

## Electronic Supplementary Information

# **Fe<sub>3</sub>O<sub>4</sub>@MOF core-shell magnetic microspheres as excellent catalysts for the Claisen-Schmidt condensation reaction**

Fei Ke,<sup>ab</sup> Ling-Guang Qiu<sup>\*c</sup> and Junfa Zhu<sup>\*ab</sup>

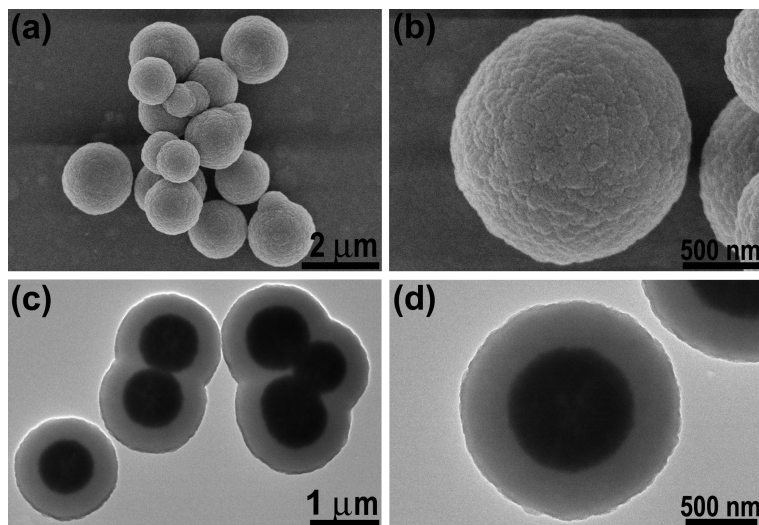
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**Fig. S1** SEM images (a,b) and TEM images (c,d) of the Fe<sub>3</sub>O<sub>4</sub>@MIL-100(Fe) core-shell magnetic catalysts after the catalytic reaction.

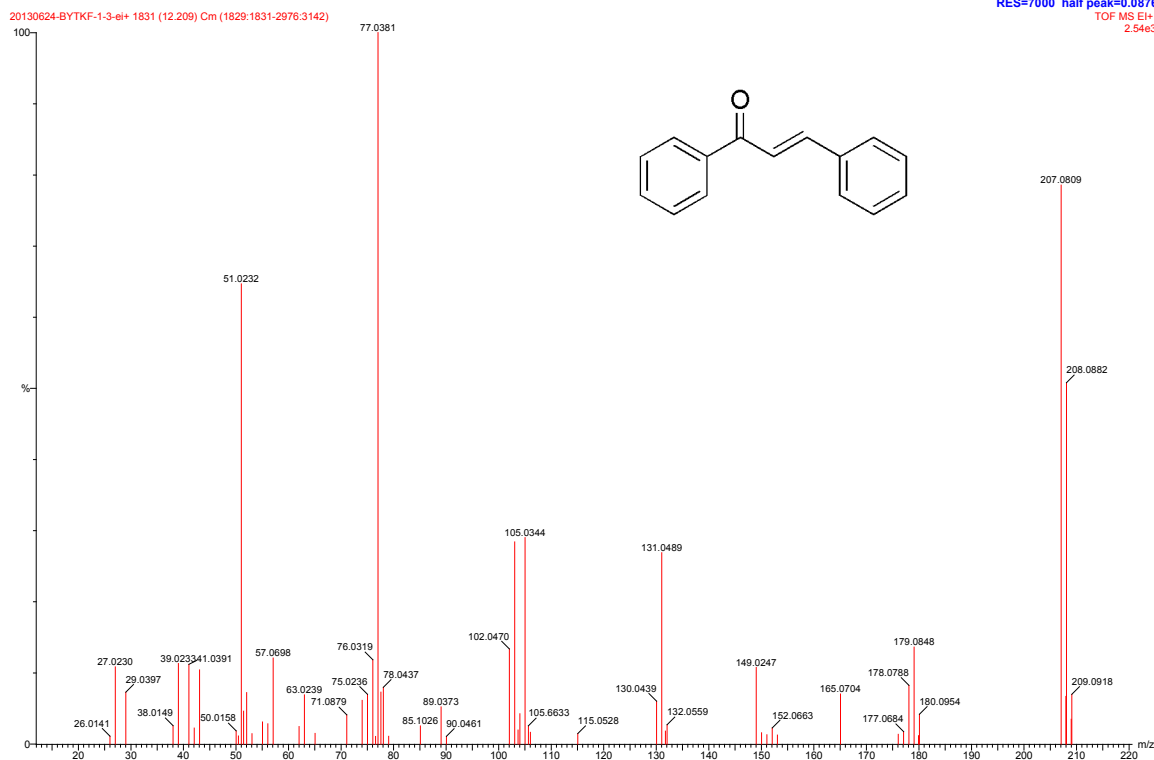
## GC-MS spectra for Chalcones

### 1. (*E*)-Chalcone, White solid.

Micromass GCT-MS

USTC-MASS CA064

24-Jun-2013 15:28:23  
 RES=7000 half peak=0.0876  
 TOF MS EI+  
 2.54e3



#### Elemental Composition Report

Multiple Mass Analysis: 61 mass(es) processed - displaying only valid results  
 Tolerance = 4.0 mDa / DBE: min = 0.0, max = 50.0

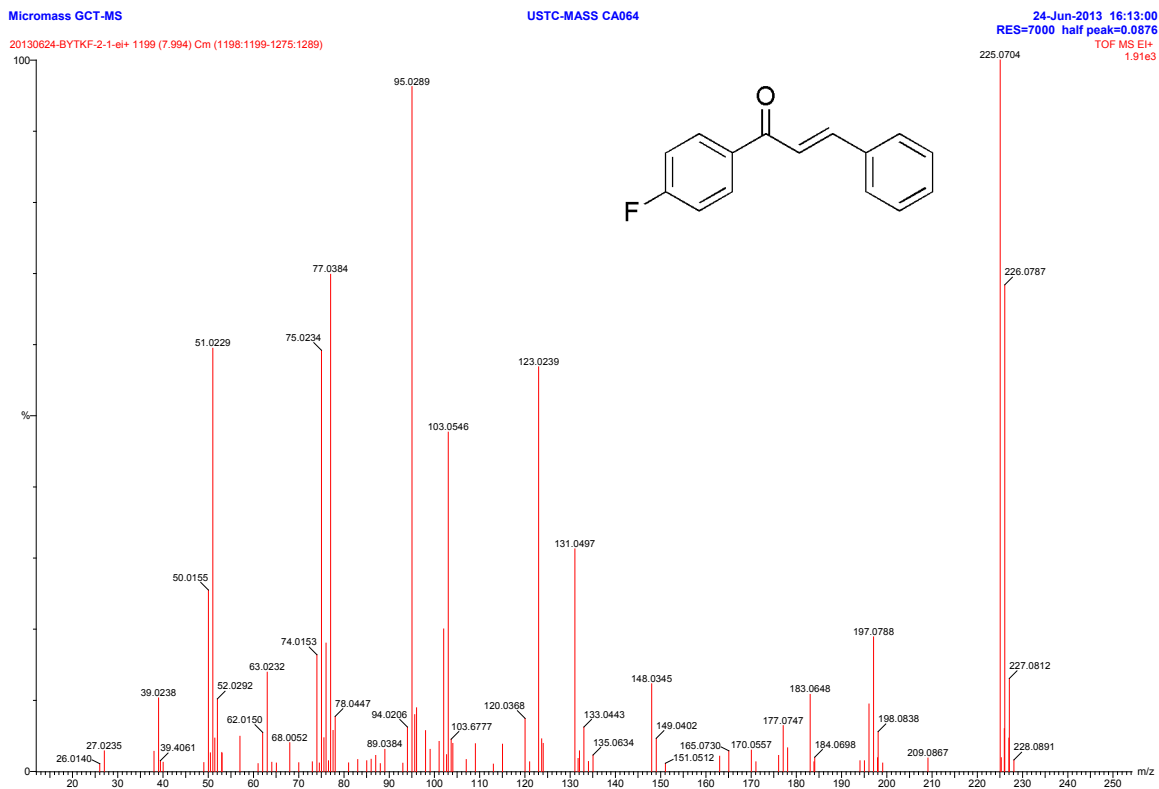
#### Monoisotopic Mass, Odd and Even Electron Ions

