Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Aqueous Sonogashira Coupling of Aryl Halides with 1-Alkynes Under Mild Conditions: Use of Surfactants in Cross-Coupling Reactions

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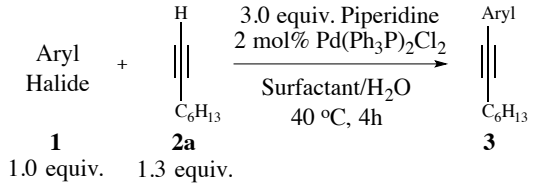
Table S1. The Effect of CTAB concentration on Sonogashira coupling yields for aryl-iodide and bromide reagents at 40 °C.

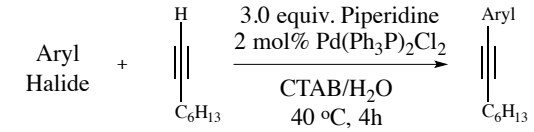


1 1.0 equiv. **2a** 1.3 equiv. **3**

Entry	Aryl Halide	CTAB (w/v%)	% Yield **3** (No CuI)	(CuI)[b]
1	1-iodoanisole	0.0	-	30
2	1-iodoanisole	0.5	-	44
3	1-iodoanisole	1.0	-	71
4	1-iodoanisole	1.5	-	86
5	1-iodoanisole	2.0	-	92
6	4-bromonbenzonitrile	0.0	0	-
7	4-bromonbenzonitrile	0.5	9	-
8	4-bromonbenzonitrile	1.0	38	-
9	4-bromonbenzonitrile	1.5	42	-
10	4-bromonbenzonitrile	2.0	57	-

Reaction conditions: 0.08 mmol aryl halide, 0.1 mmol 1-octyne, 0.24 mmol piperidine, 2.0 mol% $Pd(PPh_3)_2Cl_2$, 0.8 mL CTAB in H_2O, 40 ºC, 4 h; [a]Average ^1H NMR yields for duplicate runs (±3). [b] 5 mol% CuI.

Table S2. The Effect of SDS concentration on Sonogashira coupling yields for aryl-iodide and bromide reagents at 40 °C.

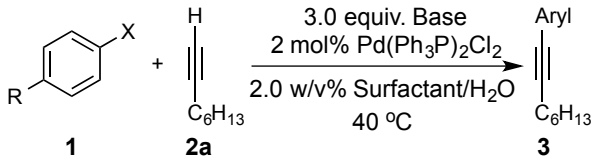


1 1.0 equiv. **2a** 1.3 equiv. **3**

Entry	Aryl Halide	SDS (w/v%)	% Yield **3** (No CuI)	(CuI)[b]
1	1-iodoanisole	0.0	-	30
2	1-iodoanisole	0.5	-	32
3	1-iodoanisole	1.0	-	68
4	1-iodoanisole	2.0	-	85
5	1-iodoanisole	4.0	-	88
6	1-iodoanisole	8.0	-	79
7	4-bromonbenzonitrile	0.0	0	-
8	4-bromonbenzonitrile	0.5	11	-
9	4-bromonbenzonitrile	1.0	34	-
10	4-bromonbenzonitrile	2.0	55	-
11	4-bromonbenzonitrile	4.0	52	-
12	4-bromonbenzonitrile	8.0	49	-

Reaction conditions: 0.08 mmol aryl halide, 0.1 mmol 1-octyne, 0.24 mmol piperidine, 2.0 mol% $Pd(PPh_3)_2Cl_2$, 0.8 mL SDS in H_2O, 40 ºC, 4 h; [a]Average ^1H NMR yields for duplicate runs (±3). [b] 5 mol% CuI.

Table S3. Base Screening for the Sonogashira Coupling of Aryl Halides with 1-Octyne.



1 **2a** **3**

1.0 equiv. 1.3 equiv.

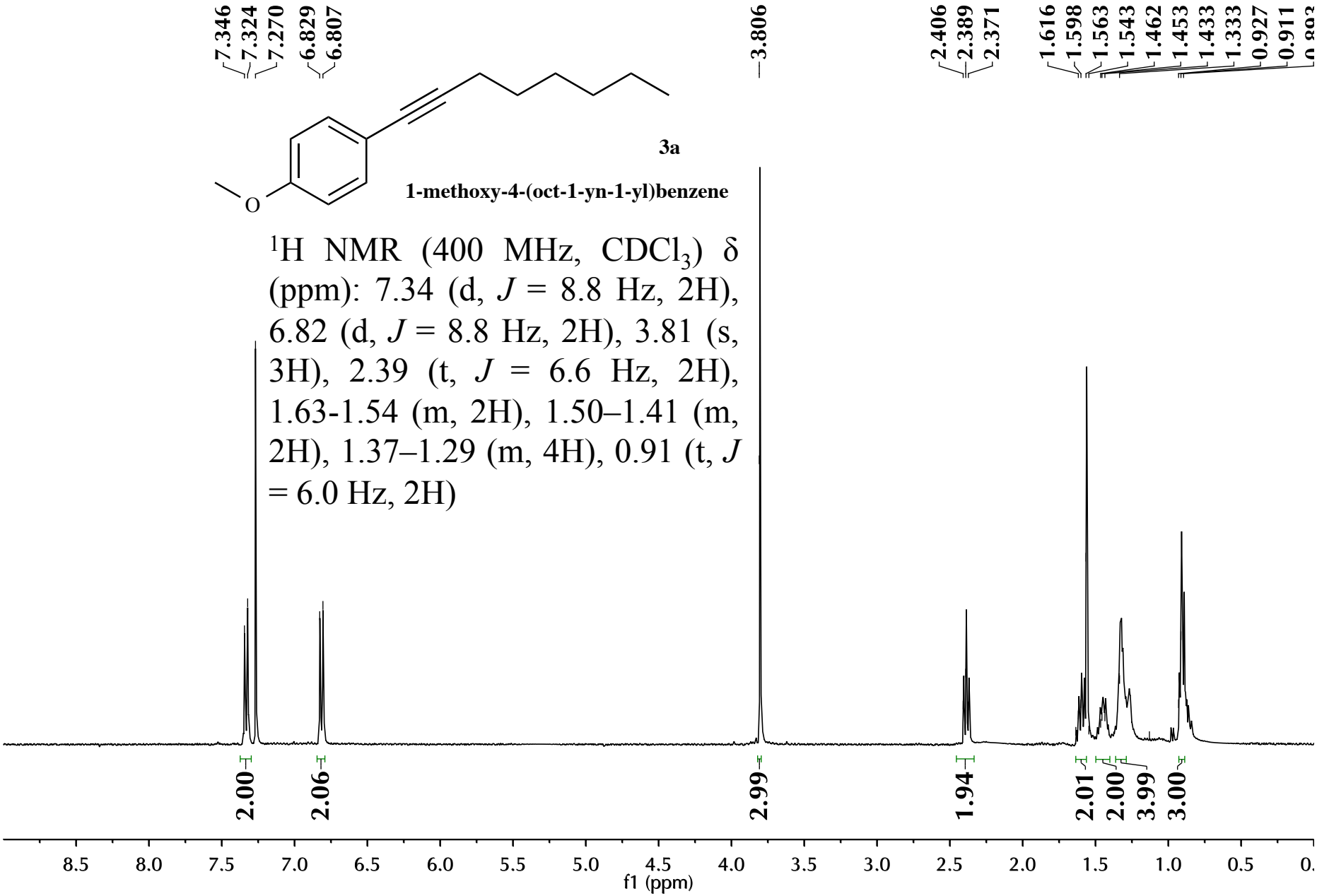
Entry[a]	R	X	Surfactant	Base	% Yield **3**[b] (CuI)[c]	% Yield **3**[b] (No CuI)
1	OMe	I	SDS	Piperidine	85	30
2	OMe	I	CTAB	Piperidine	92	38
3	OMe	I	SDS	Pyrrolidine	81	32
4	OMe	I	CTAB	Pyrrolidine	75	33
5	OMe	I	SDS	NEt_3	87	22
6	OMe	I	CTAB	NEt_3	90	17
7	OMe	I	SDS	Cs_2CO_3	21	15
8	OMe	I	CTAB	Cs_2CO_3	10	12
9	CN	Br	SDS	Piperidine	18	40
10	CN	Br	CTAB	Piperidine	31	59
11	CN	Br	SDS	Pyrrolidine	20	26
12	CN	Br	CTAB	Pyrrolidine	18	55
13	CN	Br	SDS	NEt_3	23	57
14	CN	Br	CTAB	NEt_3	20	60
15	CN	Br	SDS	Cs_2CO_3	9	10
16	CN	Br	CTAB	Cs_2CO_3	24	17

Reaction conditions: 0.08 mmol aryl halide, 0.1 mmol 1-octyne, 0.24 mmol base, 2.0 mol% $Pd(PPh_3)_2Cl_2$, 0.8 mL surfactant (2.0 w/v% in H_2O), 40 ºC; [a] Rxn 1-8 ran 4 h, Rxn 9-16 ran 12 h; [b] Average ^{1}H NMR yields for duplicate runs (±3). [c] 5 mol% CuI.

Table S4. Solution pH values for SDS, CTAB, Sodium Cholate and Triton X-100 for Sonogashira Reactions.

Surfactant	Temp (^{o}C)	Piperidine (mmol)	pH
Sodium Cholate	RT	-	7.8
Sodium Cholate	40	-	8.3
Sodium Cholate	RT	2.4	11.6
Sodium Cholate	40	2.4	11.1
CTAB	RT	-	6.5
CTAB	40	-	6.2
CTAB	RT	2.4	11.5
CTAB	40	2.4	11.1
SDS	RT	-	8.4
SDS	40	-	8.5
SDS	RT	2.4	11.7
SDS	40	2.4	10.7
Triton X-100	RT	-	6.0
Triton X-100	40	-	7.2
Triton X-100	RT	2.4	11.6
Triton X-100	40	2.4	11.0

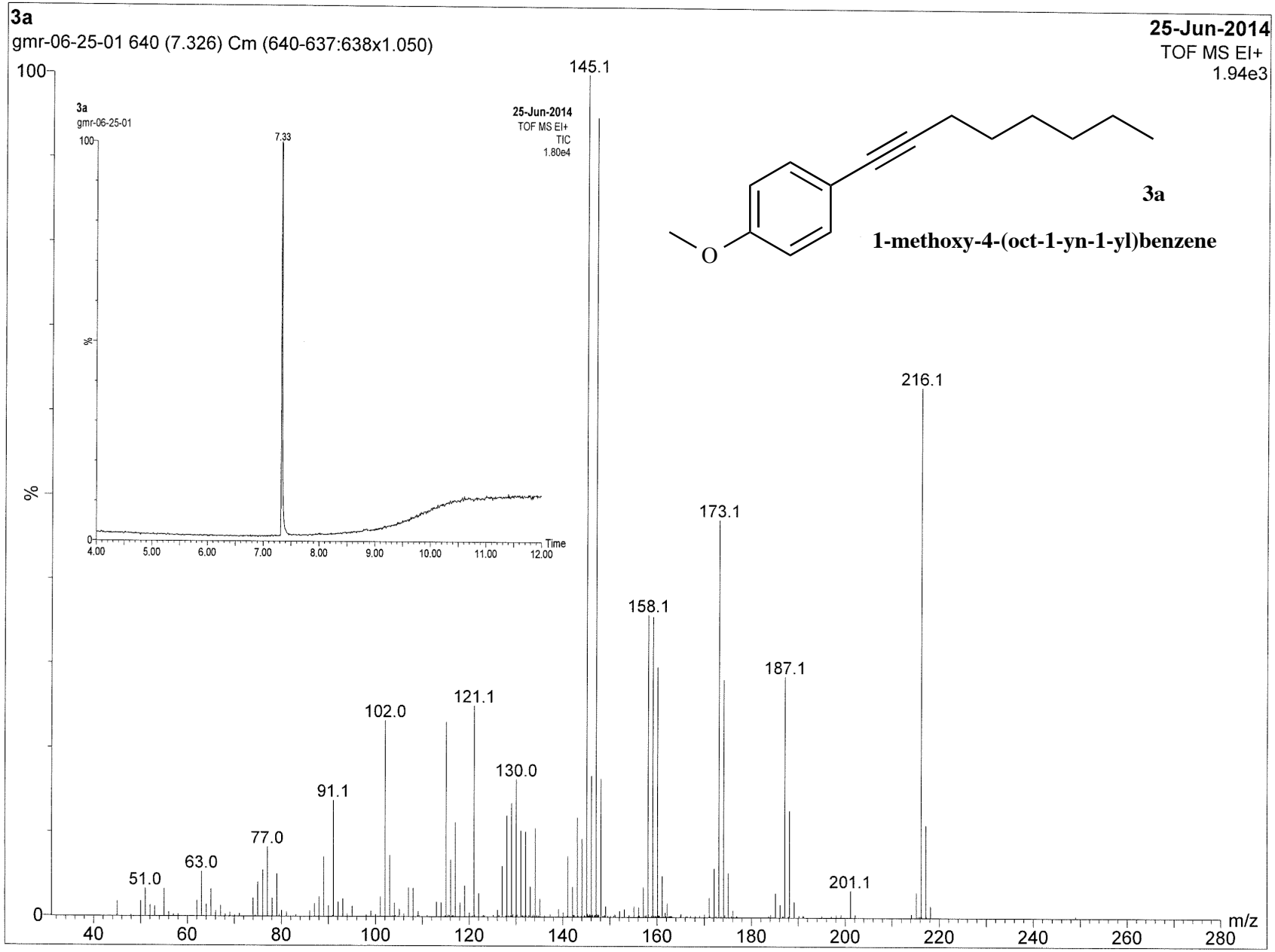
Conditions: 2.0 w/v% solution of surfactant in water with and without piperidine. The pH remained constant over 5 h at RT and 40 ^{o}C for each entry.

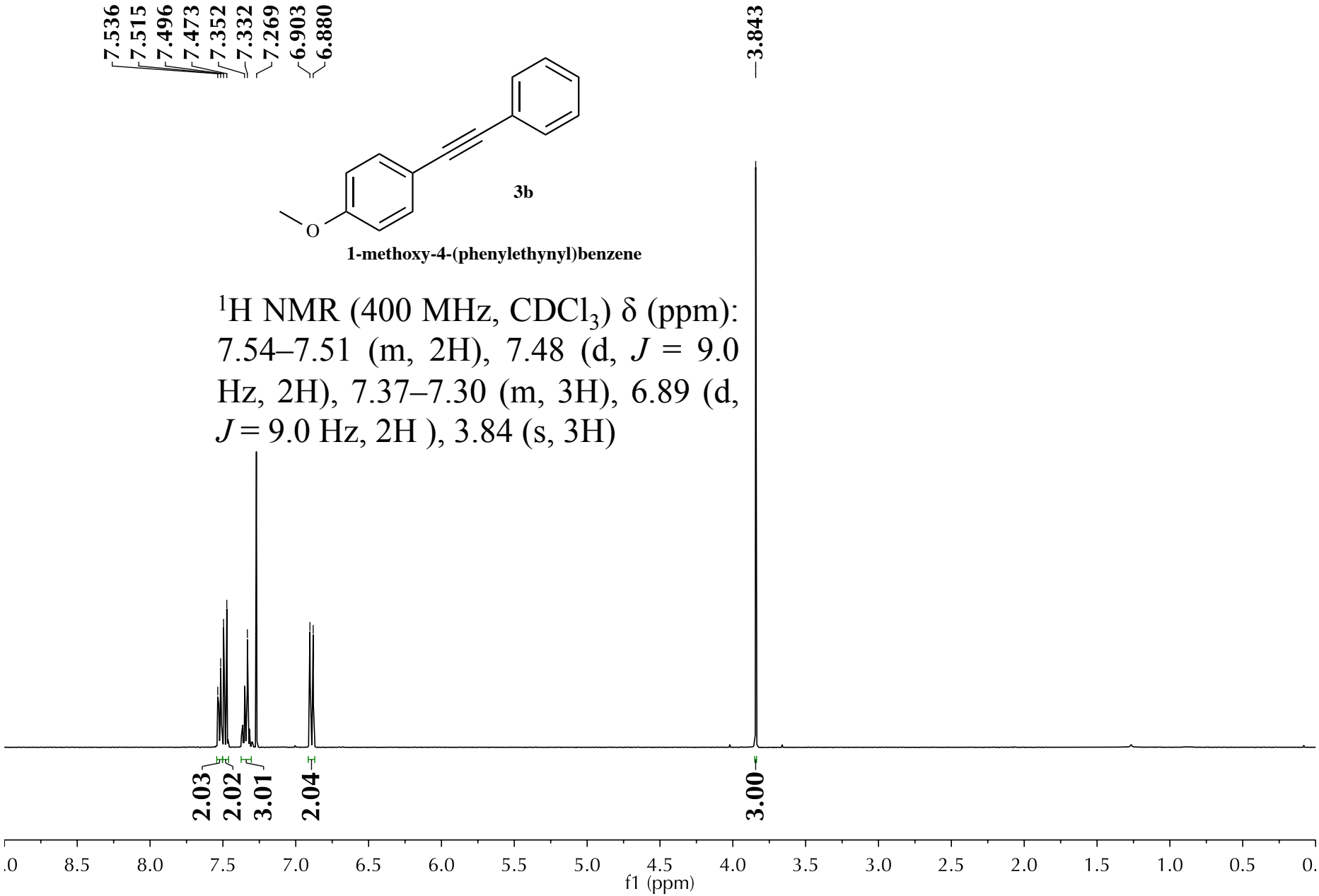


3a

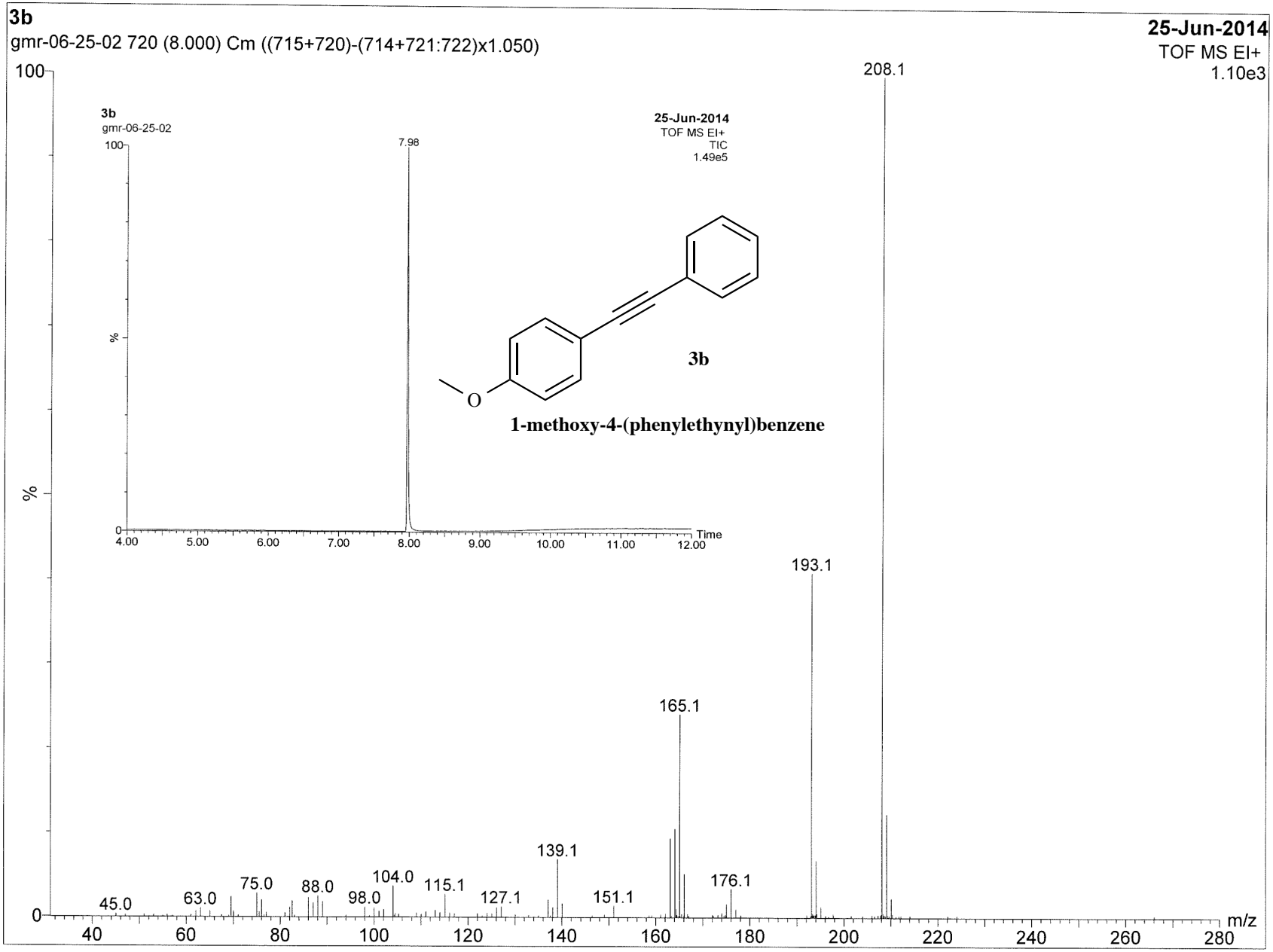
1-methoxy-4-(oct-1-yn-1-yl)benzene

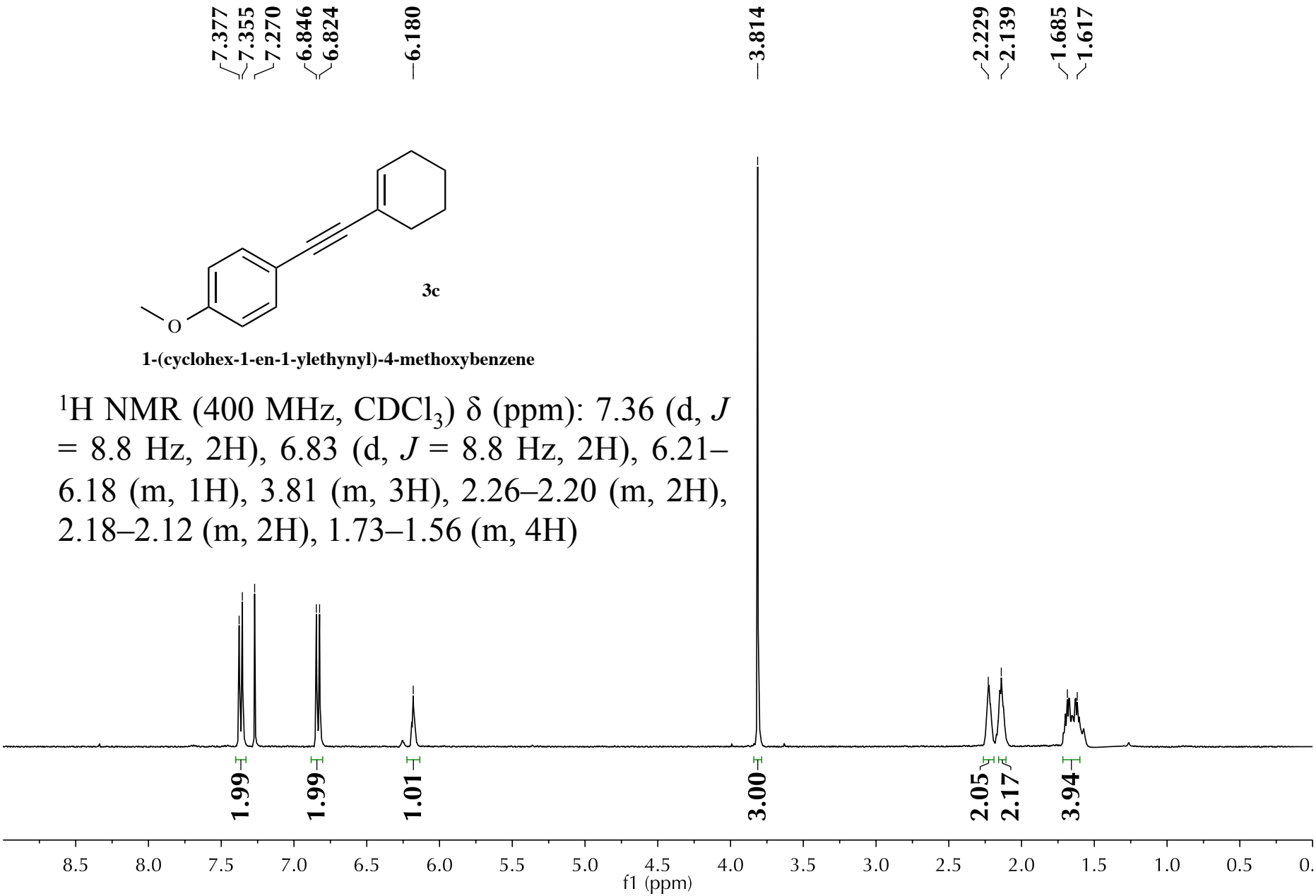
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.34 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 2.39 (t, *J* = 6.6 Hz, 2H), 1.63-1.54 (m, 2H), 1.50–1.41 (m, 2H), 1.37–1.29 (m, 4H), 0.91 (t, *J* = 6.0 Hz, 2H)


