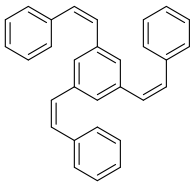


42

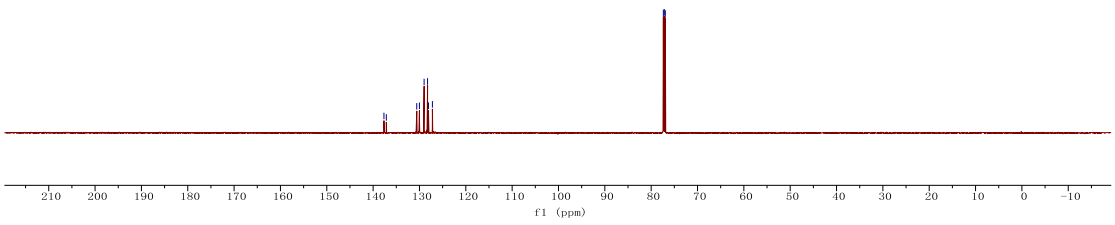


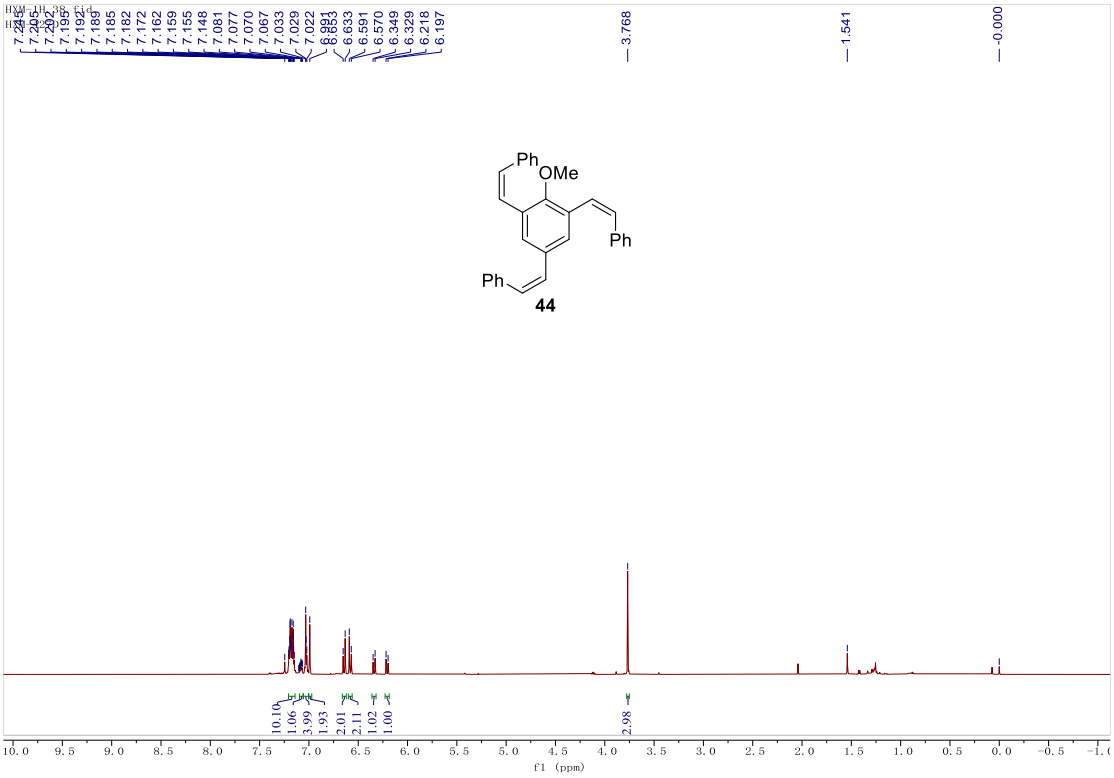
