Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Rhodium-Catalyzed Intermolecular Hydroarylation of Internal Alkynes with *N*-1-Phenylbenzotriazoles

Supporting Information

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Contents:

General Remarks

^{1}H-NMR spectra were recorded on a Bruker AVIII-400 spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ as an internal standard. ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and calibrated with $CDCl_3$ (δ = 77.0 ppm). Mass spectra were recorded using an Agilent 5975 GC-MS. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification.

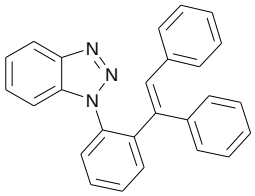
Experimental Procedures

Typical procedure

A sealed tube was charged with substrate **1** (0.2 mmol), **2** (0.3 mmol), $RhCl(PPh_3)_3$ (0.005 mmol), AgOTf (0.01 mmol) in mesitylene (1.6 mL). The mixture was stirred at 160 ^oC under N_2 for 12 h. Then, the reaction was cooled down to room temperature, diluted with ethyl acetate (50 mL), filtered, and dried under vaccum. The crude product was purified by column chromatography on silica gel to obtain the desired products **3** (petroleum ether:ethyl acetate = 20:1).

Analytical Data for Compounds 3

1) 1-(2-((E)-1,2-Diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3aa)



3aa

The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 73 mg (98%) of **3aa** as solid. m.p.: 129-130 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.88 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.3 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.42 (d, *J* = 7.3 Hz, 1H), 7.37-7.16 (m, 3H), 7.15-7.07 (m, 3H), 7.02-6.96 (m, 2H), 6.84 (s, 1H), 6.81-6.66 (m, 3H), 6.52 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.2, 142.2, 139.7, 137.9, 136.6, 134.5, 133.5, 131.8, 131.5, 129.9, 129.2, 128.7, 128.6, 127.8, 127.6, 127.5, 127.02, 127.0, 126.9, 123.5, 119.4, 110.1 ppm; IR (KBr): ν_{max} = 1612, 1593, 1502, 1495, 1458, 1271, 1072, 1007, 785, 767, 758, 748, 706, 698 cm^{-1}; MS (70 eV): m/z (%) 271.1 (M^+, 100); HRMS m/z (ESI) calcd for $C_{26}H_{20}N_3$ $(M + H)^+$: 374.1652, found 374.1643.

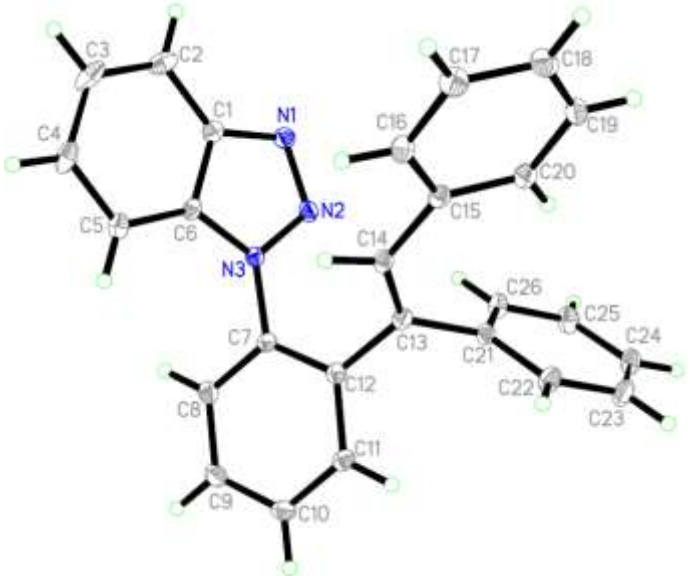
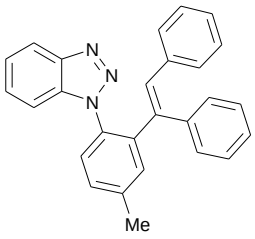


Figure S1. ORTEP drawing of **3aa**

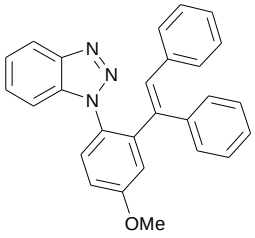
2) 1-(4-Methyl-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ba)



3ba

The reaction of 1-(4-methylphenyl)-1H-benzo[d][1,2,3]triazole (**1b**, 0.2 mmol, 41.9 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 75 mg (97%) of **3ba** as solid. m.p.: 150-151 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.85 (d, *J* = 8.4 Hz, 1H), 7.55 (s, 1H), 7.39-7.15 (m, 6H), 7.09-7.02 (m, 3H), 6.97-6.91 (m, 2H), 6.8 (s, 1H), 6.78-6.68 (m, 3H), 6.52 (d, *J* = 8.0 Hz, 1H), 2.54 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.1, 141.9, 140.1, 139.8, 138.0, 136.7, 133.6, 132.3, 132.0, 131.2, 129.23, 129.20, 128.6, 127.8, 127.7, 127.5, 127.4, 126.9, 126.8, 123.4, 119.3, 110.1, 21.2 ppm; IR (KBr): ν_{max} = 1501, 1444, 1273, 1066, 833, 768, 752, 717, 700 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{22}N_3$ $(M + H)^+$: 388.1808, found 388.1803.

3) 1-(4-Methoxy-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ca)

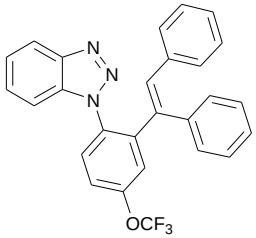


3ca

The reaction of 1-(4-methoxyphenyl)-1H-benzo[d][1,2,3]triazole (**1c**, 0.2 mmol, 45.1 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 72 mg (89%) of **3ca** as solid. m.p.: 132-133 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.86 (d, *J* = 8.0 Hz, 1H), 7.39-7.18 (m, 4H), 7.18-7.12 (m, 1H), 7.11-7.01 (m, 4H), 6.99-6.89 (m, 2H), 6.83 (s, 1H), 6.80-6.66 (m, 3H), 6.53 (d, *J* = 6.8 Hz, 2H), 3.96 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 160.5, 145.1, 143.7, 139.7, 137.7, 136.5,

133.8, 131.5, 129.3, 129.2, 128.9, 128.6, 127.8, 127.5, 127.4, 127.1, 126.9, 123.4, 119.3, 116.9, 113.7, 110.1, 55.7 ppm; IR (KBr): ν_{max} = 1610, 1571, 1502, 1453, 1284, 1249, 1216, 1068, 750, 699 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{22}N_3O$ $(M + H)^+$: 404.1757, found 404.1748.

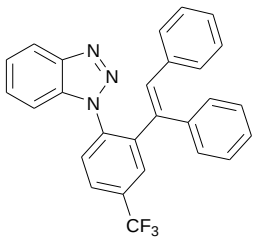
4) 1-(2-((E)-1,2-Diphenylvinyl)-4-(trifluoromethoxy)phenyl)-1H-benzo[d][1,2,3] triazole (3da)



3da

The reaction of 1-(4-(trifluoromethoxy)phenyl)-1H-benzo[d][1,2,3]triazole (**1d**, 0.2 mmol, 55.8 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 87 mg (95%) of **3da** as solid. m.p.: 126-127 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.89 (d, *J* = 6.0 Hz, 1H), 7.62 (s, 1H), 7.51-7.38 (m, 2H), 7.37-7.15 (m, 3H), 7.14-7.04 (m, 3H), 7.01-6.92 (m, 2H), 6.86 (s, 1H), 6.82-6.67 (m, 3H), 6.51 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 149.9, 145.2, 144.3, 138.5, 137.1, 136.1, 133.5, 132.9, 132.6, 129.3, 129.2, 128.6, 127.9, 127.7, 127.42, 127.37, 127.2, 123.9, 123.7, 120.5, 120.4 (q, J_{C-F} = 257.6 Hz), 119.6 ppm; IR (KBr): ν_{max} = 1503, 1453, 1256, 1220, 1169, 1068, 738, 698 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{19}F_3N_3O$ $(M + H)^+$: 458.1475, found 458.1466.

5)1-(4-(Trifluoromethyl)-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]tria zole (3ea)



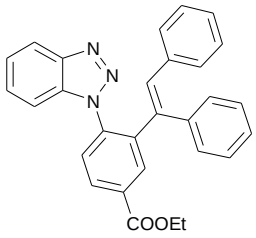
3ea

The reaction of 1-(4-(trifluoromethyl)phenyl)-1H-benzo[d][1,2,3]triazole (**1e**, 0.2

mmol, 52.6 mg), diphenylacetylene **(2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 80 mg (91%) of **3ea** as solid. m.p.: 119-120 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.03 (s, 1H), 7.96-7.86 (m, 1H), 7.82 (d, *J* = 7.2 Hz, 1H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.41-7.15 (m, 3H), 7.14-7.04 (m, 3H), 7.02-6.94 (m, 2H), 6.91 (s, 1H), 6.82-6.65 (m, 3H), 6.49 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.3, 143.0, 138.6, 137.5, 137.1, 136.1, 133.3, 132.8, 132.3, 131.9, 129.3, 128.8 (d, J_{C-F} = 3.6 Hz), 128.6, 128.2, 127.9, 127.7, 127.51, 127.47, 127.3, 125.6 (d, J_{C-F} = 3.2 Hz), 123.6 (q, J_{C-F} = 271 Hz), 119.7, 109.8 ppm; IR (KBr): ν_{max} = 1609, 1508, 1491, 1454, 1443, 1331, 1246, 1167, 1131, 1120, 1075, 1058, 860, 724, 694 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{19}F_3N_3$ $(M + H)^+$: 442.1526, found 442.1521.