3a
gmr-06-25-01 640 (7.326) Cm (640-637:638x1.050)
25-Jun-2014
TOF MS EI+
1.94e3
145.1
3a
gmr-06-25-01
7.33
25-Jun-2014
TOF MS EI+
TIC
1.80e4
Time
3a
1-methoxy-4-(oct-1-yn-1-yl)benzene
O
216.1
173.1
158.1
187.1
121.1
102.0
130.0
91.1
77.0
63.0
51.0
201.1
%
m/z



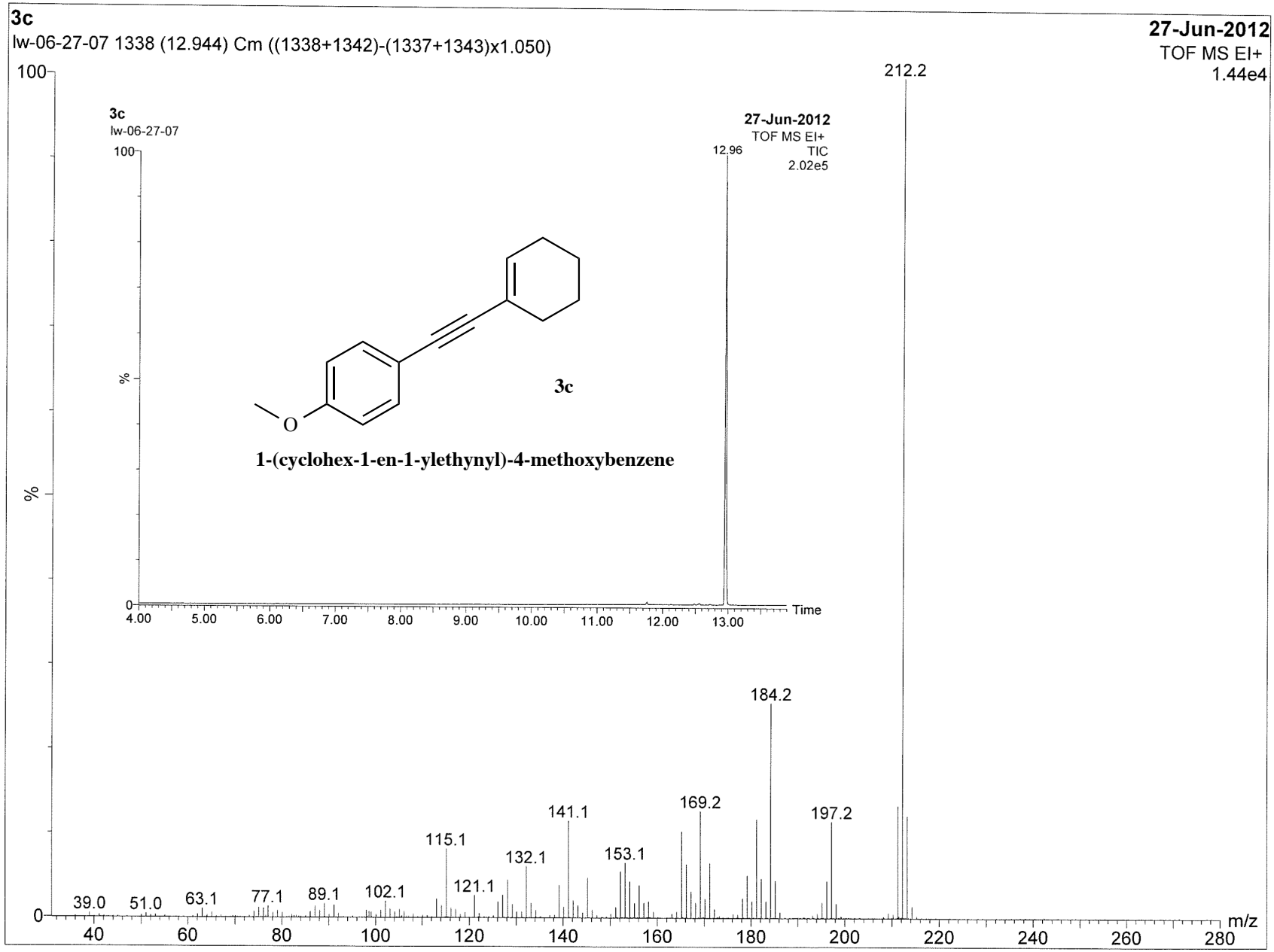
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.54–7.51 (m, 2H), 7.48 (d, J = 9.0 Hz, 2H), 7.37–7.30 (m, 3H), 6.89 (d, J = 9.0 Hz, 2H), 3.84 (s, 3H)

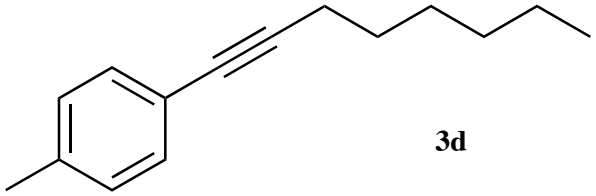

3b
gmr-06-25-02 720 (8.000) Cm ((715+720)-(714+721:722)x1.050)
25-Jun-2014
TOF MS EI+
1.10e3
208.1
193.1
165.1
139.1
176.1
104.0
75.0
88.0
98.0
115.1
127.1
151.1
63.0
45.0
m/z
%
3b
gmr-06-25-02
7.98
25-Jun-2014
TOF MS EI+
TIC
1.49e5
Time
3b
O
1-methoxy-4-(phenylethynyl)benzene



1-(cyclohex-1-en-1-ylethynyl)-4-methoxybenzene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.36 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.21–6.18 (m, 1H), 3.81 (m, 3H), 2.26–2.20 (m, 2H), 2.18–2.12 (m, 2H), 1.73–1.56 (m, 4H)

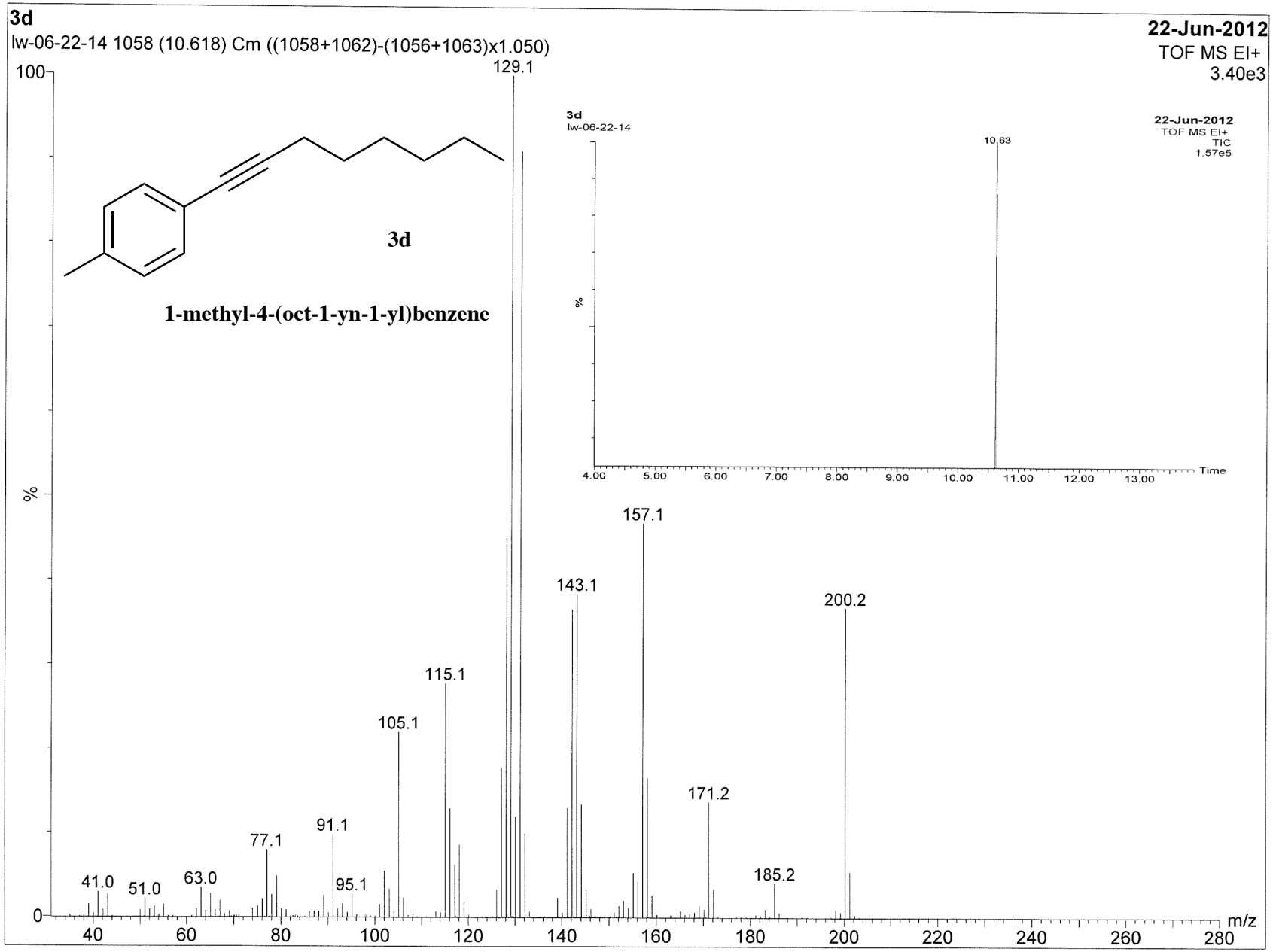

3c
lw-06-27-07 1338 (12.944) Cm ((1338+1342)-(1337+1343)x1.050)
27-Jun-2012
TOF MS EI+
1.44e4
212.2
184.2
169.2
197.2
141.1
115.1
153.1
132.1
121.1
102.1
89.1
77.1
63.1
51.0
39.0
m/z
%
3c
lw-06-27-07
27-Jun-2012
TOF MS EI+
TIC
2.02e5
12.96
Time
3c
1-(cyclohex-1-en-1-ylethynyl)-4-methoxybenzene

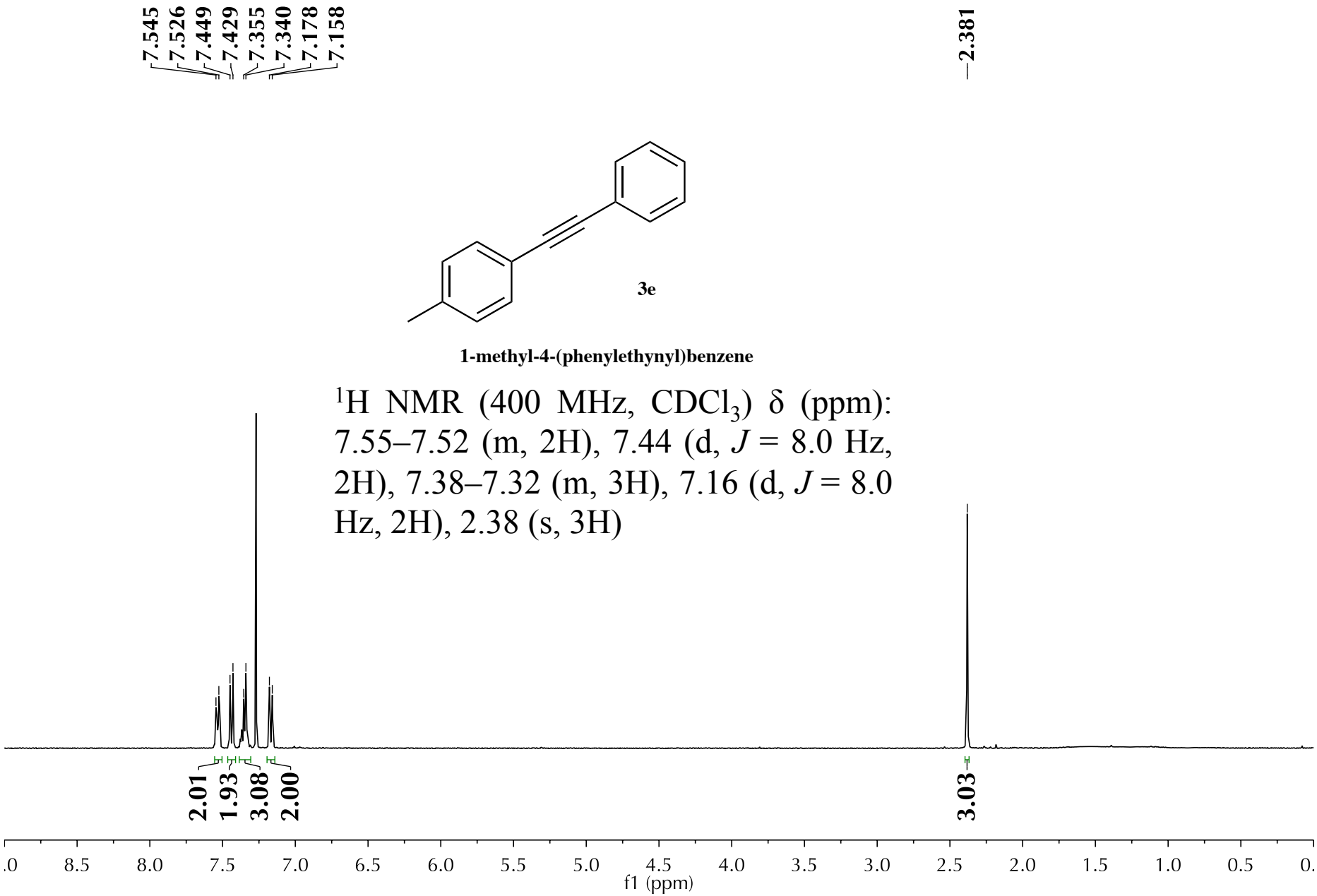


3d

1-methyl-4-(oct-1-yn-1-yl)benzene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.29 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.41 (t, *J* = 7.0 Hz, 2H), 2.34 (s, 3H), 1.67–1.58 (m, 2H), 1.48–1.44 (m, 2H), 1.36–1.28 (m, 4H), 0.92 (t, *J* = 5.6 Hz, 3H)

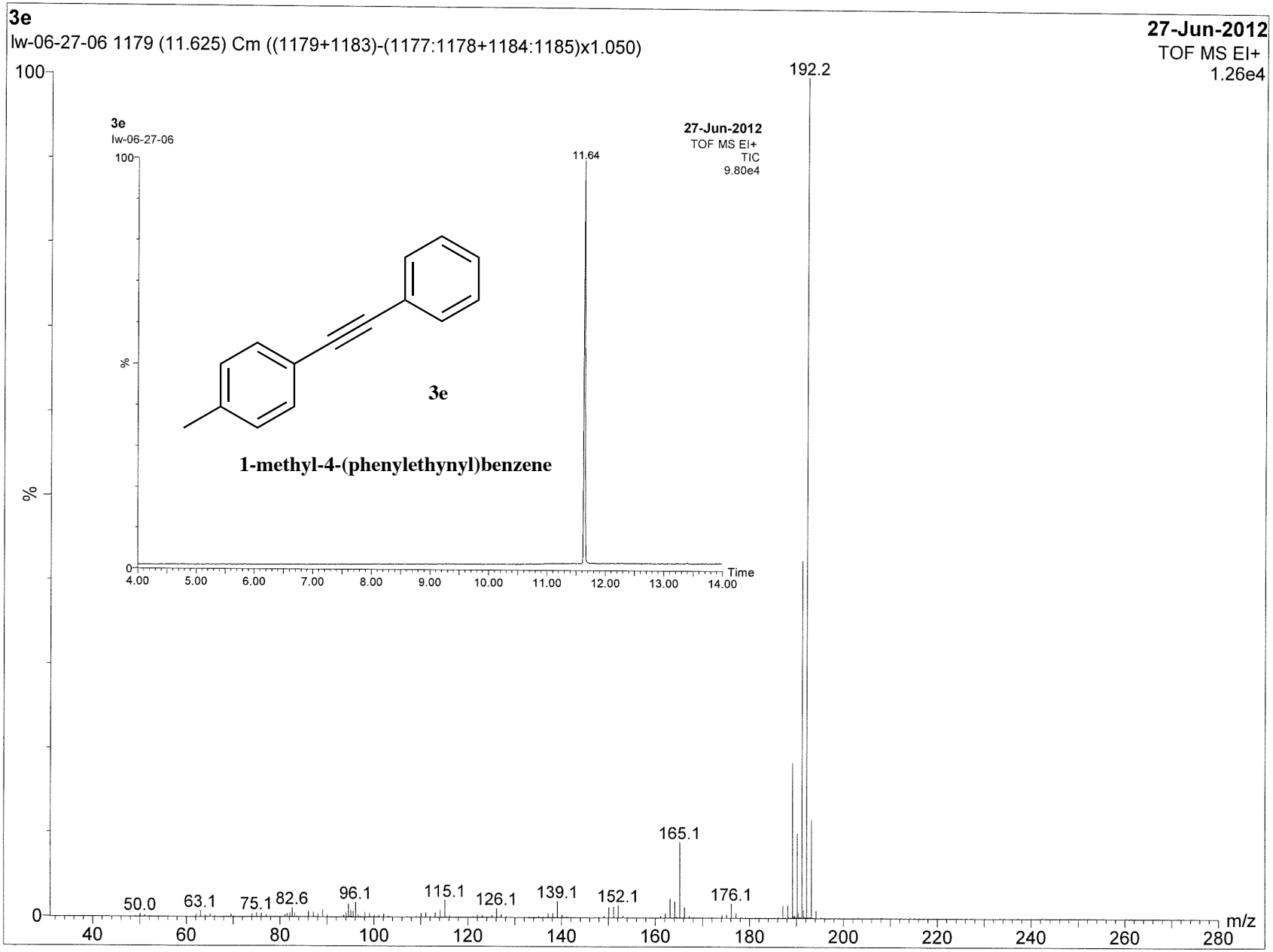

3d
lw-06-22-14 1058 (10.618) Cm ((1058+1062)-(1056+1063)x1.050)
22-Jun-2012
TOF MS EI+
3.40e3
100
%
0
129.1
157.1
143.1
200.2
115.1
105.1
171.2
91.1
77.1
185.2
41.0
51.0
63.0
95.1
40
60
80
100
120
140
160
180
200
220
240
260
280
m/z
3d
1-methyl-4-(oct-1-yn-1-yl)benzene
3d
lw-06-22-14
22-Jun-2012
TOF MS EI+
TIC
1.57e5
10.63
%
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
Time