LC-13C
LC-491-1-1

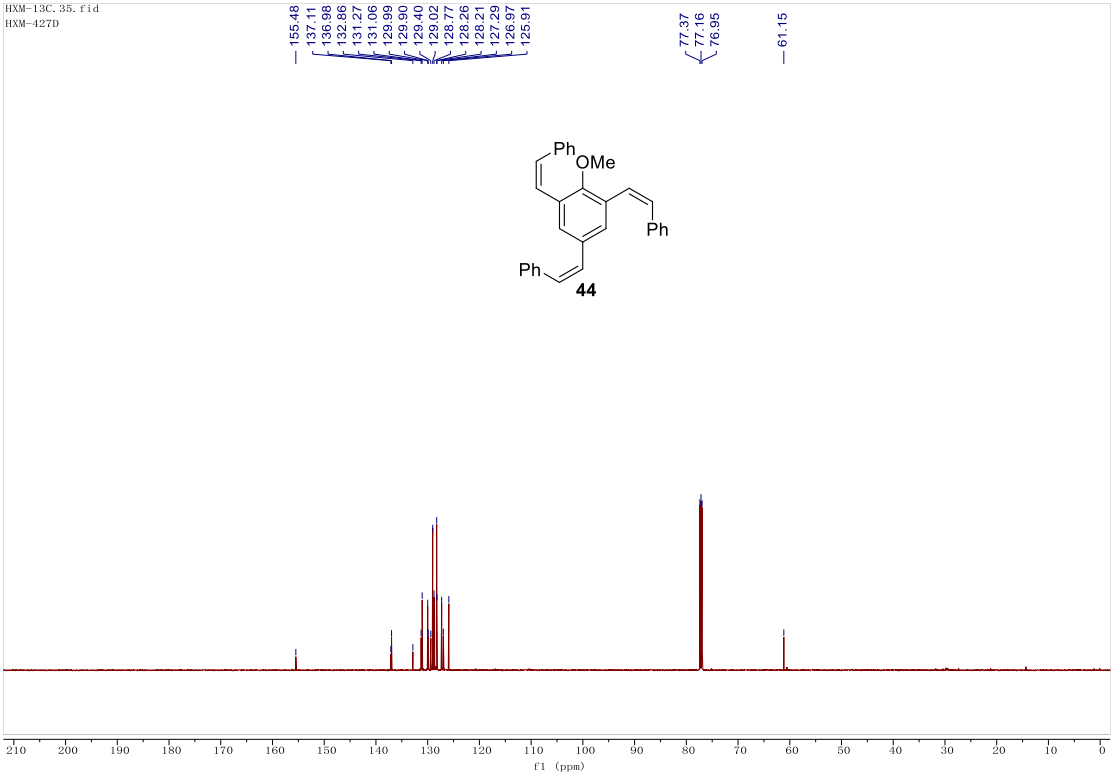
137.67
137.15
130.58
130.00
129.00
128.25
128.06
127.20
77.37
77.16
76.95