326 formula(e) evaluated with 46 results within limits (up to 50 closest results for each mass)

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
26.0141	1.06	26.0157	-1.6	-59.6	2.0	C <sub>2</sub> H <sub>2</sub>
27.0230	10.82	27.0235	-0.5	-17.6	1.5	C <sub>2</sub> H <sub>3</sub>
29.0397	7.26	29.0391	0.6	19.8	0.5	C <sub>2</sub> H <sub>5</sub>
38.0149	2.55	38.0157	-0.8	-19.7	3.0	C <sub>3</sub> H <sub>2</sub>
39.0233	11.29	39.0235	-0.2	-4.5	2.5	C <sub>3</sub> H <sub>3</sub>
41.0391	11.17	41.0391	0.0	-0.6	1.5	C <sub>3</sub> H <sub>5</sub>
42.0456	2.24	42.0470	-1.4	-32.1	1.0	C <sub>3</sub> H <sub>6</sub>
43.0537	10.39	43.0548	-1.1	-25.0	0.5	C <sub>3</sub> H <sub>7</sub>
50.0158	1.81	50.0157	0.1	3.0	4.0	C <sub>4</sub> H <sub>2</sub>
51.0232	64.64	51.0235	-0.3	-5.4	3.5	C <sub>4</sub> H <sub>3</sub>
52.0306	7.21	52.0313	-0.7	-13.5	3.0	C <sub>4</sub> H <sub>4</sub>
53.0391	1.44	53.0391	0.0	-0.5	2.5	C <sub>4</sub> H <sub>5</sub>
55.0557	3.07	55.0548	0.9	16.8	1.5	C <sub>4</sub> H <sub>7</sub>
56.0624	2.83	56.0626	-0.2	-3.6	1.0	C <sub>4</sub> H <sub>8</sub>
57.0698	12.06	57.0704	-0.6	-11.0	0.5	C <sub>4</sub> H <sub>9</sub>
62.0169	2.44	62.0157	1.2	20.2	5.0	C <sub>5</sub> H <sub>2</sub>

63.0239	6.88	63.0235	0.4	6.7	4.5	C <sub>5</sub> H <sub>3</sub>
65.0399	1.48	65.0391	0.8	11.9	3.5	C <sub>5</sub> H <sub>5</sub>
71.0879	4.07	71.0861	1.8	25.7	0.5	C <sub>5</sub> H <sub>11</sub>
74.0154	6.11	74.0157	-0.3	-3.4	6.0	C <sub>6</sub> H <sub>2</sub>
75.0236	6.96	75.0235	0.1	1.7	5.5	C <sub>6</sub> H <sub>3</sub>
76.0319	11.82	76.0313	0.6	7.9	5.0	C <sub>6</sub> H <sub>4</sub>
77.0381	100.00	77.0391	-1.0	-13.3	4.5	C <sub>6</sub> H <sub>5</sub>
78.0437	7.93	78.0470	-3.3	-41.6	4.0	C <sub>6</sub> H <sub>6</sub>
79.0532	1.08	79.0548	-1.6	-19.9	3.5	C <sub>6</sub> H <sub>7</sub>
85.1026	2.51	85.1017	0.9	10.3	0.5	C <sub>6</sub> H <sub>13</sub>
89.0373	5.19	89.0391	-1.8	-20.5	5.5	C <sub>7</sub> H <sub>5</sub>
90.0461	1.04	90.0470	-0.9	-9.4	5.0	C <sub>7</sub> H <sub>6</sub>
102.0470	13.33	102.0470	0.0	0.5	6.0	C <sub>8</sub> H <sub>6</sub>
103.0556	28.39	103.0548	0.8	8.0	5.5	C <sub>8</sub> H <sub>7</sub>
105.0344	28.99	105.0340	0.4	3.4	5.5	C <sub>7</sub> H <sub>5</sub> O
115.0528	1.44	115.0548	-2.0	-17.2	6.5	C <sub>9</sub> H <sub>7</sub>
130.0439	6.00	130.0419	2.0	15.6	7.0	C <sub>9</sub> H <sub>6</sub> O
131.0489	26.88	131.0497	-0.8	-6.0	6.5	C <sub>9</sub> H <sub>7</sub> O
132.0559	2.68	132.0575	-1.6	-12.2	6.0	C <sub>9</sub> H <sub>8</sub> O
151.0583	1.28	151.0548	3.5	23.3	9.5	C <sub>12</sub> H <sub>7</sub>
152.0663	2.24	152.0626	3.7	24.3	9.0	C <sub>12</sub> H <sub>8</sub>
153.0665	1.24	153.0704	-3.9	-25.6	8.5	C <sub>12</sub> H <sub>9</sub>
165.0704	7.03	165.0704	0.0	-0.2	9.5	C <sub>13</sub> H <sub>9</sub>
176.0600	1.36	176.0626	-2.6	-14.8	11.0	C <sub>14</sub> H <sub>8</sub>
177.0684	1.72	177.0704	-2.0	-11.4	10.5	C <sub>14</sub> H <sub>9</sub>
178.0788	8.21	178.0783	0.5	3.1	10.0	C <sub>14</sub> H <sub>10</sub>
179.0848	13.60	179.0861	-1.3	-7.1	9.5	C <sub>14</sub> H <sub>11</sub>
180.0954	4.15	180.0939	1.5	8.3	9.0	C <sub>14</sub> H <sub>12</sub>
207.0809	78.56	207.0810	-0.1	-0.4	10.5	C <sub>15</sub> H <sub>11</sub> O
208.0882	50.73	208.0888	-0.6	-3.0	10.0	C <sub>15</sub> H <sub>12</sub> O

2. (*E*)-1-(4-Fluorophenyl)-3-phenylprop-2-en-1-one, White solid.