6)

1-(4-(Ethoxycaronyl)-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3fa)

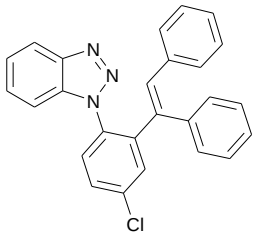


3fa

The reaction of 1-(4-ethoxycarbonylphenyl)-1H-benzo[d][1,2,3]triazole (**1f**, 0.2 mmol, 53.5 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 85 mg (95%) of **3fa** as solid. m.p.: 110-111 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.44 (s, 1H), 8.23 (d, *J* = 6.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.40-7.15 (m, 3H), 7.13-7.05 (m, 3H), 7.03-6.97 (m, 2H), 6.95 (s, 1H), 6.80-6.61 (m, 3H), 6.48 (d, *J* = 6.8 Hz, 2H), 4.49 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 165.4, 145.2, 142.2, 139.0, 138.0, 137.3, 136.3, 133.2, 133.0, 132.2, 131.8, 129.7, 129.2, 128.5, 127.8, 127.6, 127.5, 127.3, 127.2, 127.0, 123.7, 119.5, 109.9, 61.5, 14.2 ppm; IR (KBr): ν_{max} = 1720, 1599, 1495, 1448, 1299, 1279, 1242, 1229, 1122, 1053, 765, 752, 699 cm^{-1}; HRMS m/z

(ESI) calcd for $C_{29}H_{24}N_3O_2$ $(M + H)^+$: 446.1863, found 446.1858.

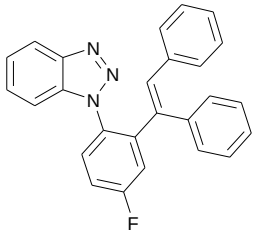
7) 1-(4-Chloro-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ga)



3ga

The reaction of 1-(4-chlorophenyl)-1H-benzo[d][1,2,3]triazole (**1g**, 0.2 mmol, 45.9 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 72 mg (88%) of **3ga** as solid. m.p.: 165-166 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.86 (d, *J* = 7.6 Hz, 1H), 7.76 (s, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.42-7.13 (m, 4H), 7.13-7.01 (m, 3H), 7.00-6.90 (m, 2H), 6.85 (s, 1H), 6.82-6.65 (m, 3H), 6.52 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.2, 143.8, 138.5, 137.3, 136.2, 135.8, 133.5, 133.1, 132.3, 131.6, 129.2, 128.9, 128.60, 128.57, 127.8, 127.6, 127.29, 127.26, 127.1, 123.6, 119.5, 109.8 ppm; IR (KBr): ν_{max} = 1493, 1442, 1059, 752, 697 cm^{-1}; HRMS m/z (ESI) calcd for $C_{26}H_{19}ClN_3$ $(M + H)^+$: 408.1262, found 408.1258.

8) 1-(4-Fluoro-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ha)

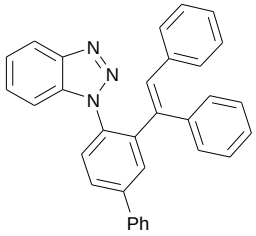


3ha

The reaction of 1-(4-fluorophenyl)-1H-benzo[d][1,2,3]triazole (**1h**, 0.2 mmol, 42.6 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 75 mg (96%) of **3ha** as solid. m.p.: 139-140 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.86 (d, *J* = 7.2 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 1H), 7.43-7.36 (m, 1H), 7.35-7.20 (m, 3H), 7.19-7.12 (m, 1H), 7.12-7.02 (m, 3H), 6.98-6.87 (m, 2H), 6.82 (s, 1H), 6.80-6.69 (m, 3H), 6.53 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 163.0

(d, $J_{C\text{-}F}$ = 249.9 Hz), 145.1, 144.6 (d, $J_{C\text{-}F}$ = 7.9 Hz), 138.6, 137.3, 136.1, 133.6, 132.3, 130.6, 129.5 (d, $J_{C\text{-}F}$ = 9.1 Hz), 129.2, 128.6, 127.9, 127.7, 127.3, 127.2, 127.1, 123.6, 119.5, 118.6 (d, $J_{C\text{-}F}$ = 23.2 Hz), 115.4 (d, $J_{C\text{-}F}$ = 22.7 Hz), 109.8 ppm; IR (KBr): ν_{max} = 1606, 1581, 1504, 1445, 1269, 1182, 1067, 865, 750, 696 cm^{-1}; HRMS m/z (ESI) calcd for $C_{26}H_{19}FN_3$ $(M + H)^+$: 392.1558, found 392.1564.

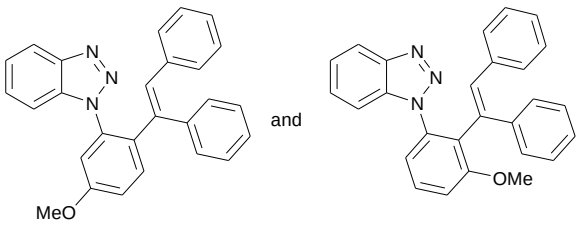
9) 1-(4-Phenyl-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ia)



3ia

The reaction of 1-(4-phenylphenyl)-1H-benzo[d][1,2,3]triazole (**1i**, 0.2 mmol, 54.3 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 87 mg (97%) of **3ia** as solid. m.p.: 101-102 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.05-7.95 (d, *J* = 1.6 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.81-7.70 (m, 3H), 7.59-7.41 (m, 4H), 7.37-7.20 (m, 3H), 7.11-6.95 (m, 5H), 6.93 (s, 1H), 6.82-6.68 (m, 3H), 6.56 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.3, 143.1, 142.6, 139.9, 139.7, 137.9, 136.7, 133.7, 131.8, 130.52, 130.51, 129.3, 129.0, 128.7, 128.2, 128.1, 127.9, 127.8, 127.6, 127.3, 127.2, 127.1, 127.0, 123.5, 119.5, 110.2 ppm; IR (KBr): ν_{max} = 1491, 1445, 1059, 784, 764, 743, 695 cm^{-1}; HRMS m/z (ESI) calcd for $C_{32}H_{24}N_3$ $(M + H)^+$: 450.1965, found 450.1956.

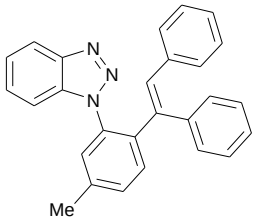
10) 1-(5-Methoxy-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ja) and
1-(3-Methoxy-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ja')



3ja **3ja'**

The reaction of 1-(3-methoxyphenyl)-1H-benzo[d][1,2,3]triazole (**1j**, 0.2 mmol, 45.1 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 58 mg (72%) of **3ja** and **3ja'** as mixtures (2.78:1.00). HRMS m/z (ESI) calcd for $C_{27}H_{22}N_3O$ $(M + H)^+$: 404.1757, found 404.1756.

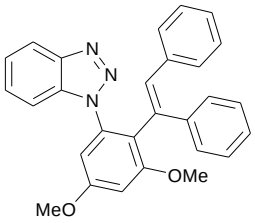
11) 1-(5-Methyl-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ka)



3ka

The reaction of 1-(3-methylphenyl)-1H-benzo[d][1,2,3]triazole (**1k**, 0.2 mmol, 41.9 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 50 mg (65%) of **3ka** as solid. m.p.: 139-140 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.89 (d, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 1H), 7.38-7.22 (m, 4H), 7.11-7.05 (m, 3H), 7.01-6.93 (m, 2H), 6.83 (s, 1H), 6.81-6.71 (m, 3H), 6.53 (d, *J* = 7.6 Hz, 2H), 2.50 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.2, 139.6, 139.2, 139.0, 138.1, 136.8, 134.4, 133.6, 131.6, 131.1, 130.6, 129.2, 128.7, 128.2, 127.8, 127.5, 127.0, 126.89, 126.85, 123.4, 119.4, 110.2, 20.9 ppm; IR (KBr): ν_{max} = 1507, 1493, 1459, 1445, 1271, 1072, 748, 721, 697 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{22}N_3$ $(M + H)^+$: 388.1808, found 388.1801.

