Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Copper(I)-Catalyzed Synthesis of 1,3-Enynes via Coupling between Vinyl Halides and Alkynes or Domino Coupling of Vinyl halides

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Experimental Section

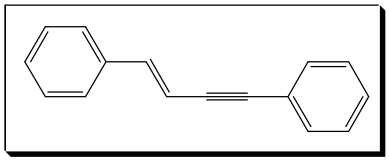
General Procedures

All reactions were carried out under an argon atmosphere condition. Solvents were dried and degassed by standard methods and all alkynes were purchased from Aldrich and Alfa. Various vinyl halides were prepared according the references. 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.

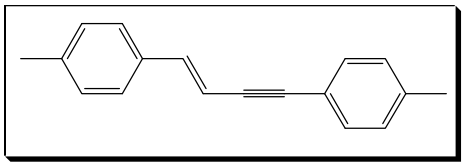
General procedure for copper-catalyzed domino coupling of (*E*)-vinyl halide: Vinyl halide (0.8 mmol), CuI (10 mol%), and K_3PO_4 (0.8 mmol) were added to a screw-capped test tube. The tube was then evacuated and backfilled with argon (3 cycles). DMSO (2 mL) was added by syringe at room temperature. The tube was again evacuated and backfilled with argon (3 cycles). The mixture was heated to 135 ^{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.

General procedure for copper-catalyzed coupling of vinyl halide and terminal alkynes: A mixture of vinyl halide (0.4 mmol), alkyne (0.5 mmol), CuI (10 mol%), and K_3PO_4 (0.8 mmol), and DMSO (2 mL) in a Schlenk tube was stirred under argon atmosphere 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.

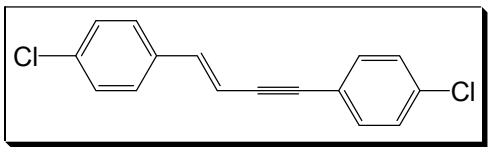
Characterization of the corresponding products:



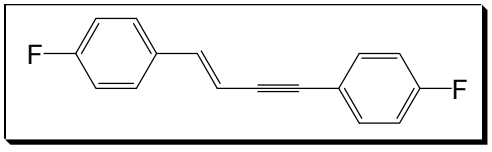
^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.48 (d, J = 7.6 Hz, 2H), 7.42 (d, J = 7.2 Hz, 2H), 7.35–7.24 (m, 6H), 7.04 (d, J = 16.0 Hz, 1H), 6.39 (d, J = 16.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) (δ, ppm) 141.7, 136.8, 132.0, 129.2, 129.0, 128.8, 128.7, 126.8, 123.8, 108.6, 92.2, 89.4; (ESI^+): HRMS calcd. for $[C_{16}H_{12}]^+$ requires m/z 204.0939, found 204.0939.



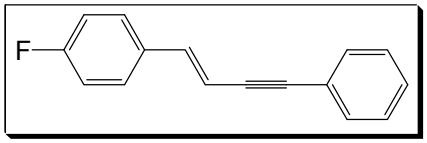
^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.37–7.31 (m, 4H), 7.16–7.12 (m, 4H), 7.00 (d, J = 16.0 Hz, 1H), 6.33 (d, J = 16.0 Hz, 1H), 2.37 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) (δ, ppm) 141.1, 138.9, 138.5, 133.9, 131.6, 129.7, 129.4, 126.5, 120.6, 107.4, 91.9, 88.7, 21.8, 21.6; HRMS calcd. for $[C_{18}H_{16}]^+$ requires m/z 232.1252, found 232.1254.



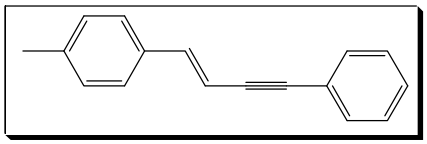
^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.40–7.34 (m, 4H), 7.33–7.30 (m, 4H), 6.99 (d, J = 16.0 Hz, 1H), 6.34 (d, J = 16.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) (δ, ppm) 140.5, 134.9, 134.7, 134.6, 133.0, 129.2, 129.0, 127.7, 122.0, 108.7, 91.4, 89.8; HRMS calcd. for $[C_{16}H_{10}Cl_2]^+$ requires m/z 272.0160, found 272.0160.



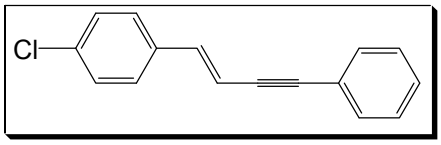
^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.46–7.37 (m, 4H), 7.05–7.01 (m, 4H), 6.97 (s, 1H), 6.27 (d, J = 16.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) (δ, ppm) 163.2 (d, ^{1}J = 247.7 Hz), 162.7 (d, ^{1}J = 248.2 Hz), 140.3, 133.6 (d, ^{3}J = 8.3 Hz), 132.7 (d, ^{4}J = 3.0 Hz), 128.2 (d, ^{3}J = 8.0 Hz), 119.6 (d, ^{4}J = 3.2 Hz), 116.0 (d, ^{2}J = 21.7 Hz), 115.9 (d, ^{2}J = 22.0 Hz), 107.9, 90.8, 88.6; HRMS calcd. for $[C_{16}H_{10}F_2]^+$ requires m/z 240.0751, found 240.0751.



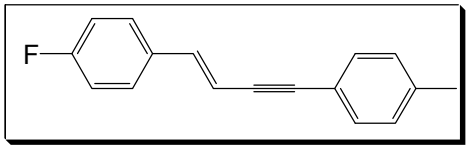
^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.48–7.46 (m, 2H), 7.41–7.38 (m, 2H), 7.35–7.32 (m, 3H), 7.06–6.98 (m, 3H), 6.30 (d, J = 16.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) (δ, ppm) 163.1 (d, ^{1}J = 247.7 Hz), 140.2, 132.8 (d, ^{4}J = 2.9 Hz), 131.7, 128.6, 128.5, 128.2 (d, ^{3}J = 8.0 Hz), 123.5, 116.0 (d, ^{2}J = 21.8 Hz), 108.1, 92.0, 88.9; HRMS calcd. for $[C_{16}H_{11}F]^+$ requires m/z 222.0845, found222.0844.



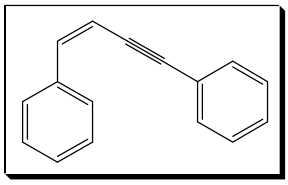
^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.47 (t, J = 2.7 Hz, 2H), 7.32 (d, J = 6.3 Hz, 5H), 7.15 (d, J = 7.8 Hz, 2H), 7.02 (d, J = 16.2 Hz, 1H), 6.33 (d, J = 16.2 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 141.7, 139.2, 134.0, 131.9, 129.9, 128.8, 128.6, 126.7, 123.9, 107.4, 91.8, 89.6, 21.8; HRMS calcd. for $[C_{17}H_{14}]^+$ requires m/z 217.1096, found 217.1061.



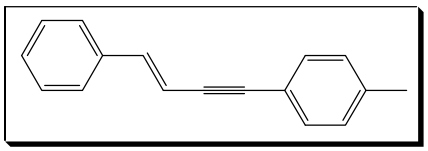
^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.49–7.46 (m, 2H), 7.41–7.25 (m, 7H), 6.98 (d, J = 16.2 Hz, 1H), 6.35 (d, J = 16.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 140.3, 135.2, 134.7, 132.0, 129.4, 128.9, 128.8, 127.9, 123.7, 109.2, 92.8, 89.0; HRMS calcd. for $[C_{16}H_{11}Cl]^+$ requires m/z 238.0549, found238.0548.



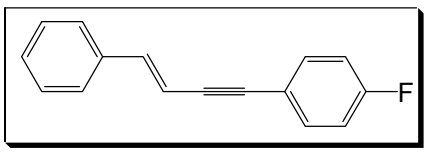
^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.37 (d, J = 6.0 Hz, 4H), 7.14 (d, J = 7.5 Hz, 2H), 7.05–6.95 (m, 3H), 6.28 (d, J = 16.2 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 163.3 (d, ^1J = 247.2 Hz), 140.0, 138.9, 133.1, 131.8, 129.6, 128.3 (d, ^3J =6.0 Hz), 120.6, 116.2 (d, ^2J = 21.6 Hz), 108.5, 92.4, 88.5, 22.0; HRMS calcd. for $[C_{17}H_{13}F]^+$ requires m/z 236.1001, found 236.1001.



^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.932 (d, J = 7.3 Hz, 2H), 7.51–7.48 (m, 2H), 7.41 (d, J = 6.9 Hz, 1H), 7.37–7.31 (m, 5H), 6.71 (d, J = 11.7 Hz, 1H), 5.93 (d, J = 11.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 139.1, 137.0, 131.9, 129.2, 129.0, 128.9, 128.8, 126.8, 123.9, 107.8, 96.3, 88.7; HRMS calcd. for $[C_{16}H_{12}]^+$ requires m/z 205.0973, found 205.0981.

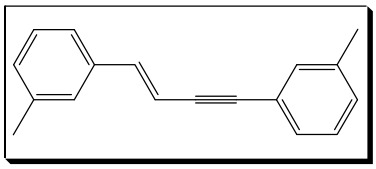


^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.43–7.24 (m, 7H), 7.13 (d, J = 7.5 Hz, 2H), 7.02 (d, J = 16.2 Hz, 1H), 6.38 (d, J = 16.2 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 141.3, 138.8, 136.8, 131.9, 129.6, 129.2, 129.0, 126.7, 120.7, 108.7, 92.5, 88.7, 22.0; HRMS calcd. for $[C_{17}H_{14}]^+$ requires m/z 218.1096, found 218.1096.

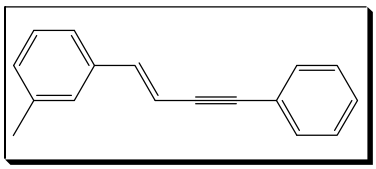


^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.46–7.40 (m, 4H), 7.36–7.28 (m, 3H), 7.05 (d,

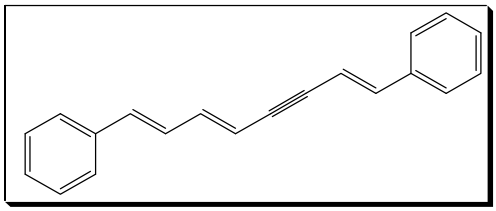
J = 3.6 Hz, 1H), 7.00 (t, *J* = 8.7 Hz, 2H), 6.35 (d, *J* = 16.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 163.0 (d, ^1J = 248.2 Hz), 141.9, 136.8, 134.0 (d, ^3J = 8.2 Hz), 129.3, 129.2, 126.9, 120.1 (d, ^4J = 3.3 Hz), 116.2 (d, ^2J = 22.0 Hz), 108.5, 91.2, 89.2; HRMS calcd. for $[C_{16}H_{11}F]^+$ requires m/z 222.0845, found 222.0844.



^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.29 (d, *J* = 8.7 Hz, 2H), 7.20 (t, *J* = 4.2 Hz, 4H), 7.12 (d, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 16.2 Hz, 1H), 6.35 (d, *J* = 16.2 Hz, 1H), 2.35 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 141.9, 138.9, 138.6, 136.9, 132.7, 130.0, 129.7, 129.2, 129.2, 128.8, 127.6, 124.0, 123.8, 108.5, 92.4, 89.3, 22.0, 21.8; HRMS calcd. for $[C_{18}H_{16}]^+$ requires m/z 232.1252, found232.1254.

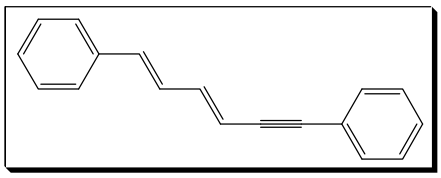


^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.48 (t, *J* = 3.3 Hz, 2H), 7.32 (d, *J* = 4.8 Hz, 3H), 7.23 (d, *J* = 3.3 Hz, 3H), 7.11 (s, 1H), 7.00 (d, *J* = 16.2 Hz, 1H), 6.37 (d, *J* = 16.2 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 142.0, 138.9, 136.8, 132.1, 130.1, 129.7, 129.2, 128.9, 128.7, 127.6, 124.1, 108.4, 92.2, 89.6, 22.0; HRMS calcd. for $[C_{17}H_{14}]^+$ requires m/z 218.1096, found 218.1095.