### Elemental Composition Report

Multiple Mass Analysis: 95 mass(es) processed - displaying only valid results  
 Tolerance = 4.0 mDa / DBE: min = 0.0, max = 50.0

### Monoisotopic Mass, Odd and Even Electron Ions

976 formula(e) evaluated with 66 results within limits (up to 50 closest results for each mass)

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
26.0140	1.05	26.0157	-1.7	-63.4	2.0	C <sub>2</sub> H <sub>2</sub>
27.0235	2.88	27.0235	0.0	0.9	1.5	C <sub>2</sub> H <sub>3</sub>
38.0155	2.81	38.0157	-0.2	-3.9	3.0	C <sub>3</sub> H <sub>2</sub>
39.0238	10.31	39.0235	0.3	8.3	2.5	C <sub>3</sub> H <sub>3</sub>
40.0282	1.27	40.0313	-3.1	-77.4	2.0	C <sub>3</sub> H <sub>4</sub>
49.0080	1.22	49.0078	0.2	3.6	4.5	C <sub>4</sub> H
50.0155	25.47	50.0157	-0.2	-3.0	4.0	C <sub>4</sub> H <sub>2</sub>
51.0229	59.45	51.0235	-0.6	-11.3	3.5	C <sub>4</sub> H <sub>3</sub>
52.0292	10.16	52.0313	-2.1	-40.4	3.0	C <sub>4</sub> H <sub>4</sub>
53.0041	2.65	53.0027	1.4	25.7	3.5	C <sub>3</sub> HO
53.0398	2.49	53.0391	0.7	12.7	2.5	C <sub>4</sub> H <sub>5</sub>
57.0143	4.93	57.0141	0.2	4.3	2.5	C <sub>3</sub> H <sub>2</sub> F
61.0069	1.06	61.0078	-0.9	-15.2	5.5	C <sub>5</sub> H
62.0150	5.46	62.0157	-0.7	-10.5	5.0	C <sub>5</sub> H <sub>2</sub>
63.0232	13.93	63.0235	-0.3	-4.4	4.5	C <sub>5</sub> H <sub>3</sub>
64.0346	1.27	64.0324	2.2	33.7	0.0	C <sub>2</sub> H <sub>5</sub> OF
65.0424	1.17	65.0391	3.3	50.3	3.5	C <sub>5</sub> H <sub>5</sub>
68.0052	4.03	68.0062	-1.0	-15.1	4.0	C <sub>4</sub> HF
73.0075	1.33	73.0078	-0.3	-4.5	6.5	C <sub>6</sub> H
74.0153	16.37	74.0157	-0.4	-4.7	6.0	C <sub>6</sub> H <sub>2</sub>

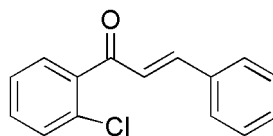
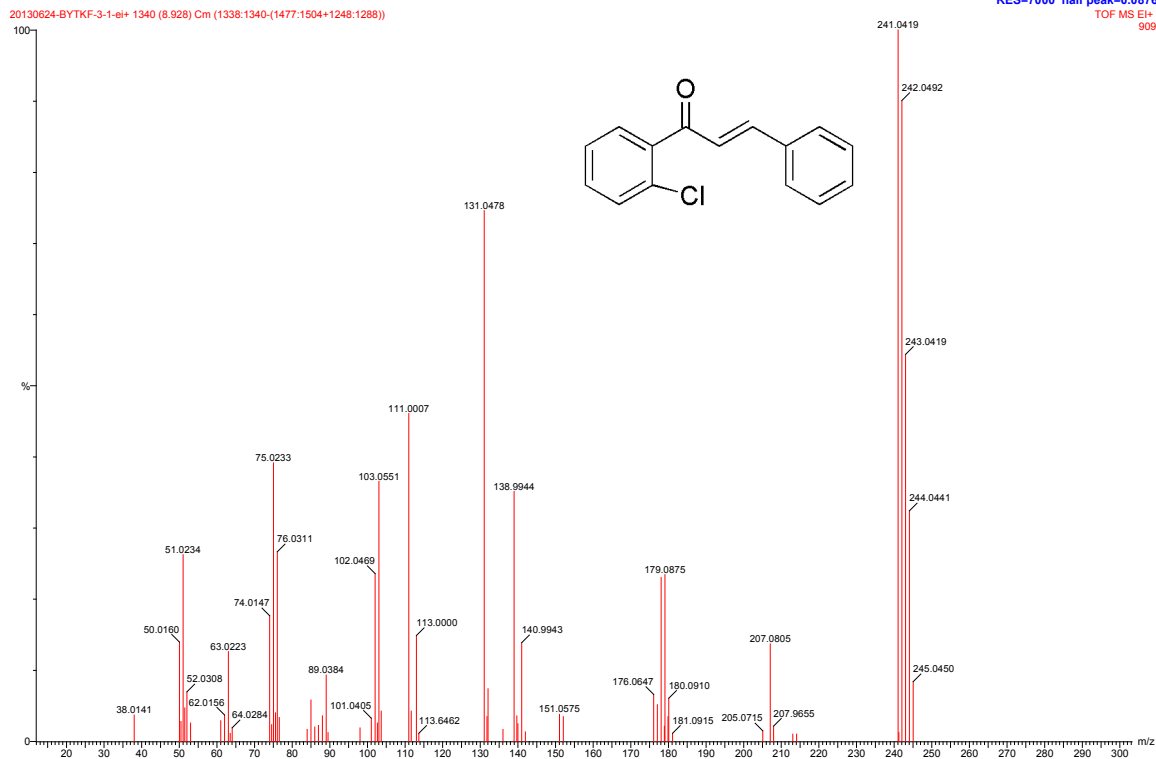
75.0234	59.18	75.0235	-0.1	-1.0	5.5	C <sub>6</sub> H <sub>3</sub>
76.0313	18.01	76.0313	0.0	0.0	5.0	C <sub>6</sub> H <sub>4</sub>
77.0384	69.86	77.0391	-0.7	-9.4	4.5	C <sub>6</sub> H <sub>5</sub>
78.0447	7.71	78.0470	-2.3	-28.8	4.0	C <sub>6</sub> H <sub>6</sub>
81.0135	1.18	81.0141	-0.6	-6.8	4.5	C <sub>5</sub> H <sub>2</sub> F
83.0310	1.64	83.0297	1.3	15.6	3.5	C <sub>5</sub> H <sub>4</sub> F
86.0165	1.70	86.0168	-0.3	-3.4	3.0	C <sub>4</sub> H <sub>3</sub> OF
87.0219	2.23	87.0235	-1.6	-18.1	6.5	C <sub>7</sub> H <sub>3</sub>
88.0291	1.06	88.0313	-2.2	-25.0	6.0	C <sub>7</sub> H <sub>4</sub>
89.0384	3.07	89.0391	-0.7	-8.1	5.5	C <sub>7</sub> H <sub>5</sub>
93.0126	1.13	93.0141	-1.5	-15.6	5.5	C <sub>6</sub> H <sub>2</sub> F
94.0206	6.20	94.0219	-1.3	-13.6	5.0	C <sub>6</sub> H <sub>3</sub> F
95.0289	96.23	95.0297	-0.8	-8.5	4.5	C <sub>6</sub> H <sub>4</sub> F
96.0339	8.91	96.0375	-3.6	-37.8	4.0	C <sub>6</sub> H <sub>5</sub> F
101.0407	4.19	101.0403	0.4	4.3	2.5	C <sub>5</sub> H <sub>6</sub> OF
102.0464	20.01	102.0470	-0.6	-5.4	6.0	C <sub>8</sub> H <sub>6</sub>
103.0546	47.67	103.0548	-0.2	-1.7	5.5	C <sub>8</sub> H <sub>7</sub>
107.0299	1.64	107.0297	0.2	1.8	5.5	C <sub>7</sub> H <sub>4</sub> F
109.0440	3.87	109.0454	-1.4	-12.4	4.5	C <sub>7</sub> H <sub>6</sub> F
113.0367	1.01	113.0391	-2.4	-21.5	7.5	C <sub>9</sub> H <sub>5</sub>
115.0544	3.82	115.0548	-0.4	-3.3	6.5	C <sub>9</sub> H <sub>7</sub>
120.0368	7.42	120.0375	-0.7	-6.1	6.0	C <sub>8</sub> H <sub>5</sub> F
121.0440	1.32	121.0454	-1.4	-11.2	5.5	C <sub>8</sub> H <sub>6</sub> F
123.0239	56.83	123.0235	0.4	3.5	9.5	C <sub>10</sub> H <sub>3</sub>
131.0497	31.27	131.0497	0.0	0.1	6.5	C <sub>9</sub> H <sub>7</sub> O
133.0443	6.20	133.0454	-1.1	-7.9	6.5	C <sub>9</sub> H <sub>6</sub> F
134.0551	1.38	134.0532	1.9	14.3	6.0	C <sub>9</sub> H <sub>7</sub> F
135.0634	2.28	135.0610	2.4	17.7	5.5	C <sub>9</sub> H <sub>8</sub> F
148.0345	12.31	148.0324	2.1	13.9	7.0	C <sub>9</sub> H <sub>5</sub> OF
149.0402	4.61	149.0403	-0.1	-0.5	6.5	C <sub>9</sub> H <sub>6</sub> OF
151.0512	1.11	151.0548	-3.6	-23.7	9.5	C <sub>12</sub> H <sub>7</sub>
163.0539	2.12	163.0548	-0.9	-5.4	10.5	C <sub>13</sub> H <sub>7</sub>
165.0730	2.87	165.0716	1.4	8.7	5.5	C <sub>10</sub> H <sub>10</sub> OF
170.0557	2.97	170.0532	2.5	14.8	9.0	C <sub>12</sub> H <sub>7</sub> F
176.0663	2.23	176.0637	2.6	14.5	7.0	C <sub>11</sub> H <sub>9</sub> OF
177.0747	6.41	177.0716	3.1	17.7	6.5	C <sub>11</sub> H <sub>10</sub> OF
178.0804	3.29	178.0794	1.0	5.7	6.0	C <sub>11</sub> H <sub>11</sub> OF
183.0648	10.80	183.0610	3.8	20.7	9.5	C <sub>13</sub> H <sub>8</sub> F
184.0698	1.96	184.0688	1.0	5.3	9.0	C <sub>13</sub> H <sub>9</sub> F
194.0539	1.48	194.0532	0.7	3.7	11.0	C <sub>14</sub> H <sub>7</sub> F
195.0600	1.48	195.0610	-1.0	-5.1	10.5	C <sub>14</sub> H <sub>8</sub> F
196.0704	9.46	196.0688	1.6	8.0	10.0	C <sub>14</sub> H <sub>9</sub> F
197.0788	18.89	197.0767	2.1	10.9	9.5	C <sub>14</sub> H <sub>10</sub> F
198.0838	5.57	198.0845	-0.7	-3.4	9.0	C <sub>14</sub> H <sub>11</sub> F
225.0704	100.00	225.0716	-1.2	-5.2	10.5	C <sub>15</sub> H <sub>10</sub> OF
226.0787	68.34	226.0794	-0.7	-3.1	10.0	C <sub>15</sub> H <sub>11</sub> OF