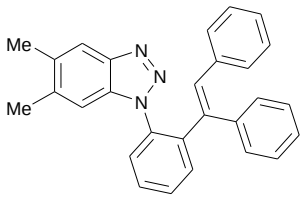
12) 1-(3,5-Dimethoxy-2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3la)



3la

The reaction of 1-(3,5-dimethoxyphenyl)-1H-benzo[d][1,2,3]triazole (**1l**, 0.2 mmol, 51.1 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.01 mmol, 9.3 mg), AgOTf (0.02 mmol, 5.1 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 34 mg (39%) of **3la** as solid. m.p.: 69-70 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.91 (d, *J* = 8.4 Hz, 1H), 7.33-7.17 (m, 1H), 7.16-7.00 (m, 9H), 6.94-6.89 (m, 2H), 6.88-6.79 (m, 1H), 6.78-6.68 (m, 1H), 6.66-6.57 (m, 1H), 3.88 (s, 3H), 3.63 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 160.8, 159.8, 145.0, 142.1, 137.7, 136.8, 133.9, 133.4, 130.9, 128.3, 127.8, 127.7, 127.0, 126.9, 126.3, 123.2, 120.3, 119.2, 110.0, 103.8, 100.5, 56.0, 55.7 ppm; IR (KBr): ν_{max} = 1606, 1575, 1492, 1459, 1277, 1163, 1047, 1023, 745, 694 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{24}N_3O_2$ $(M + H)^+$: 434.1863, found 434.1856.

13) 5,6-Dimethyl-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ma)

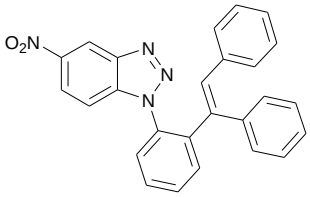


3ma

The reaction of 1-phenyl-5,6-dimethyl-1H-benzo[d][1,2,3]triazole (**1m**, 0.2 mmol, 44.7 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 70 mg (87%) of **3ma** as solid. m.p.: 181-182 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.72 (d, *J* = 7.1 Hz, 1H), 7.66-7.58 (m, 2H), 7.54 (t, *J* = 7.1 Hz, 1H), 7.40 (d, *J* = 7.1 Hz, 1H), 7.12-7.02 (m, 3H), 7.00-6.89 (m, 3H), 6.86-6.68 (m, 4H), 6.52 (d, *J* = 7.2 Hz, 2H), 2.33 (s, 3H), 2.32 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 144.4,

142.1, 139.8, 138.1, 137.2, 136.7, 134.8, 133.1, 132.7, 131.6, 131.4, 129.7, 129.2, 128.7, 128.5, 127.8, 127.7, 127.5, 126.9, 126.8, 118.4, 109.7, 20.5, 20.1 ppm; IR (KBr): ν_{max} = 1496, 1443, 1245, 1104, 1058, 837, 770, 695 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{24}N_3$ $(M + H)^+$: 402.1965, found 402.1967.

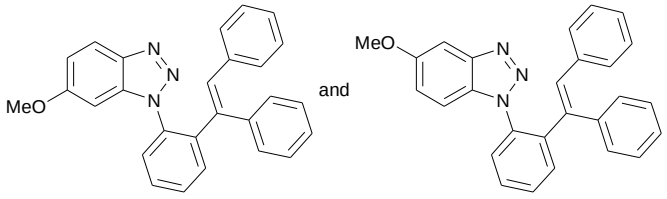
14) 5-Nitro-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3na)



3na

The reaction of 1-phenyl-5-nitro-1H-benzo[d][1,2,3]triazole (**1n**, 0.2 mmol, 48.0 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 31 mg (37%) of **3na** as solid. m.p.: 147-148 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.81 (s, 1H), 8.18 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 7.47 Hz, 1H), 7.71 (t, *J* = 7.47 Hz, 1H), 7.60 (t, *J* = 7.47 Hz, 1H), 7.40 (d, *J* = 7.47 Hz, 1H), 7.28-7.20 (m, 2H), 7.15-7.02 (m, 4H), 7.01-6.93 (m, 2H), 6.90 (s, 1H), 6.78-6.66 (m, 2H), 6.50 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 144.5, 144.3, 142.6, 139.1, 137.9, 136.3, 136.2, 133.7, 132.3, 132.2, 130.9, 129.3, 129.0, 128.6, 128.0, 127.8, 127.6, 127.5, 127.2, 122.1, 116.8, 110.7 ppm; IR (KBr): ν_{max} = 1526, 1346, 1071, 801 cm^{-1}; HRMS m/z (ESI) calcd for $C_{26}H_{19}N_4O_2$ $(M + H)^+$: 419.1503, found 419.1502.

15) 6-Methoxy-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3oa) and 5-Methoxy-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3] triazole (3oa')

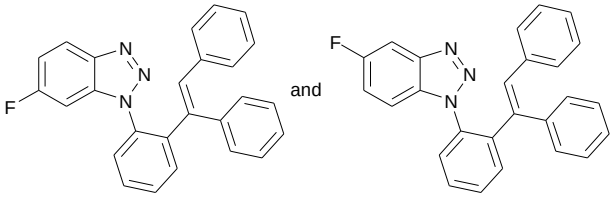


3oa **3oa'**

The reaction of 1-phenyl-6 or 5-methoxy-1H-benzo[d][1,2,3]triazole **1o** and **1o'**

(**1o**/**1o'** = 2.57:1.00, 0.2 mmol, 45.1 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 43 mg (53%) of **3oa** and **3oa'** as mixtures (2.23:1.00). HRMS m/z (ESI) calcd for $C_{27}H_{22}N_3O$ $(M + H)^+$: 404.1757, found 404.1749.

16) 6-Fluoro-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3] triazole (3pa) and 5-Fluoro-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3] triazole (3pa')



3pa **3pa'**

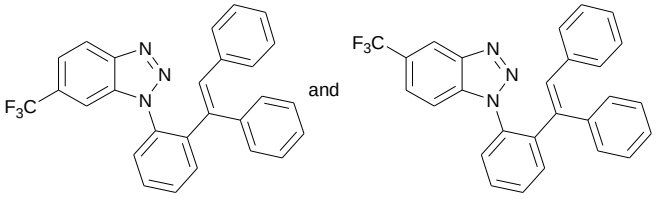
The reaction of 1-phenyl-5 or 6-fluoro-1H-benzo[d][1,2,3]triazole **1p** and **1p'** (**1p**/**1p'** = 1.50:1.00, 0.2 mmol, 42.6 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 70 mg (89%) of **3pa** and **3pa'** (1.83:1.00) as mixture. HRMS m/z (ESI) calcd for $C_{26}H_{19}FN_3$ $(M + H)^+$: 392.1558, found 392.1556.

17)

6-(Trifluoromethyl)-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3qa)

and

5-(Trifluoromethyl)-1-(2-((E)-1,2-diphenylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3qa')

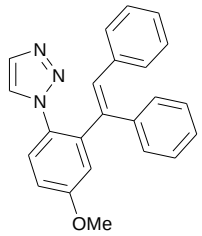


3qa **3qa'**

The reaction of 1-phenyl-6 or 5-trifluoromethyl-1H-benzo[d][1,2,3]triazole **1q** and

1q' (**1q**/**1q'** = 1.38:1.00, 0.15 mmol, 39.5 mg), diphenylacetylene (**2a**, 0.225 mmol, 40.1 mg), $RhCl(PPh_3)_3$ (0.00375 mmol, 3.5 mg), AgOTf (0.0075 mmol, 1.9 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 46 mg (69%) of **3qa** and **3qa'** (1.52:1.00) as mixtures. HRMS m/z (ESI) calcd for $C_{27}H_{19}F_3N_3$ $(M + H)^+$: 442.1526, found 442.1527.

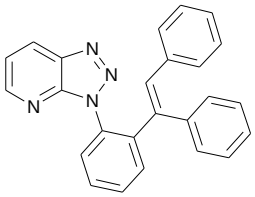
18) 1-(4-Methoxy-2-((E)-1,2-diphenylvinyl)phenyl)-1H-1,2,3-triazole (3ra)



3ra

The reaction of 1-(4-methoxyphenyl)-1H-[1,2,3]triazole (**1n**, 0.2 mmol, 35.0 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under N_2 for 50 h afforded 34 mg (48%) of **3ra** as solid. m.p.: 143-144 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.50 (s, 2H), 7.42 (d, J = 8.4 Hz, 1H), 7.14-6.92 (m, 12H), 6.59 (s, 1H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.8, 142.0, 139.5, 139.0, 137.1, 134.7, 132.6, 130.6, 129.8, 129.3, 127.84, 127.80, 127.72, 127.68, 127.1, 126.9, 116.5, 113.3, 55.6 ppm; IR (KBr): ν_{max} = 1607, 1575, 1504, 1462, 1421, 1294, 1205, 1061, 1028, 952, 810, 775, 699 cm^{-1}; HRMS m/z (ESI) calcd for $C_{23}H_{20}N_3O$ $(M + H)^+$: 354.1601, found 354.1601.