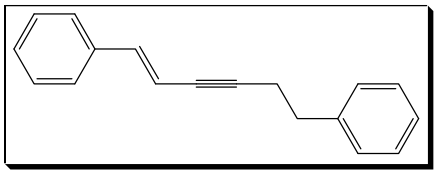


^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.41 (t, *J* = 5.7 Hz, 4H), 7.33 (t, *J* = 6.6 Hz, 4H), 7.26 (d, *J* = 7.5 Hz, 2H), 6.96 (d, *J* = 16.2 Hz, 1H), 6.85 (d, *J* = 13.8 Hz, 1H), 6.76 (d, *J* = 10.8 Hz, 1H), 6.64 (d, *J* = 14.4 Hz, 1H), 6.34 (dd, *J* = 16.2 Hz, 1H), 5.90 (d, *J* =

12.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 142.4, 141.6, 137.3, 136.9, 135.3, 129.3, 129.3, 129.2, 128.8, 128.7, 127.2, 126.9, 112.1, 108.9, 93.4, 92.6; HRMS calcd. for $[C_{20}H_{16}]^+$ requires m/z 256.1252, found 256.1251.

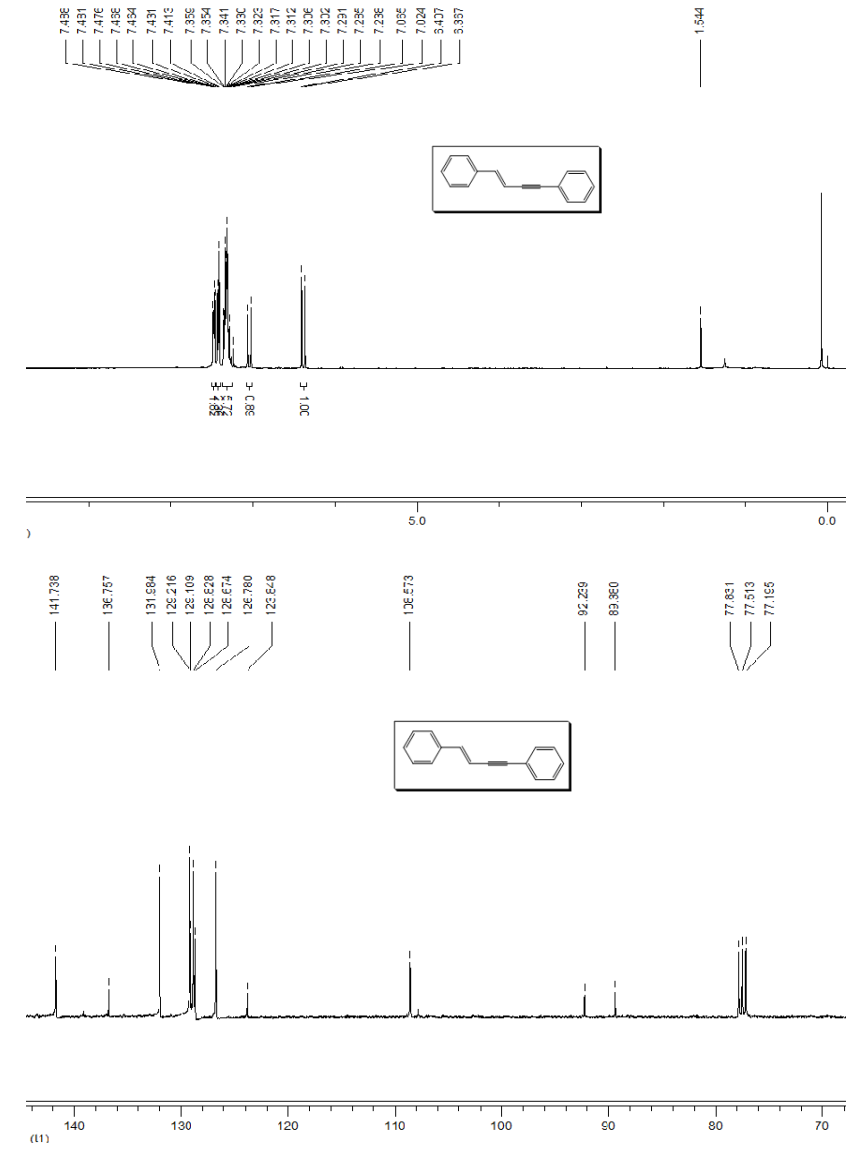


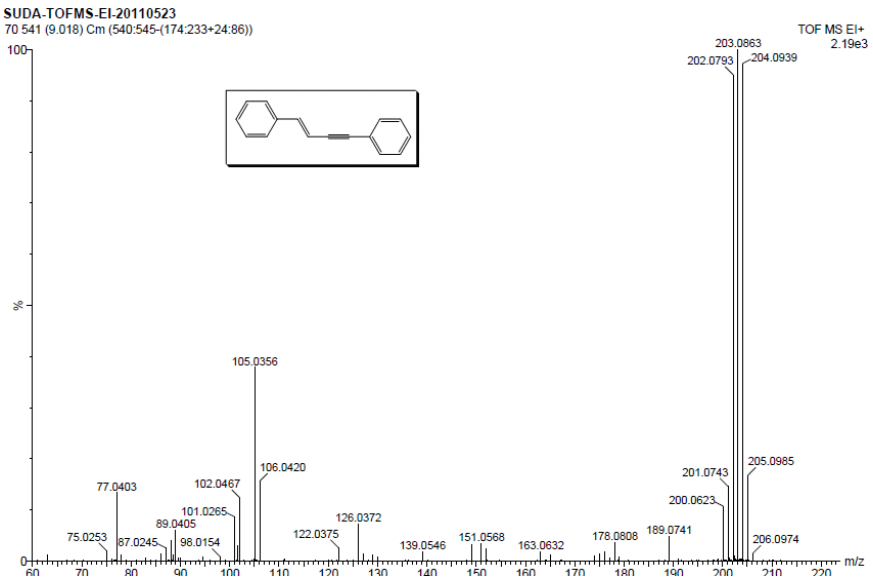
^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.45 (t, J = 7.2 Hz, 4H), 7.36–7.28 (m, 6H), 6.89–6.84 (m, 2H), 6.65 (d, J = 14.7 Hz, 1H), 5.95 (d, J = 13.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 142.5, 137.3, 135.3, 132.0, 129.3, 128.9, 128.7, 128.7, 127.2, 126.9, 124.0, 111.9, 93.5, 90.0; HRMS calcd. for $[C_{18}H_{14}]^+$ requires m/z 230.1096, found 230.1094.

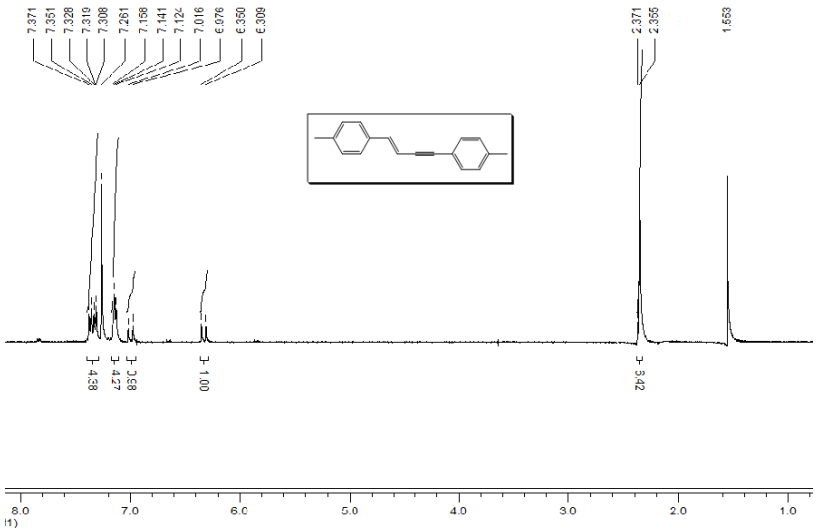


^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm) 7.48–7.41 (m, 2H), 7.33 (t, J = 3.0 Hz, 3H), 7.31 (d, J = 2.4 Hz, 2H), 7.22 (d, J = 6.3 Hz, 2H), 7.05 (d, J = 16.2 Hz, 1H), 6.38 (d, J = 16.2 Hz, 1H), 2.85 (t, J = 7.5 Hz, 2H), 2.51–2.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 141.9, 132.1, 130.5, 129.3, 129.2, 129.0, 128.9, 127.0, 126.9, 108.7, 92.3, 89.5, 69.5, 35.4; HRMS calcd. for $[C_{18}H_{16}]^+$ requires m/z 232.1252, found 232.1252.

Copy of HRMS and NMR Spectra for desired products:



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7.319
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7.261
7.156
7.141
7.016
6.676
6.350
6.309
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2.355
1.553
4.58
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6.0
5.0
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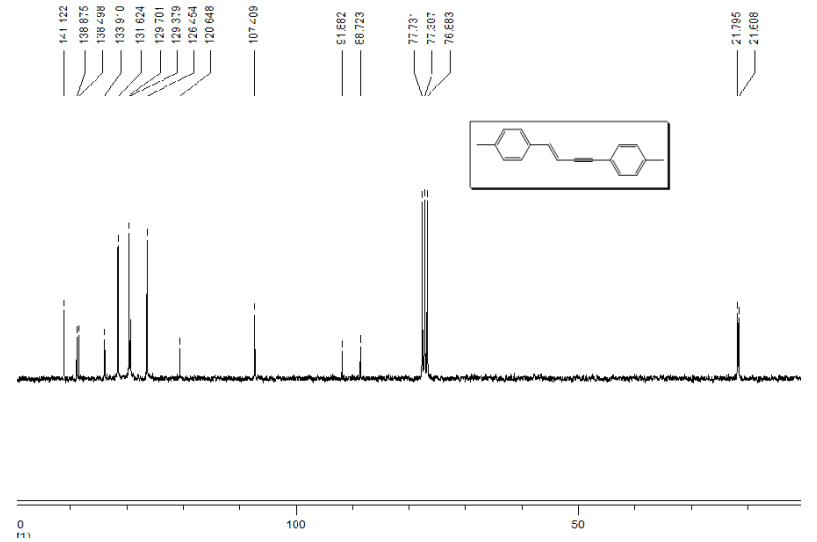
3.0
2.0
1.0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138.498
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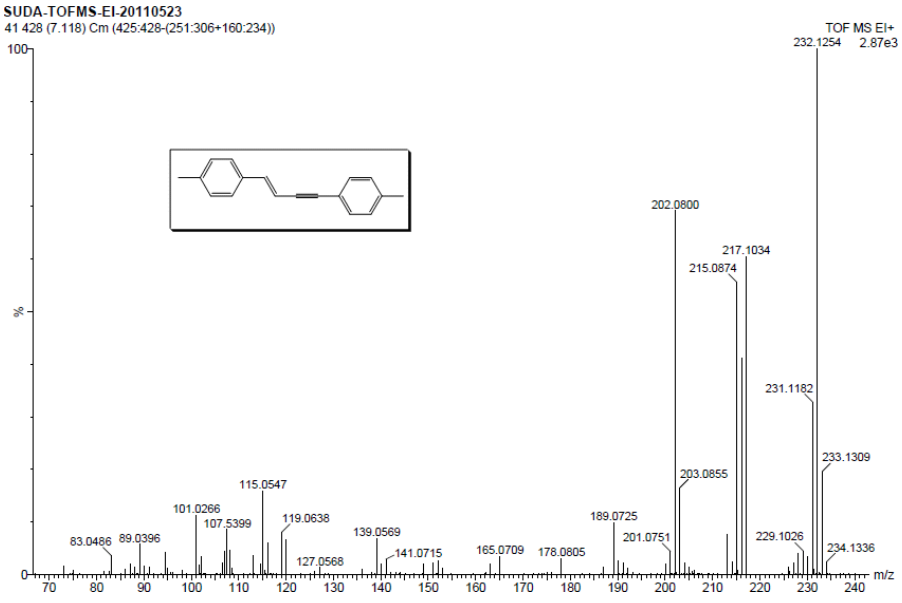
129.701
129.379
126.454
120.648
107.409
91.682
88.723
77.737
77.307
76.883
21.795
21.608
0
100
50