3. (*E*)-1-(2-Chlorophenyl)-3-phenylprop-2-en-1-one, White solid.

Micromass GCT-MS

USTC-MASS CA064

24-Jun-2013 16:37:30  
 RES=7000 half peak=0.0876  
 TOF MS EI+  
 909



### Elemental Composition Report

Multiple Mass Analysis: 65 mass(es) processed - displaying only valid results  
 Tolerance = 4.0 mDa / DBE: min = 0.0, max = 50.0

### Monoisotopic Mass, Odd and Even Electron Ions

1128 formula(e) evaluated with 38 results within limits (up to 50 closest results for each mass)

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
38.0141	3.68	38.0157	-1.6	-40.8	3.0	C <sub>3</sub> H <sub>2</sub>
50.0160	13.94	50.0157	0.3	7.0	4.0	C <sub>4</sub> H <sub>2</sub>
51.0234	26.23	51.0235	-0.1	-1.5	3.5	C <sub>4</sub> H <sub>3</sub>
52.0308	6.94	52.0313	-0.5	-9.6	3.0	C <sub>4</sub> H <sub>4</sub>
53.0050	2.56	53.0027	2.3	42.6	3.5	C <sub>3</sub> HO
62.0156	3.68	62.0157	-0.1	-0.8	5.0	C <sub>5</sub> H <sub>2</sub>
63.0223	12.61	63.0235	-1.2	-18.6	4.5	C <sub>5</sub> H <sub>3</sub>
64.0284	1.89	64.0313	-2.9	-45.3	4.0	C <sub>5</sub> H <sub>4</sub>
74.0147	17.63	74.0157	-1.0	-12.8	6.0	C <sub>6</sub> H <sub>2</sub>
75.0233	39.13	75.0235	-0.2	-2.3	5.5	C <sub>6</sub> H <sub>3</sub>
76.0311	26.62	76.0313	-0.2	-2.6	5.0	C <sub>6</sub> H <sub>4</sub>
84.9840	5.79	84.9845	-0.5	-5.9	3.5	C <sub>4</sub> H <sub>2</sub> <sup>35</sup> Cl
86.9820	2.23	86.9816	0.4	5.1	3.5	C <sub>4</sub> H <sub>2</sub> <sup>37</sup> Cl
88.0309	3.57	88.0313	-0.4	-4.5	6.0	C <sub>7</sub> H <sub>4</sub>
89.0384	9.30	89.0391	-0.7	-8.1	5.5	C <sub>7</sub> H <sub>5</sub>
101.0405	3.24	101.0391	1.4	13.6	6.5	C <sub>8</sub> H <sub>5</sub>
102.0469	23.55	102.0470	-0.1	-0.5	6.0	C <sub>8</sub> H <sub>6</sub>
103.0551	36.53	103.0548	0.3	3.2	5.5	C <sub>8</sub> H <sub>7</sub>
111.0007	46.07	111.0002	0.5	4.9	4.5	C <sub>6</sub> H <sub>4</sub> <sup>35</sup> Cl
113.0000	14.84	113.0027	-2.7	-24.2	8.5	C <sub>8</sub> HO