19) 3-(2-((E)-1,2-Diphenylvinyl)phenyl)-3H-[1,2,3]triazolo[4,5-b]pyridine (3sa)

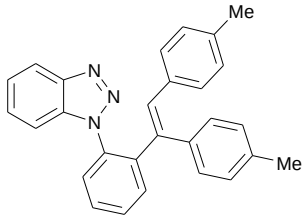


3sa

The reaction of 1-phenyl-1H-7-azabenzo[d][1,2,3]triazole (**1s**, 0.2 mmol, 39.2 mg), diphenylacetylene (**2a**, 0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure**

afforded 65 mg (87%) of **3sa** as solid. m.p.: 139-140 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.58-8.46 (m, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 7.07 Hz, 1H), 7.63 (t, *J* = 7.07 Hz, 1H), 7.57 (t, *J* = 7.07 Hz, 1H), 7.48 (d, *J* = 7.07 Hz, 1H), 7.30-7.16 (m, 1H), 7.09-7.02 (m, 3H), 6.96-6.86 (m, 2H), 6.79 (s, 1H), 6.77-6.68 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 150.2, 146.2, 142.5, 139.3, 138.3, 136.8, 136.2, 133.3, 131.7, 131.5, 130.2, 129.3, 129.1, 128.6, 128.2, 128.0, 127.8, 127.5, 126.9, 126.7, 119.4 ppm; IR (KBr): ν_{max} = 2156, 1589, 1496, 1455, 1259, 764, 701 cm^{-1}; HRMS m/z (ESI) calcd for $C_{25}H_{19}N_4$ $(M + H)^+$: 375.1604, found 375.1602.

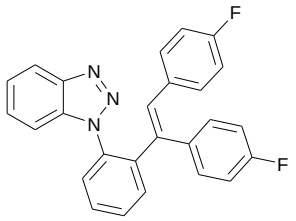
20) 1-(2-((E)-1,2-Dip-tolylvinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ab)



3ab

The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39.0 mg), bis(4-methylphenyl)acetylene (**2b**, 0.3 mmol, 61.9 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 77 mg (96%) of **3ab** as solid. m.p.: 138-139 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.90 (d, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 7.47 Hz, 1H), 7.65 (t, *J* = 7.47 Hz, 1H), 7.56 (t, *J* = 7.47 Hz, 1H), 7.43 (d, *J* = 7.47 Hz, 1H), 7.37-7.17 (m, 3H), 7.96-7.86 (m, 4H), 6.78 (s, 1H), 6.57 (d, *J* = 8.4 Hz, 2H), 6.46 (d, *J* = 8.0 Hz, 2H), 2.26 (s, 3H), 2.05 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.3, 142.8, 138.8, 136.8, 136.6, 135.4, 134.6, 134.0, 133.6, 131.8, 131.2, 129.9, 129.2, 128.6, 128.5, 128.4, 128.3, 127.8, 126.9, 123.4, 119.4, 110.4, 21.1, 20.9 ppm; IR (KBr): ν_{max} = 1509, 1458, 1271, 1065, 784, 741 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{24}N_3$ $(M + H)^+$: 402.1965, found 402.1966.

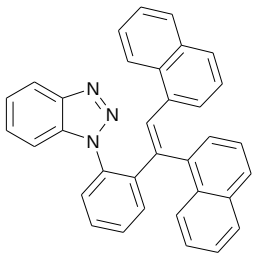
21) 1-(2-((E)-1,2-Bis(4-fluorophenyl)vinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ac)



3ac

The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39.0 mg), bis(4-fluorophenyl)acetylene (**2c**, 0.3 mmol, 64.3 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 72 mg (88%) of **3ac** as solid. m.p.: 158-159 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.89 (d, *J* = 8.8 Hz, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.39-7.21 (m, 2H), 7.21-7.11 (m, 1H), 6.86-7.01 (m, 2H), 6.84-6.66 (m, 2H), 6.60-6.29 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 161.6 (d, J_{C-F} = 246.2 Hz), 161.5 (d, J_{C-F} = 246.0 Hz), 145.1, 141.9, 138.5, 134.4, 133.7 (d, J_{C-F} = 3.5 Hz), 133.4, 132.5 (d, J_{C-F} = 3.4 Hz), 131.7, 130.9, 130.8 130.4 (d, J_{C-F} = 19 Hz), 130.2 (d, J_{C-F} = 22.5 Hz), 128.9, 127.6, 127.2, 123.7, 119.4, 114.9 (d, J_{C-F} = 21.4 Hz), 114.6 (d, J_{C-F} = 21.5 Hz), 109.9 ppm; IR (KBr): ν_{max} = 1599, 1507, 1459, 1223, 1158, 1068, 837, 788, 744 cm^{-1}; HRMS m/z (ESI) calcd for $C_{26}H_{18}F_2N_3$ $(M + H)^+$: 410.1463, found 410.1457.

22) 1-(2-((E)-1,2-Di(naphthalen-1-yl)vinyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ad)

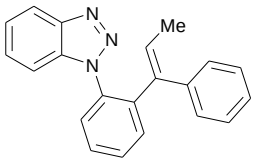


3ad

The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39.0 mg), bis(1-naphthyl)acetylene (**2d**, 0.3 mmol, 83.5 mg), $RhCl(PPh_3)_3$ (0.01 mmol, 9.3 mg), AgOTf (0.02 mmol, 5.1 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 41 mg (43%) of **3ad** as solid. m.p.: 105-106 ^oC; ^1H NMR ($CDCl_3$, 400 MHz):

δ = 8.21 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.83-7.65 (m, 4H), 7.64-7.42 (m, 6H), 7.30-7.19 (m, 2H), 7.17-7.05 (m, 3H), 7.05-6.93 (m, 1H), 6.90-6.77 (m, 1H), 6.76-6.66 (m, 1H), 6.64-6.45 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.1, 143.2, 140.5, 135.4, 134.3, 133.9, 133.4, 133.3, 132.6, 132.1, 131.7, 131.0, 130.7, 128.7, 128.4, 128.2, 128.1, 127.6, 127.13, 127.09, 126.8, 126.2, 125.8, 125.4, 125.3, 125.0, 124.9, 124.8, 124.5, 123.4, 119.2, 109.10 ppm; IR (KBr): ν_{max} = 1498, 1273, 1063, 797, 777, 744 cm^{-1}; HRMS m/z (ESI) calcd for $C_{34}H_{24}N_3$ $(M + H)^+$: 474.1965, found 474.1957.

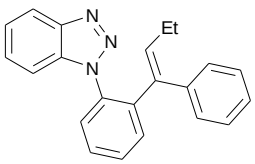
23) 1-(2-((E)-1-Phenylprop-1-enyl)phenyl)-1H-benzo[d][1,2,3]triazole (3ae)



3ae

The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39.0 mg), 1-phenyl-1-propyne (**2e**, 0.3 mmol, 37 μL), $RhCl(PPh_3)_3$ (0.01 mmol, 9.3 mg), AgOTf (0.02 mmol, 5.1 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 30 mg (48%) of **3ae** as liquid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.05-7.84 (m, 1H), 7.69-7.46 (m, 3H), 7.40-7.21 (m, 3H), 7.18-7.01 (m, 1H), 6.88-6.73 (m, 3H), 6.63-6.44 (m, 2H), 6.04 (d, *J* = 6.8 Hz, 1H), 1.68 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.2, 142.2, 139.4, 137.7, 134.4, 133.6, 131.6, 129.9, 128.3, 128.2, 128.1, 127.5, 127.2, 127.0, 126.4, 123.4, 119.4, 110.2, 15.3 ppm; IR (KBr): ν_{max} = 1496, 1458, 1441, 1274, 1185, 1062, 1006, 786, 765, 745, 701 cm^{-1}; HRMS m/z (ESI) calcd for $C_{21}H_{18}N_3$ $(M + H)^+$: 312.1495, found 312.1503.

24) 1-(2-((E)-1-Phenylbut-1-enyl)phenyl)-1H-benzo[d][1,2,3]triazole (3af)

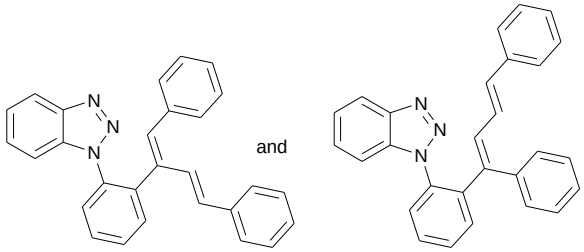


3af

The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39.0 mg),

1-phenyl-1-butyne (**2f**, 0.3 mmol, 43 μL), $RhCl(PPh_3)_3$ (0.01 mmol, 9.3 mg), AgOTf (0.02 mmol, 5.1 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 43 mg (66%) of **3af** as solid. m.p.: 77-78 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.93 (d, *J* = 8.0 Hz, 1H), 7.66-7.55 (m, 2H), 7.55-7.45 (m, 1H), 7.44-7.23 (m, 3H), 7.22-7.13 (m, 1H), 6.97-6.81 (m, 3H), 6.64-6.50 (m, 2H), 5.83 (t, *J* = 7.5 Hz, 1H), 2.03 (m, *J* = 7.5 Hz, 2H), 0.84 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.3, 142.1, 138.1, 137.8, 135.9, 134.5, 133.8, 131.7, 129.9, 128.3, 128.2, 127.7, 127.3, 127.0, 126.6, 123.5, 119.5, 110.4, 22.7, 14.0 ppm; IR (KBr): ν_{max} = 1613, 1497, 1458, 1444, 1272, 1062, 1005, 785, 773, 760, 743, 710 cm^{-1}; HRMS m/z (ESI) calcd for $C_{22}H_{20}N_3$ $(M + H)^+$: 326.1652, found 326.1654.