SUDA-TOFMS-EI-20110523
41 428 (7.118) Cm (425:428-(251:306+160:234))
TOF MS EI+
232.1254 2.87e3
100
%
0
202.0800
217.1034
215.0874
231.1182
233.1309
203.0855
115.0547
101.0266
107.5399
119.0638
83.0486
89.0396
139.0569
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150
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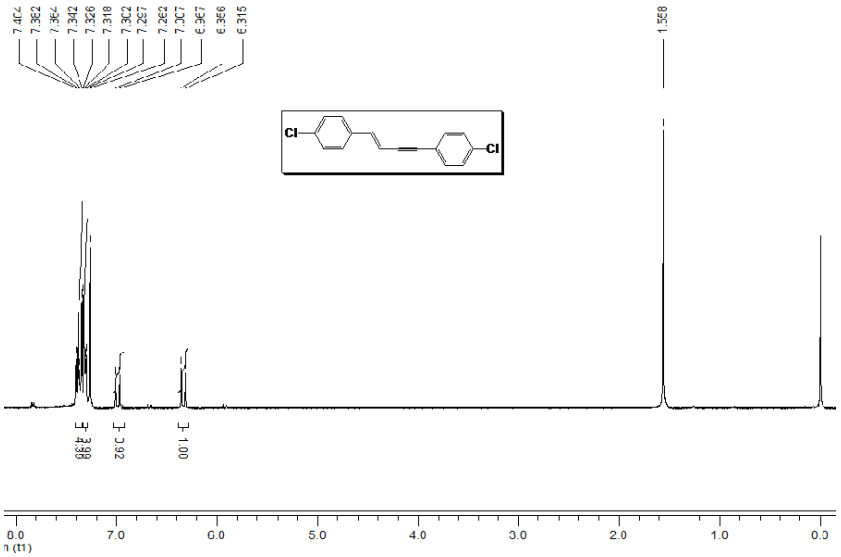
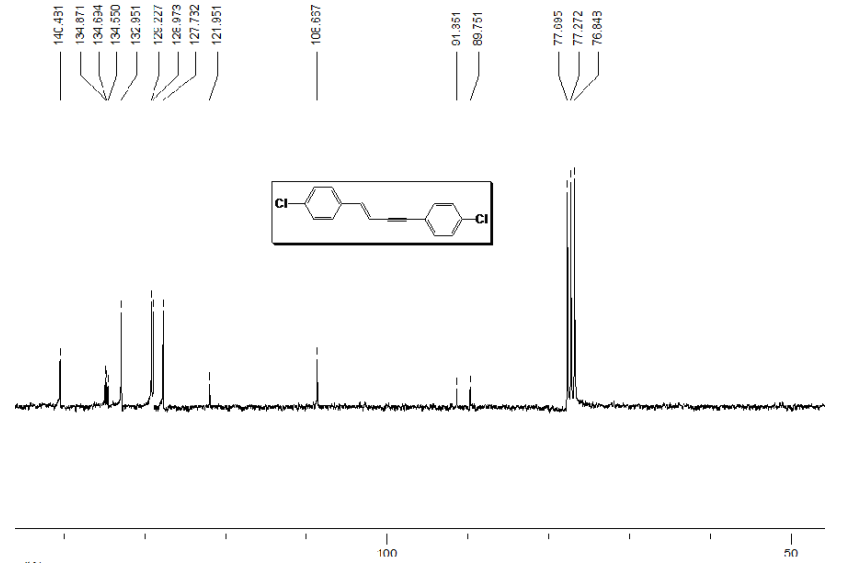
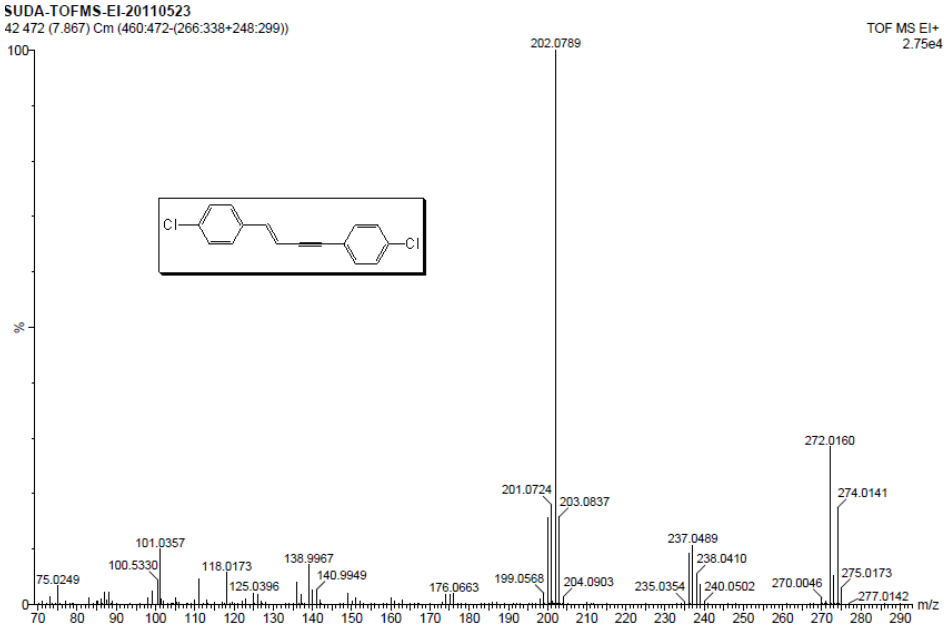
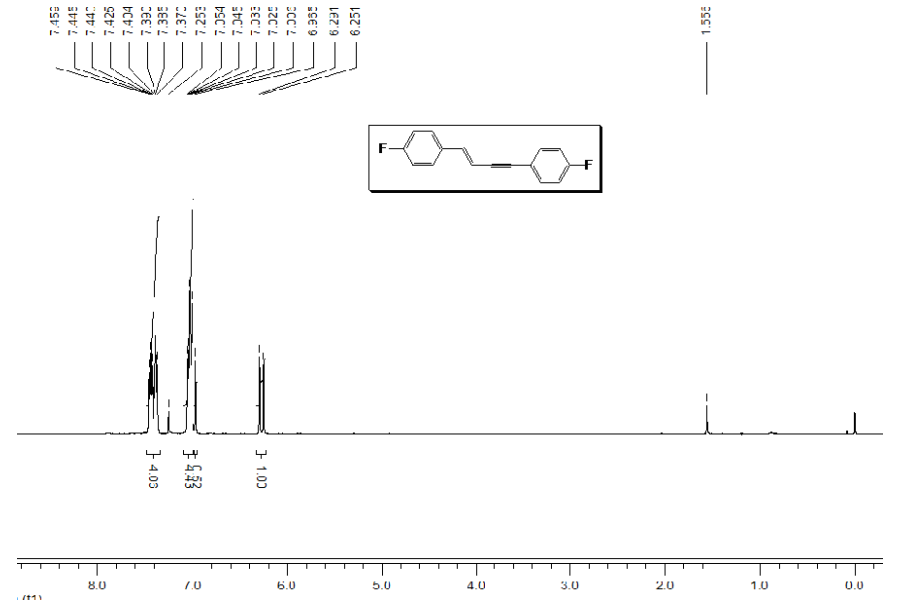
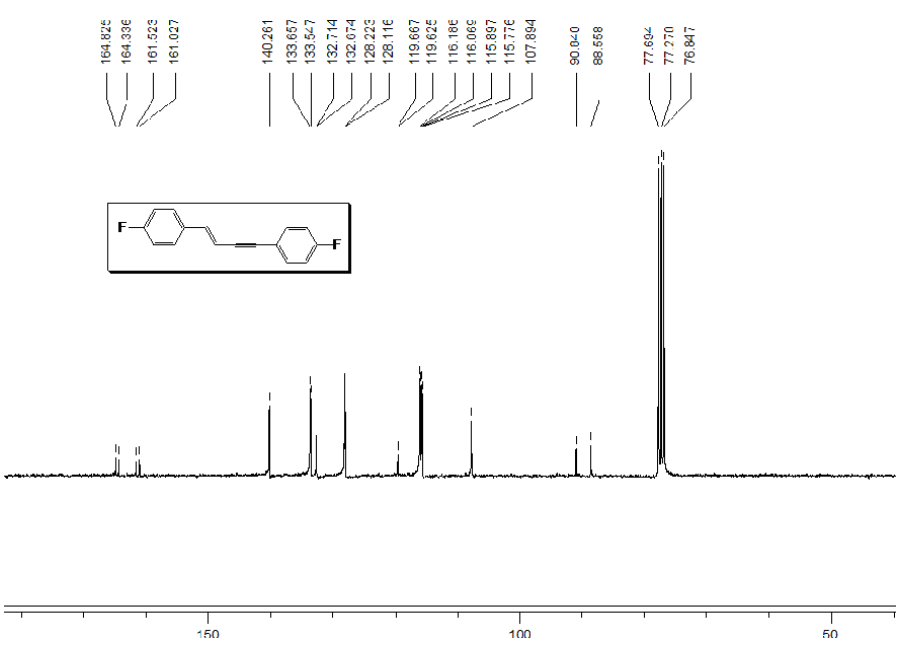
190
200
210
220
230
240

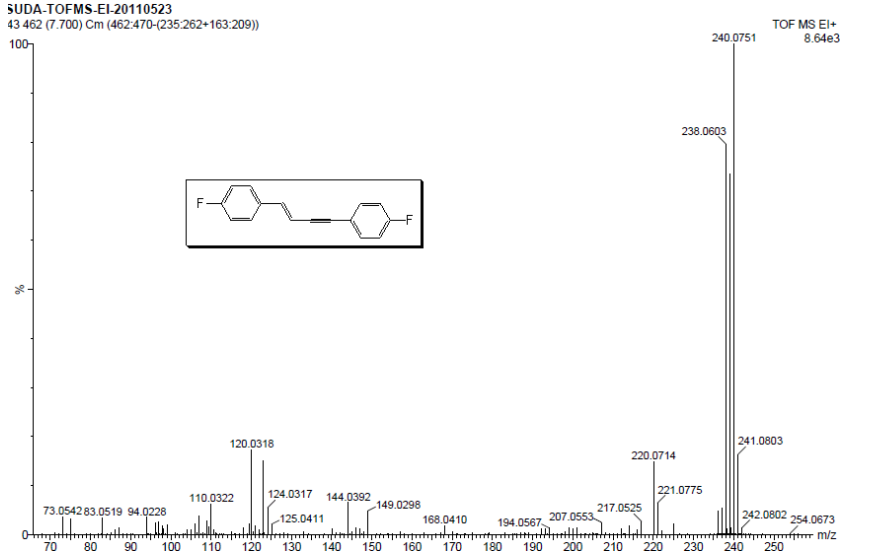


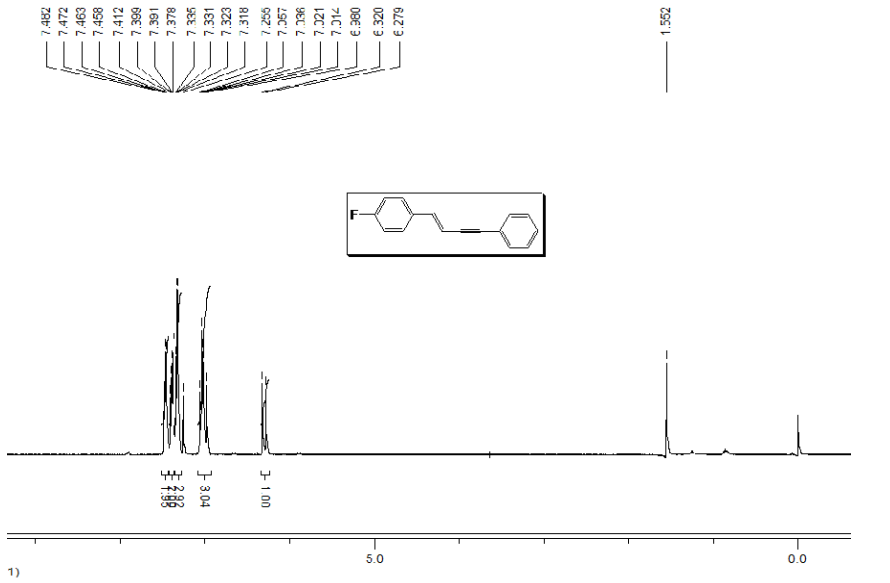


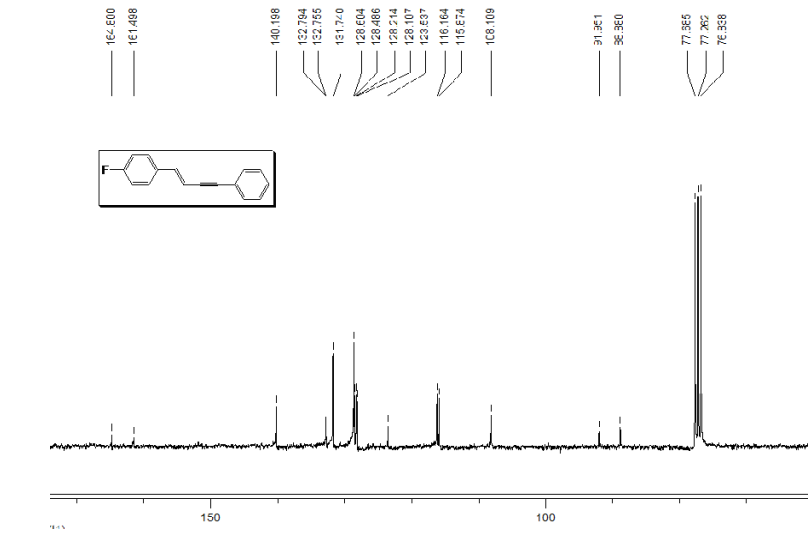


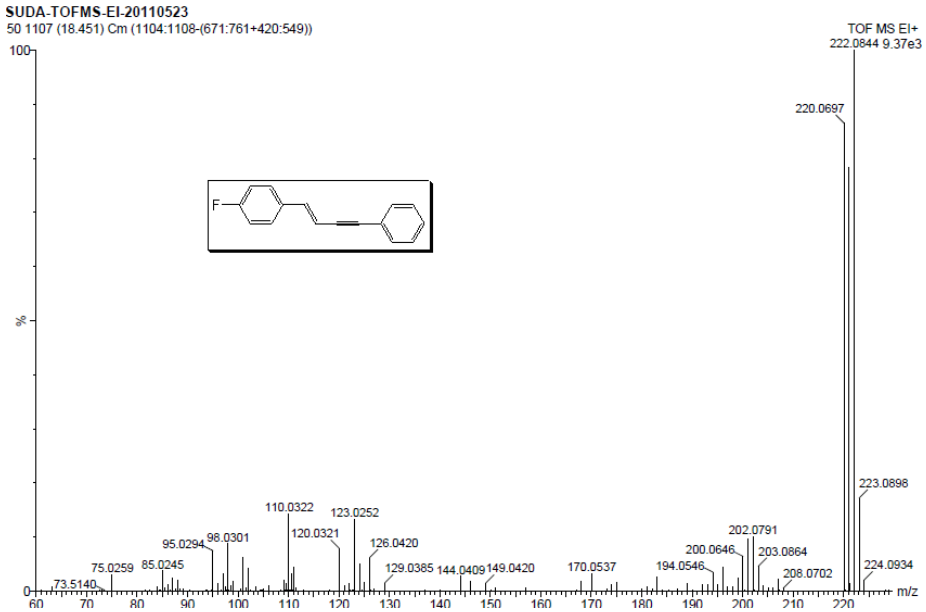

7.455
7.445
7.441
7.426
7.404
7.392
7.388
7.372
7.253
7.354
7.345
7.333
7.325
7.305
6.395
6.291
6.251
1.553
F
F
4.00
4.33
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