131.0478	74.59	131.0497	-1.9	-14.4	6.5	C <sub>9</sub> H <sub>7</sub> O
132.0503	7.38	132.0520	-1.7	-12.7	2.0	C <sub>7</sub> H <sub>11</sub> <sup>37</sup> Cl
138.9944	35.11	138.9951	-0.7	-4.8	5.5	C <sub>7</sub> H <sub>4</sub> O <sup>35</sup> Cl
139.9992	2.45	139.9974	1.8	13.2	1.0	C <sub>5</sub> H <sub>8</sub> <sup>35</sup> Cl <sup>37</sup> Cl
140.9943	13.84	140.9921	2.2	15.5	5.5	C <sub>7</sub> H <sub>4</sub> O <sup>37</sup> Cl
141.9962	1.34	141.9999	-3.7	-26.4	5.0	C <sub>7</sub> H <sub>5</sub> O <sup>37</sup> Cl
151.0575	3.79	151.0548	2.7	18.0	9.5	C <sub>12</sub> H <sub>7</sub>
176.0647	6.58	176.0626	2.1	11.9	11.0	C <sub>14</sub> H <sub>8</sub>
177.0723	5.13	177.0704	1.9	10.6	10.5	C <sub>14</sub> H <sub>9</sub>
178.0779	23.02	178.0783	-0.4	-2.0	10.0	C <sub>14</sub> H <sub>10</sub>
179.0875	23.43	179.0861	1.4	8.0	9.5	C <sub>14</sub> H <sub>11</sub>
207.0805	13.68	207.0810	-0.5	-2.4	10.5	C <sub>15</sub> H <sub>11</sub> O
207.9655	2.12	207.9661	-0.6	-2.7	9.0	C <sub>11</sub> H <sub>4</sub> <sup>35</sup> Cl <sup>37</sup> Cl
213.0619	1.00	213.0627	-0.8	-3.7	0.5	C <sub>9</sub> H <sub>17</sub> O <sup>35</sup> Cl <sup>37</sup> Cl
241.0419	100.00	241.0420	-0.1	-0.5	10.5	C <sub>15</sub> H <sub>10</sub> O <sup>35</sup> Cl
242.0492	90.07	242.0498	-0.6	-2.7	10.0	C <sub>15</sub> H <sub>11</sub> O <sup>35</sup> Cl
243.0419	54.37	243.0391	2.8	11.7	10.5	C <sub>15</sub> H <sub>10</sub> O <sup>37</sup> Cl
244.0441	32.38	244.0469	-2.8	-11.4	10.0	C <sub>15</sub> H <sub>11</sub> O <sup>37</sup> Cl

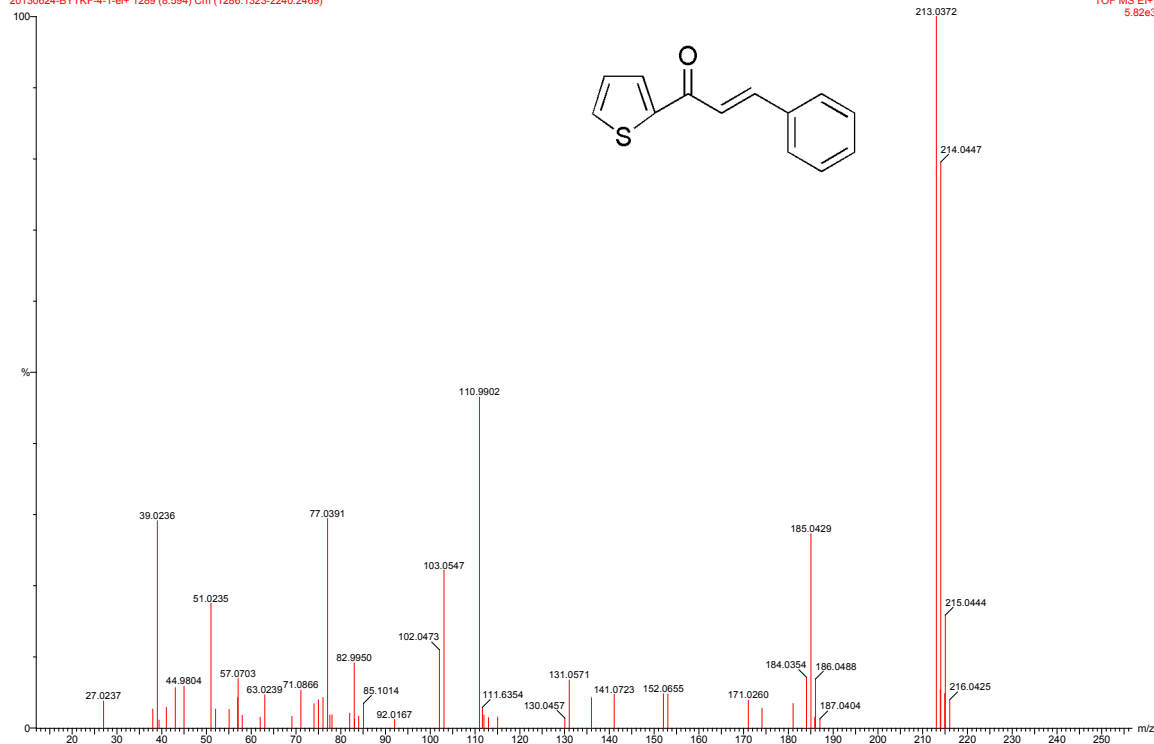
#### 4. (*E*)-3-Phenyl-1-(thiophen-3-yl)prop-2-en-1-one, Grey solid.

Micromass GCT-MS

USTC-MASS CA064

24-Jun-2013 17:02:14  
 RES=7000 half peak=0.0876  
 TOF MS EI+  
 5.82e3

20130624-BYTKF-4-1-ei+ 1289 (8.594) Cm (1286:1323-2240:2469)



#### Elemental Composition Report

Multiple Mass Analysis: 56 mass(es) processed - displaying only valid results

Tolerance = 4.0 mDa / DBE: min = 0.0, max = 50.0

Monoisotopic Mass, Odd and Even Electron Ions

473 formula(e) evaluated with 43 results within limits (up to 50 closest results for each mass)