25)1-(2-((1E,3E)-1,4-diphenylbuta-1,3-dien-2-yl)phenyl)-1H-benzo[d][1,2,3]triazole/1-(2-((1E,3E)-1,4-diphenylbuta-1,3-dienyl)phenyl)-1H-benzo[d][1,2,3]triazole

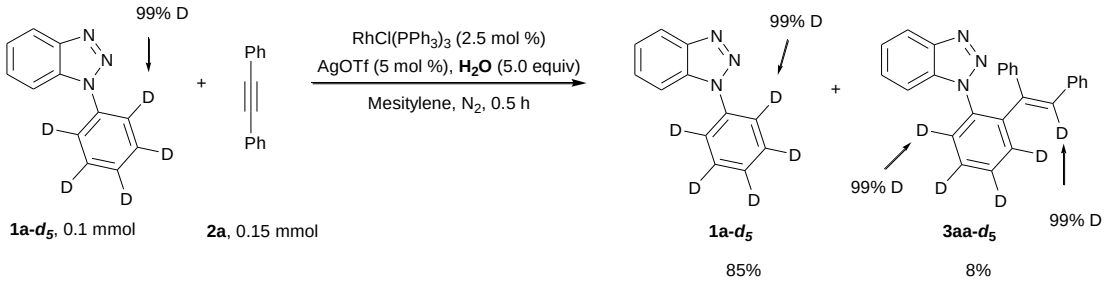


3ag **3ag'**

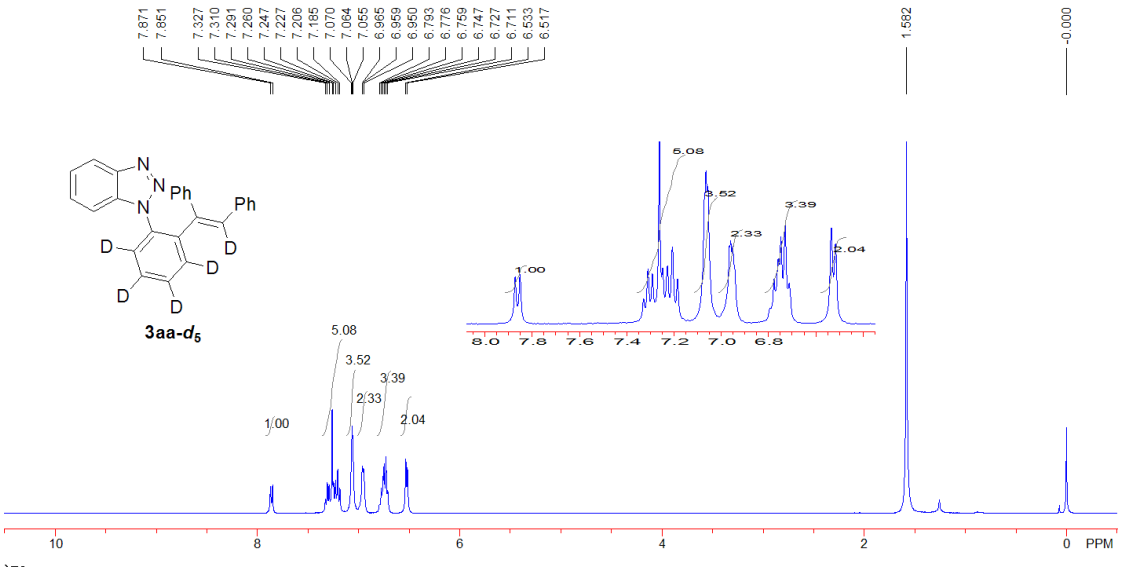
The reaction of 1-phenyl-1H-benzo[d][1,2,3]triazole (**1a**, 0.2 mmol, 39.0 mg), (E)-1,4-diphenylbut-1-en-3-yne（**2g**，0.3 mmol, 61.3 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol,2.6 mg) in mesitylene (1.6 mL) under **typical procedure** afforded 60 mg (75%) of **3ag** and **3ag'** (1.26:1.00) as a mixtures. HRMS m/z (ESI) calcd for $C_{28}H_{22}N_3$ $(M + H)^+$: 400.1808, found 400.1805.

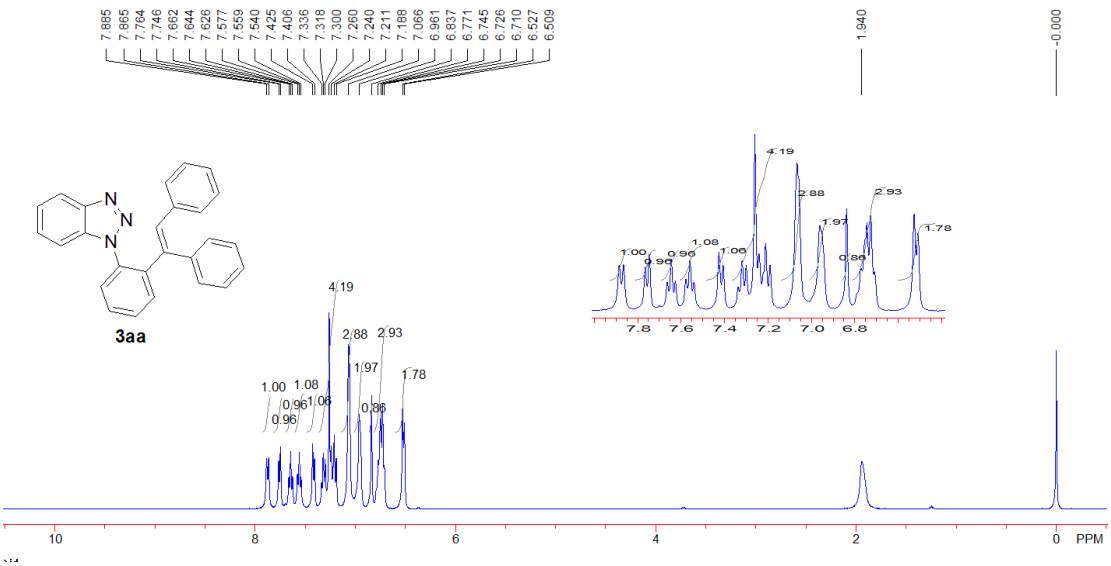
Deuterium-Labeling Experiments

1)



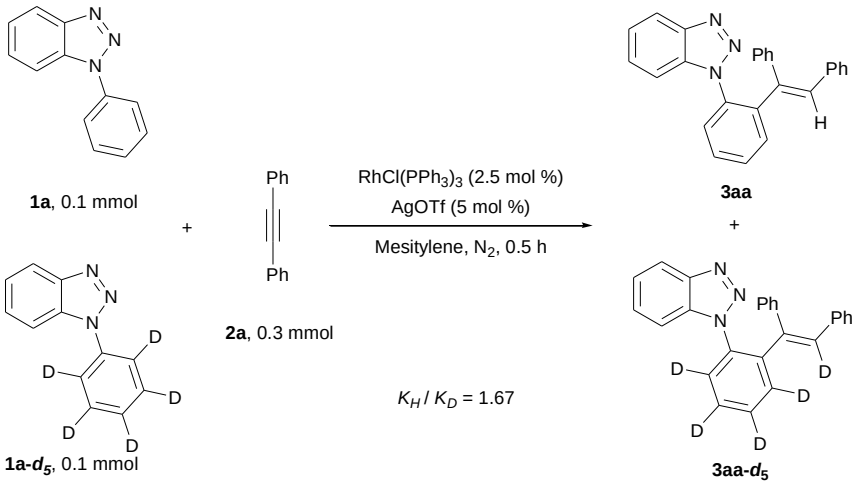
The reaction of **1a-*d*$_5$** (0.1 mmol, 20 mg), **2a** (0.15 mmol, 26.7 mg), RhCl(PPh$_3$)$_3$ (0.0025 mmol, 2.3 mg), AgOTf (0.005 mmol, 1.3 mg), H_2O (0.5 mmol, 9 μL) in mesitylene (0.8 mL) at 160 ^{o}C under N_2 for 0.5 h afforded **3aa-*d*$_5$** (3 mg, 8%) with the recovery of **1a-*d*$_5$** (17 mg, 85%).