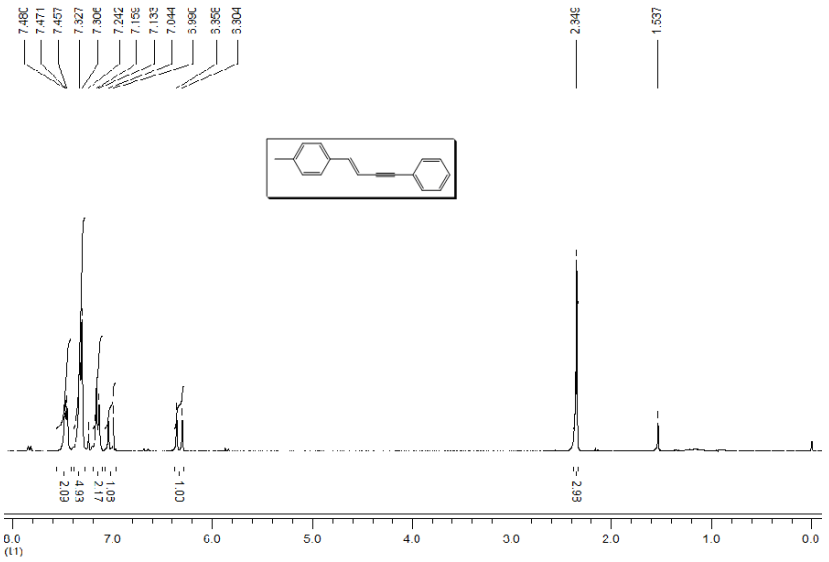

164.825
164.336
161.523
161.027
140.261
133.657
133.547
132.714
132.674
128.223
128.116
119.667
119.625
116.186
116.069
115.897
115.776
107.894
90.040
88.568
77.604
77.270
76.847
F
F
150
100
50

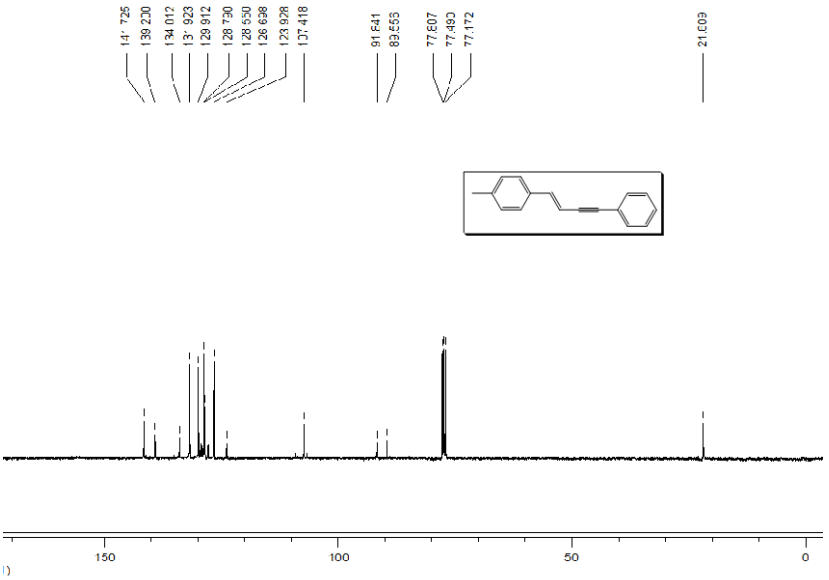

SUDA-TOFMS-EI-20110523
43 462 (7.700) Cm (462:470-(235:262+163:209))
TOF MS EI+
8.64e3
240.0751
238.0603
F
F
%
120.0318
110.0322
124.0317
144.0392
149.0298
125.0411
168.0410
73.0542
83.0519
94.0228
194.0567
207.0553
217.0525
220.0714
221.0775
241.0803
242.0802
254.0673
m/z
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250

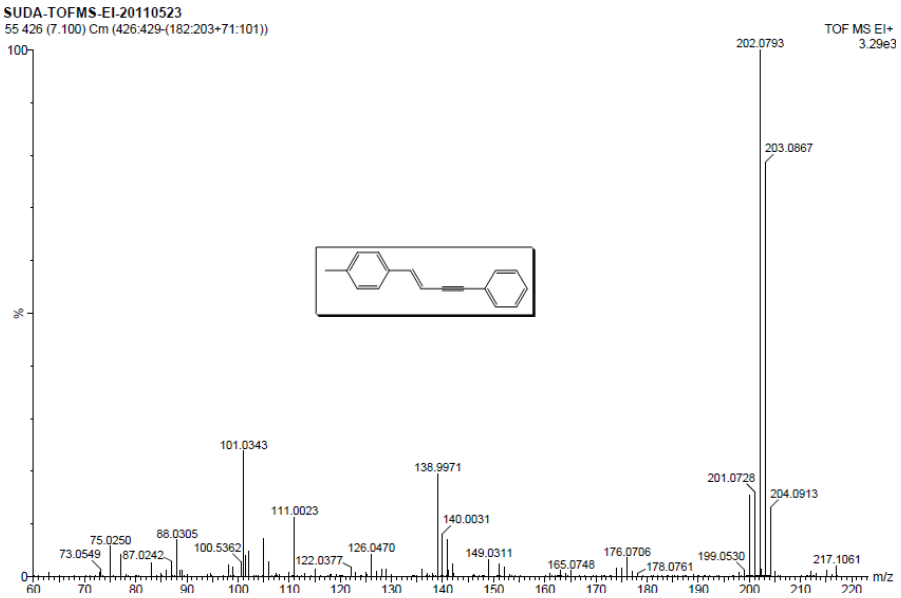

7.462
7.472
7.463
7.458
7.412
7.399
7.391
7.378
7.335
7.331
7.323
7.318
7.256
7.057
7.036
7.021
7.014
6.980
6.320
6.279
1.552
F
2.00
2.96
3.04
1.00
5.0
0.0

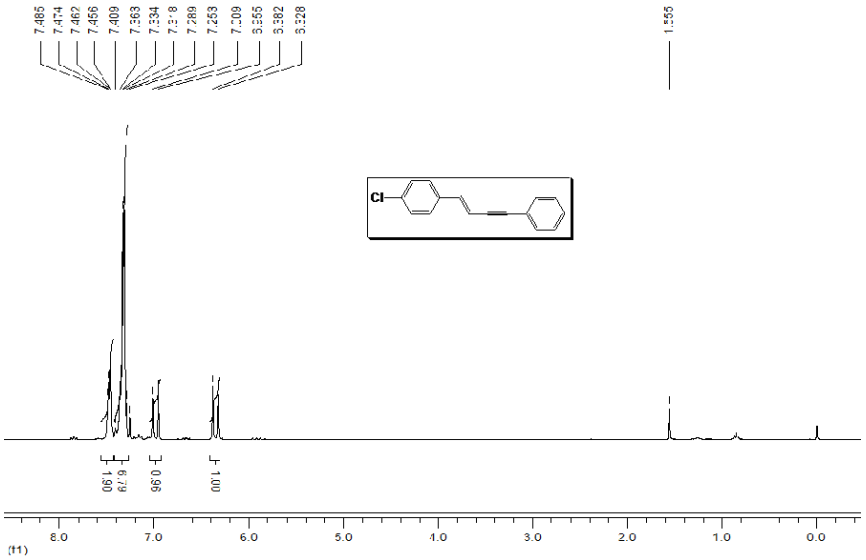

164.600
161.488
140.188
132.794
132.755
131.740
128.604
128.486
128.214
128.107
123.637
116.164
115.674
108.109
91.951
91.360
77.365
77.262
76.838
F
150
100

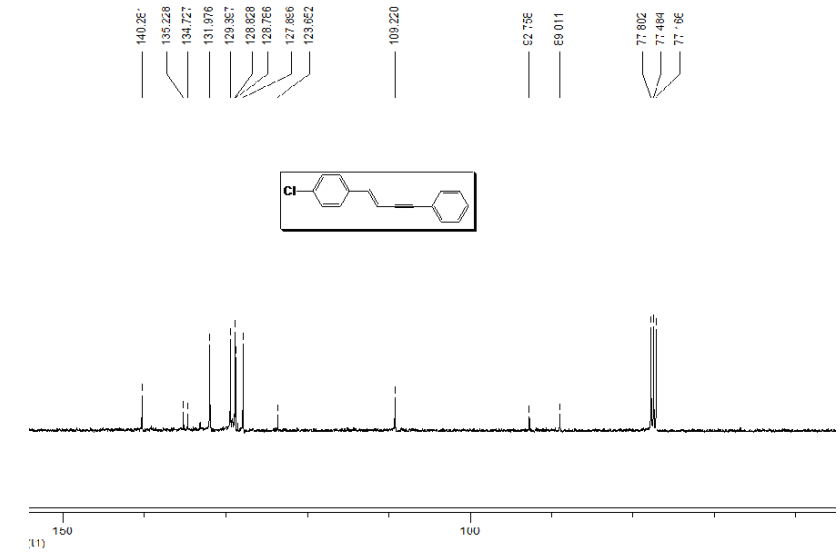

SUDA-TOFMS-EI-20110523
50 1107 (18.451) Cm (1104:1108-(671:761+420:549))
TOF MS EI+
222.0844 9.37e3
100
%
F
220.0697
223.0898
224.0934
202.0791
203.0864
200.0646
208.0702
194.0546
170.0537
149.0420
144.0409
129.0385
126.0420
123.0252
120.0321
110.0322
98.0301
95.0294
85.0245
75.0259
73.5140
0
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
m/z

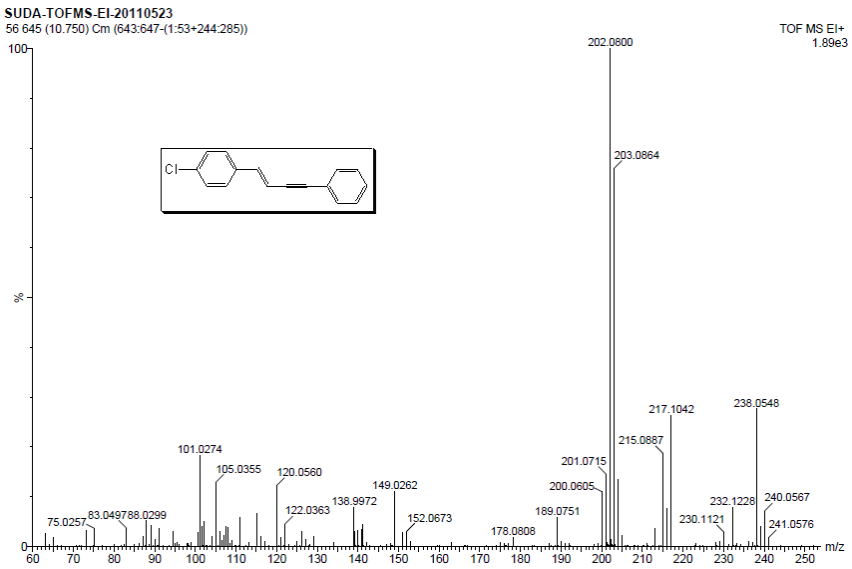

7.480
7.471
7.457
7.327
7.306
7.242
7.156
7.133
7.044
5.996
5.356
3.904
2.348
1.537
2.09
4.93
2.17
1.09
1.00
2.39
0.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(t1)