Minimum:	1.00			0.0
Maximum:	100.00	4.0	5.0	50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
27.0237	3.75	27.0235	0.2	8.3	1.5	C <sub>2</sub> H <sub>3</sub>
38.0167	2.63	38.0157	1.0	27.6	3.0	C <sub>3</sub> H <sub>2</sub>
39.0236	29.08	39.0235	0.1	3.2	2.5	C <sub>3</sub> H <sub>3</sub>
41.0392	2.85	41.0391	0.1	1.8	1.5	C <sub>3</sub> H <sub>5</sub>
43.0551	5.64	43.0548	0.3	7.5	0.5	C <sub>3</sub> H <sub>7</sub>
44.9804	5.83	44.9799	0.5	11.2	1.5	CHS
51.0235	17.48	51.0235	0.0	0.5	3.5	C <sub>4</sub> H <sub>3</sub>
52.0300	2.61	52.0313	-1.3	-25.0	3.0	C <sub>4</sub> H <sub>4</sub>
55.0549	2.56	55.0548	0.1	2.3	1.5	C <sub>4</sub> H <sub>7</sub>
56.9813	4.25	56.9799	1.4	24.6	2.5	C <sub>2</sub> HS
57.0703	6.89	57.0704	-0.1	-2.2	0.5	C <sub>4</sub> H <sub>9</sub>
57.9881	1.74	57.9877	0.4	6.5	2.0	C <sub>2</sub> H <sub>2</sub> S
62.0146	1.50	62.0157	-1.1	-16.9	5.0	C <sub>5</sub> H <sub>2</sub>
63.0239	4.61	63.0235	0.4	6.7	4.5	C <sub>5</sub> H <sub>3</sub>
69.0717	1.57	69.0704	1.3	18.5	1.5	C <sub>5</sub> H <sub>9</sub>
71.0866	5.27	71.0861	0.5	7.4	0.5	C <sub>5</sub> H <sub>11</sub>
74.0160	3.36	74.0157	0.3	4.7	6.0	C <sub>6</sub> H <sub>2</sub>
75.0249	3.91	75.0235	1.4	19.0	5.5	C <sub>6</sub> H <sub>3</sub>
76.0303	4.23	76.0313	-1.0	-13.2	5.0	C <sub>6</sub> H <sub>4</sub>
77.0391	29.39	77.0391	0.0	-0.3	4.5	C <sub>6</sub> H <sub>5</sub>
78.0444	1.83	78.0470	-2.6	-32.7	4.0	C <sub>6</sub> H <sub>6</sub>
81.9892	2.04	81.9877	1.5	18.0	4.0	C <sub>4</sub> H <sub>2</sub> S
82.9950	9.10	82.9955	-0.5	-6.6	3.5	C <sub>4</sub> H <sub>3</sub> S
83.0868	1.17	83.0861	0.7	8.7	1.5	C <sub>6</sub> H <sub>11</sub>
84.0021	1.60	84.0034	-1.3	-15.1	3.0	C <sub>4</sub> H <sub>4</sub> S
85.1014	3.43	85.1017	-0.3	-3.8	0.5	C <sub>6</sub> H <sub>13</sub>
102.0473	10.96	102.0470	0.3	3.4	6.0	C <sub>8</sub> H <sub>6</sub>
103.0547	22.12	103.0548	-0.1	-0.7	5.5	C <sub>8</sub> H <sub>7</sub>
110.9902	46.45	110.9905	-0.3	-2.4	4.5	C <sub>5</sub> H <sub>3</sub> OS
111.9949	1.78	111.9949	0.0	-0.1	9.0	C <sub>8</sub> O
115.0537	1.50	115.0548	-1.1	-9.3	6.5	C <sub>9</sub> H <sub>7</sub>
130.0457	1.34	130.0452	0.5	3.6	2.0	C <sub>6</sub> H <sub>10</sub> OS
135.9984	4.21	135.9983	0.1	0.8	6.0	C <sub>7</sub> H <sub>4</sub> OS
141.0723	4.68	141.0738	-1.5	-10.6	2.5	C <sub>8</sub> H <sub>13</sub> S
152.0655	4.77	152.0660	-0.5	-3.1	4.0	C <sub>9</sub> H <sub>12</sub> S
153.0700	4.70	153.0704	-0.4	-2.8	8.5	C <sub>12</sub> H <sub>9</sub>
171.0260	3.86	171.0268	-0.8	-5.0	8.5	C <sub>11</sub> H <sub>7</sub> S
181.0649	3.39	181.0653	-0.4	-2.4	9.5	C <sub>13</sub> H <sub>9</sub> O
184.0354	7.08	184.0347	0.7	4.0	9.0	C <sub>12</sub> H <sub>8</sub> S
185.0429	27.26	185.0425	0.4	2.2	8.5	C <sub>12</sub> H <sub>9</sub> S
186.0488	6.84	186.0503	-1.5	-8.2	8.0	C <sub>12</sub> H <sub>10</sub> S
213.0372	100.00	213.0374	-0.2	-1.0	9.5	C <sub>13</sub> H <sub>9</sub> OS
214.0447	79.53	214.0452	-0.5	-2.5	9.0	C <sub>13</sub> H <sub>10</sub> OS

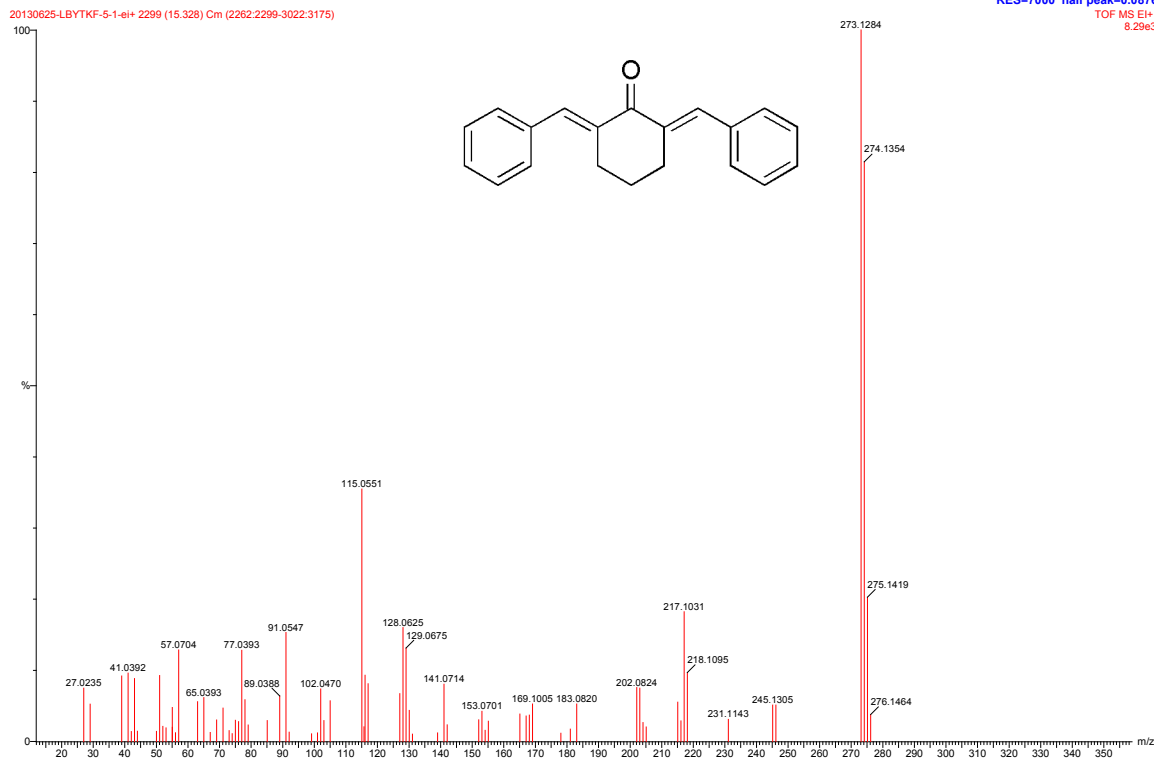
#### 5. 2.6-Dibenzalicyclohexanone, Yellow solid