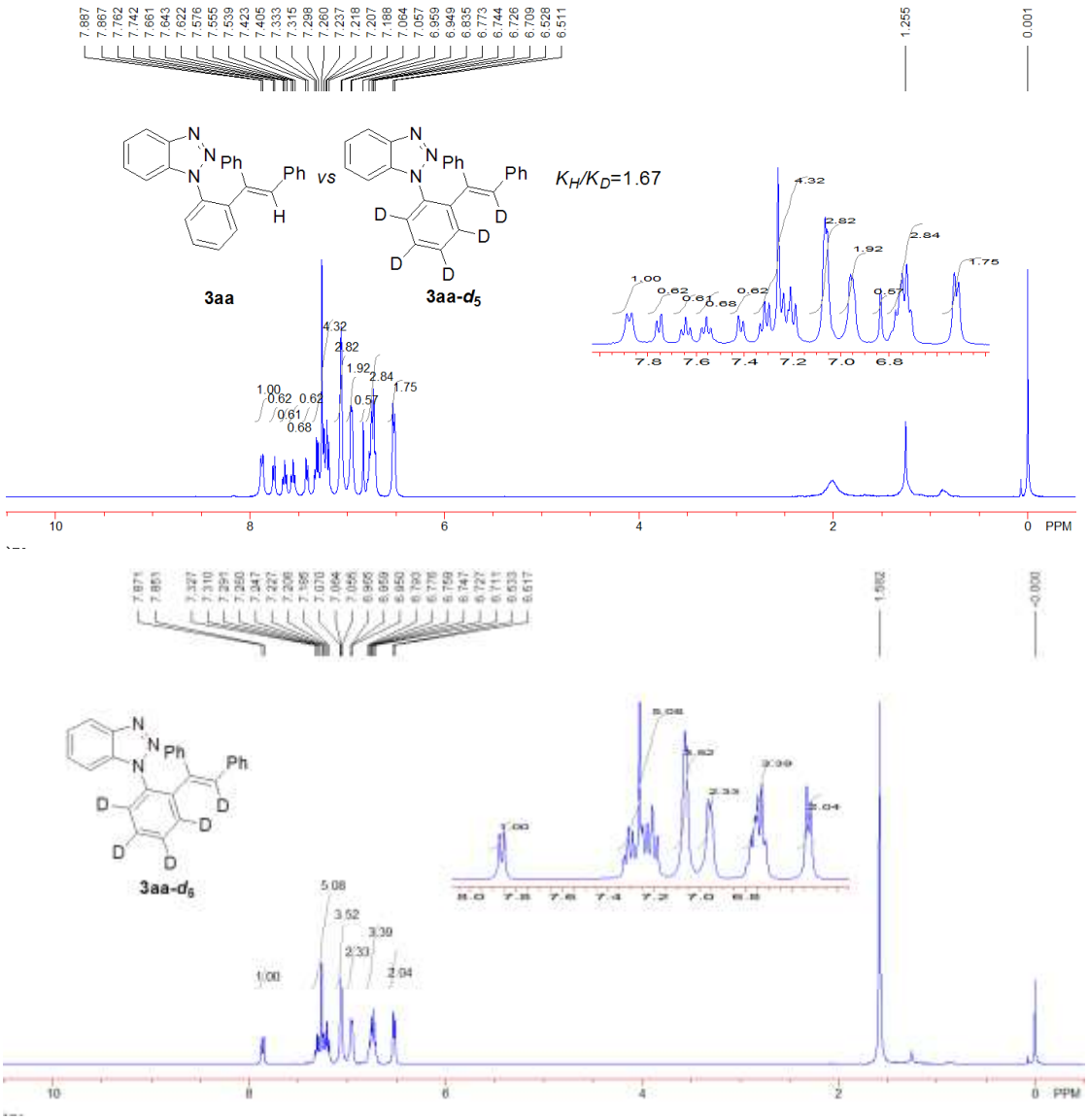


2) Kinetic Isotope Effect (KIE) Experiment:

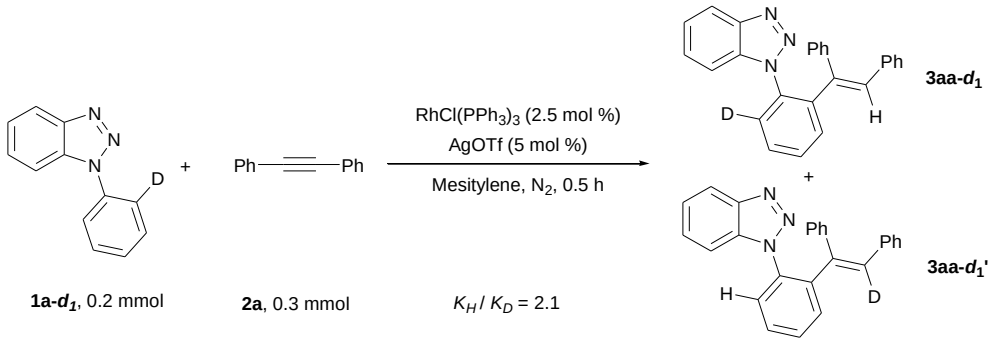
(1) Intermolecular KIE



The reaction of **1a** (0.1 mmol, 19.5 mg), **1a-*d*$_5$** (0.1 mmol, 20.0 mg), **2a** (0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) at 160 ^{o}C under N_2 for 0.5 h afforded **3aa** and **3aa-*d*$_5$** (**3aa** + **3aa-*d*$_5$**, 8 mg, 11%) with the ratio of 1.67:1.00 (**3aa**/**3aa-*d*$_5$**), which was determined by ^{1}H NMR.