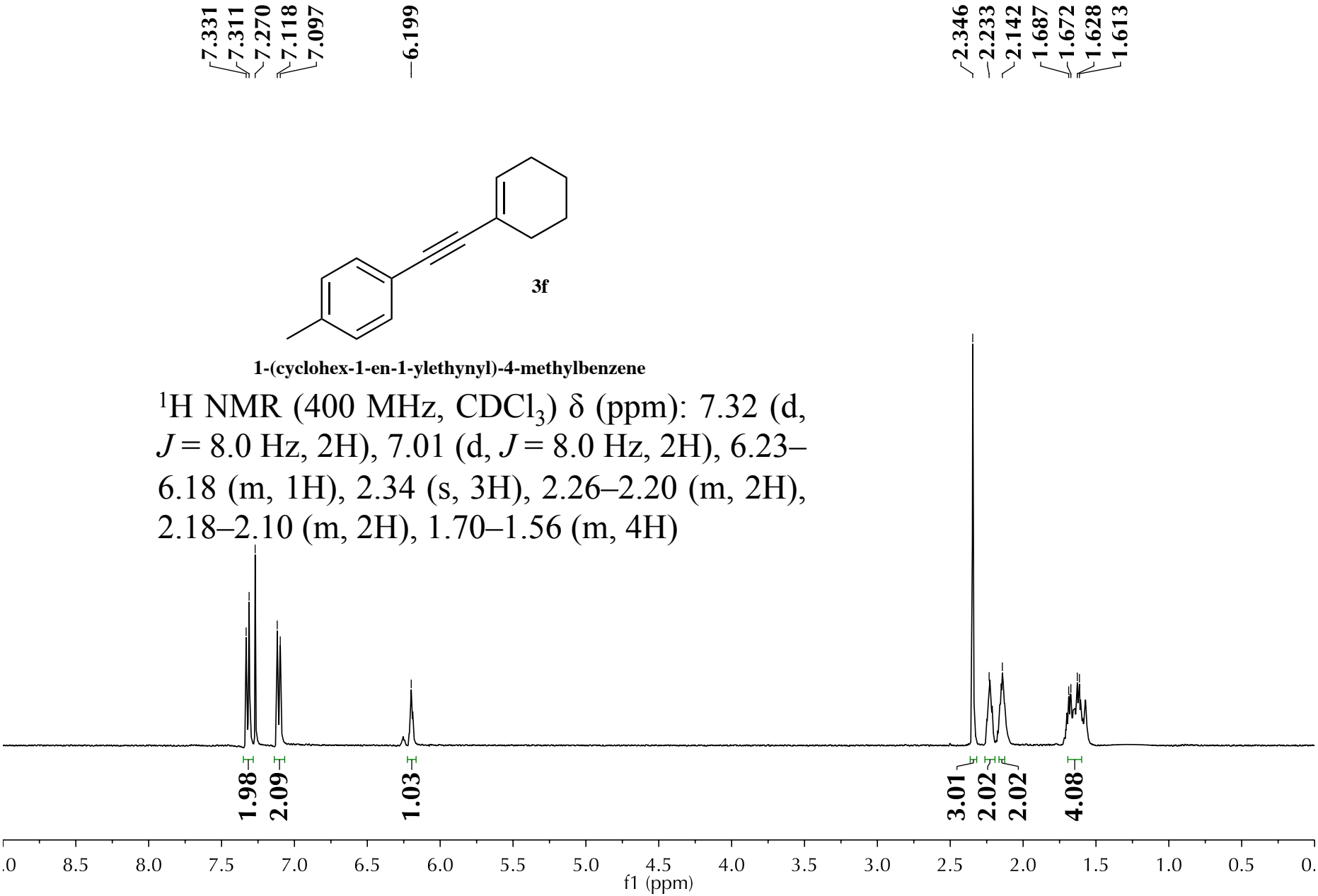


3e

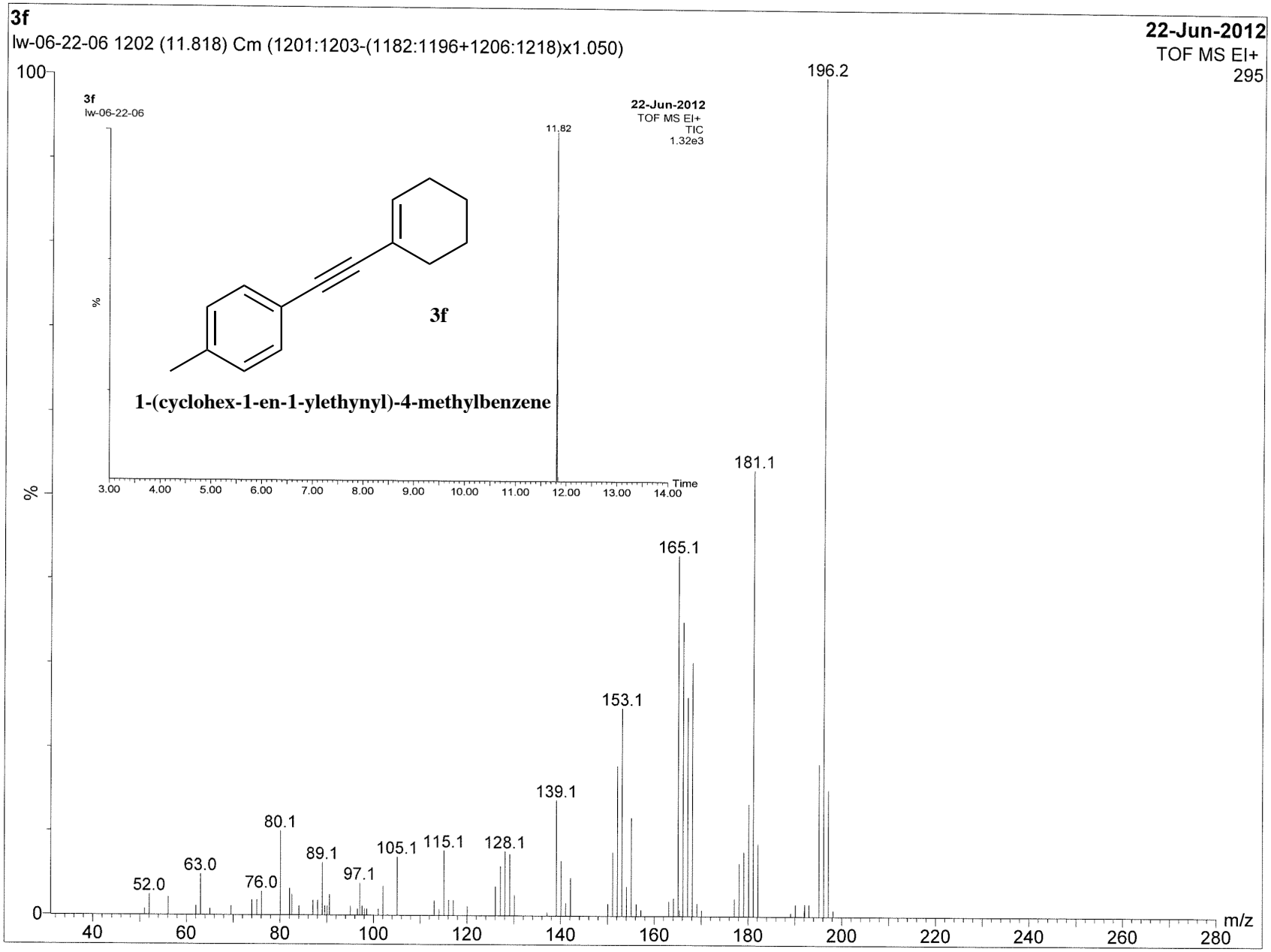
1-methyl-4-(phenylethynyl)benzene

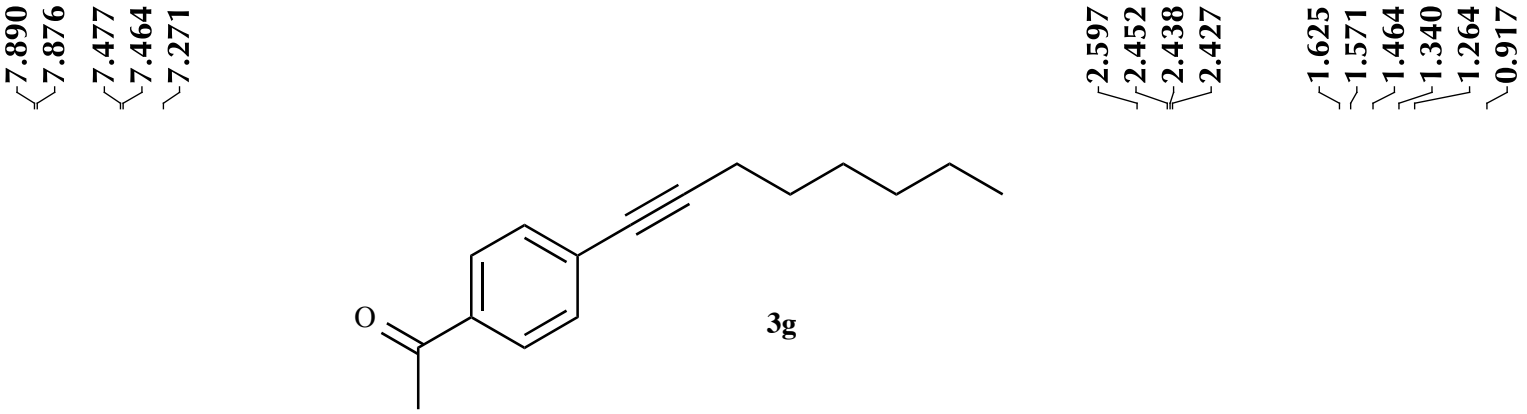
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.55–7.52 (m, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.38–7.32 (m, 3H), 7.16 (d, *J* = 8.0 Hz, 2H), 2.38 (s, 3H)


3e
lw-06-27-06 1179 (11.625) Cm ((1179+1183)-(1177:1178+1184:1185)x1.050)
27-Jun-2012
TOF MS EI+
1.26e4
192.2
3e
lw-06-27-06
27-Jun-2012
TOF MS EI+
TIC
9.80e4
11.64
3e
1-methyl-4-(phenylethynyl)benzene
Time
m/z
%
165.1
50.0
63.1
75.1
82.6
96.1
115.1
126.1
139.1
152.1
176.1



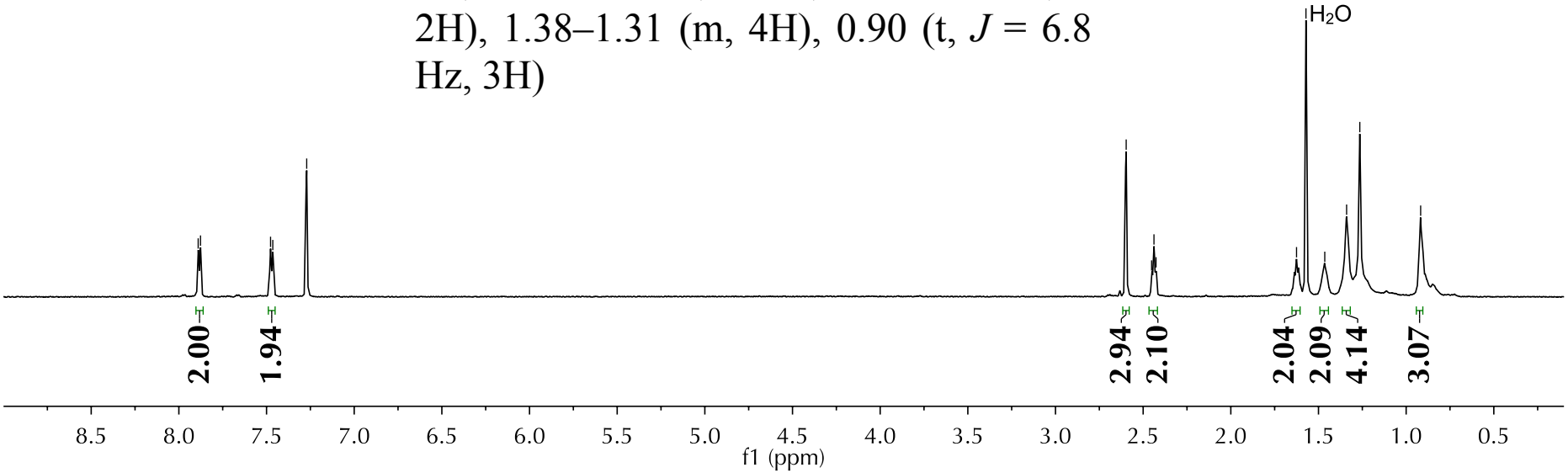
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.32 (d, J = 8.0 Hz, 2H), 7.01 (d, J = 8.0 Hz, 2H), 6.23–6.18 (m, 1H), 2.34 (s, 3H), 2.26–2.20 (m, 2H), 2.18–2.10 (m, 2H), 1.70–1.56 (m, 4H)

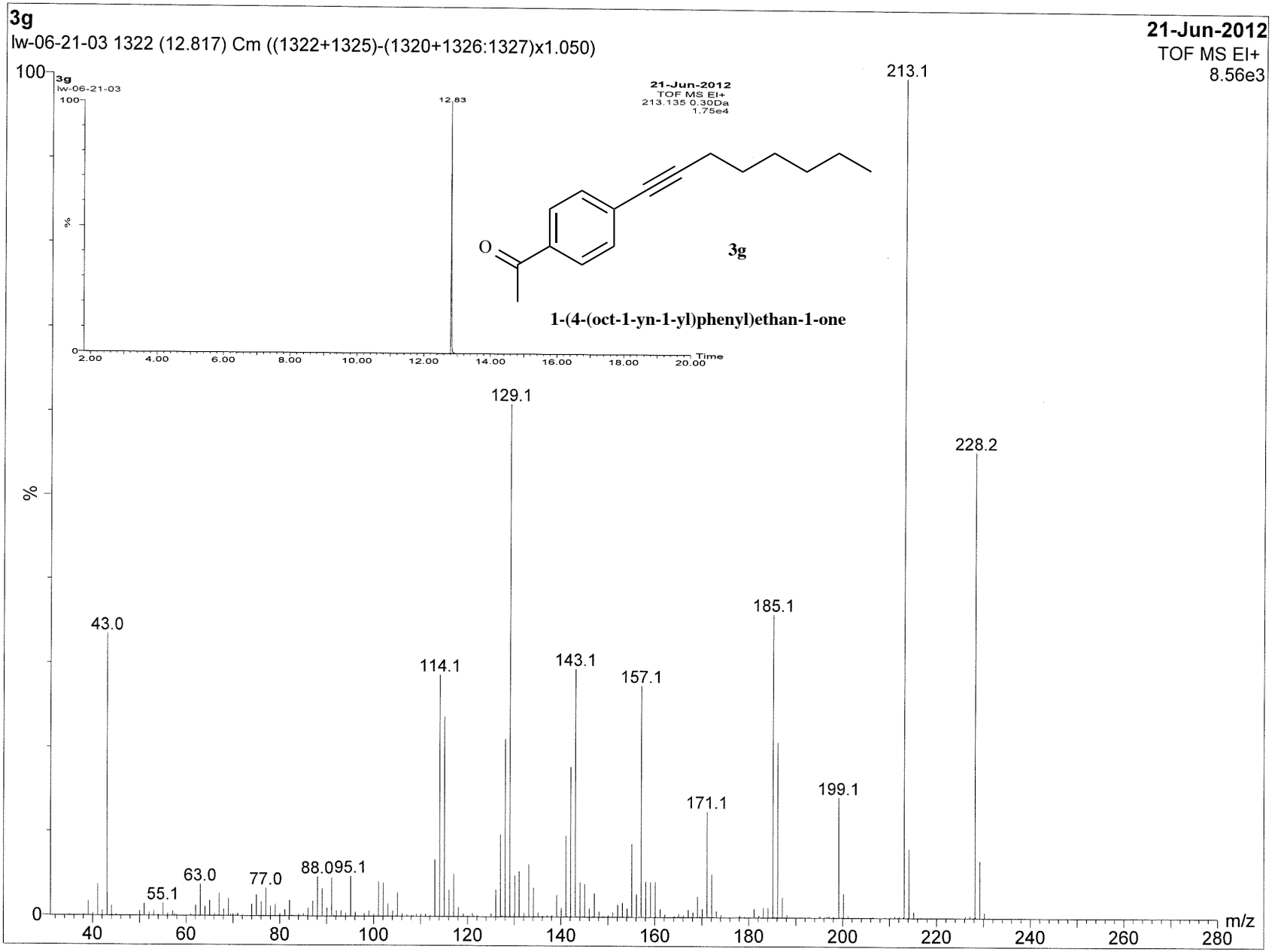

3f
lw-06-22-06 1202 (11.818) Cm (1201:1203-(1182:1196+1206:1218)x1.050)
22-Jun-2012
TOF MS EI+
295
100
%
0
196.2
181.1
165.1
153.1
139.1
80.1
89.1
105.1
115.1
128.1
63.0
52.0
76.0
97.1
40
60
80
100
120
140
160
180
200
220
240
260
280
m/z
3f
lw-06-22-06
22-Jun-2012
TOF MS EI+
TIC
1.32e3
11.82
%
3f
1-(cyclohex-1-en-1-ylethynyl)-4-methylbenzene
3.00
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
Time

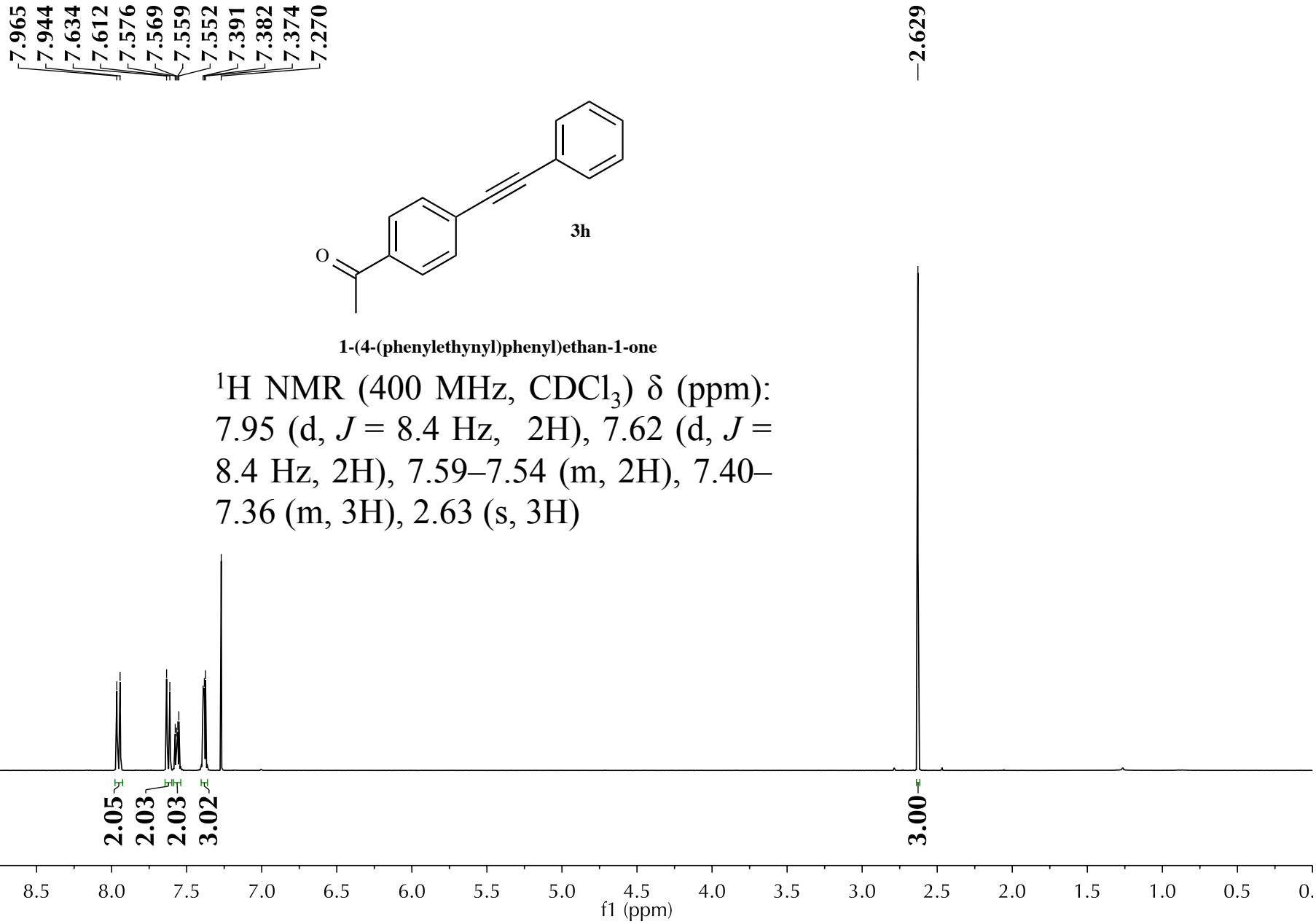


1-(4-(oct-1-yn-1-yl)phenyl)ethan-1-one

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.87 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 2.60 (s, 3H), 2.44 (t, *J* = 7.2 Hz, 2H), 1.65–1.59 (m, 4H), 1.50–1.44 (m, 2H), 1.38–1.31 (m, 4H), 0.90 (t, *J* = 6.8 Hz, 3H)

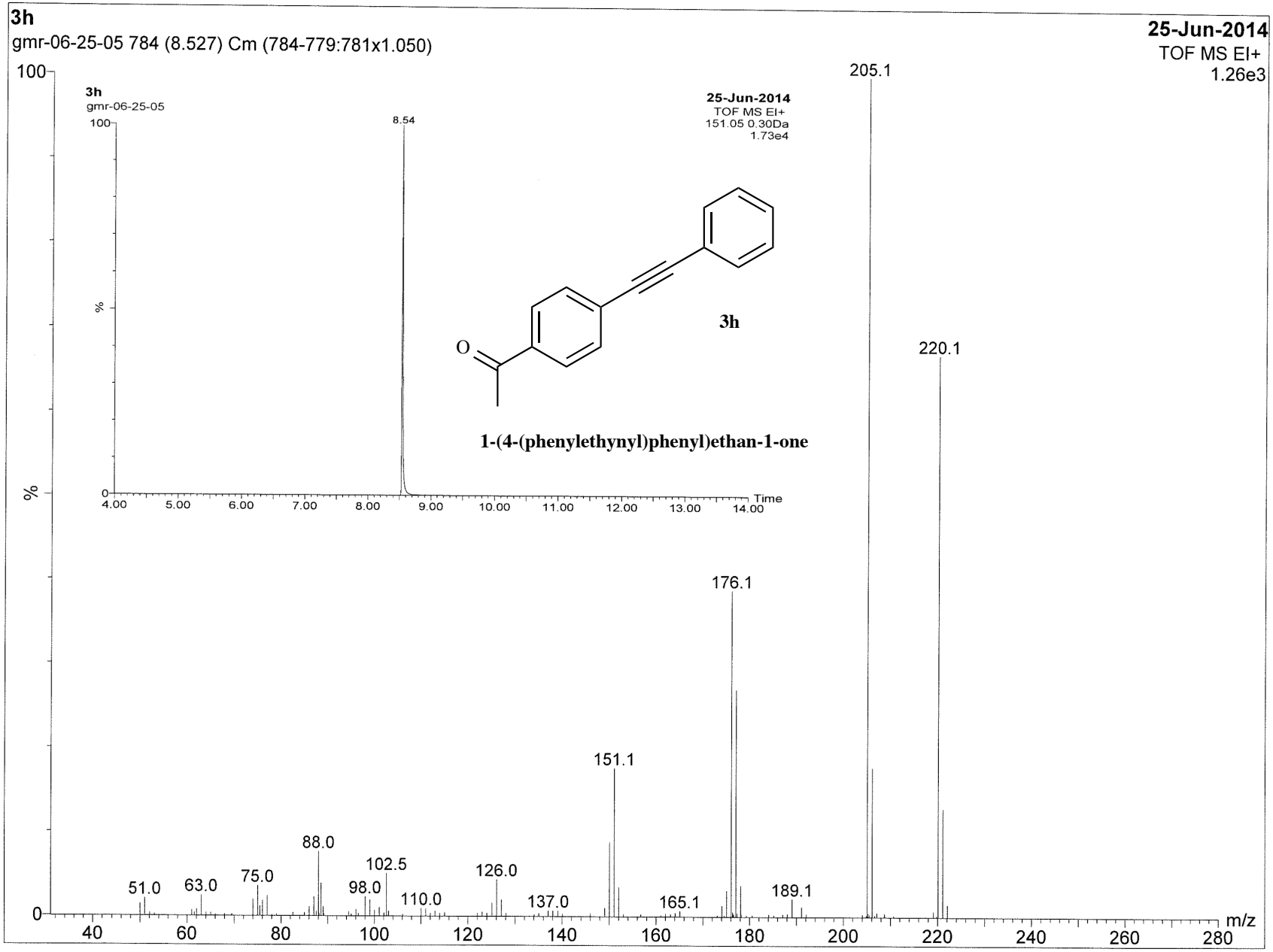


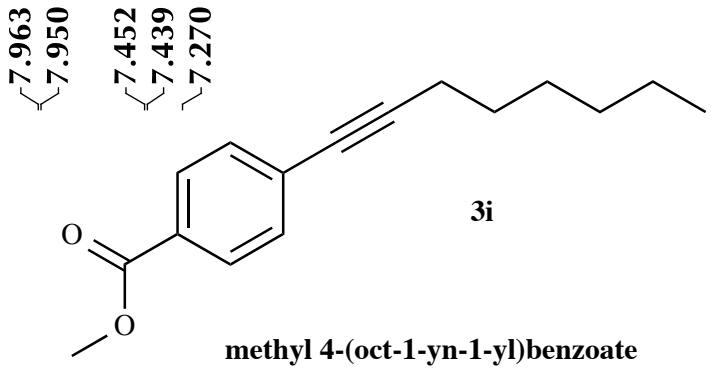

3g
lw-06-21-03 1322 (12.817) Cm ((1322+1325)-(1320+1326:1327)x1.050)
21-Jun-2012
TOF MS EI+
8.56e3
213.1
129.1
228.2
43.0
185.1
114.1
143.1
157.1
171.1
199.1
63.0
77.0
88.095.1
55.1
%
m/z
0
40
60
80
100
120
140
160
180
200
220
240
260
280
3g
lw-06-21-03
12.83
Time
21-Jun-2012
TOF MS EI+
213.135 0.30Da
1.75e4
O
3g
1-(4-(oct-1-yn-1-yl)phenyl)ethan-1-one



1-(4-(phenylethynyl)phenyl)ethan-1-one

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.95 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.59–7.54 (m, 2H), 7.40–7.36 (m, 3H), 2.63 (s, 3H)