Micromass GCT-MS

USTC-MASS CA064

25-Jun-2013 11:05:48  
 RES=7000 half peak=0.0876  
 TOF MS EI+  
 6.29e3



Multiple Mass Analysis: 74 mass(es) processed - displaying only valid results  
 Tolerance = 4.0 mDa / DBE: min = 0.0, max = 50.0

Monoisotopic Mass, Odd and Even Electron Ions

327 formula(e) evaluated with 64 results within limits (up to 50 closest results for each mass)

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
27.0235	7.47	27.0235	0.0	0.9	1.5	C <sub>2</sub> H <sub>3</sub>
29.0388	5.21	29.0391	-0.3	-11.2	0.5	C <sub>2</sub> H <sub>5</sub>
39.0236	9.19	39.0235	0.1	3.2	2.5	C <sub>3</sub> H <sub>3</sub>
41.0392	9.58	41.0391	0.1	1.8	1.5	C <sub>3</sub> H <sub>5</sub>
42.0456	1.37	42.0470	-1.4	-32.1	1.0	C <sub>3</sub> H <sub>6</sub>
43.0547	8.82	43.0548	-0.1	-1.7	0.5	C <sub>3</sub> H <sub>7</sub>
50.0142	1.40	50.0157	-1.5	-29.0	4.0	C <sub>4</sub> H <sub>2</sub>
51.0235	9.25	51.0235	0.0	0.5	3.5	C <sub>4</sub> H <sub>3</sub>
52.0310	2.10	52.0313	-0.3	-5.8	3.0	C <sub>4</sub> H <sub>4</sub>
53.0400	1.88	53.0391	0.9	16.5	2.5	C <sub>4</sub> H <sub>5</sub>
55.0185	1.98	55.0184	0.1	2.0	2.5	C <sub>3</sub> H <sub>3</sub> O
55.0558	4.74	55.0548	1.0	18.6	1.5	C <sub>4</sub> H <sub>7</sub>
56.0619	1.20	56.0626	-0.7	-12.5	1.0	C <sub>4</sub> H <sub>8</sub>
57.0704	12.84	57.0704	0.0	-0.4	0.5	C <sub>4</sub> H <sub>9</sub>
63.0238	5.56	63.0235	0.3	5.2	4.5	C <sub>5</sub> H <sub>3</sub>
65.0393	6.13	65.0391	0.2	2.7	3.5	C <sub>5</sub> H <sub>5</sub>
67.0560	1.25	67.0548	1.2	18.3	2.5	C <sub>5</sub> H <sub>7</sub>
69.0705	3.00	69.0704	0.1	1.1	1.5	C <sub>5</sub> H <sub>9</sub>
71.0863	4.67	71.0861	0.2	3.2	0.5	C <sub>5</sub> H <sub>11</sub>
74.0180	1.06	74.0157	2.3	31.7	6.0	C <sub>6</sub> H <sub>2</sub>

75.0254	2.94	75.0235	1.9	25.7	5.5	C <sub>6</sub> H <sub>3</sub>
76.0309	2.76	76.0313	-0.4	-5.3	5.0	C <sub>6</sub> H <sub>4</sub>
77.0393	12.79	77.0391	0.2	2.3	4.5	C <sub>6</sub> H <sub>5</sub>
78.0468	5.84	78.0470	-0.2	-1.9	4.0	C <sub>6</sub> H <sub>6</sub>
79.0549	2.28	79.0548	0.1	1.6	3.5	C <sub>6</sub> H <sub>7</sub>
85.1026	2.92	85.1017	0.9	10.3	0.5	C <sub>6</sub> H <sub>13</sub>
89.0388	6.35	89.0391	-0.3	-3.7	5.5	C <sub>7</sub> H <sub>5</sub>
91.0547	15.31	91.0548	-0.1	-0.8	4.5	C <sub>7</sub> H <sub>7</sub>
92.0590	1.28	92.0626	-3.6	-39.1	4.0	C <sub>7</sub> H <sub>8</sub>
99.1202	1.04	99.1174	2.8	28.5	0.5	C <sub>7</sub> H <sub>15</sub>
101.0397	1.18	101.0391	0.6	5.7	6.5	C <sub>8</sub> H <sub>5</sub>
102.0470	7.37	102.0470	0.0	0.5	6.0	C <sub>8</sub> H <sub>6</sub>
103.0559	2.91	103.0548	1.1	10.9	5.5	C <sub>8</sub> H <sub>7</sub>
105.0367	5.69	105.0340	2.7	25.3	5.5	C <sub>7</sub> H <sub>5</sub> O
115.0551	35.47	115.0548	0.3	2.8	6.5	C <sub>9</sub> H <sub>7</sub>
116.0602	9.28	116.0626	-2.4	-20.7	6.0	C <sub>9</sub> H <sub>8</sub>
127.0559	6.71	127.0548	1.1	8.9	7.5	C <sub>10</sub> H <sub>7</sub>
128.0625	15.99	128.0626	-0.1	-0.8	7.0	C <sub>10</sub> H <sub>8</sub>
129.0675	13.10	129.0704	-2.9	-22.7	6.5	C <sub>10</sub> H <sub>9</sub>
139.0560	1.17	139.0548	1.2	8.8	8.5	C <sub>11</sub> H <sub>7</sub>
141.0714	8.01	141.0704	1.0	6.9	7.5	C <sub>11</sub> H <sub>9</sub>
142.0784	2.32	142.0783	0.1	1.1	7.0	C <sub>11</sub> H <sub>10</sub>
152.0629	3.02	152.0626	0.3	2.0	9.0	C <sub>12</sub> H <sub>8</sub>
153.0701	4.22	153.0704	-0.3	-2.1	8.5	C <sub>12</sub> H <sub>9</sub>
154.0765	1.54	154.0783	-1.8	-11.4	8.0	C <sub>12</sub> H <sub>10</sub>
155.0867	2.82	155.0861	0.6	4.0	7.5	C <sub>12</sub> H <sub>11</sub>
165.0719	3.84	165.0704	1.5	8.9	9.5	C <sub>13</sub> H <sub>9</sub>
167.0865	3.56	167.0861	0.4	2.5	8.5	C <sub>13</sub> H <sub>11</sub>
168.0923	3.69	168.0939	-1.6	-9.5	8.0	C <sub>13</sub> H <sub>12</sub>
169.1005	5.25	169.1017	-1.2	-7.2	7.5	C <sub>13</sub> H <sub>13</sub>
178.0807	1.12	178.0783	2.4	13.8	10.0	C <sub>14</sub> H <sub>10</sub>
181.0679	1.72	181.0653	2.6	14.1	9.5	C <sub>13</sub> H <sub>9</sub> O
183.0820	5.24	183.0810	1.0	5.5	8.5	C <sub>13</sub> H <sub>11</sub> O
203.0871	7.46	203.0861	1.0	5.0	11.5	C <sub>16</sub> H <sub>11</sub>
204.0914	2.63	204.0939	-2.5	-12.3	11.0	C <sub>16</sub> H <sub>12</sub>
205.1010	2.00	205.1017	-0.7	-3.5	10.5	C <sub>16</sub> H <sub>13</sub>
215.0858	5.51	215.0861	-0.3	-1.3	12.5	C <sub>17</sub> H <sub>11</sub>
216.0936	2.87	216.0939	-0.3	-1.4	12.0	C <sub>17</sub> H <sub>12</sub>
217.1031	18.22	217.1017	1.4	6.3	11.5	C <sub>17</sub> H <sub>13</sub>
218.1095	9.65	218.1096	-0.1	-0.2	11.0	C <sub>17</sub> H <sub>14</sub>
231.1143	3.08	231.1174	-3.1	-13.3	11.5	C <sub>18</sub> H <sub>15</sub>
245.1305	5.09	245.1330	-2.5	-10.3	11.5	C <sub>19</sub> H <sub>17</sub>
273.1284	100.00	273.1279	0.5	1.7	12.5	C <sub>20</sub> H <sub>17</sub> O
274.1354	81.43	274.1358	-0.4	-1.3	12.0	C <sub>20</sub> H <sub>18</sub> O