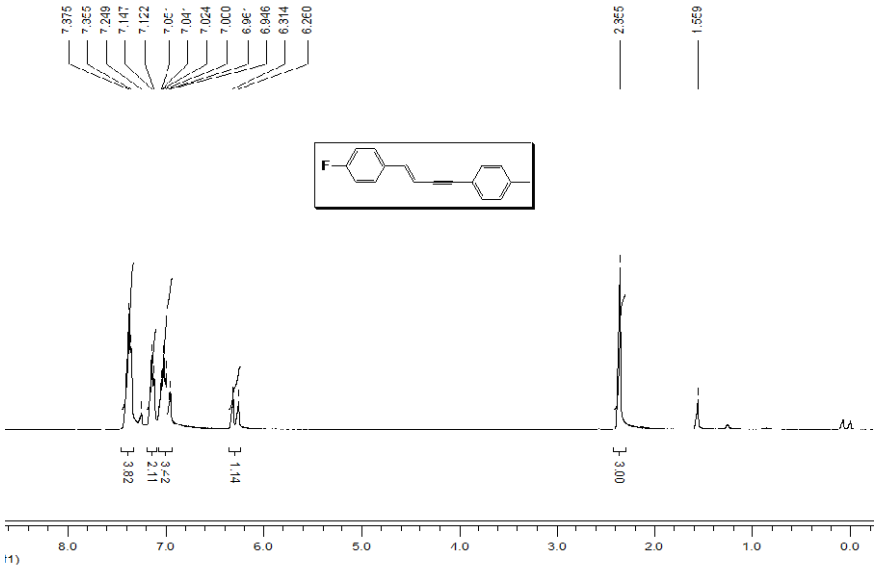

139.220
134.012
131.923
129.912
128.790
128.550
126.698
123.926
137.418
91.641
89.553
77.607
77.490
77.172
21.009
150
100
50
0

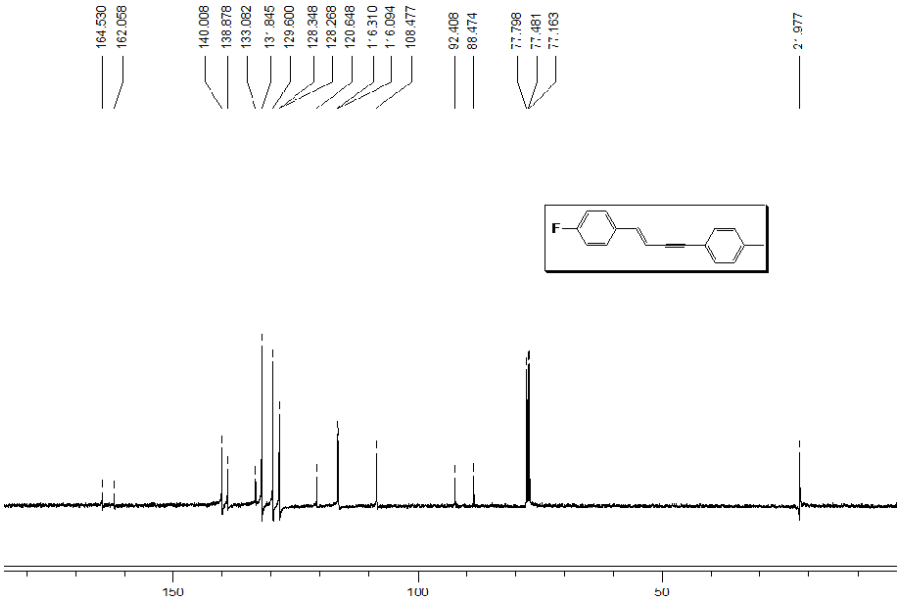

SUDA-TOFMS-EI-20110523
55 426 (7.100) Cm (426:429-(182:203+71:101))
TOF MS EI+
3.29e3
100
%
202.0793
203.0867
101.0343
138.9971
201.0728
204.0913
111.0023
140.0031
75.0250
88.0305
73.0549
87.0242
100.5362
122.0377
126.0470
149.0311
165.0748
176.0706
178.0761
199.0530
217.1061
0
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
m/z

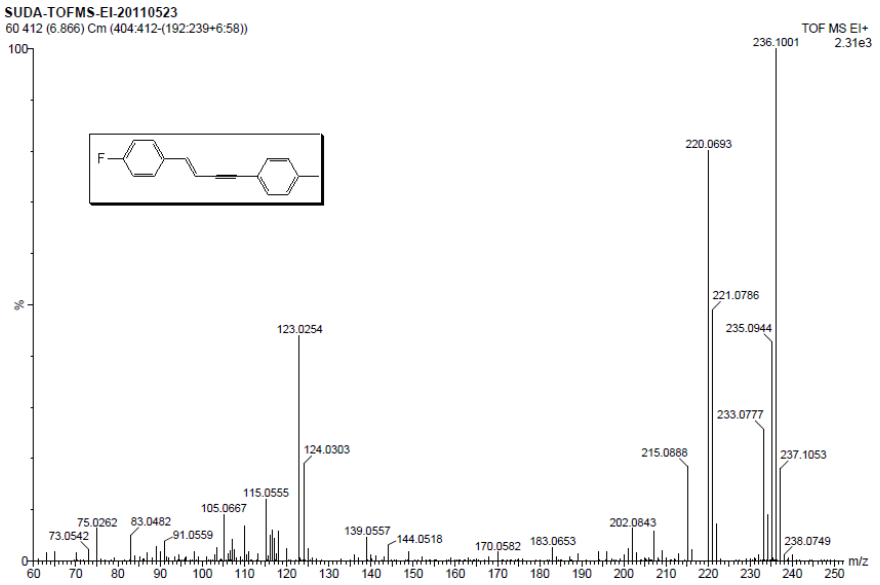


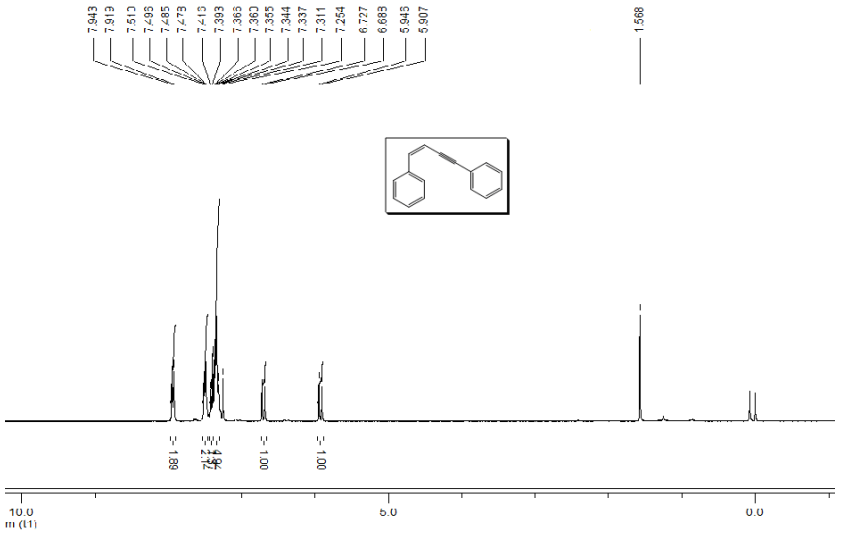


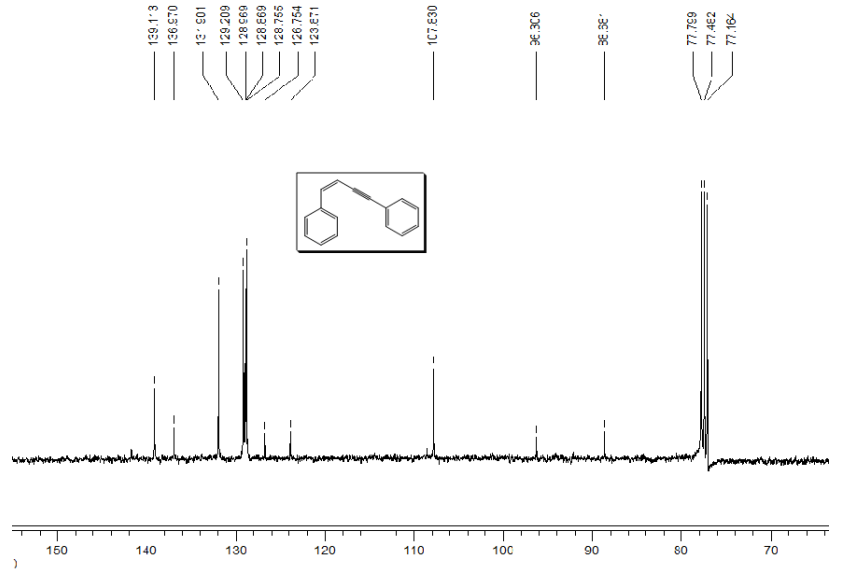


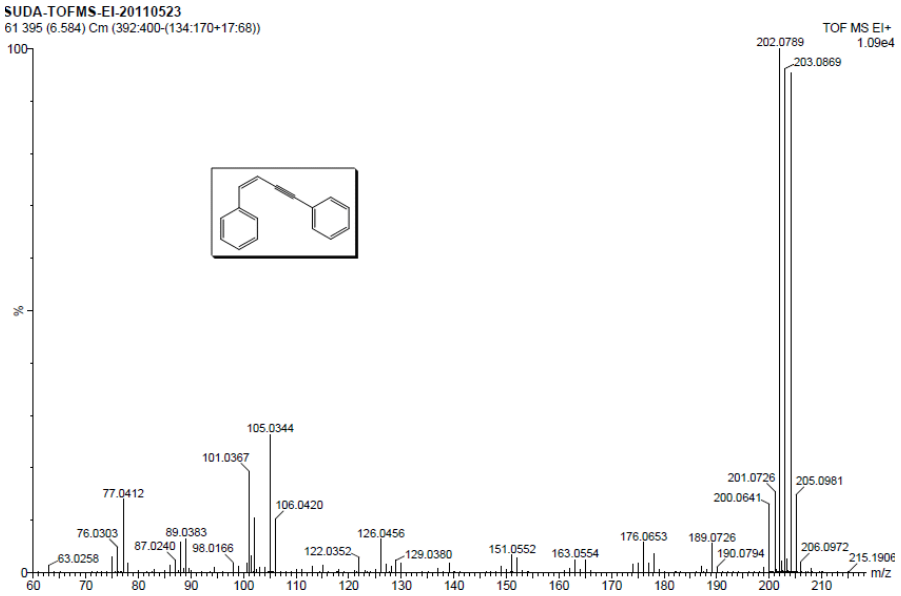

7.375
7.365
7.249
7.147
7.122
7.024
7.000
6.946
6.314
6.260
2.365
1.569
F
3.82
2.11
1.14
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

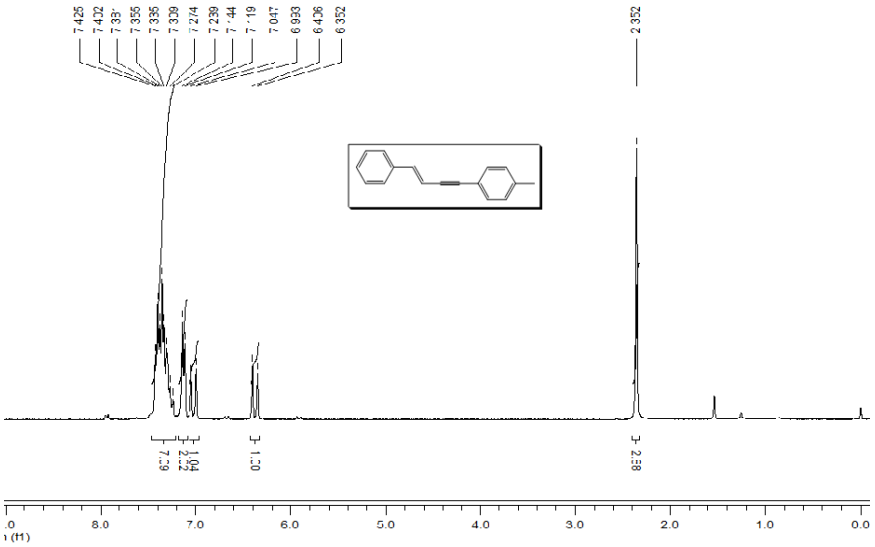

164.530
162.058
140.008
138.878
133.062
129.600
128.348
128.268
120.648
116.310
116.094
108.477
92.406
88.474
77.796
77.481
77.163
21.977
F
150
100
50