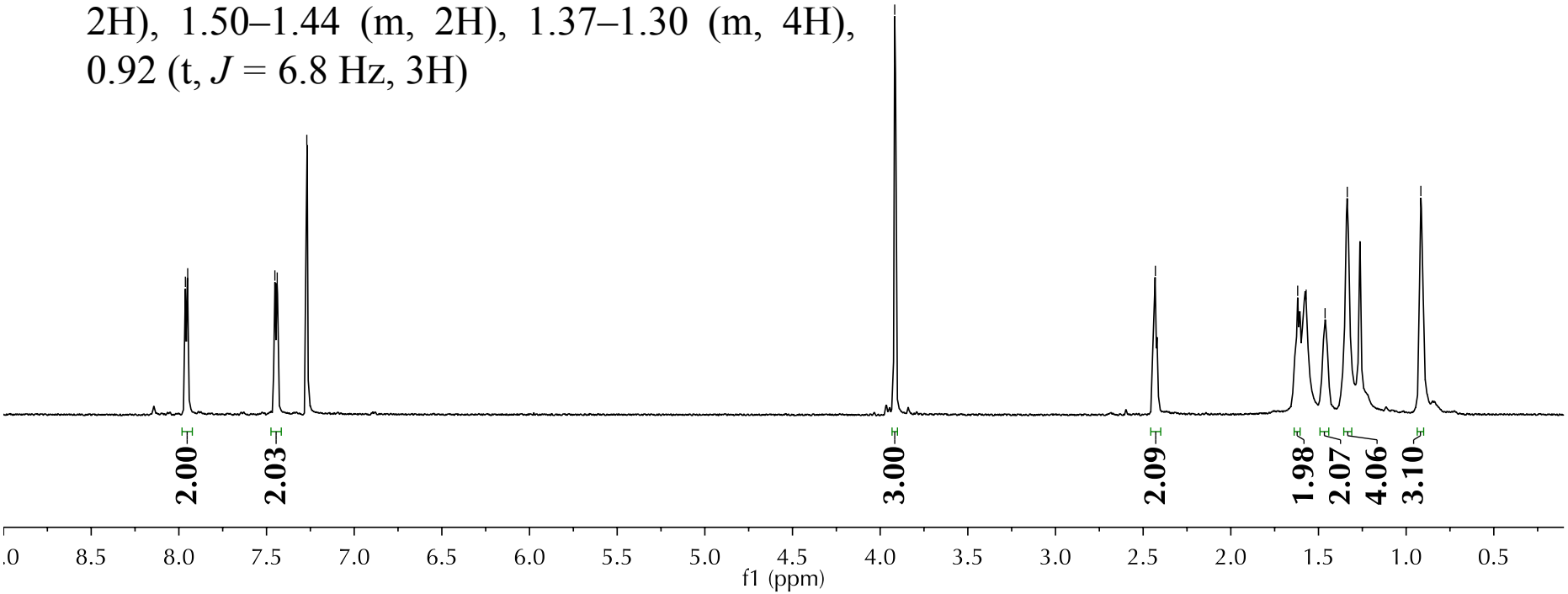

3h
gmr-06-25-05 784 (8.527) Cm (784-779:781x1.050)
25-Jun-2014
TOF MS EI+
1.26e3
205.1
220.1
176.1
151.1
88.0
102.5
126.0
51.0
63.0
75.0
98.0
110.0
137.0
165.1
189.1
m/z
%
3h
gmr-06-25-05
8.54
Time
25-Jun-2014
TOF MS EI+
151.05 0.30Da
1.73e4
3h
1-(4-(phenylethynyl)phenyl)ethan-1-one

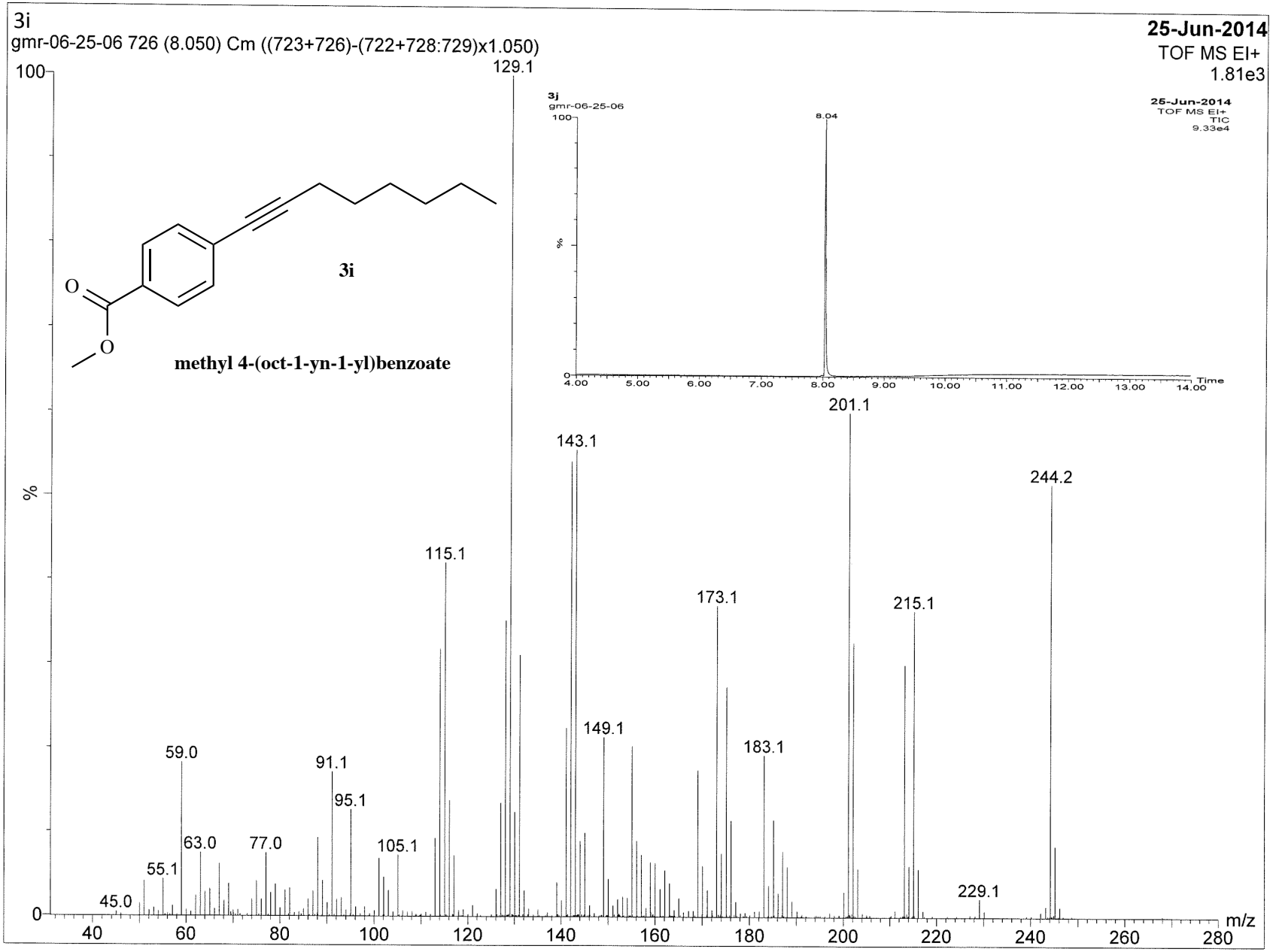


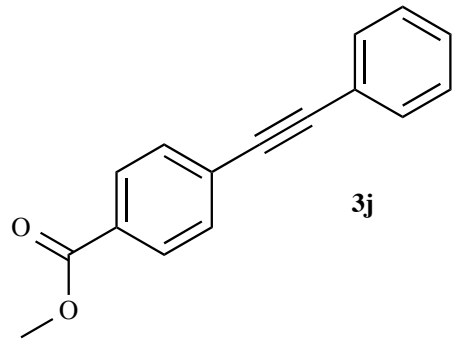
3i

methyl 4-(oct-1-yn-1-yl)benzoate

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.96 (d, J = 8.8 Hz, 2H), 7.45 (d, J = 8.8 Hz, 2H), 3.92 (s, 3H), 2.43 (t, J = 7.0 Hz, 2H), 1.65–1.60 (m, 2H), 1.50–1.44 (m, 2H), 1.37–1.30 (m, 4H), 0.92 (t, J = 6.8 Hz, 3H)



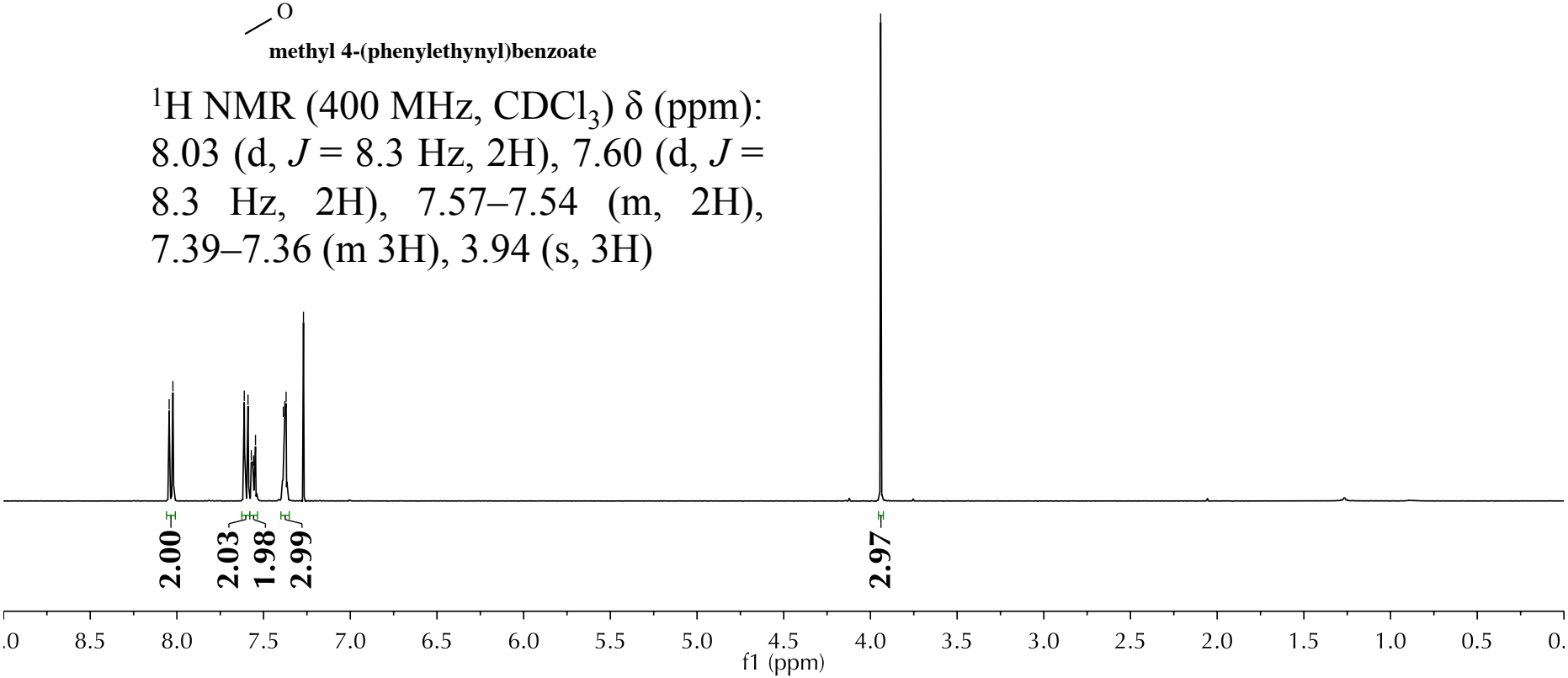

3i
gmr-06-25-06 726 (8.050) Cm ((723+726)-(722+728:729)x1.050)
25-Jun-2014
TOF MS EI+
1.81e3
3i
methyl 4-(oct-1-yn-1-yl)benzoate
3j
gmr-06-25-06
25-Jun-2014
TOF MS EI+
TIC
9.33e4
8.04
Time
%
m/z
129.1
201.1
143.1
244.2
115.1
173.1
215.1
149.1
183.1
59.0
91.1
95.1
63.0
77.0
105.1
55.1
45.0
229.1

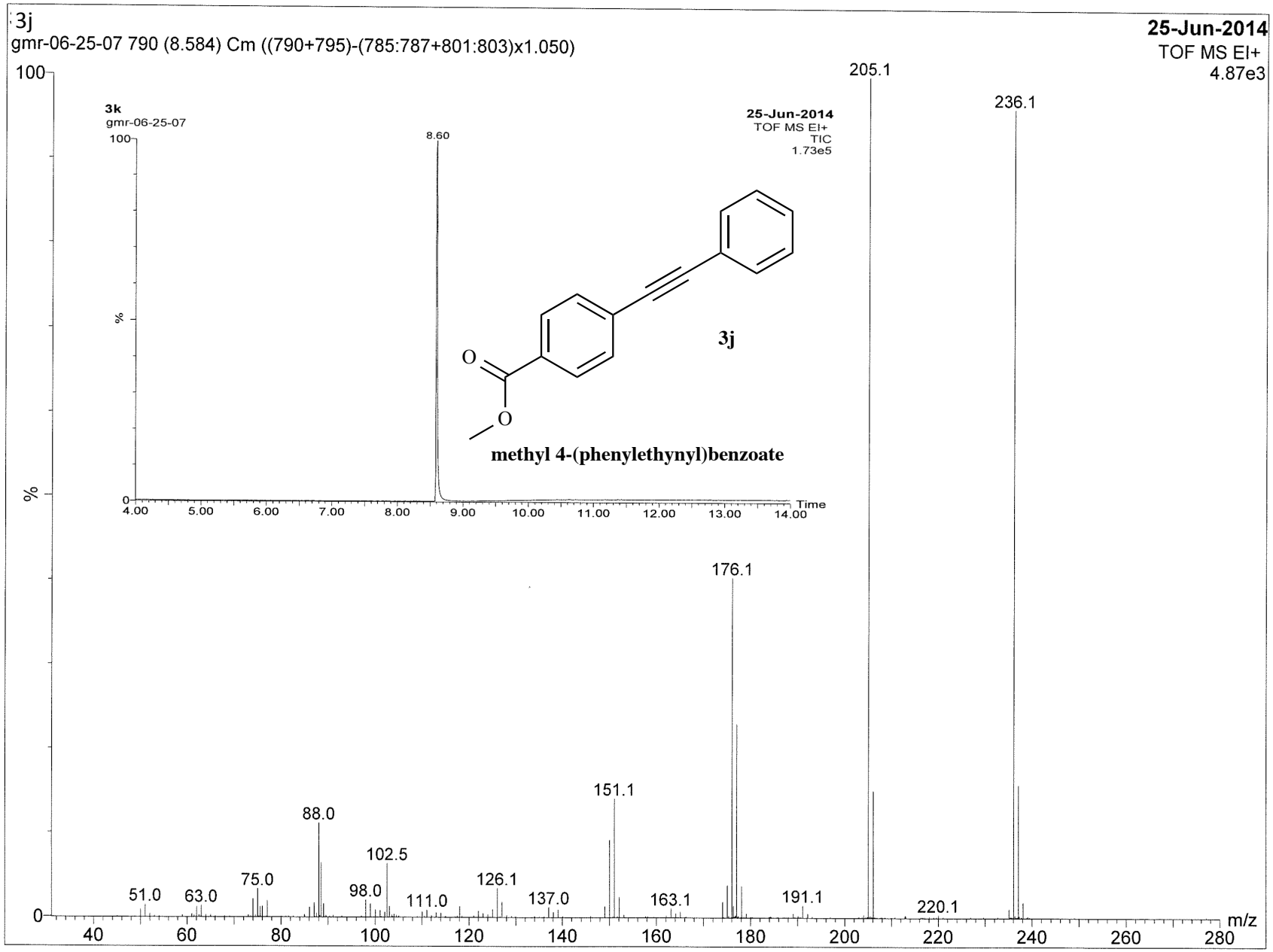


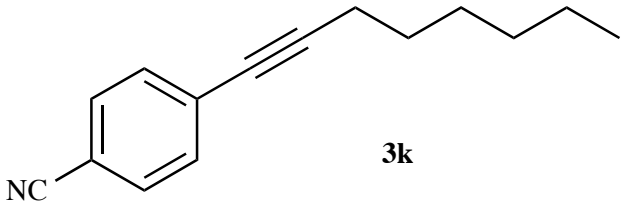
3j

methyl 4-(phenylethynyl)benzoate

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.03 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.57–7.54 (m, 2H), 7.39–7.36 (m 3H), 3.94 (s, 3H)



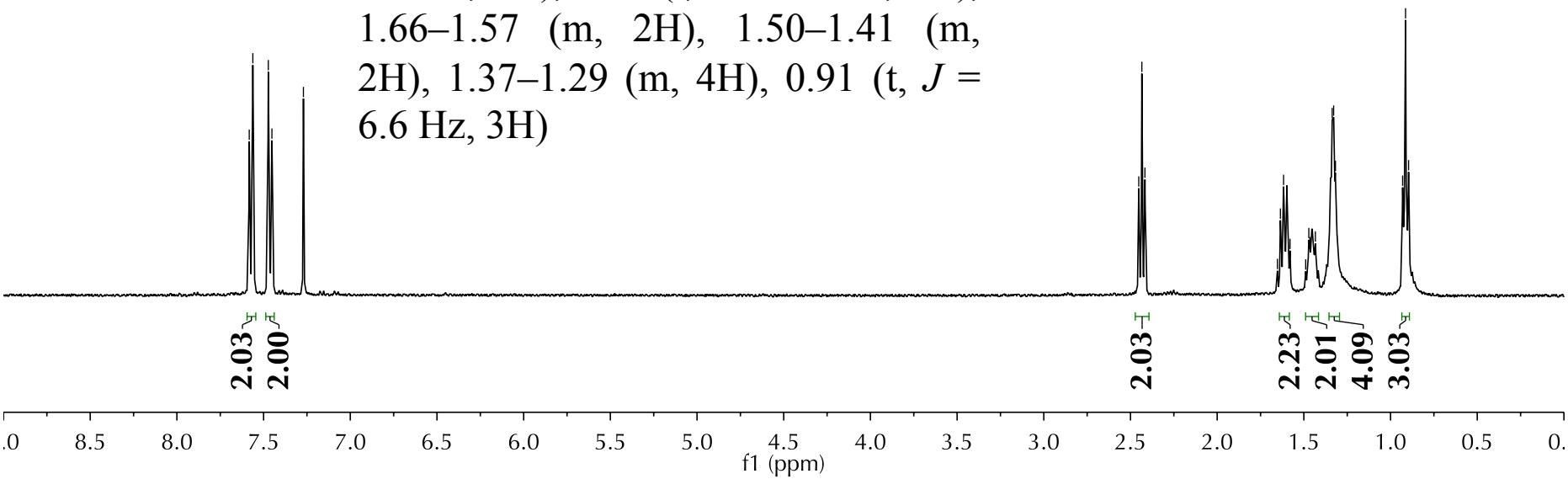

3j
gmr-06-25-07 790 (8.584) Cm ((790+795)-(785:787+801:803)x1.050)
25-Jun-2014
TOF MS EI+
4.87e3
100
%
0
205.1
236.1
176.1
151.1
88.0
102.5
75.0
51.0
63.0
98.0
111.0
126.1
137.0
163.1
191.1
220.1
40
60
80
100
120
140
160
180
200
220
240
260
280
m/z
3k
gmr-06-25-07
8.60
25-Jun-2014
TOF MS EI+
TIC
1.73e5
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
Time
O
O
3j
methyl 4-(phenylethynyl)benzoate

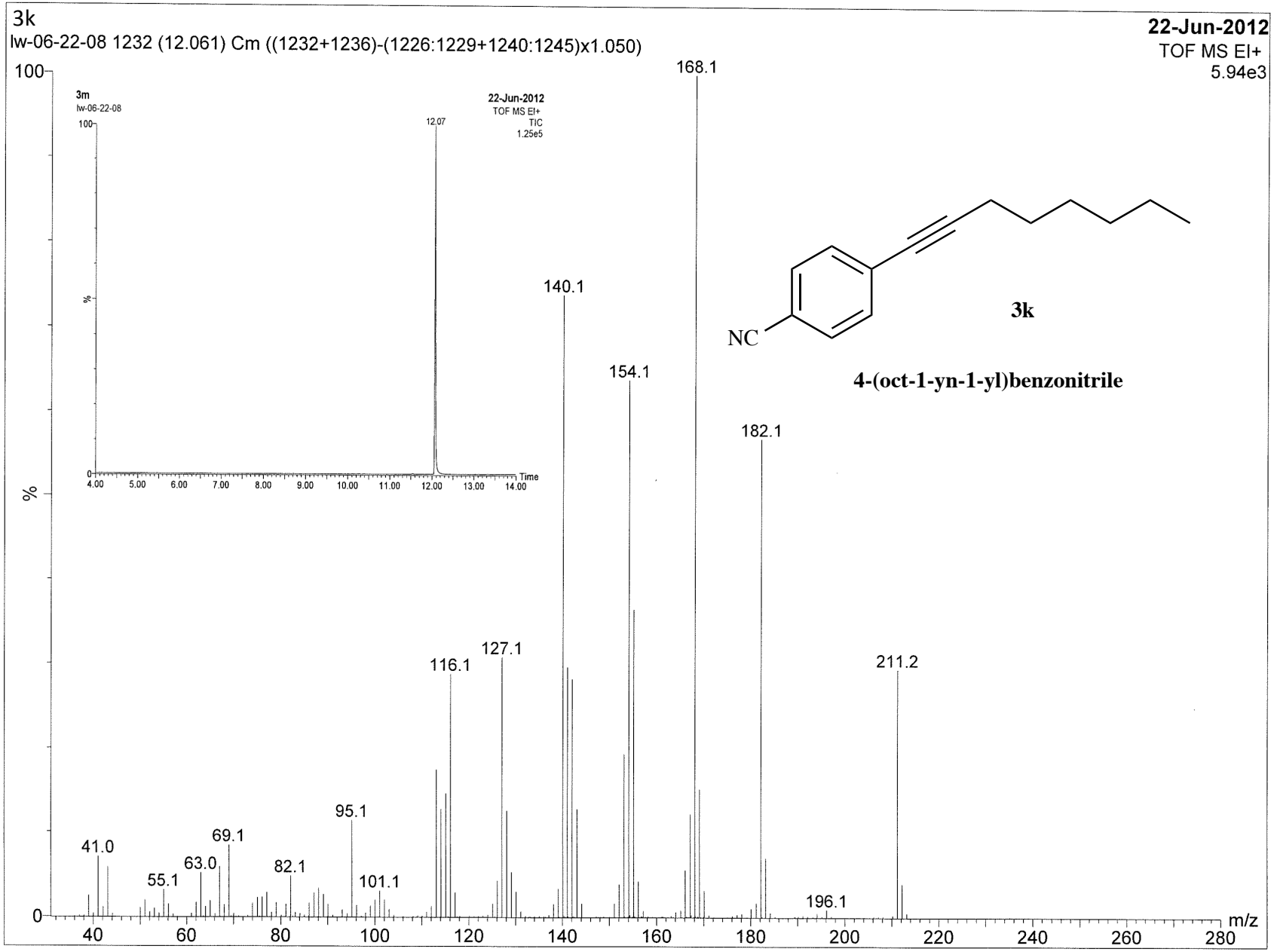


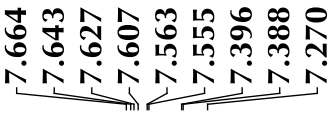
3k

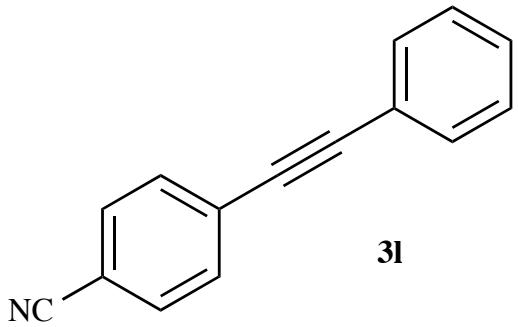
4-(oct-1-yn-1-yl)benzonitrile

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.57 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 1.66–1.57 (m, 2H), 1.50–1.41 (m, 2H), 1.37–1.29 (m, 4H), 0.91 (t, *J* = 6.6 Hz, 3H)