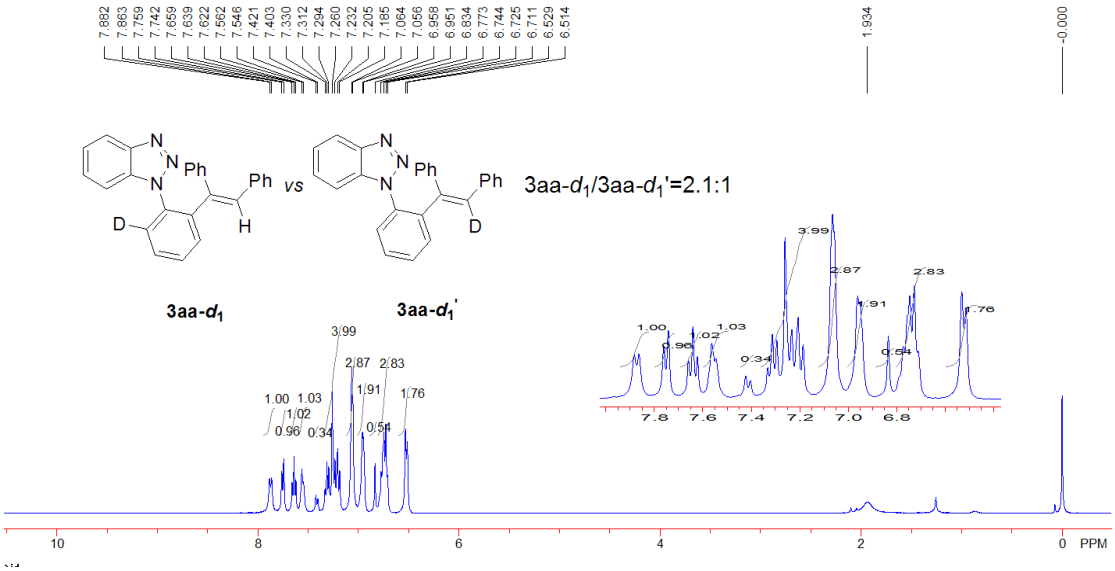


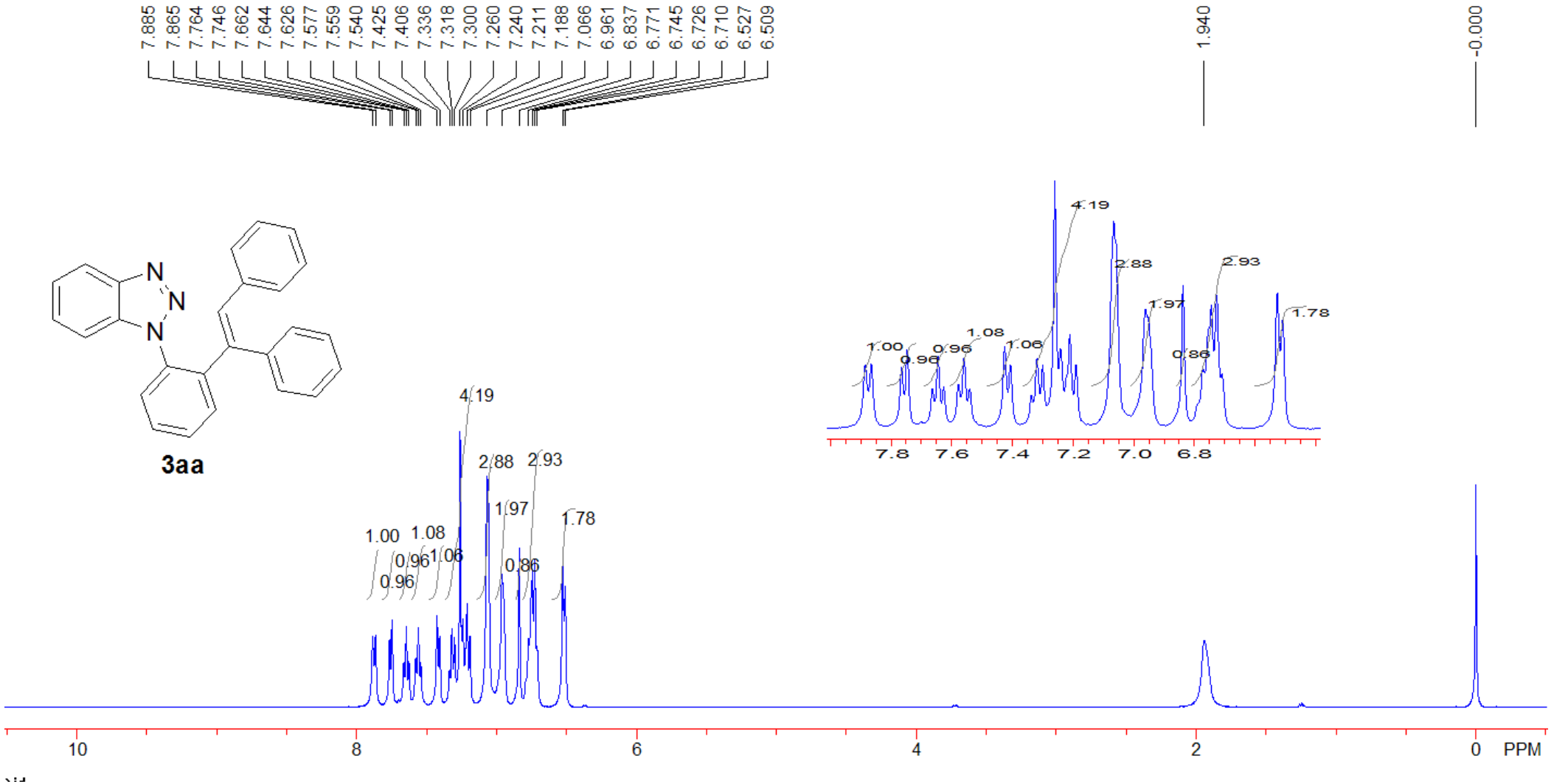
(2) Intramolecular KIE

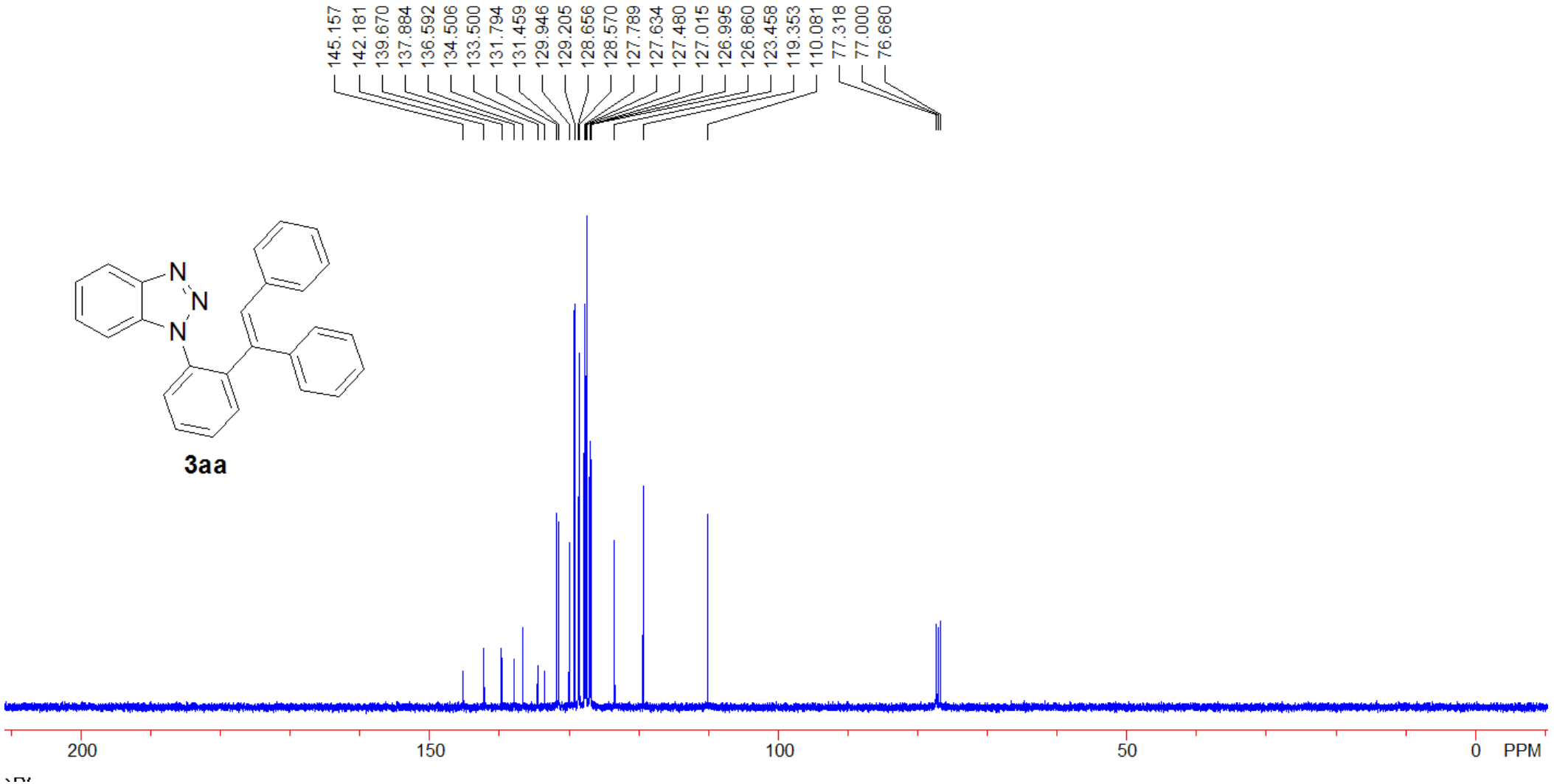


The reaction of **1a-*d*$_1$** (0.2 mmol, 39.2 mg), **2a** (0.3 mmol, 53.5 mg), $RhCl(PPh_3)_3$ (0.005 mmol, 4.6 mg), AgOTf (0.01 mmol, 2.6 mg) in mesitylene (1.6 mL) at 160 ^oC under N_2 for 0.5 h afforded **3aa-*d*$_1$** and **3aa-*d*$_1$'** (**3aa-*d*$_1$ + 3aa-*d*$_1$'**, 21 mg, 28 %) with

the ratio of 2.10:1.00 (**3aa-*d*$_1$/3aa-*d*$_1$'**).