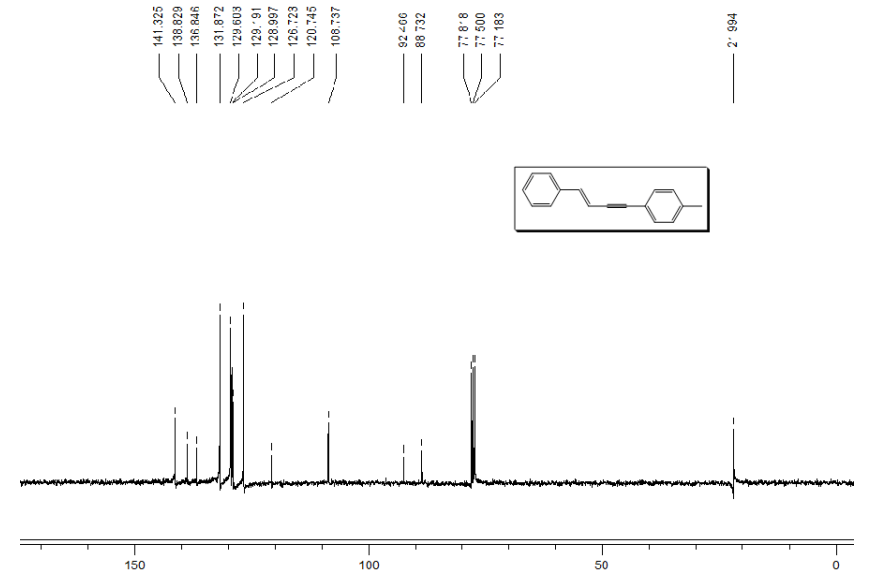

SUDA-TOFMS-EI-20110523
60 412 (6.866) Cm (404:412-(192:239+6:58))
TOF MS EI+
2.31e3
236.1001
220.0693
221.0786
235.0944
233.0777
237.1053
238.0749
215.0888
202.0843
123.0254
124.0303
115.0555
105.0667
75.0262
83.0482
73.0542
91.0559
139.0557
144.0518
170.0582
183.0653
F
%
m/z

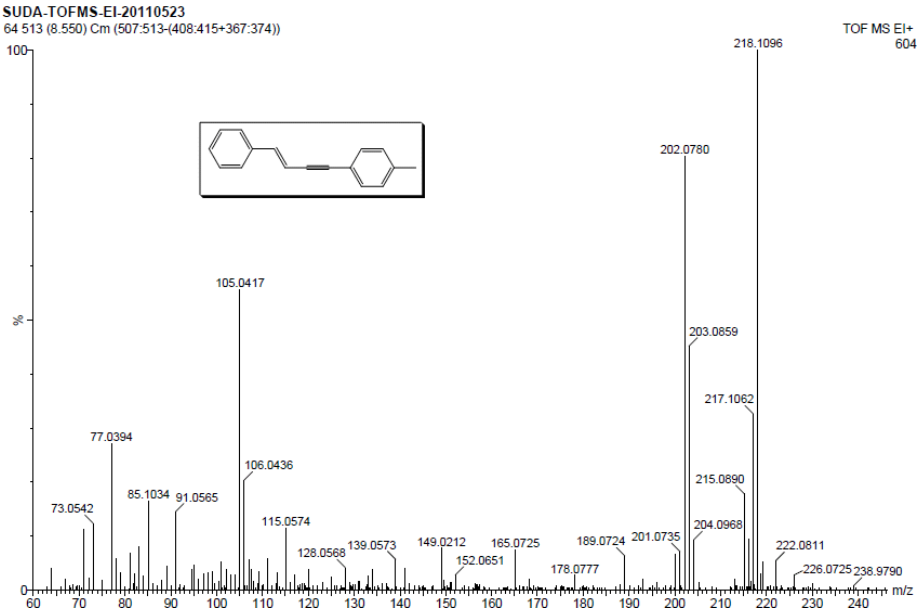

7.943
7.919
7.513
7.493
7.485
7.479
7.413
7.393
7.363
7.353
7.344
7.337
7.311
7.254
6.727
6.683
5.943
5.907
1.568
10.0
5.0
0.0

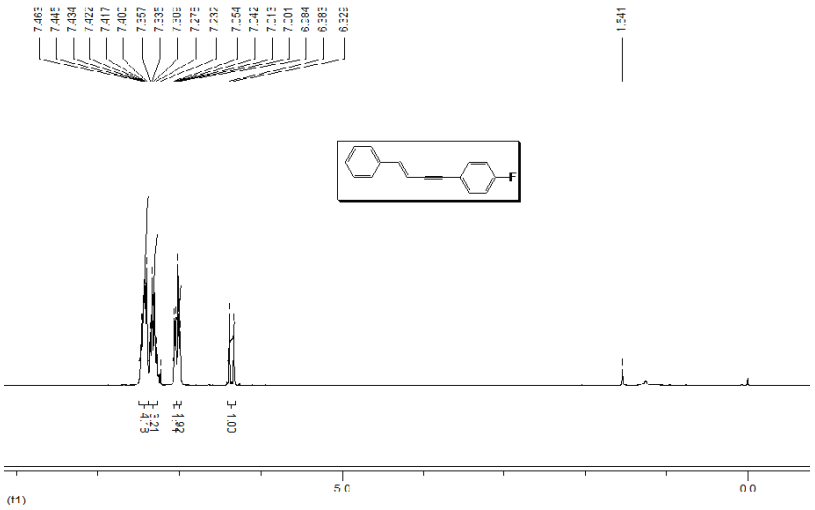

139.13
136.670
129.209
128.669
128.569
128.755
126.754
123.671
107.830
96.306
77.759
77.452
77.164
150
140
130
120
110
100
90
80
70

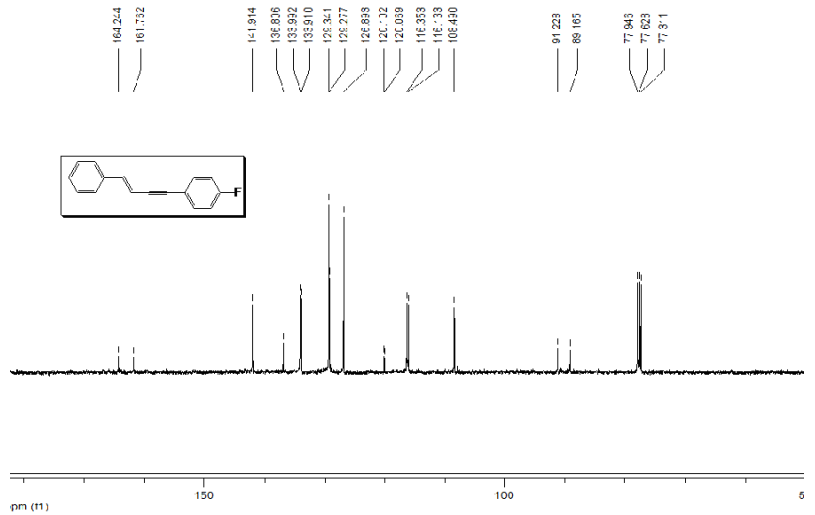

SUDA-TOFMS-EI-20110523
61 395 (6.584) Cm (392:400-(134:170+17:68))
TOF MS EI+
1.09e4
202.0789
203.0869
105.0344
101.0367
77.0412
106.0420
76.0303
89.0383
87.0240
98.0166
63.0258
122.0352
126.0456
129.0380
151.0552
163.0554
176.0653
189.0726
190.0794
201.0726
205.0981
200.0641
206.0972
215.1906
m/z

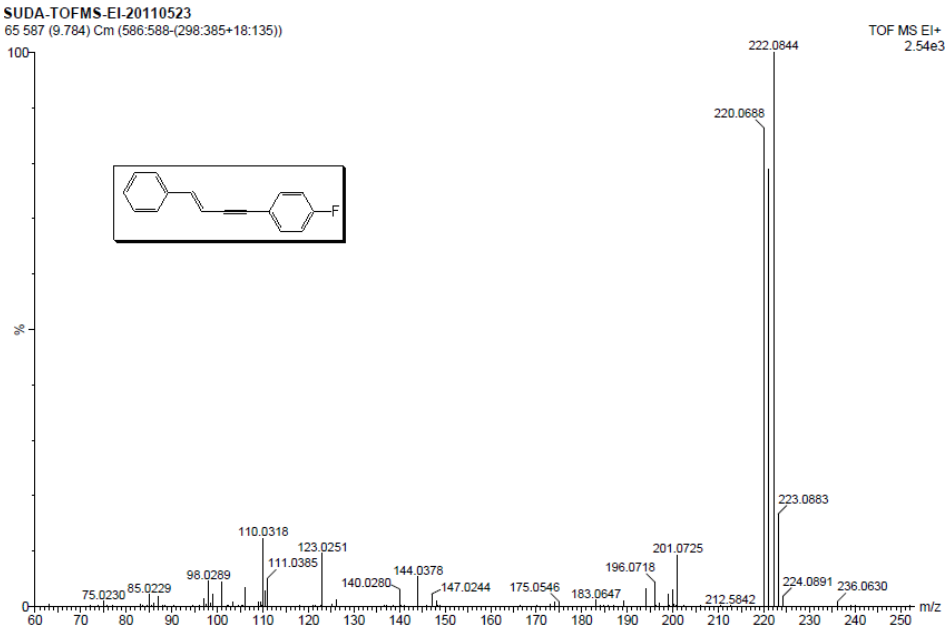

7.425
7.432
7.355
7.336
7.339
7.274
7.239
7.044
7.019
7.047
6.993
6.436
6.352
2.352
6.74
2.22
1.04
1.00
2.38
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

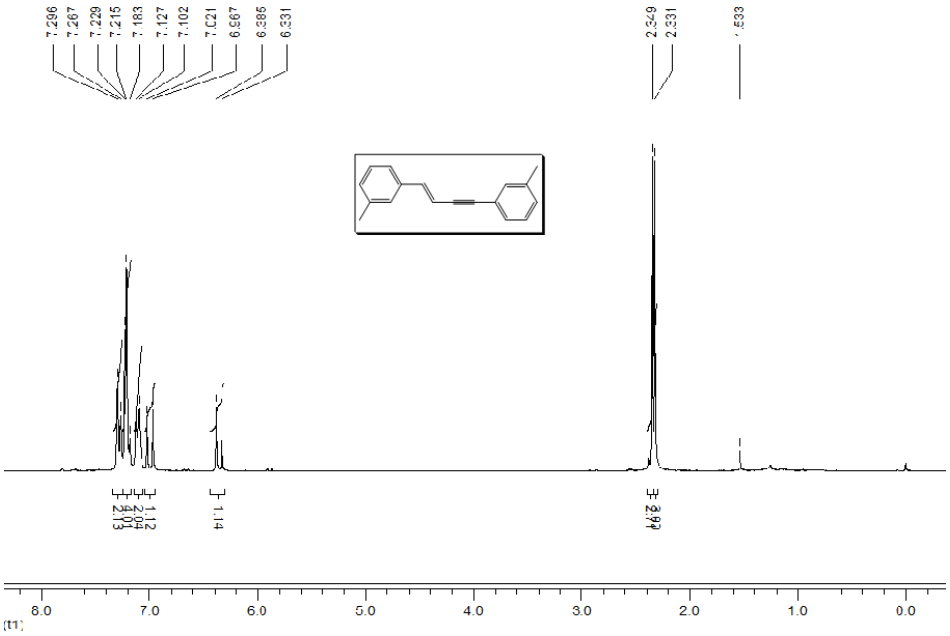

141.325
138.829
136.846
131.872
129.603
129.191
128.997
126.723
120.745
108.737
92.466
88.732
77.818
77.500
77.183
21.994
150
100
50
0

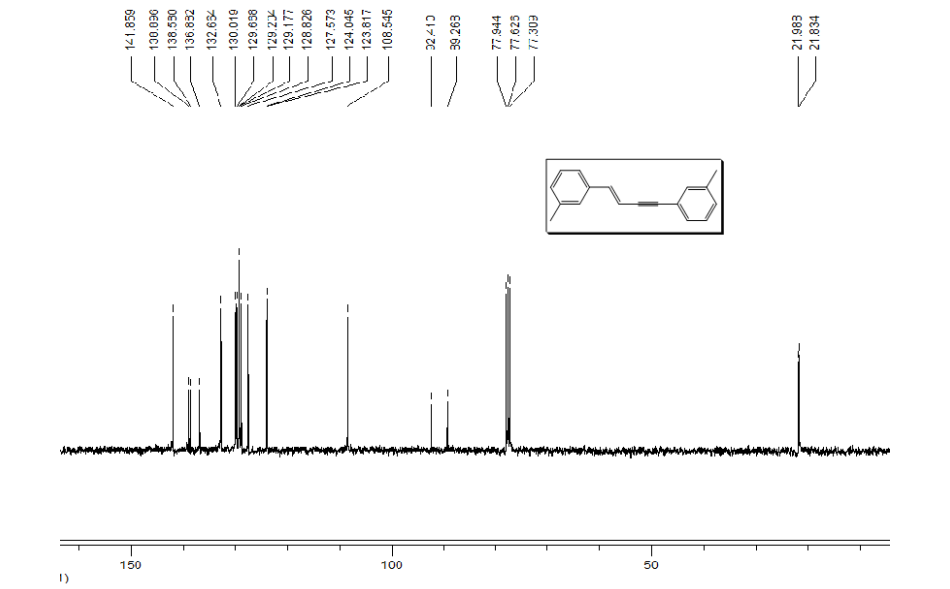

SUDA-TOFMS-EI-20110523
64 513 (8.550) Cm (507:513-(408:415+367:374))
TOF MS EI+
604
100
%
218.1096
202.0780
105.0417
203.0859
217.1062
77.0394
106.0436
215.0890
85.1034
91.0565
73.0542
115.0574
204.0968
128.0568
139.0573
149.0212
165.0725
189.0724
201.0735
222.0811
152.0651
178.0777
226.0725
238.9790
m/z
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240