3k
lw-06-22-08 1232 (12.061) Cm ((1232+1236)-(1226:1229+1240:1245)x1.050)
22-Jun-2012
TOF MS EI+
5.94e3
100
%
0
168.1
140.1
154.1
182.1
127.1
116.1
211.2
95.1
69.1
41.0
63.0
82.1
55.1
101.1
196.1
m/z
40
60
80
100
120
140
160
180
200
220
240
260
280
3m
lw-06-22-08
22-Jun-2012
TOF MS EI+
TIC
1.25e5
12.07
Time
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
NC
3k
4-(oct-1-yn-1-yl)benzonitrile

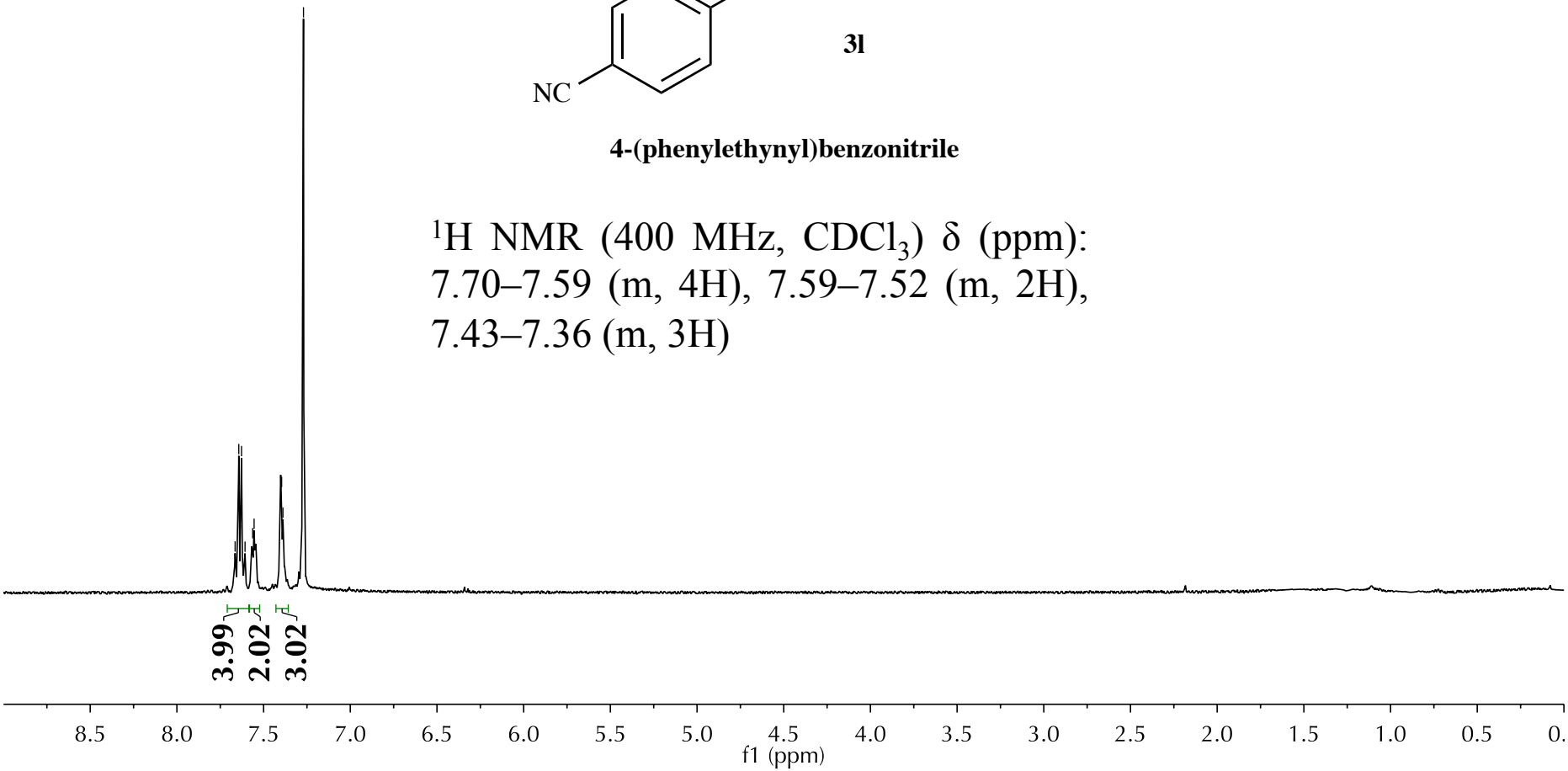


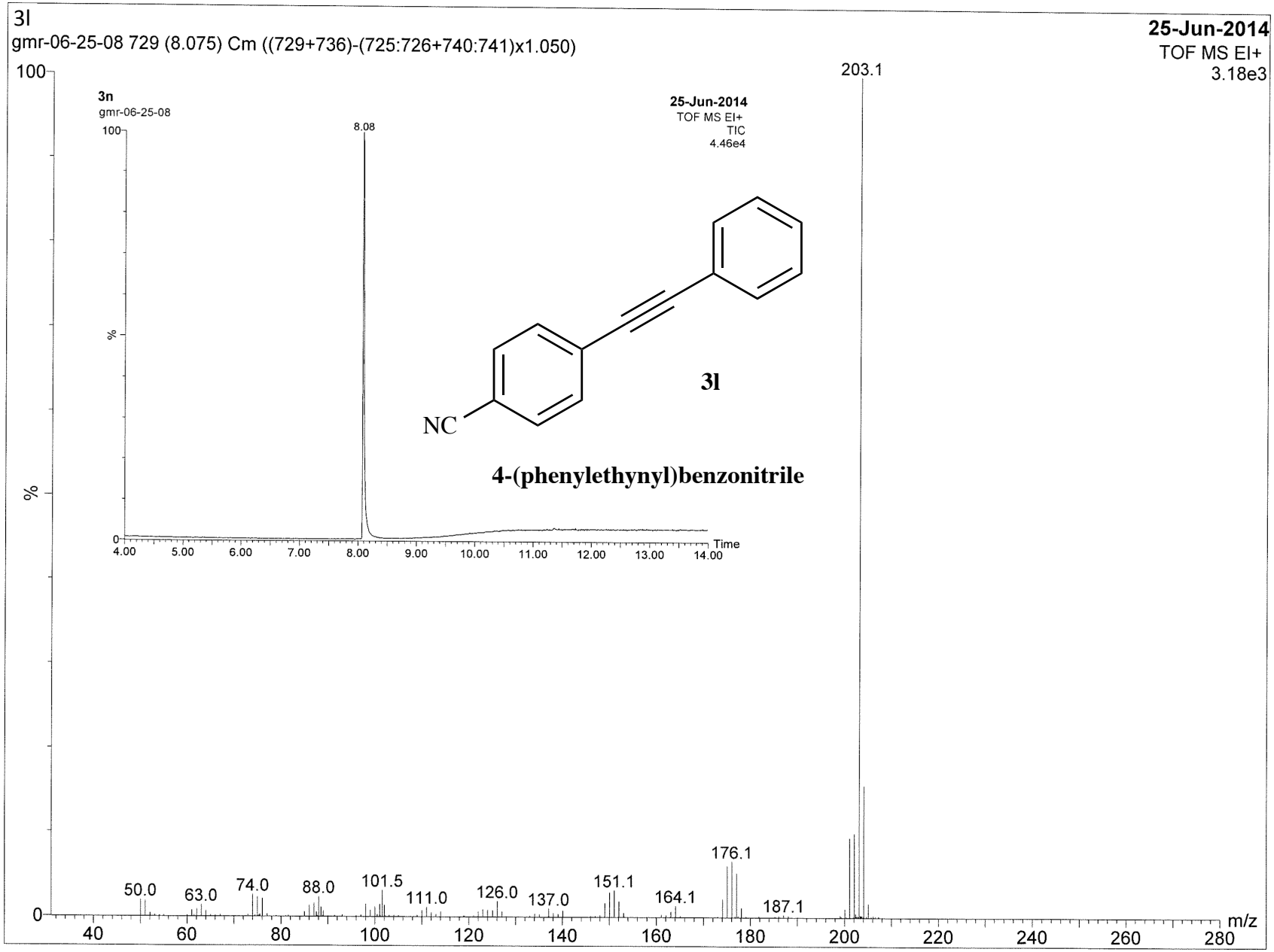


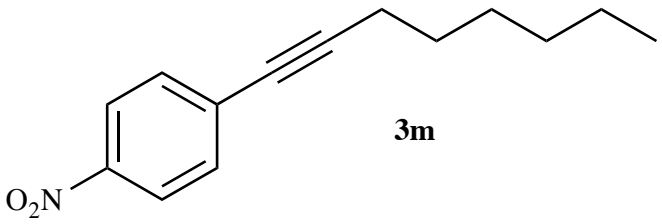
3l

4-(phenylethynyl)benzonitrile

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm):
7.70–7.59 (m, 4H), 7.59–7.52 (m, 2H),
7.43–7.36 (m, 3H)



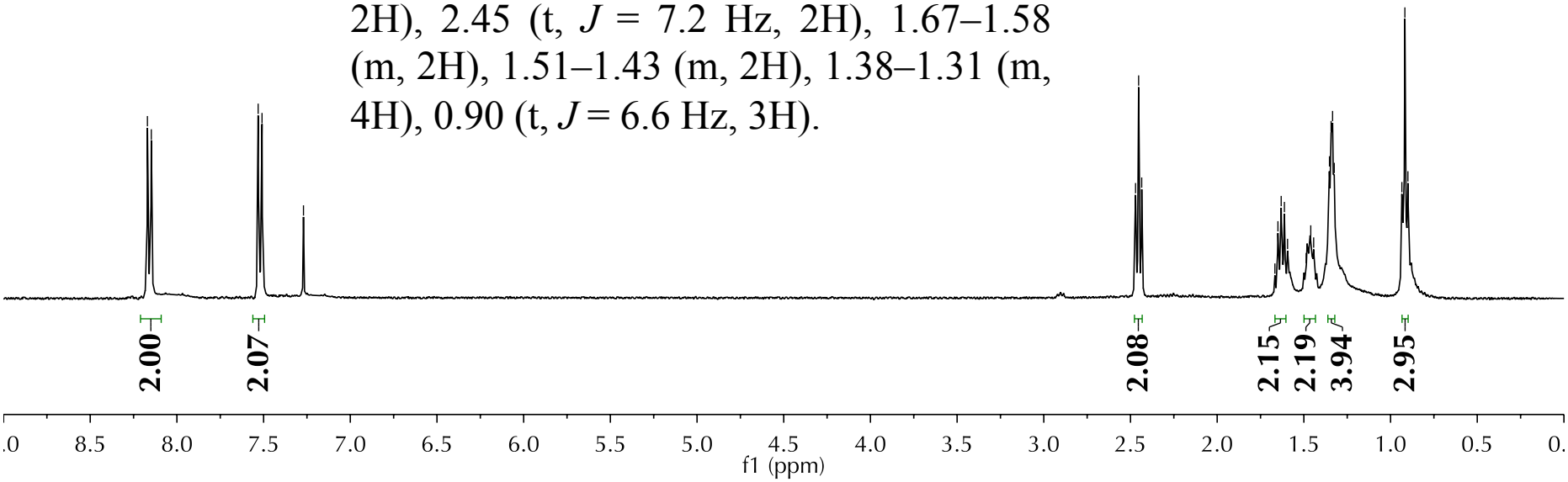

3l
gmr-06-25-08 729 (8.075) Cm ((729+736)-(725:726+740:741)x1.050)
25-Jun-2014
TOF MS EI+
3.18e3
203.1
3n
gmr-06-25-08
8.08
25-Jun-2014
TOF MS EI+
TIC
4.46e4
NC
3l
4-(phenylethynyl)benzonitrile
Time
m/z
%
176.1
151.1
101.5
88.0
74.0
63.0
50.0
111.0
126.0
137.0
164.1
187.1

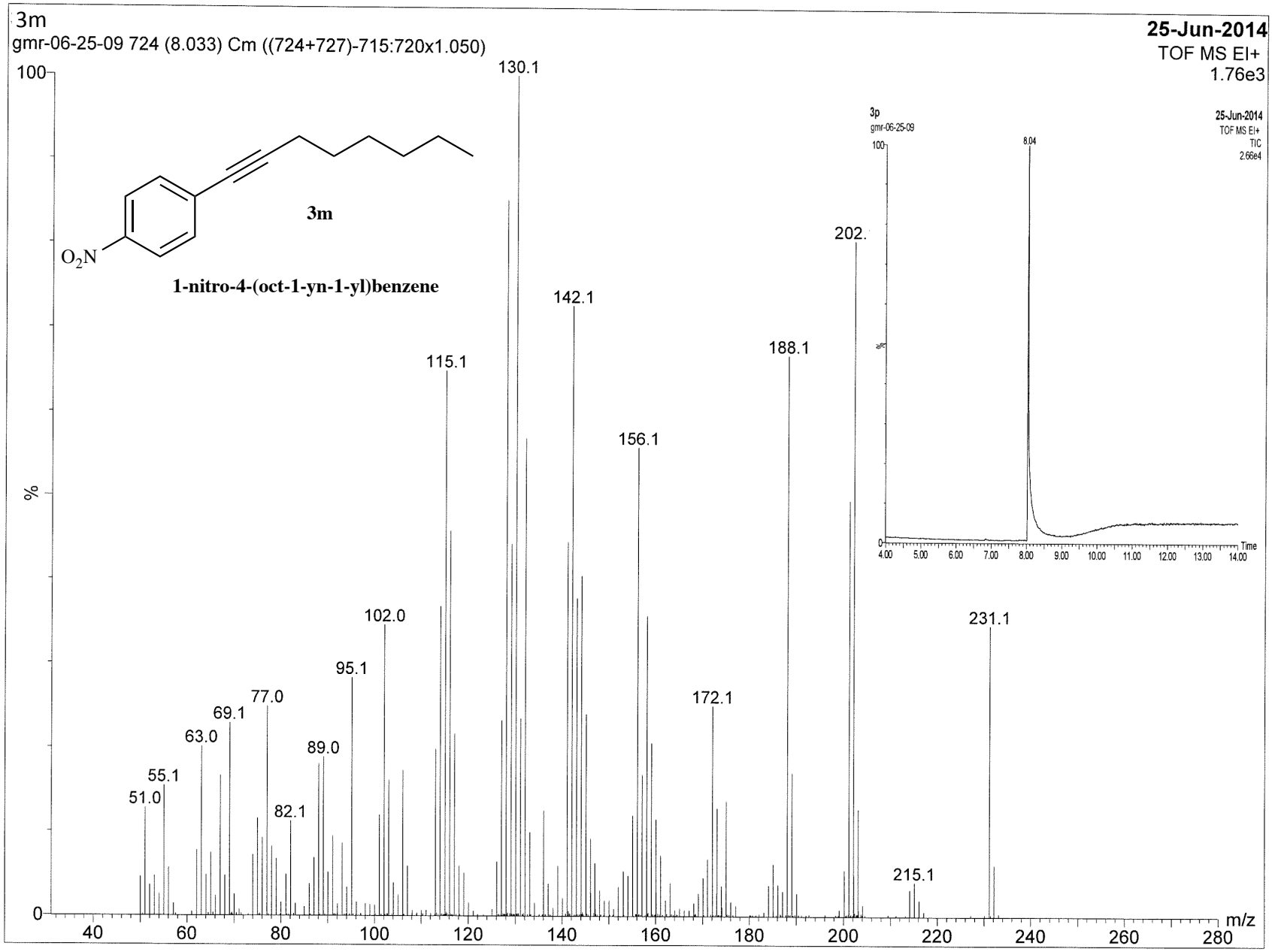


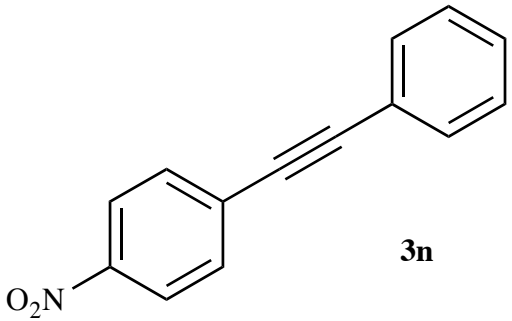
3m

1-nitro-4-(oct-1-yn-1-yl)benzene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.16 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 2.45 (t, *J* = 7.2 Hz, 2H), 1.67–1.58 (m, 2H), 1.51–1.43 (m, 2H), 1.38–1.31 (m, 4H), 0.90 (t, *J* = 6.6 Hz, 3H).



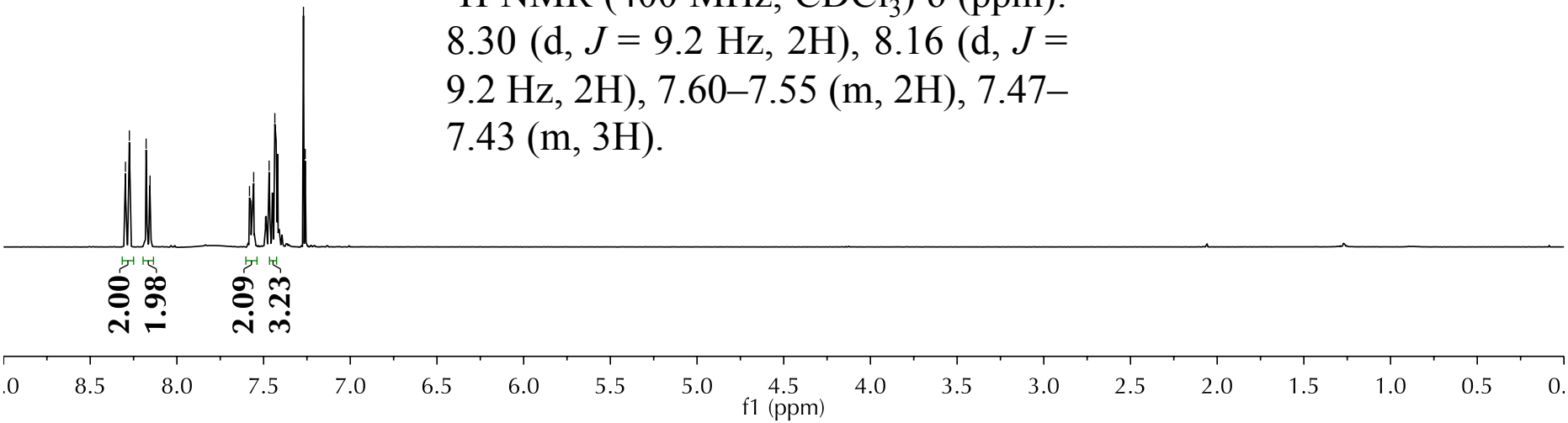

3m
gmr-06-25-09 724 (8.033) Cm ((724+727)-715:720x1.050)
25-Jun-2014
TOF MS EI+
1.76e3
3m
1-nitro-4-(oct-1-yn-1-yl)benzene
130.1
202.
142.1
188.1
115.1
156.1
102.0
231.1
95.1
77.0
172.1
69.1
63.0
89.0
55.1
51.0
82.1
215.1
m/z
%
3p
gmr-06-25-09
25-Jun-2014
TOF MS EI+
TIC
2.66e4
8.04
Time