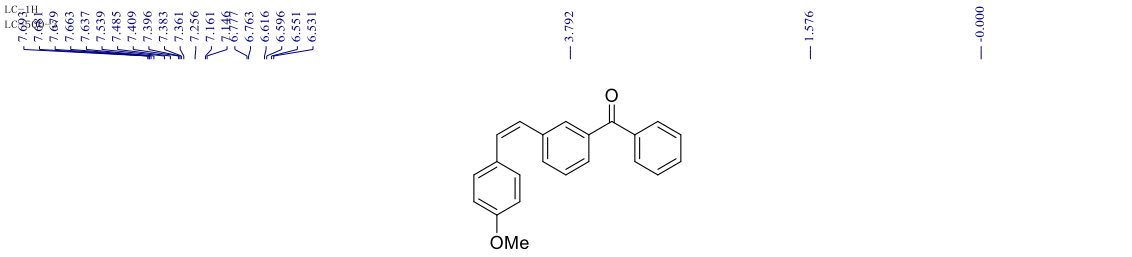


42

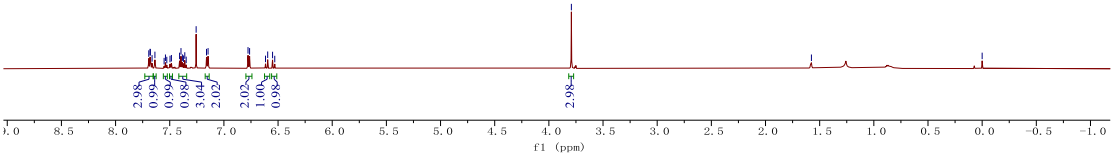


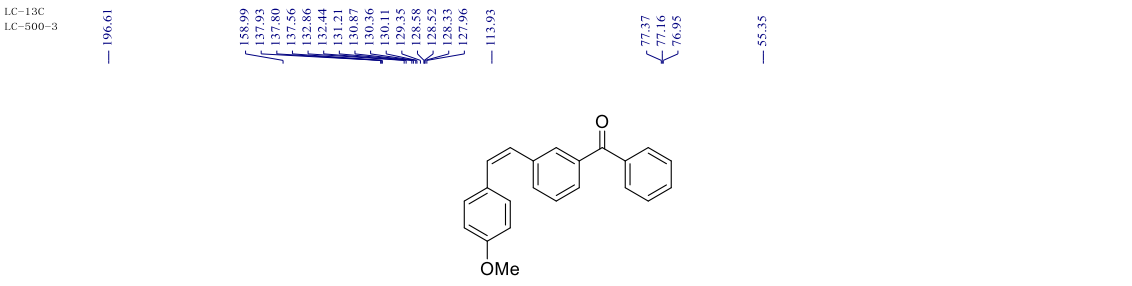

HXM-1H-38.fid
7.244
7.205
7.202
7.195
7.192
7.185
7.185
7.182
7.172
7.162
7.159
7.155
7.148
7.081
7.077
7.070
7.067
7.033
7.029
7.022
6.883
6.633
6.591
6.570
6.349
6.329
6.218
6.197
3.768
1.541
-0.000
Ph
OMe
Ph
Ph
44
10.10
1.06
3.99
1.93
2.01
2.11
1.02
1.00
2.98
f1 (ppm)


HXM-13C.35.fid
HXM-427D
155.48
137.11
136.98
132.86
131.27
131.06
129.99
129.90
129.40
129.02
128.77
128.26
128.21
127.29
126.97
125.91
77.37
77.16
76.95
61.15
Ph
OMe
Ph
Ph
44
f1 (ppm)

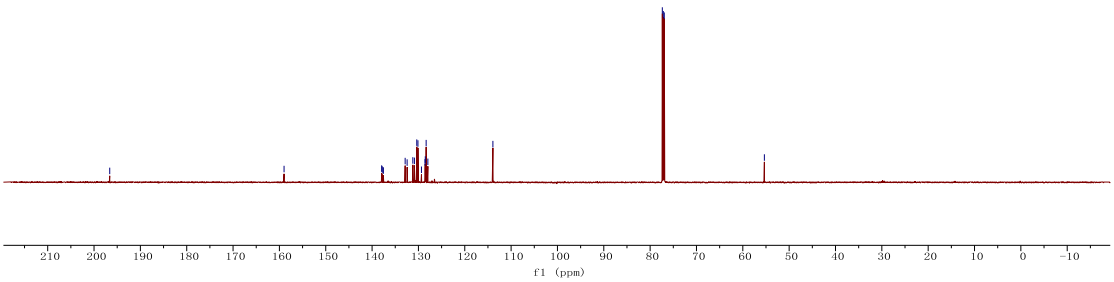

LC-1H
LC-500-3
7.693
7.690
7.679
7.663
7.637
7.539
7.485
7.409
7.396
7.383
7.361
7.256
7.161
6.763
6.616
6.596
6.551
6.531
3.792
1.576
0.000
O
OMe

47


2.98
0.99
0.99
0.98
3.04
2.02
2.02
1.00
0.98
2.98
f1 (ppm)


LC-13C
LC-500-3
196.61
158.99
137.93
137.80
137.56
132.86
132.44
131.21
130.87
130.36
130.11
129.35
128.58
128.52
128.33
127.96
113.93
77.37
77.16
76.95
55.35
O
OMe

47


f1 (ppm)