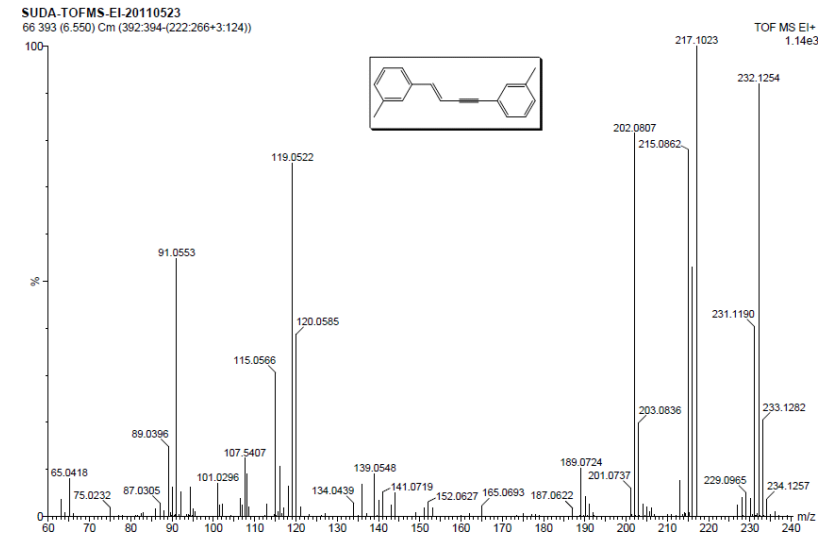


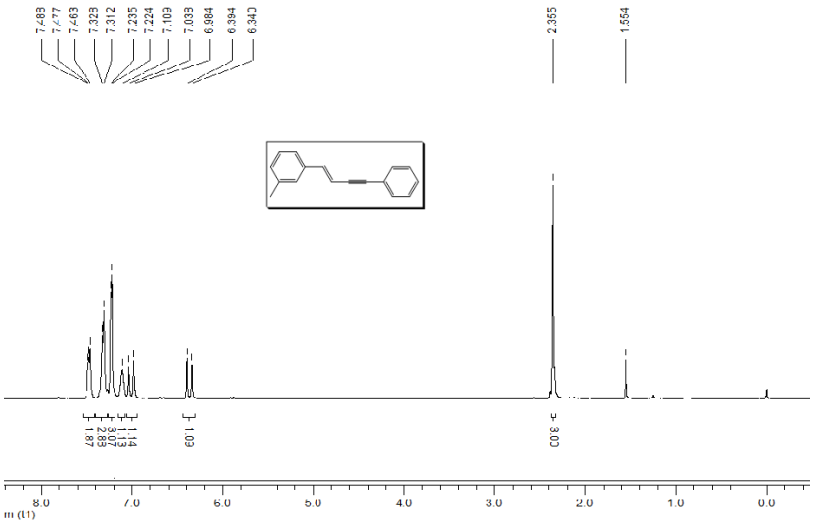


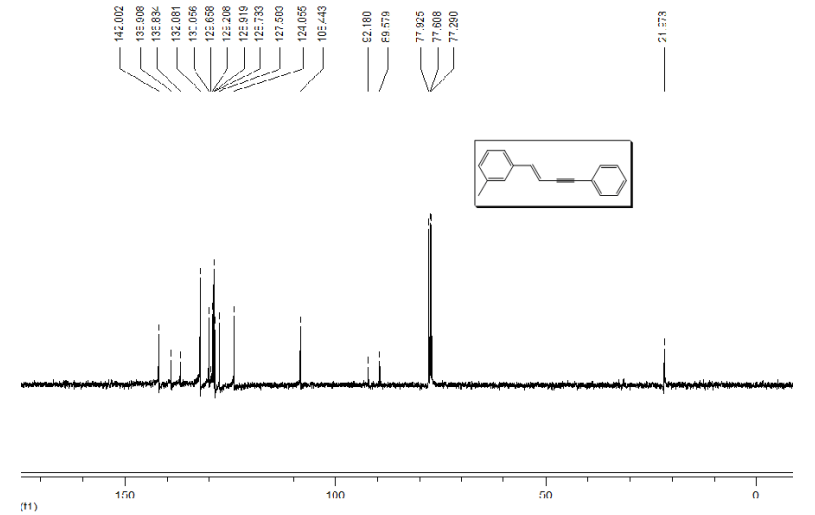

SUDA-TOFMS-EI-20110523
65 587 (9.784) Cm (586:588-(298:385+18:135))
TOF MS EI+
2.54e3
222.0844
220.0688
223.0883
110.0318
123.0251
111.0385
201.0725
98.0289
144.0378
196.0718
140.0280
224.0891
236.0630
75.0230
85.0229
147.0244
175.0546
183.0647
212.5842
%
m/z

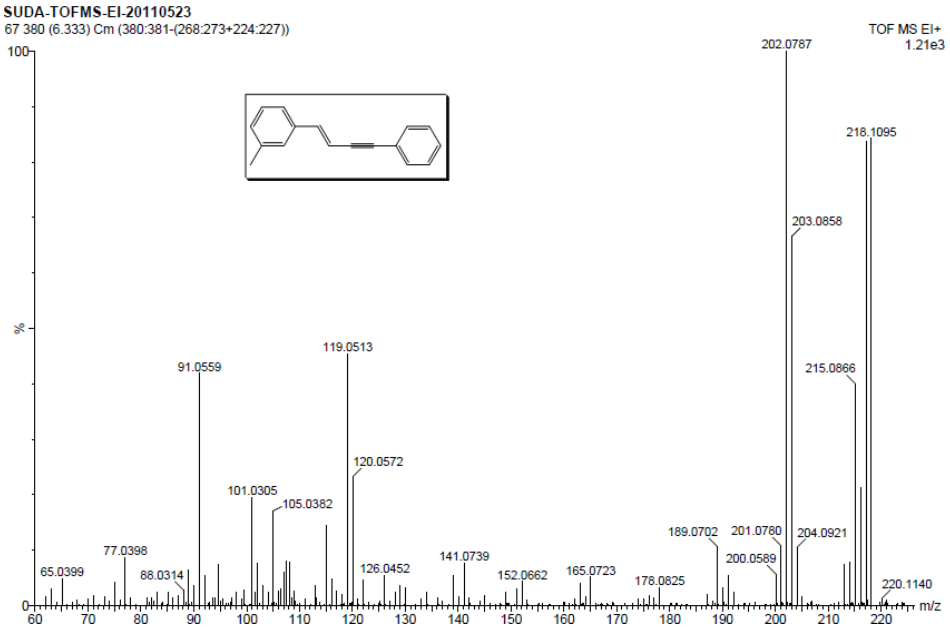


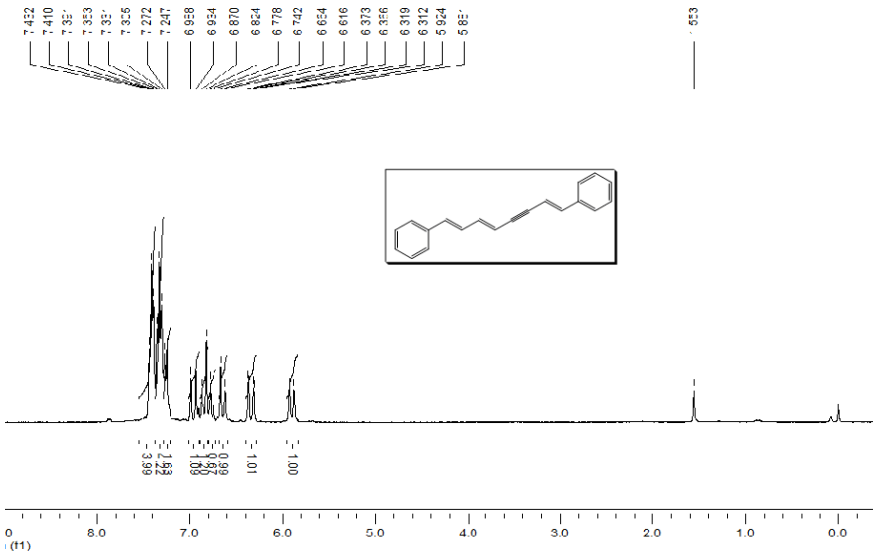


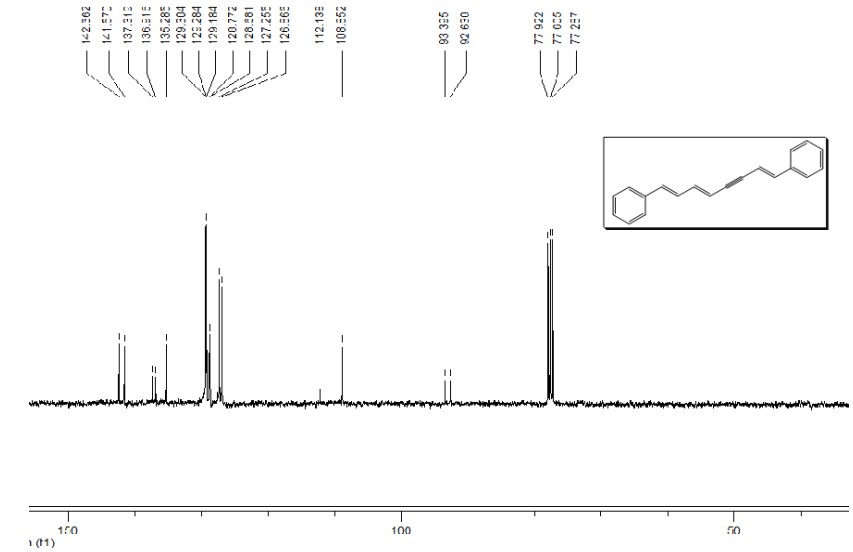


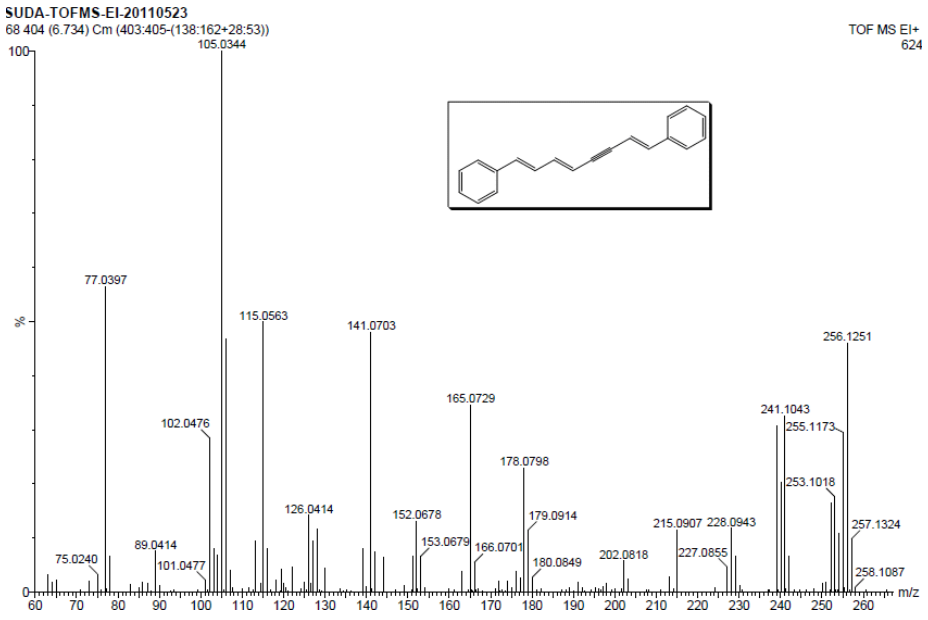

7.483
7.477
7.463
7.323
7.312
7.235
7.224
7.109
7.039
6.984
6.394
6.343
2.355
1.564
3.02
1.09
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