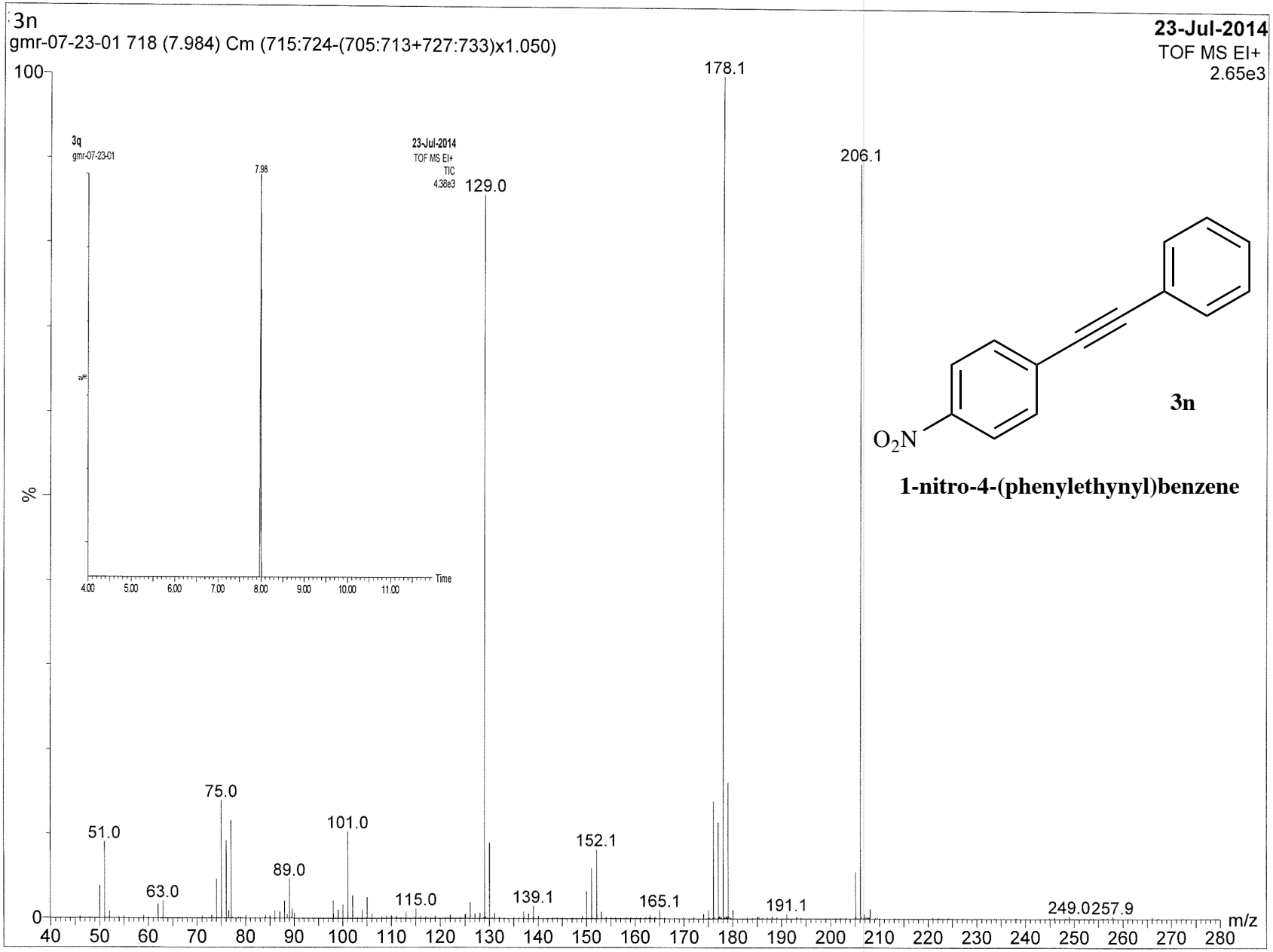


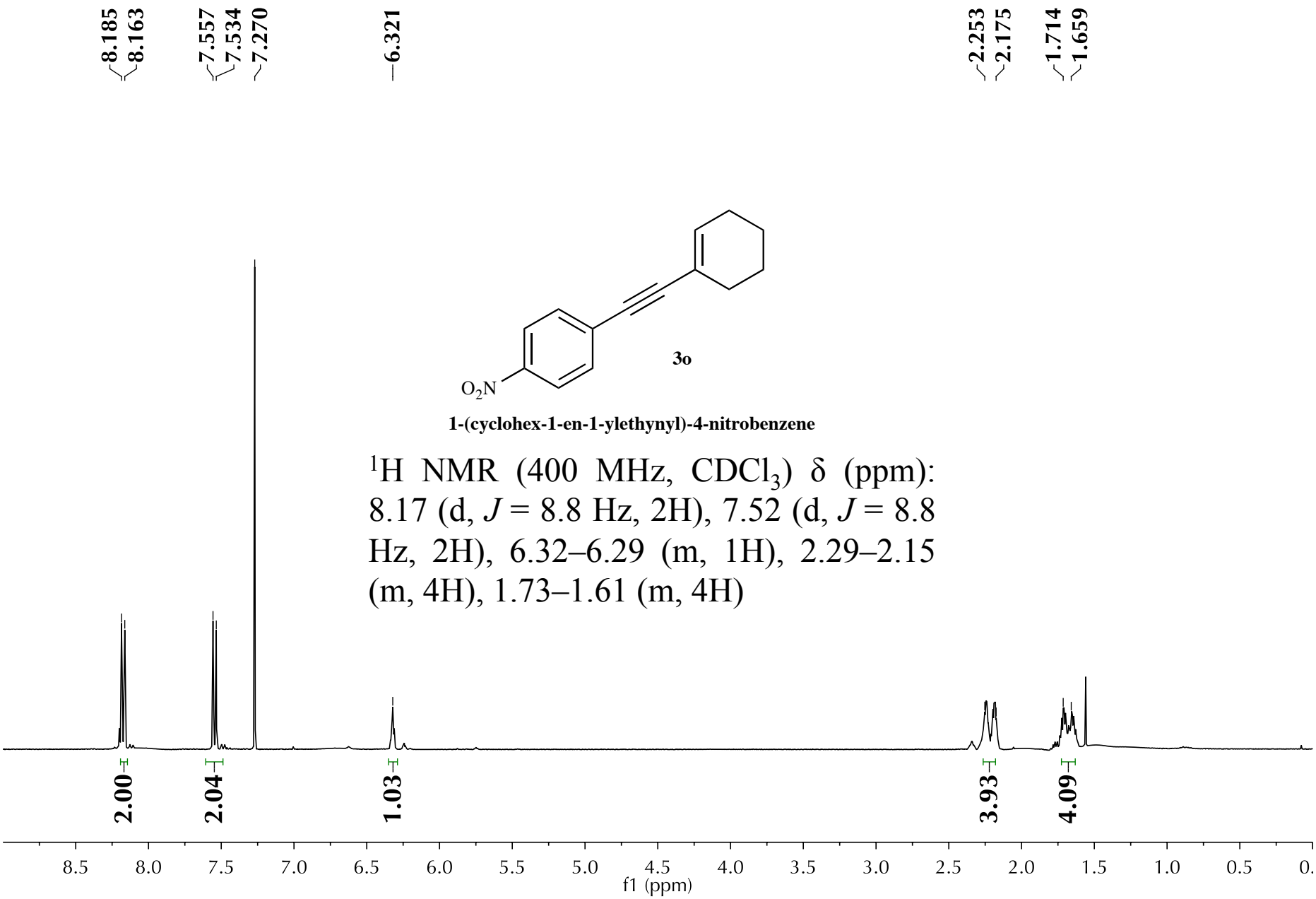
3n

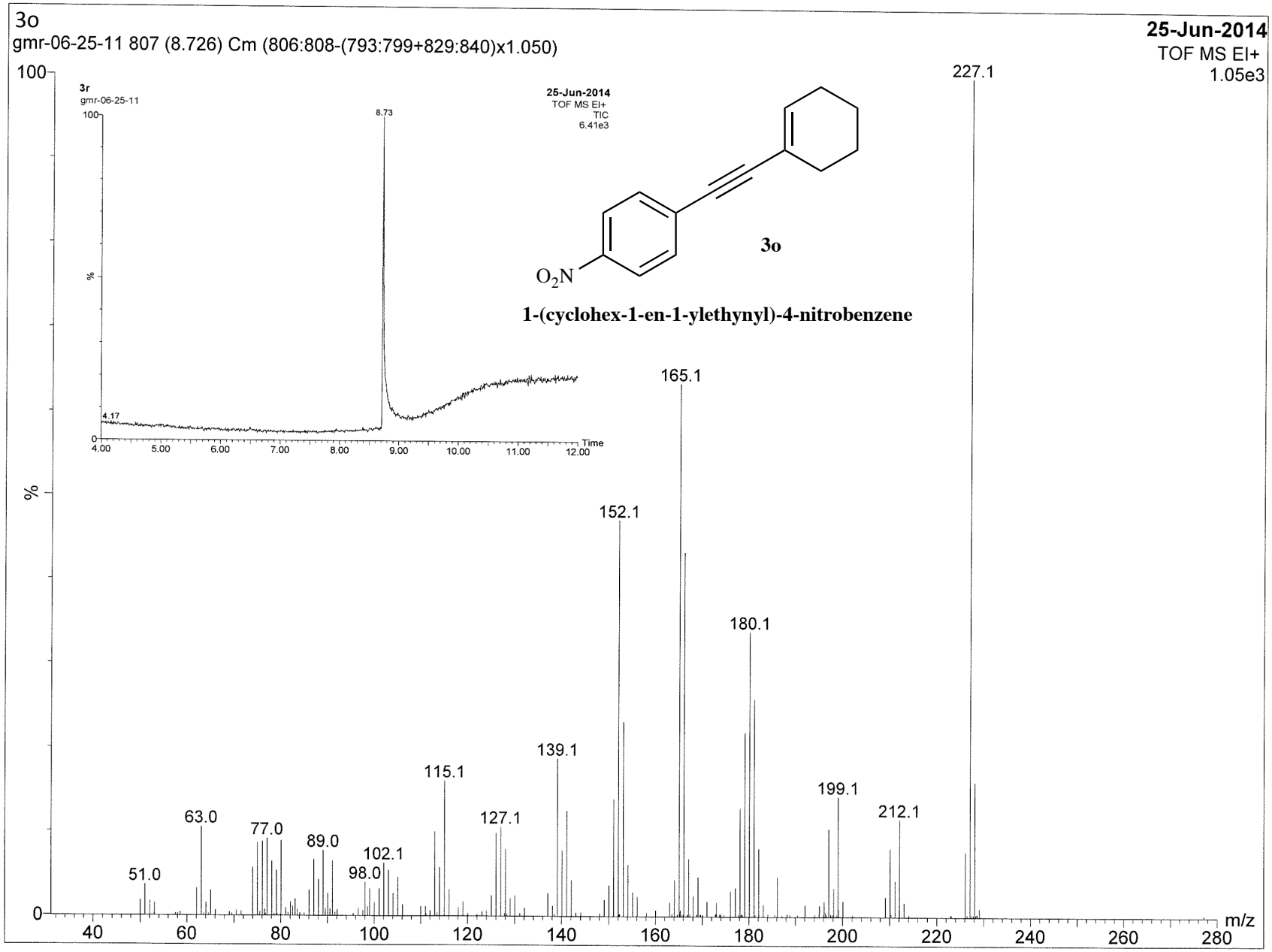
1-nitro-4-(phenylethynyl)benzene

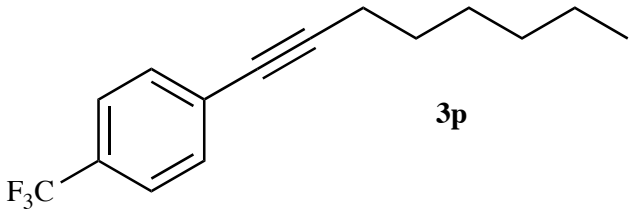
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.30 (d, *J* = 9.2 Hz, 2H), 8.16 (d, *J* = 9.2 Hz, 2H), 7.60–7.55 (m, 2H), 7.47–7.43 (m, 3H).




3n
gmr-07-23-01 718 (7.984) Cm (715:724-(705:713+727:733)x1.050)
23-Jul-2014
TOF MS EI+
2.65e3
100
%
0
178.1
206.1
129.0
75.0
51.0
101.0
152.1
89.0
63.0
115.0
139.1
165.1
191.1
249.0257.9
m/z
40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280
3q
gmr-07-23-01
7.98
Time
4.00 5.00 6.00 7.00 8.00 9.00 10.00 11.00
23-Jul-2014
TOF MS EI+
TIC
4.38e3
O_2N
3n
1-nitro-4-(phenylethynyl)benzene

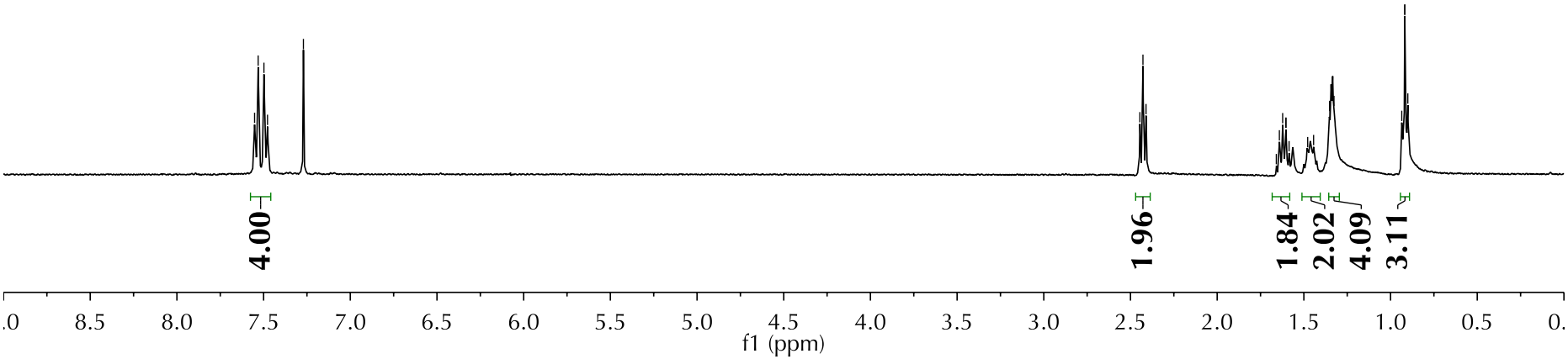

8.185
8.163
7.557
7.534
7.270
6.321
2.253
2.175
1.714
1.659
O2N
3o
1-(cyclohex-1-en-1-ylethynyl)-4-nitrobenzene
1H NMR (400 MHz, CDCl3) δ (ppm): 8.17 (d, J = 8.8 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H), 6.32–6.29 (m, 1H), 2.29–2.15 (m, 4H), 1.73–1.61 (m, 4H)
2.00
2.04
1.03
3.93
4.09
f1 (ppm)

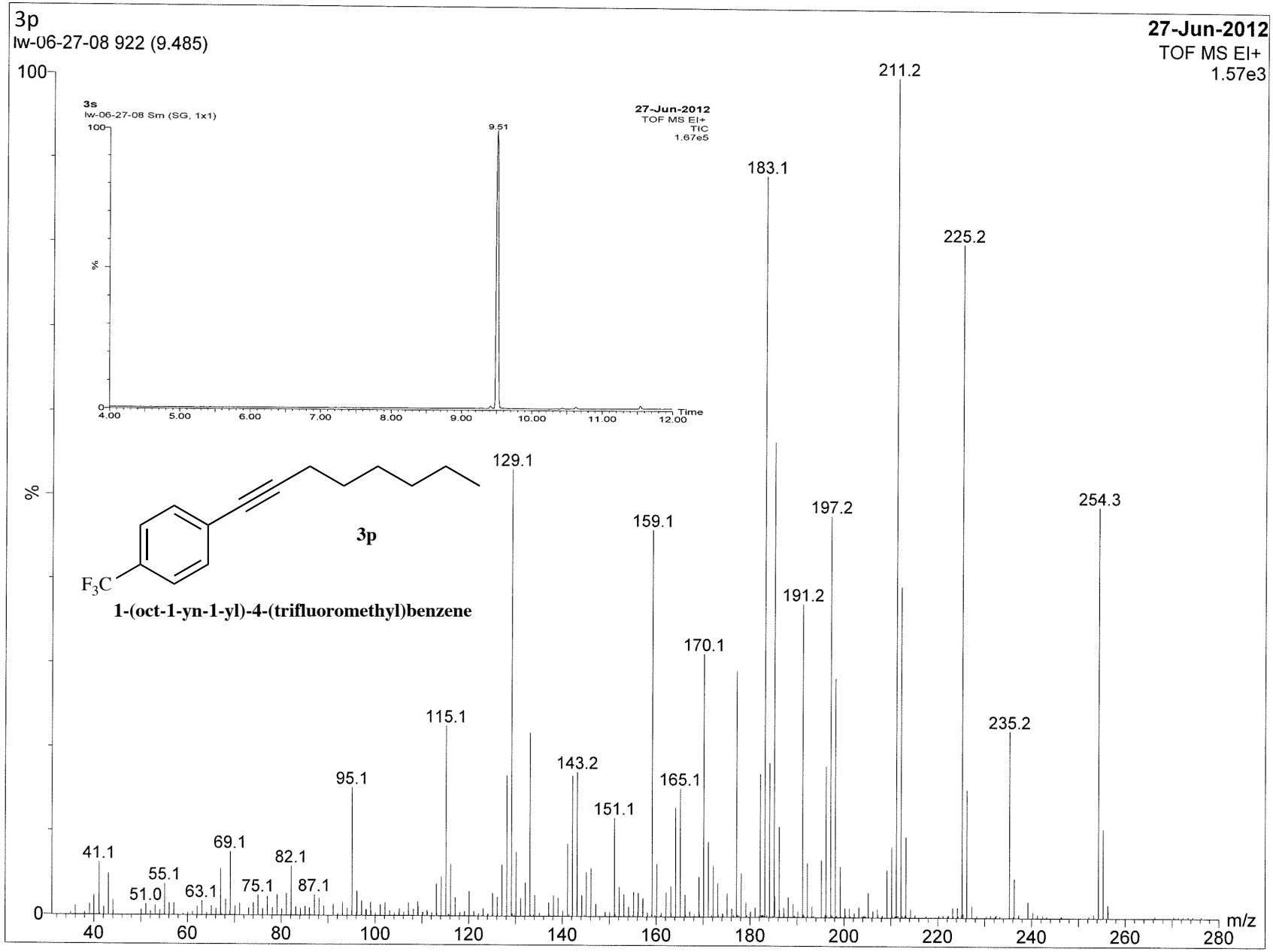

3o
gmr-06-25-11 807 (8.726) Cm (806:808-(793:799+829:840)x1.050)
25-Jun-2014
TOF MS EI+
1.05e3
227.1
165.1
152.1
180.1
139.1
115.1
199.1
212.1
127.1
63.0
77.0
89.0
102.1
98.0
51.0
m/z
%
3r
gmr-06-25-11
8.73
4.17
Time
25-Jun-2014
TOF MS EI+
TIC
6.41e3
O2N
3o
1-(cyclohex-1-en-1-ylethynyl)-4-nitrobenzene

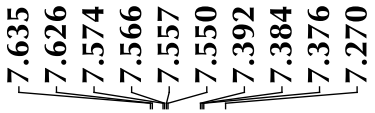


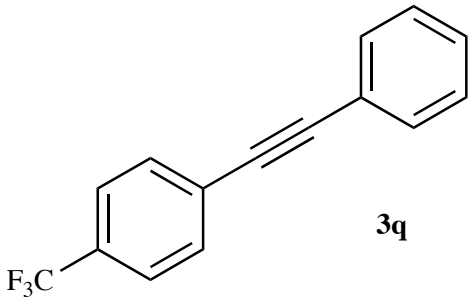
1-(oct-1-yn-1-yl)-4-(trifluoromethyl)benzene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.54 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 2.43 (t, *J* = 7.0 Hz, 2H), 1.67–1.58 (m, 2H), 1.45–1.43 (m, 2H), 1.33–1.29 (m, 4H), 0.90 (t, *J* = 6.6 Hz, 3H)




3p
lw-06-27-08 922 (9.485)
27-Jun-2012
TOF MS EI+
1.57e3
3s
lw-06-27-08 Sm (SG, 1x1)
27-Jun-2012
TOF MS EI+
TIC
1.67e5
9.51
Time
3p
1-(oct-1-yn-1-yl)-4-(trifluoromethyl)benzene
211.2
183.1
225.2
129.1
254.3
197.2
159.1
191.2
170.1
115.1
235.2
143.2
95.1
165.1
151.1
69.1
41.1
82.1
55.1
51.0
63.1
75.1
87.1
%
m/z

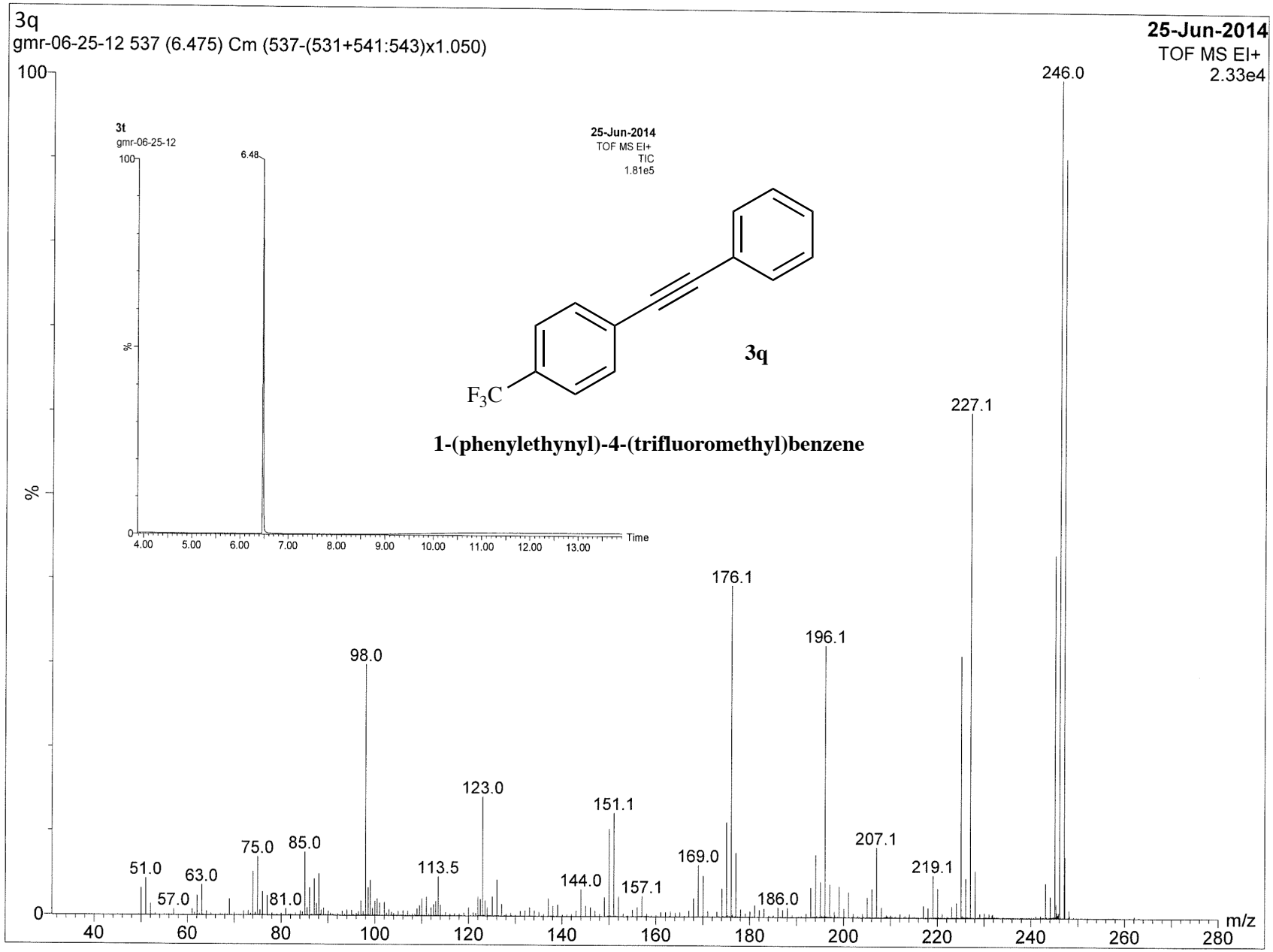


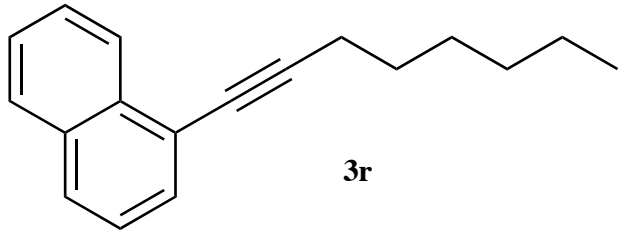


3q

1-(phenylethynyl)-4-(trifluoromethyl)benzene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.67–7.60 (m, 4H), 7.57–7.54 (m, 2H), 7.40–7.36 (m, 3H)

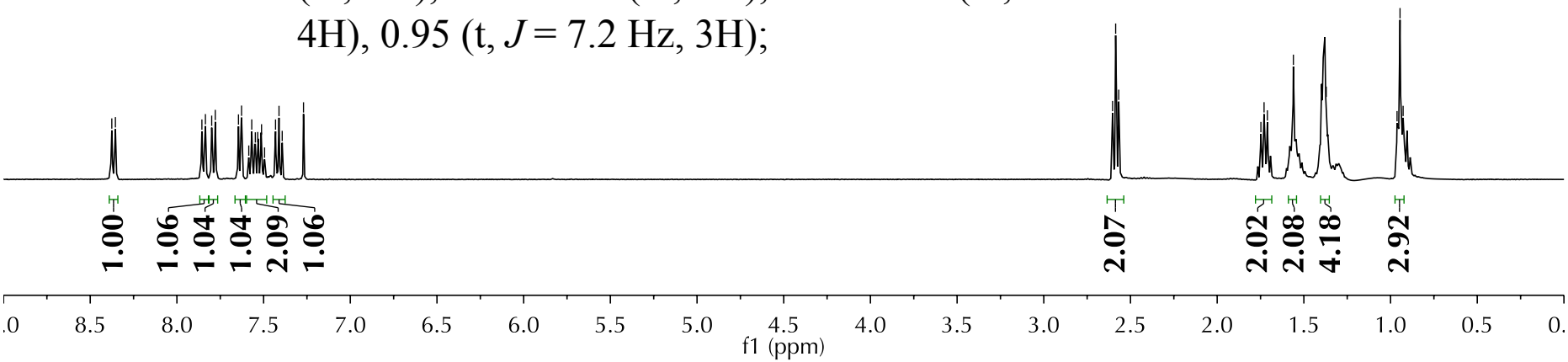

3q
gmr-06-25-12 537 (6.475) Cm (537-(531+541:543)x1.050)
25-Jun-2014
TOF MS EI+
2.33e4
246.0
227.1
176.1
196.1
98.0
123.0
151.1
207.1
169.0
219.1
75.0
85.0
51.0
63.0
57.0
81.0
113.5
144.0
157.1
186.0
m/z
%
3t
gmr-06-25-12
6.48
Time
25-Jun-2014
TOF MS EI+
TIC
1.81e5
F_3C
3q
1-(phenylethynyl)-4-(trifluoromethyl)benzene