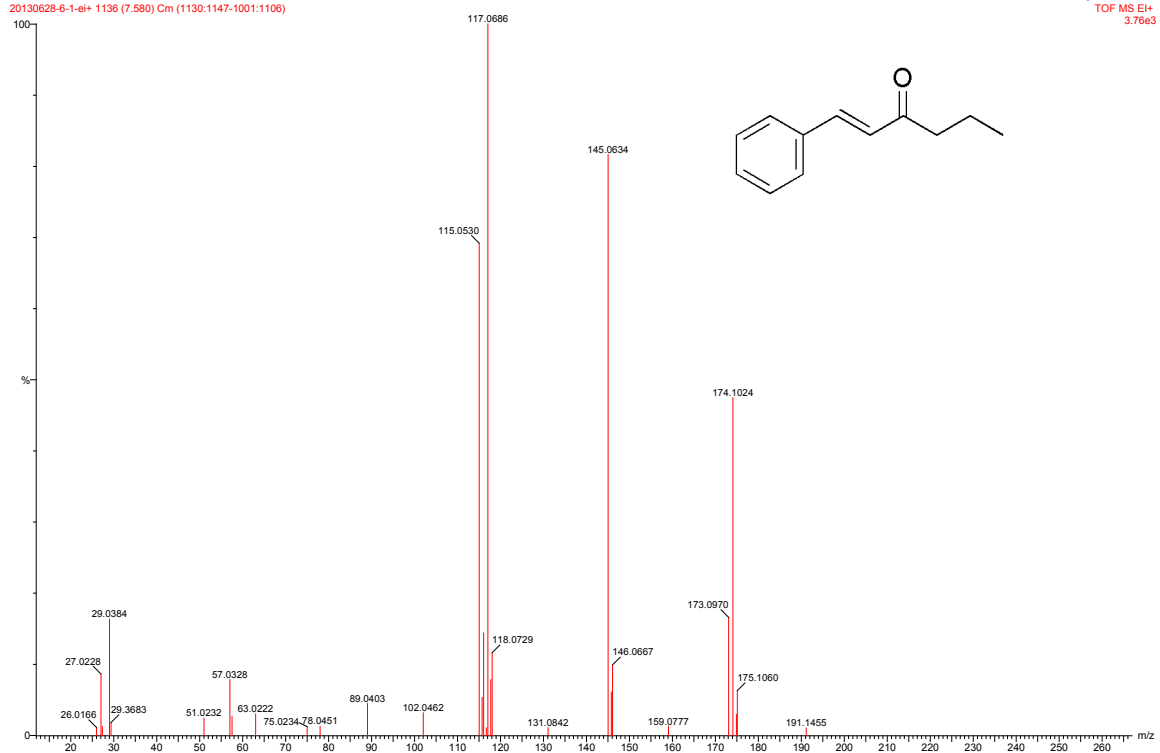
6. (*E*)-1-phenyloct-1-en-3-one, White solid.

Micromass GCT-MS

USTC-MASS CA064

28-Jun-2013 15:53:26  
RES=7000 half peak=0.0876  
TOF MS EI+  
3.7663

20130628-6-1-ei+ 1136 (7.580) Cm (1130:1147-1001:1106)



## Elemental Composition Report

Multiple Mass Analysis: 30 mass(es) processed - displaying only valid results

Tolerance = 4.0 mDa / DBE: min = 0.0, max = 50.0

### Monoisotopic Mass, Odd and Even Electron Ions

201 formula(e) evaluated with 18 results within limits (up to 50 closest results for each mass)

Minimum:	1.00				0.0	
Maximum:	100.00		4.0	5.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
26.0166	1.06	26.0157	0.9	36.5	2.0	C <sub>2</sub> H <sub>2</sub>
27.0228	8.61	27.0235	-0.7	-25.0	1.5	C <sub>2</sub> H <sub>3</sub>
29.0384	16.30	29.0391	-0.7	-25.0	0.5	C <sub>2</sub> H <sub>5</sub>
51.0232	2.38	51.0235	-0.3	-5.4	3.5	C <sub>4</sub> H <sub>3</sub>
57.0328	7.83	57.0340	-1.2	-21.7	1.5	C <sub>3</sub> H <sub>5</sub> O
63.0222	2.99	63.0235	-1.3	-20.2	4.5	C <sub>5</sub> H <sub>3</sub>
75.0234	1.19	75.0235	-0.1	-1.0	5.5	C <sub>6</sub> H <sub>3</sub>
78.0451	1.27	78.0470	-1.9	-23.7	4.0	C <sub>6</sub> H <sub>6</sub>
89.0403	4.47	89.0391	1.2	13.2	5.5	C <sub>7</sub> H <sub>5</sub>
102.0462	3.18	102.0470	-0.8	-7.4	6.0	C <sub>8</sub> H <sub>6</sub>
115.0530	69.15	115.0548	-1.8	-15.4	6.5	C <sub>9</sub> H <sub>7</sub>
116.0600	14.38	116.0626	-2.6	-22.4	6.0	C <sub>9</sub> H <sub>8</sub>
117.0686	100.00	117.0704	-1.8	-15.6	5.5	C <sub>9</sub> H <sub>9</sub>
131.0842	1.05	131.0861	-1.9	-14.3	5.5	C <sub>10</sub> H <sub>11</sub>
145.0634	81.61	145.0653	-1.9	-13.4	6.5	C <sub>10</sub> H <sub>9</sub> O
159.0777	1.24	159.0810	-3.3	-20.7	6.5	C <sub>11</sub> H <sub>11</sub> O
173.0970	16.57	173.0966	0.4	2.1	6.5	C <sub>12</sub> H <sub>13</sub> O
174.1024	47.46	174.1045	-2.1	-11.9	6.0	C <sub>12</sub> H <sub>14</sub> O