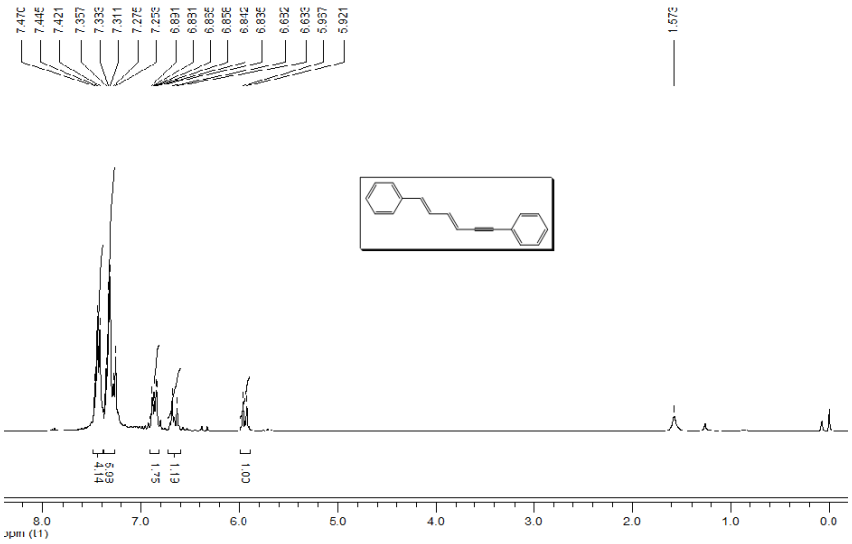

142.002
135.098
132.081
131.056
128.688
128.208
127.919
127.733
127.503
124.055
105.443
92.180
89.579
77.925
77.608
77.290
21.373
150
100
50
0

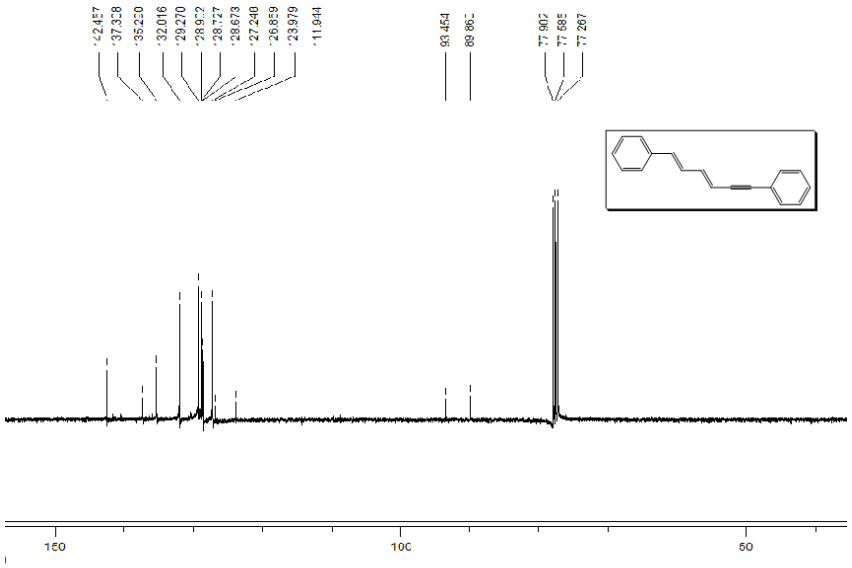

SUDA-TOFMS-EI-20110523
67 380 (6.333) Cm (380:381-(268:273+224:227))
TOF MS EI+
1.21e3
100
%
0
202.0787
218.1095
203.0858
215.0866
119.0513
91.0559
120.0572
101.0305
105.0382
189.0702
201.0780
204.0921
200.0589
77.0398
65.0399
88.0314
126.0452
141.0739
152.0662
165.0723
178.0825
220.1140
m/z
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220

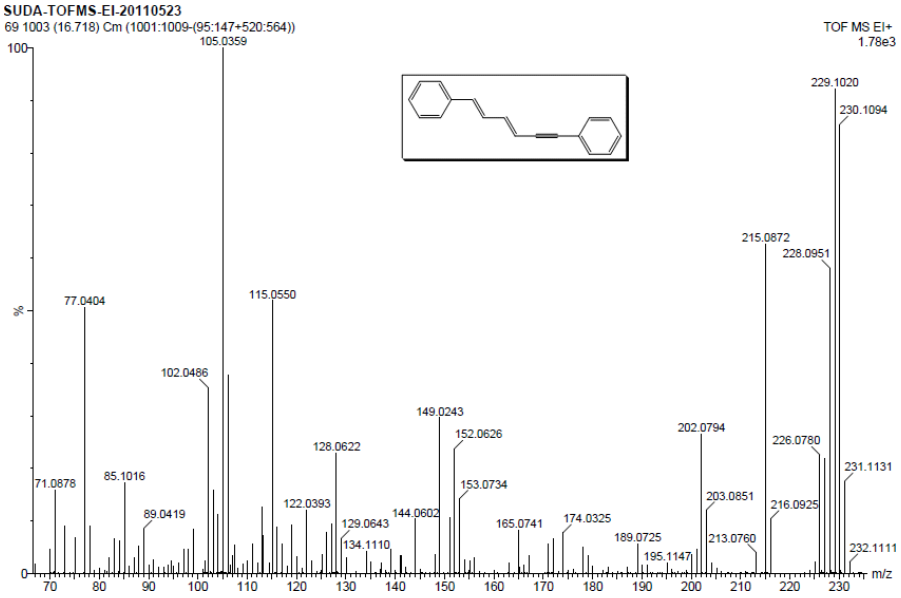


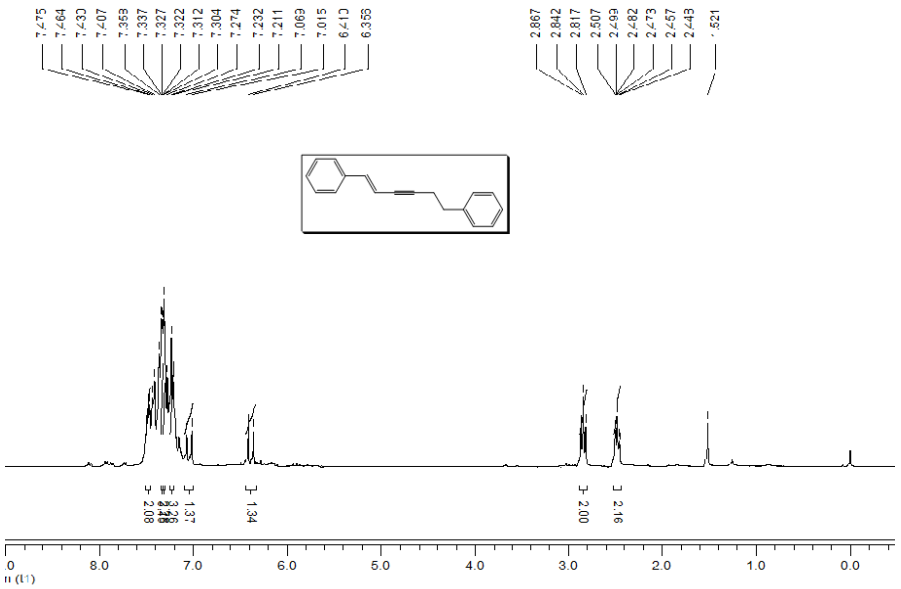


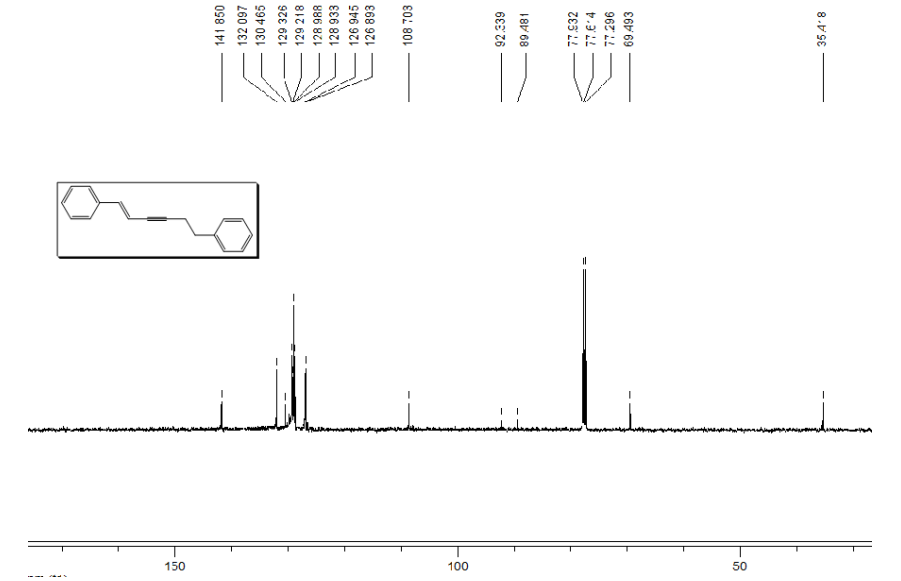

SUDA-TOFMS-EI-20110523
68 404 (6.734) Cm (403:405-(138:162+28:53))
TOF MS EI+
624
105.0344
77.0397
115.0563
141.0703
256.1251
165.0729
102.0476
241.1043
255.1173
178.0798
253.1018
126.0414
152.0678
179.0914
257.1324
89.0414
153.0679
166.0701
215.0907
228.0943
75.0240
101.0477
180.0849
202.0818
227.0855
258.1087
%
m/z

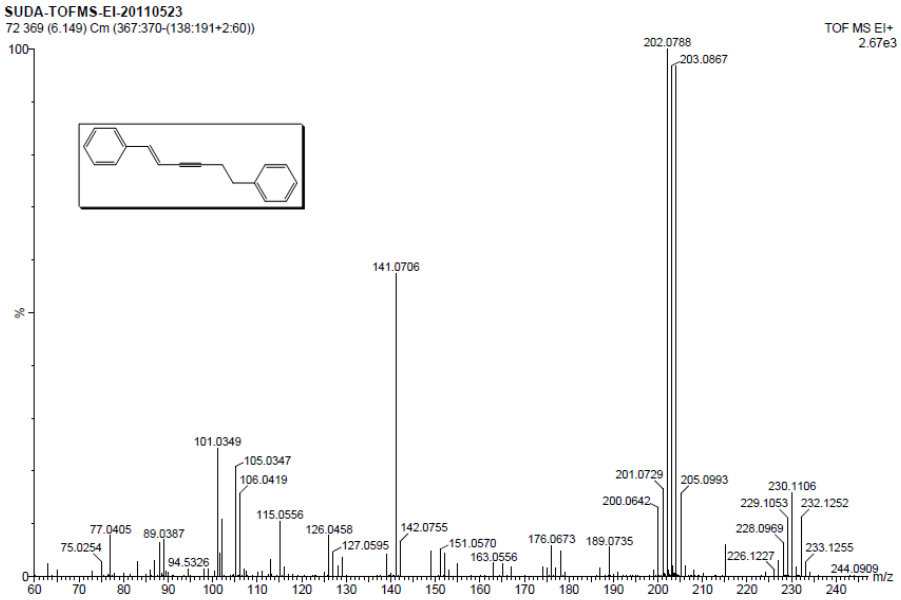

7.470
7.448
7.421
7.357
7.335
7.311
7.275
7.255
6.891
6.881
6.858
6.856
6.842
6.835
6.632
6.633
5.957
5.921
1.572
4.14
1.75
1.13
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


62.457
37.328
35.220
32.016
29.270
28.972
28.727
28.673
27.240
26.859
23.979
11.944
93.454
89.862
77.902
77.688
77.267
150
100
50


SUDA-TOFMS-EI-20110523
69 1003 (16.718) Cm (1001:1009-(95:147+520:564))
TOF MS EI+
1.78e3
105.0359
229.1020
230.1094
215.0872
228.0951
77.0404
115.0550
102.0486
149.0243
152.0626
128.0622
202.0794
226.0780
231.1131
71.0878
85.1016
153.0734
203.0851
216.0925
122.0393
144.0602
89.0419
129.0643
165.0741
174.0325
189.0725
213.0760
134.1110
195.1147
232.1111
%
m/z


7.475
7.464
7.430
7.407
7.359
7.337
7.327
7.322
7.312
7.304
7.274
7.232
7.211
7.069
7.015
6.410
6.356
2.867
2.842
2.817
2.507
2.499
2.482
2.473
2.457
2.443
2.08
1.37
1.34
2.00
2.16
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


141.850
132.097
130.465
129.326
129.218
128.988
128.933
126.945
126.893
108.703
92.339
89.481
77.532
77.296
69.493
35.418
150
100
50


SUDA-TOFMS-EI-20110523
72 369 (6.149) Cm (367:370-(138:191+2:60))
TOF MS EI+
2.67e3
100
%
202.0788
203.0867
141.0706
101.0349
105.0347
106.0419
115.0556
126.0458
142.0755
127.0595
151.0570
163.0556
176.0673
189.0735
201.0729
205.0993
200.0642
230.1106
229.1053
232.1252
228.0969
233.1255
226.1227
244.0909
77.0405
89.0387
75.0254
94.5326
0
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
m/z