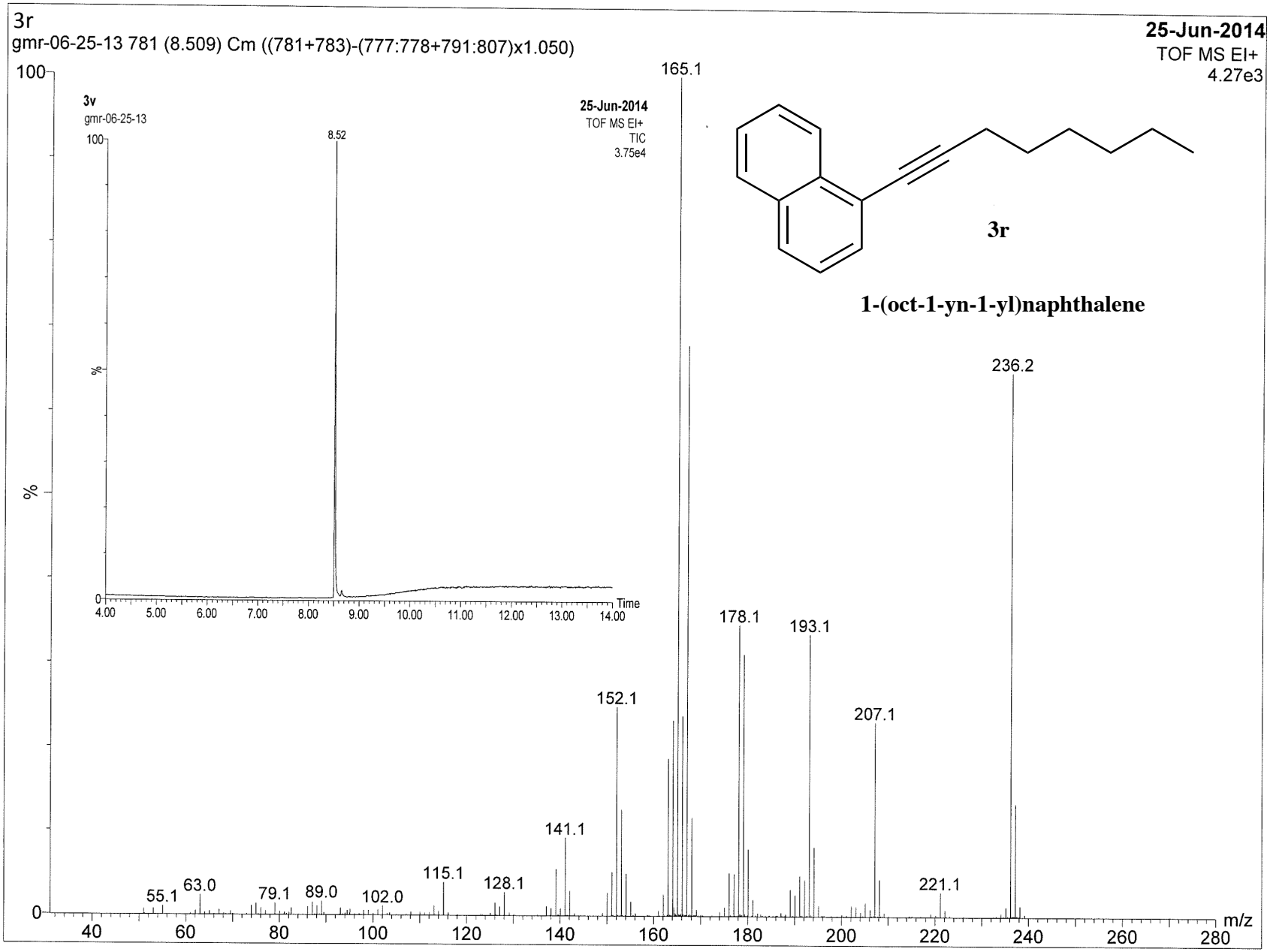


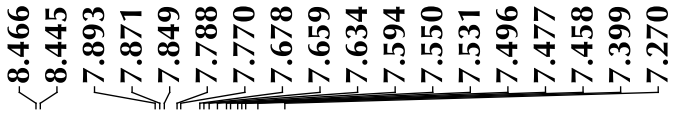
3r

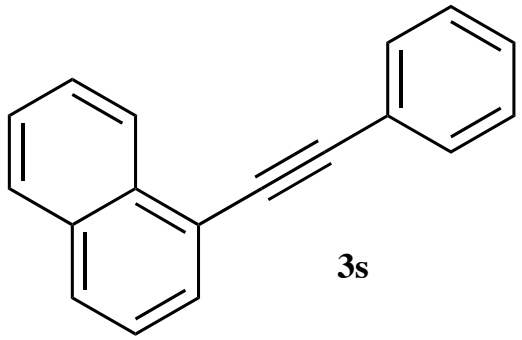
1-(oct-1-yn-1-yl)naphthalene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.36 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 7.2 Hz, 1H), 7.60–7.48 (m, 2H), 7.45–7.38 (m, 1H), 2.58 (t, *J* = 7.0 Hz, 2H), 1.78–1.67 (m, 2H), 1.61–1.55 (m, 2H), 1.42–1.35 (m, 4H), 0.95 (t, *J* = 7.2 Hz, 3H);




3r
gmr-06-25-13 781 (8.509) Cm ((781+783)-(777:778+791:807)x1.050)
25-Jun-2014
TOF MS EI+
4.27e3
3v
gmr-06-25-13
25-Jun-2014
TOF MS EI+
TIC
3.75e4
8.52
Time
3r
1-(oct-1-yn-1-yl)naphthalene
165.1
236.2
178.1
193.1
152.1
207.1
141.1
115.1
128.1
55.1
63.0
79.1
89.0
102.0
221.1
m/z

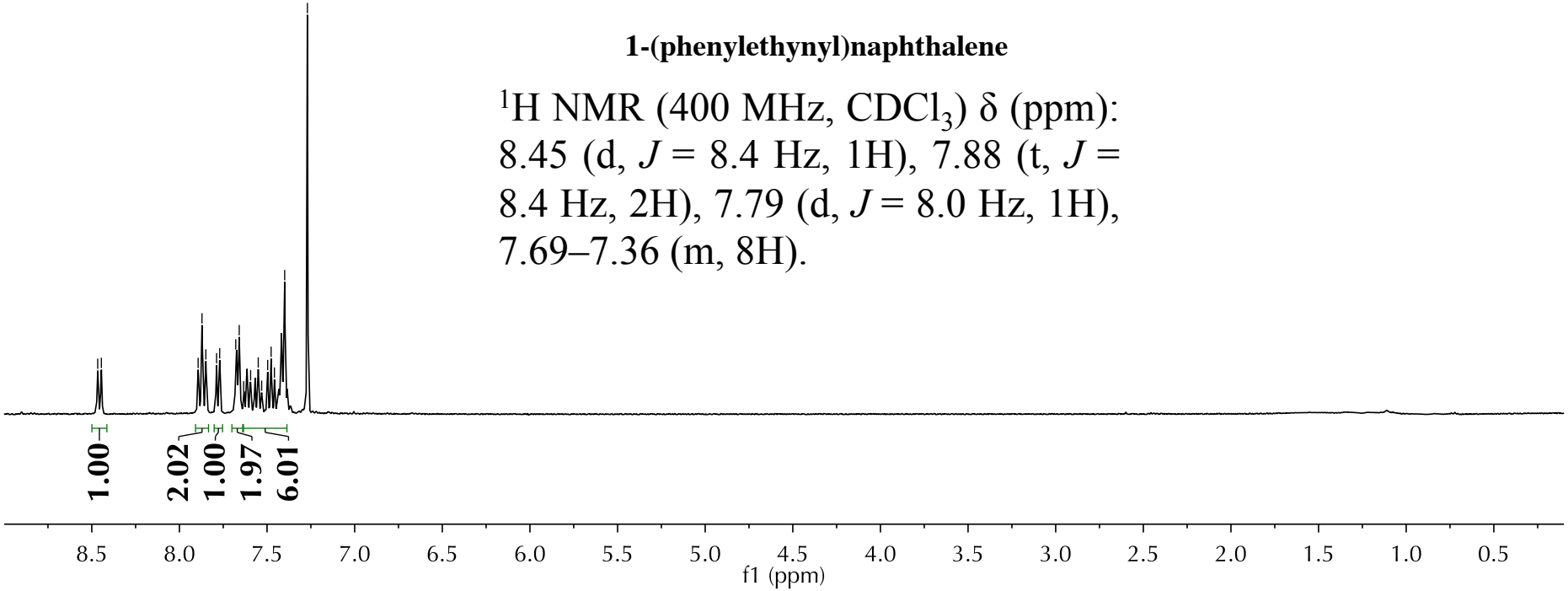


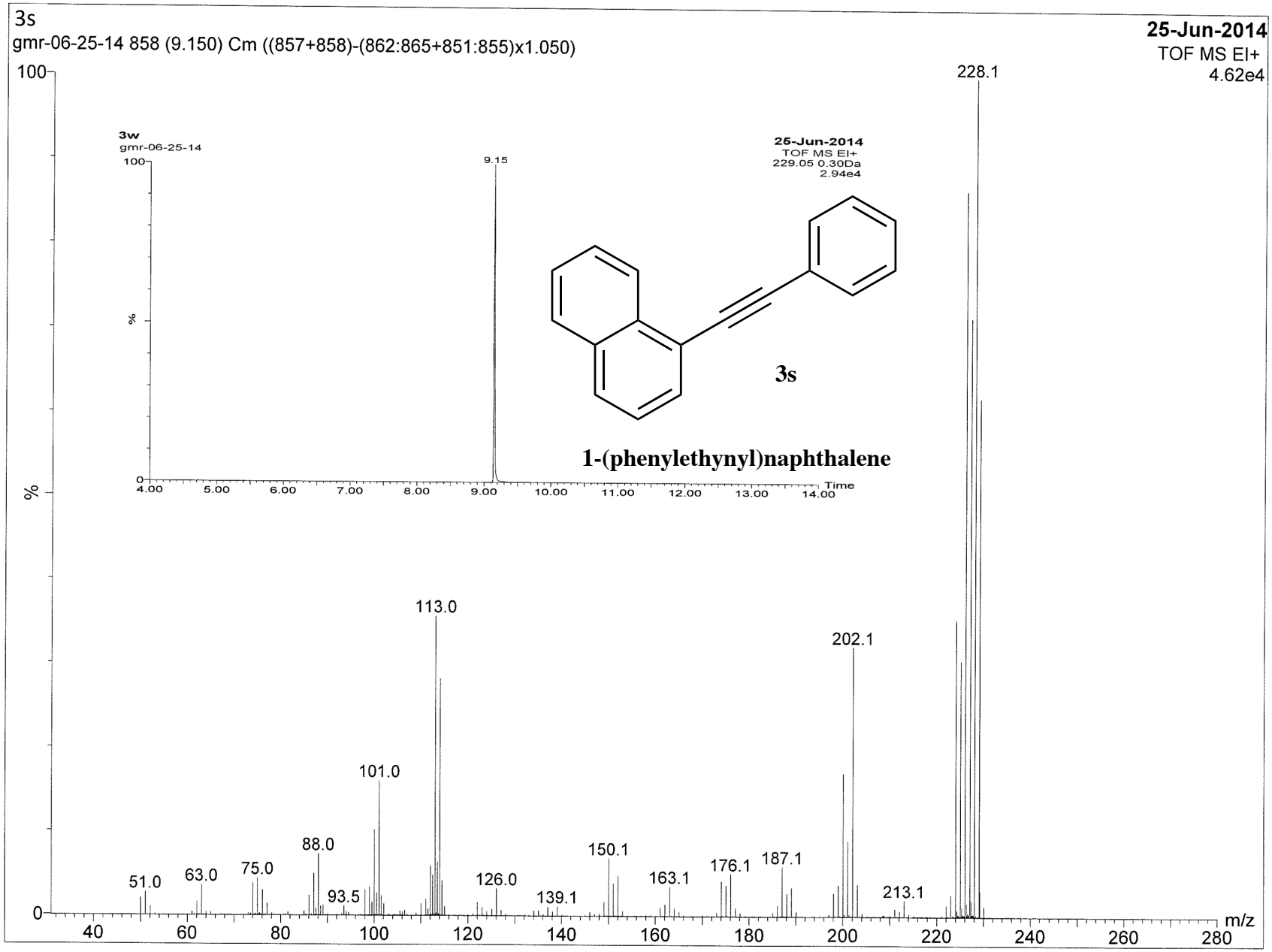


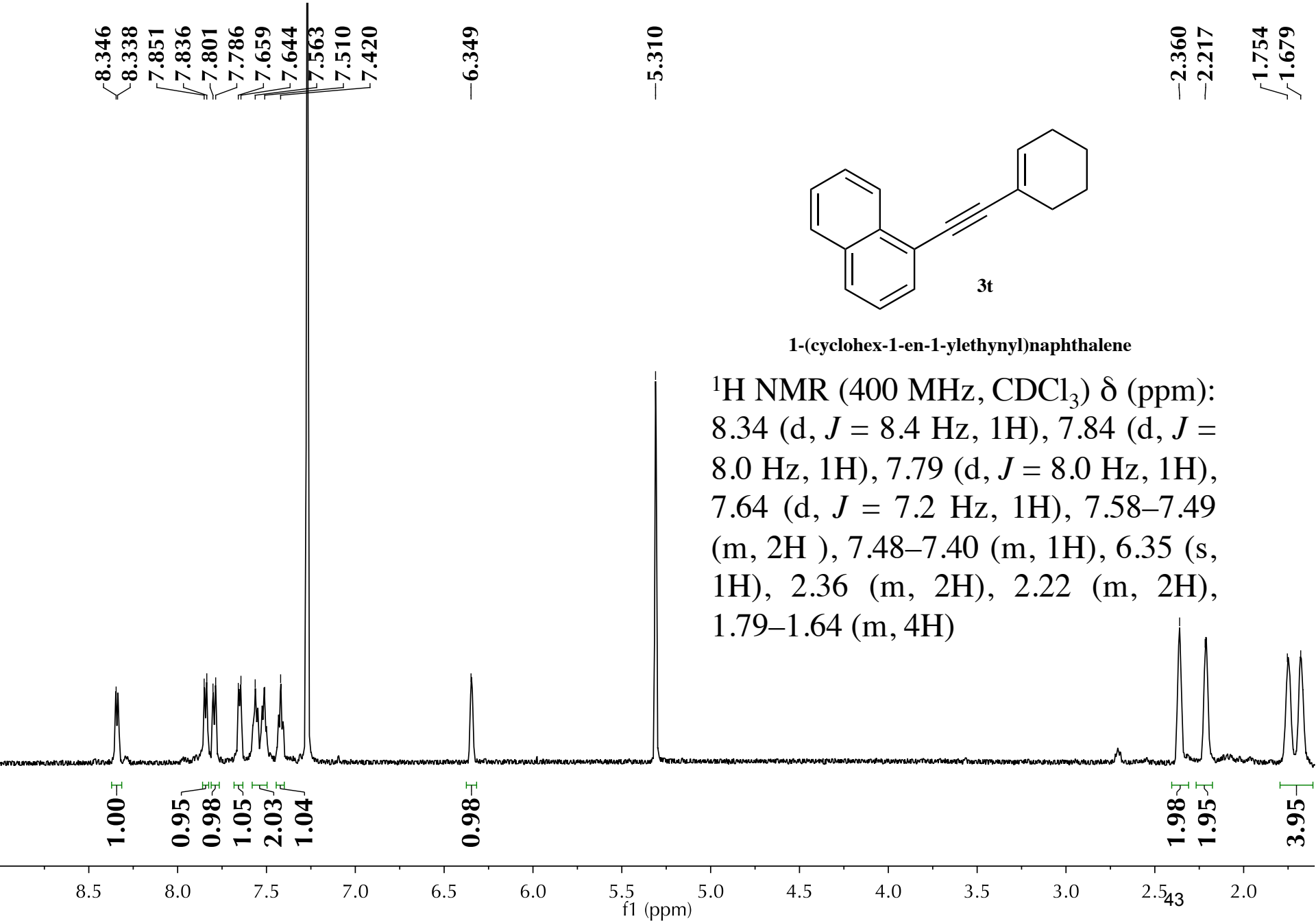
3s

1-(phenylethynyl)naphthalene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.45 (d, *J* = 8.4 Hz, 1H), 7.88 (t, *J* = 8.4 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.69–7.36 (m, 8H).



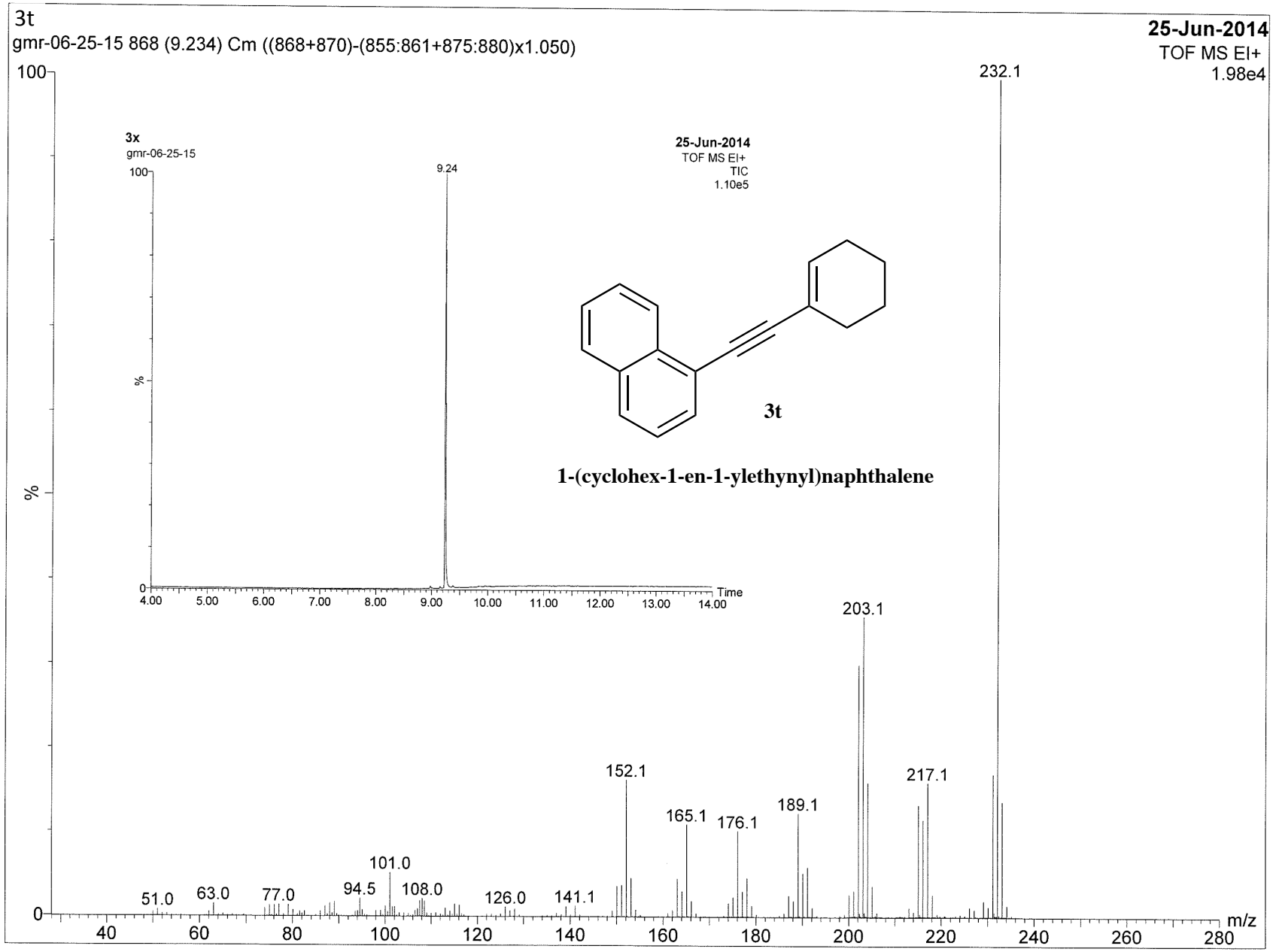

3s
gmr-06-25-14 858 (9.150) Cm ((857+858)-(862:865+851:855)x1.050)
25-Jun-2014
TOF MS EI+
4.62e4
228.1
3w
gmr-06-25-14
9.15
25-Jun-2014
TOF MS EI+
229.05 0.30Da
2.94e4
3s
1-(phenylethynyl)naphthalene
Time
%
m/z
113.0
202.1
101.0
88.0
150.1
51.0
63.0
75.0
93.5
126.0
139.1
163.1
176.1
187.1
213.1

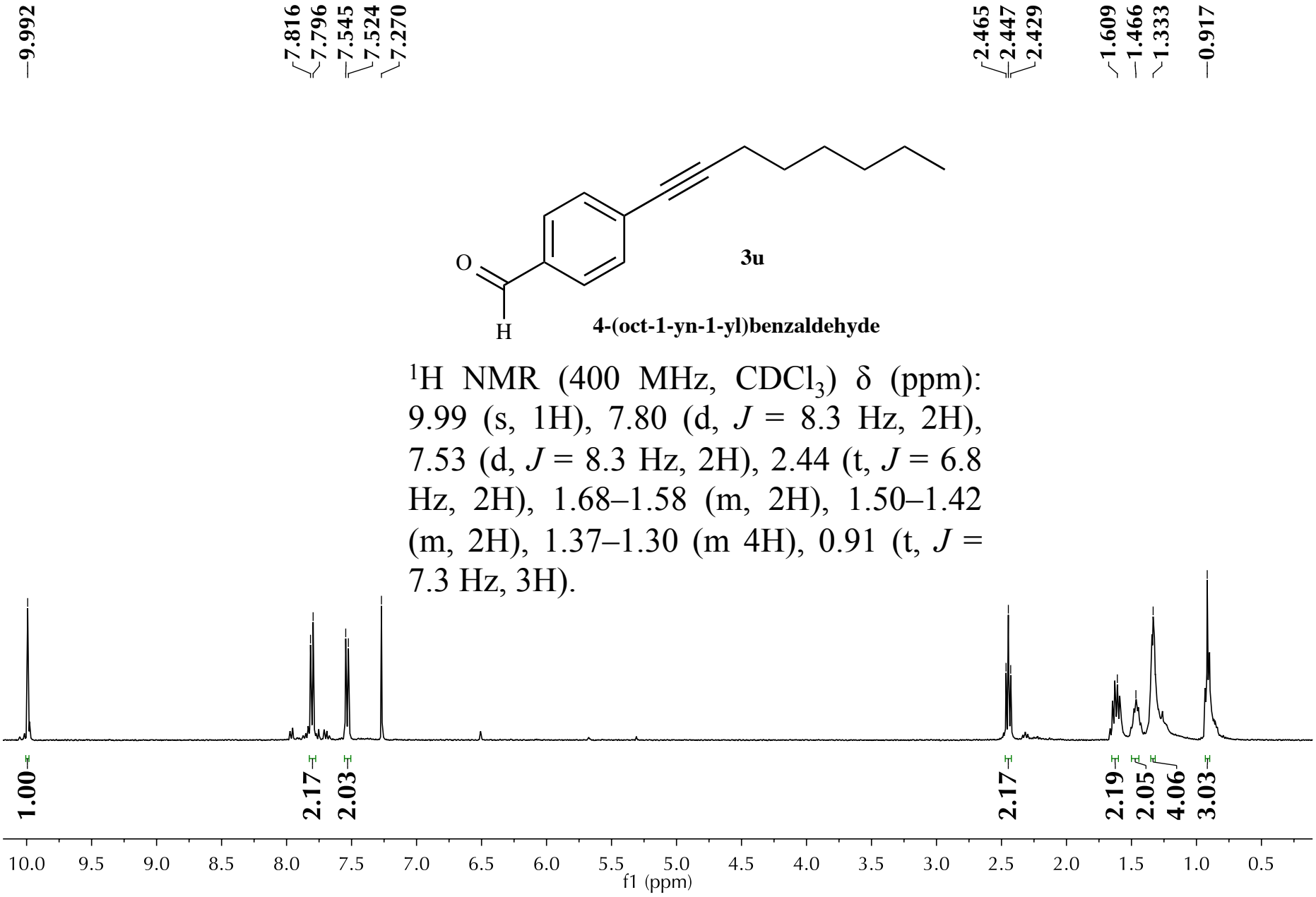


3t

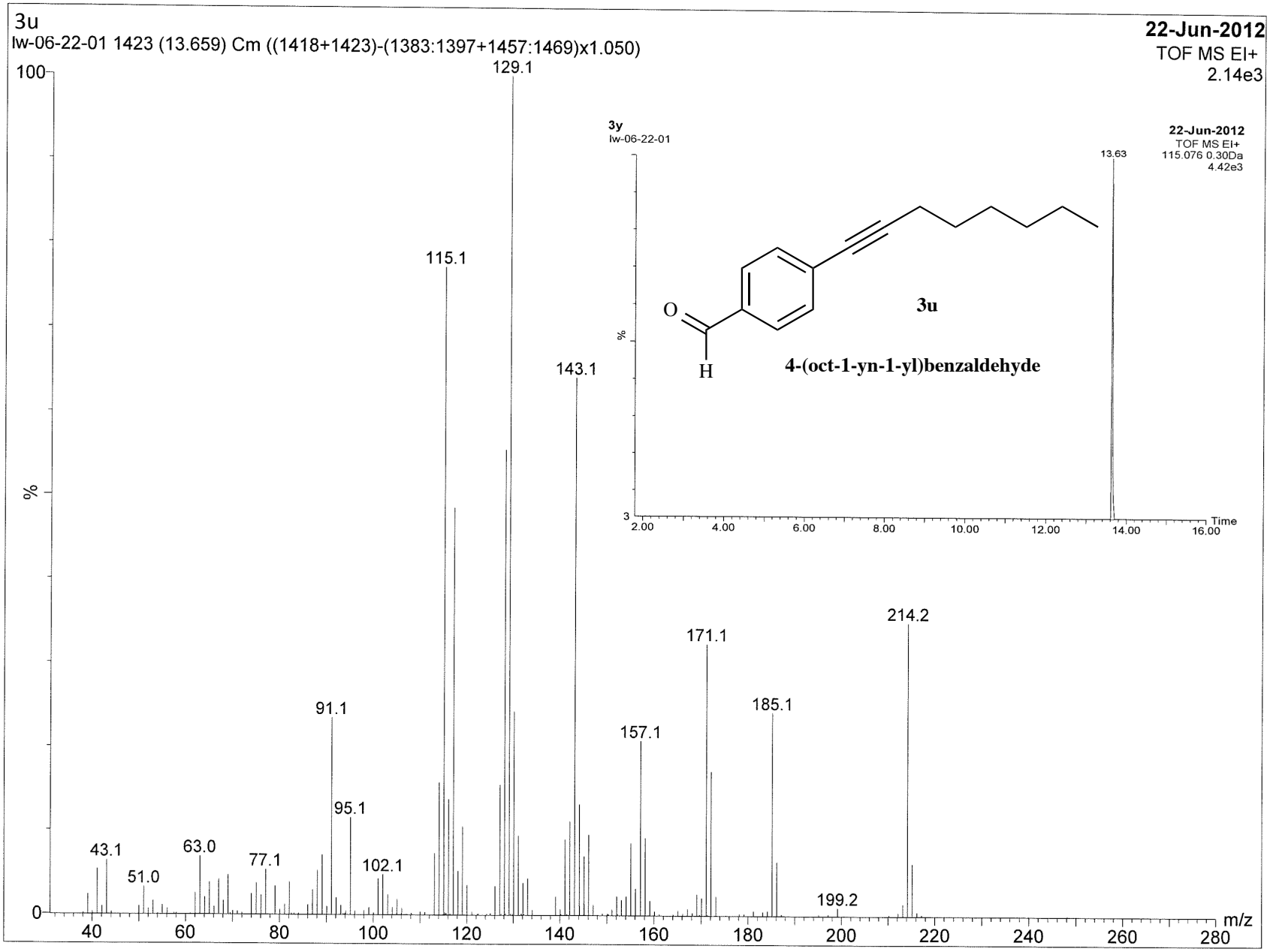
1-(cyclohex-1-en-1-ylethynyl)naphthalene

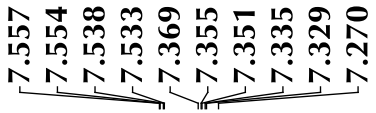
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.34 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.2 Hz, 1H), 7.58–7.49 (m, 2H), 7.48–7.40 (m, 1H), 6.35 (s, 1H), 2.36 (m, 2H), 2.22 (m, 2H), 1.79–1.64 (m, 4H)

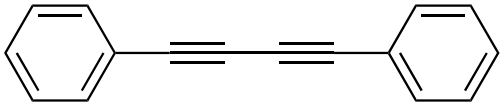

3t
gmr-06-25-15 868 (9.234) Cm ((868+870)-(855:861+875:880)x1.050)
25-Jun-2014
TOF MS EI+
1.98e4
232.1
3x
gmr-06-25-15
9.24
25-Jun-2014
TOF MS EI+
TIC
1.10e5
3t
1-(cyclohex-1-en-1-ylethynyl)naphthalene
Time
203.1
152.1
217.1
165.1
176.1
189.1
101.0
51.0
63.0
77.0
94.5
108.0
126.0
141.1
m/z



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.99 (s, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 2.44 (t, *J* = 6.8 Hz, 2H), 1.68–1.58 (m, 2H), 1.50–1.42 (m, 2H), 1.37–1.30 (m 4H), 0.91 (t, *J* = 7.3 Hz, 3H).


3u
lw-06-22-01 1423 (13.659) Cm ((1418+1423)-(1383:1397+1457:1469)x1.050)
22-Jun-2012
TOF MS EI+
2.14e3
100
%
0
129.1
115.1
143.1
91.1
95.1
43.1
63.0
51.0
77.1
102.1
157.1
171.1
185.1
214.2
199.2
40
60
80
100
120
140
160
180
200
220
240
260
280
m/z
3y
lw-06-22-01
22-Jun-2012
TOF MS EI+
115.076 0.30Da
4.42e3
13.63
3
%
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
Time
O
H
3u
4-(oct-1-yn-1-yl)benzaldehyde

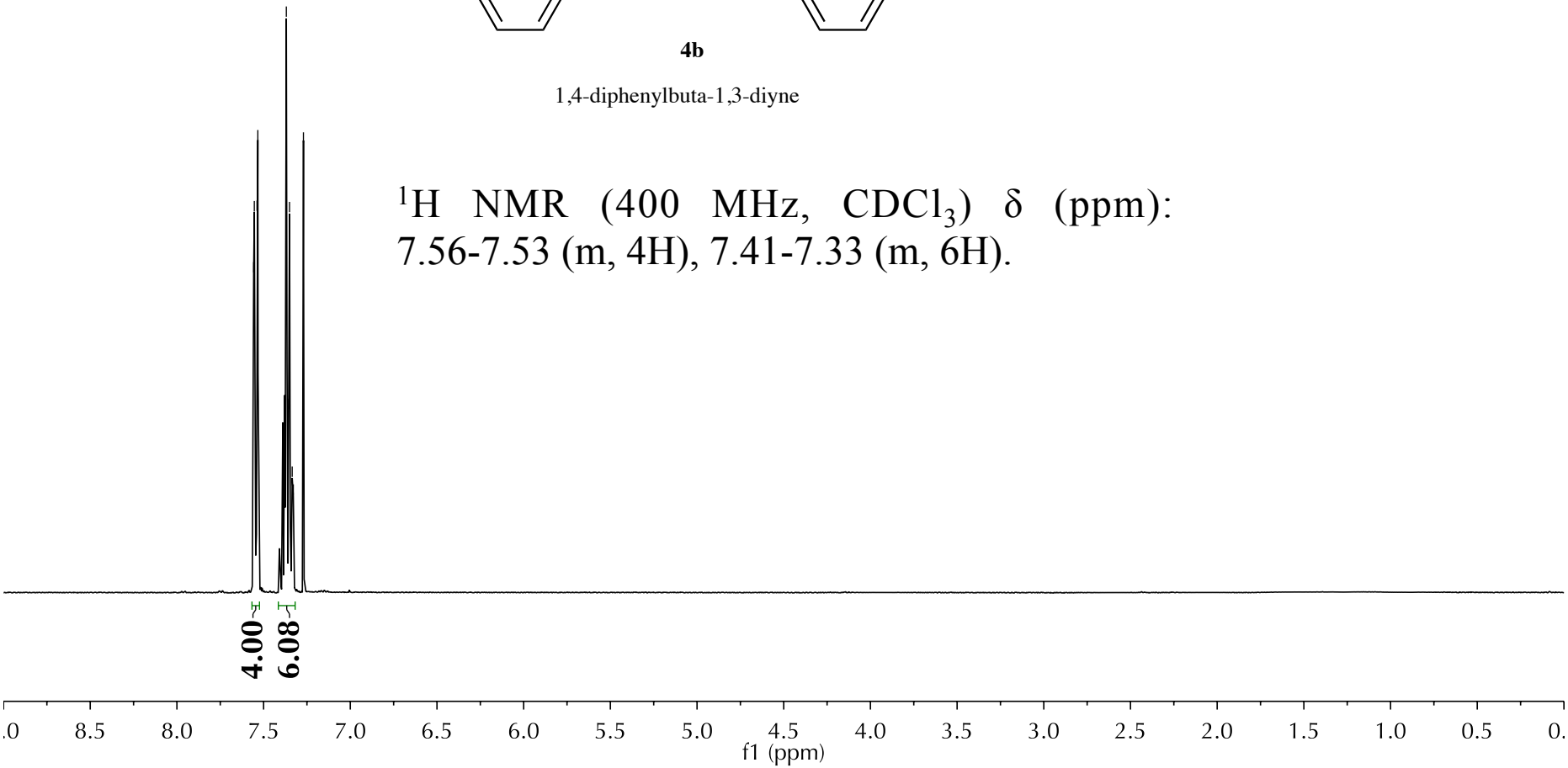


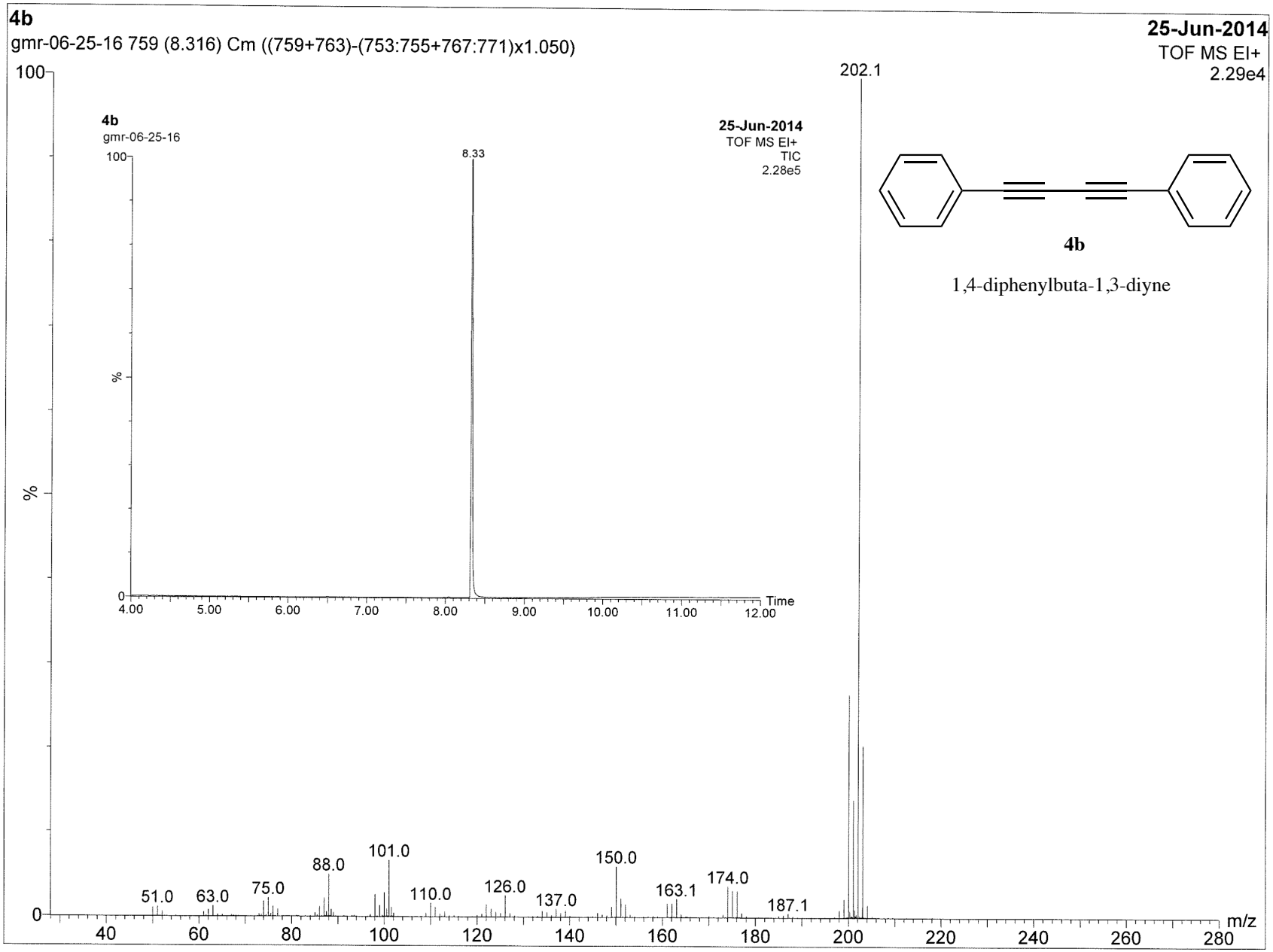


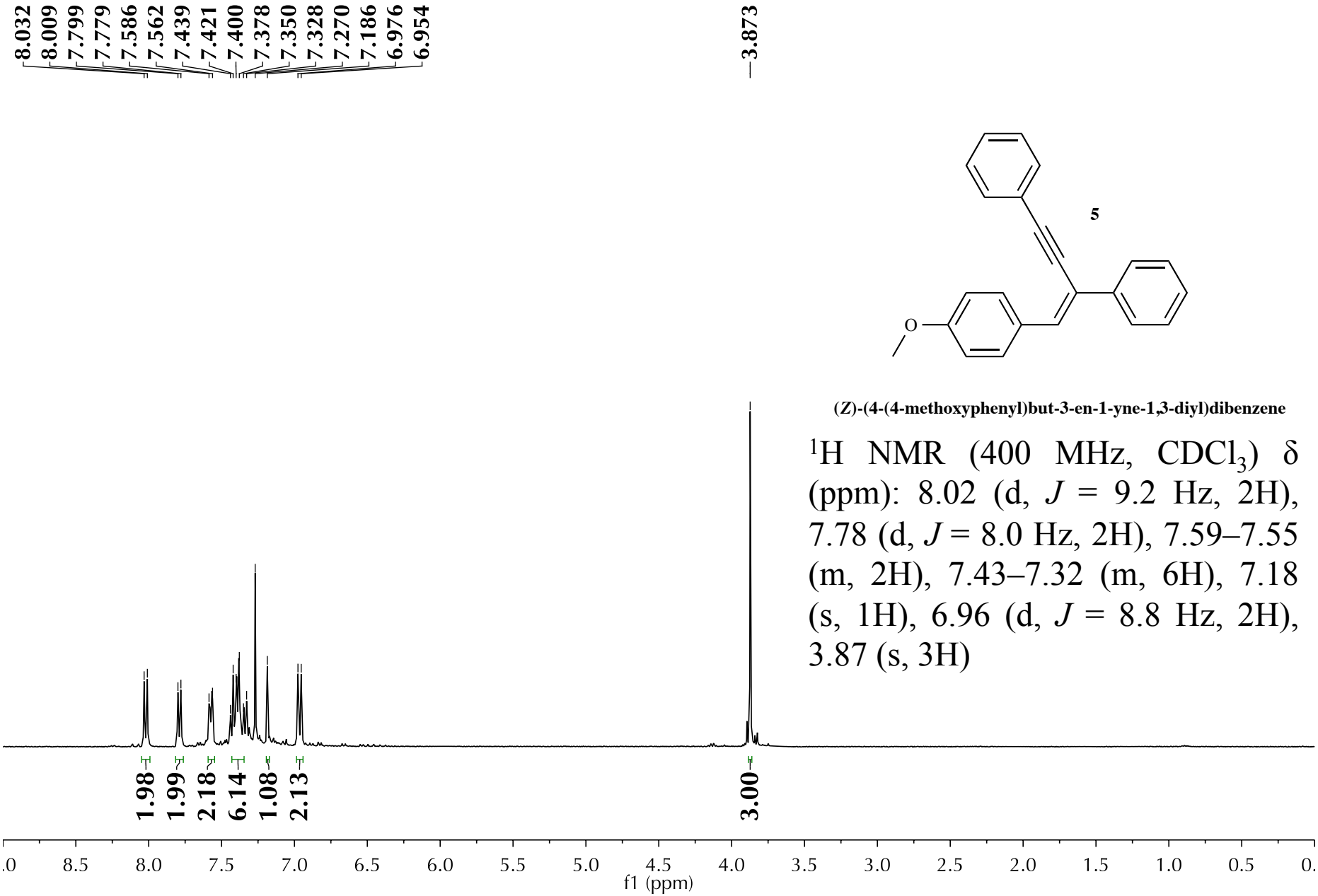
4b

1,4-diphenylbuta-1,3-diyne

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.56-7.53 (m, 4H), 7.41-7.33 (m, 6H).

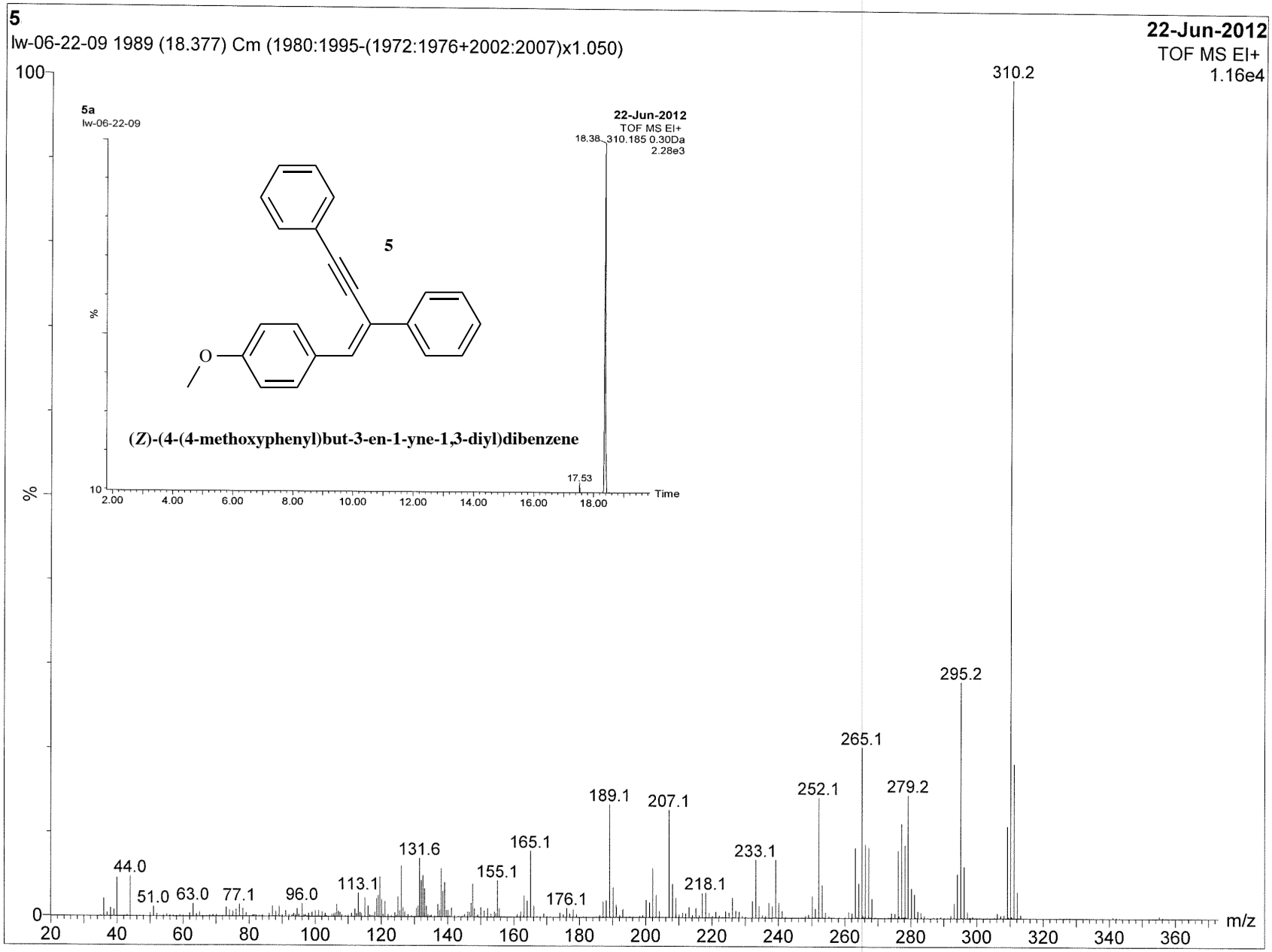



4b
gmr-06-25-16 759 (8.316) Cm ((759+763)-(753:755+767:771)x1.050)
25-Jun-2014
TOF MS EI+
2.29e4
202.1
4b
gmr-06-25-16
8.33
25-Jun-2014
TOF MS EI+
TIC
2.28e5
Time
4b
1,4-diphenylbuta-1,3-diyne
51.0
63.0
75.0
88.0
101.0
110.0
126.0
137.0
150.0
163.1
174.0
187.1
m/z



(*Z*)-(4-(4-methoxyphenyl)but-3-en-1-yne-1,3-diyl)dibenzene

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.02 (d, *J* = 9.2 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.59–7.55 (m, 2H), 7.43–7.32 (m, 6H), 7.18 (s, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H)


5
lw-06-22-09 1989 (18.377) Cm (1980:1995-(1972:1976+2002:2007)x1.050)
22-Jun-2012
TOF MS EI+
1.16e4
5a
lw-06-22-09
22-Jun-2012
TOF MS EI+
18.38 310.185 0.30Da
2.28e3
5
(Z)-(4-(4-methoxyphenyl)but-3-en-1-yne-1,3-diyl)dibenzene
17.53
Time
%
m/z
310.2
295.2
265.1
279.2
252.1
189.1
207.1
233.1
218.1
131.6
165.1
155.1
113.1
176.1
44.0
51.0
63.0
77.1
96.0