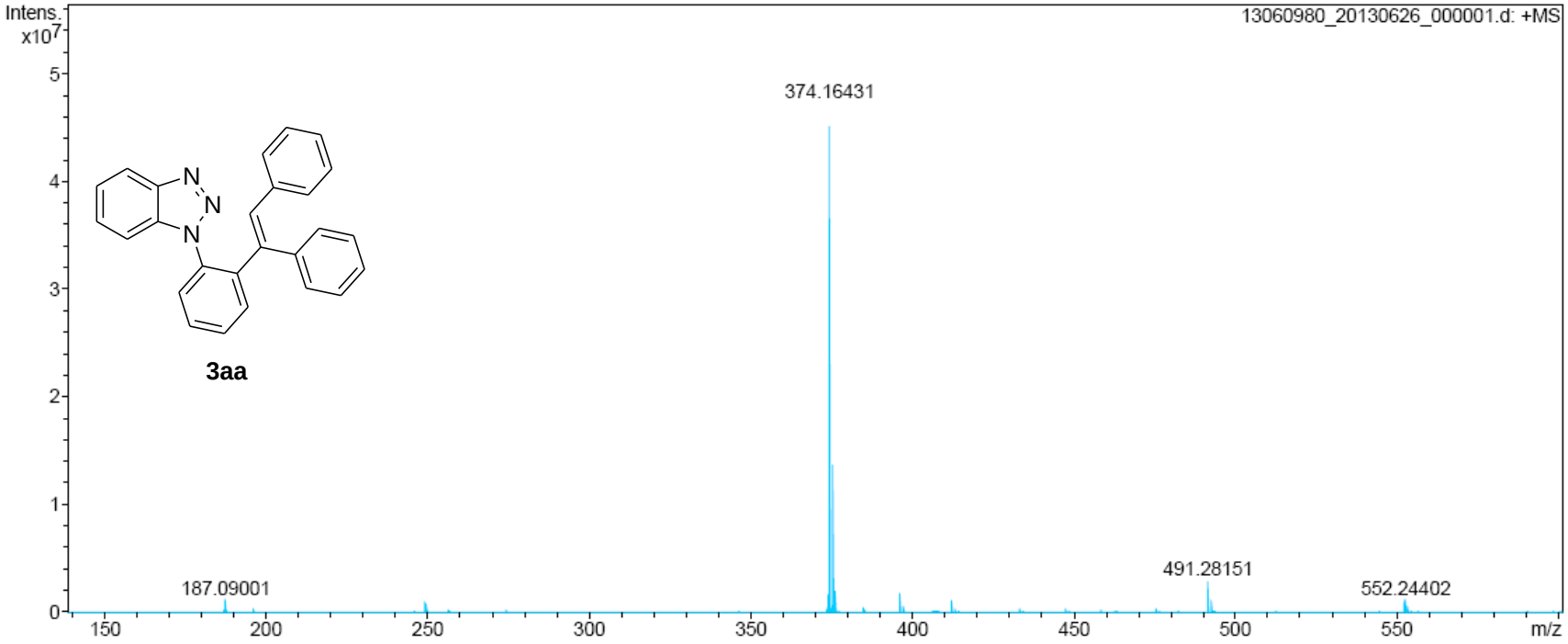




Peking University Mass Spectrometry Sample Analysis Report

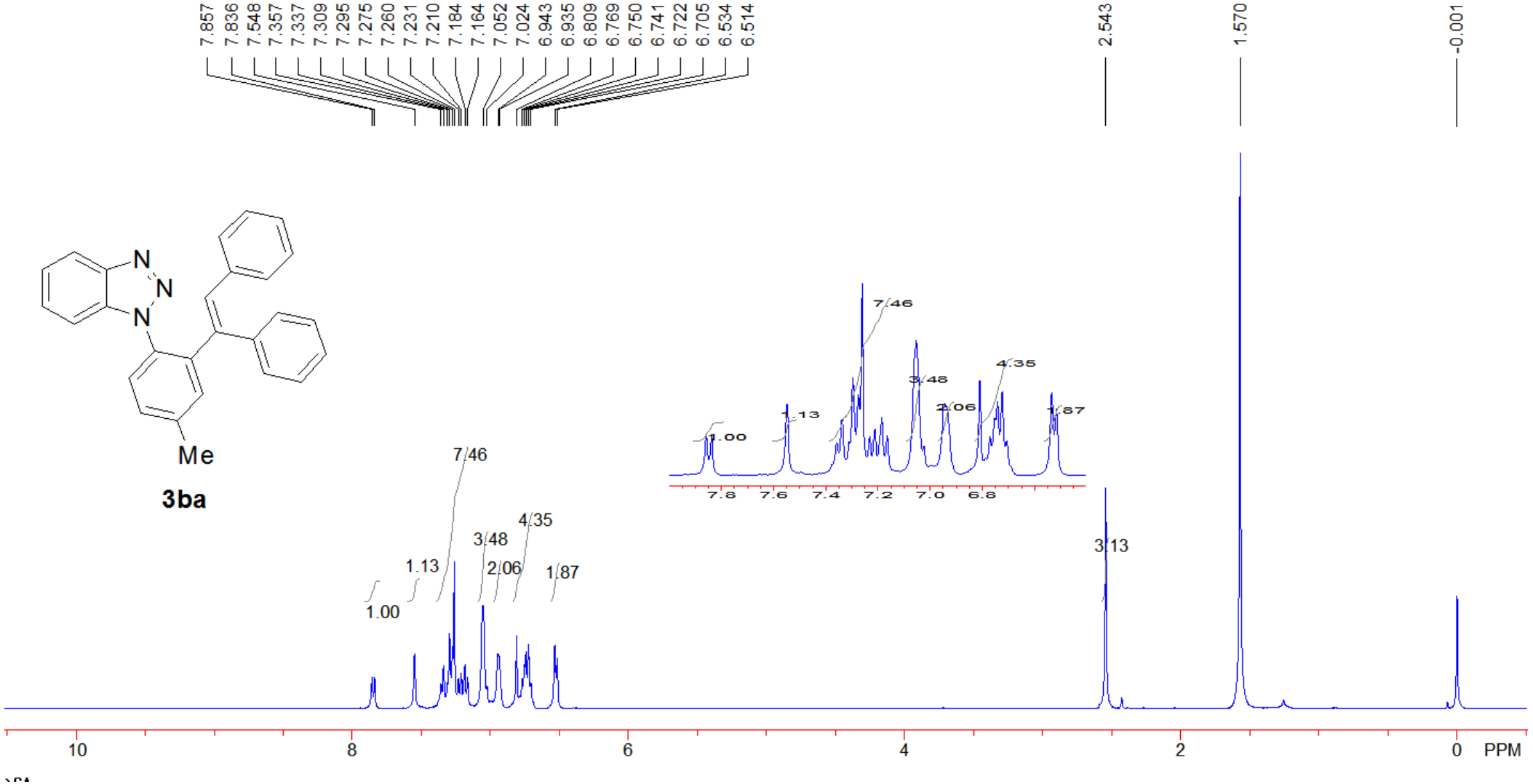
Analysis Info

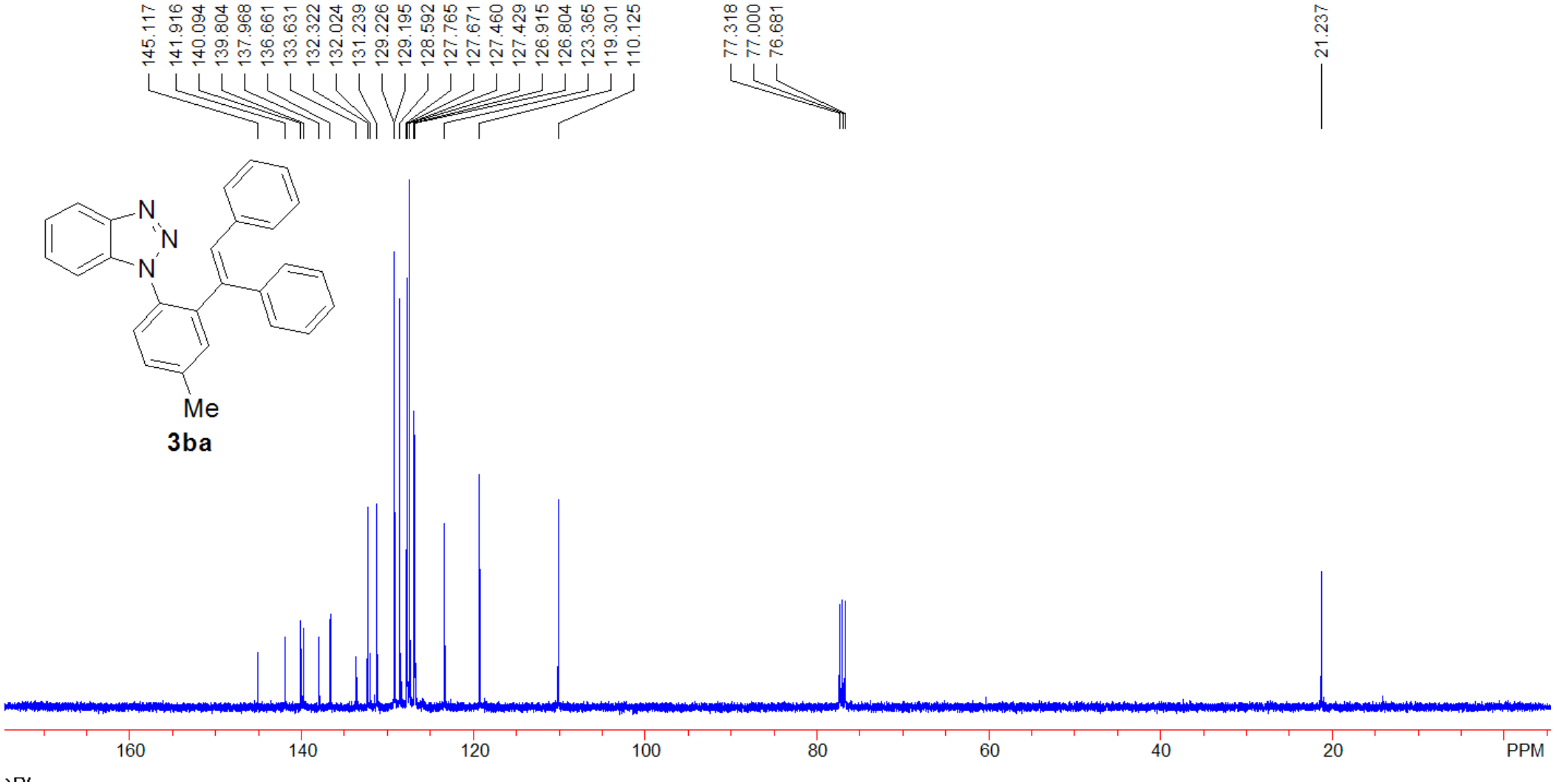
Analysis Name	13060980_20130626_000001.d	Acquisition Date	6/26/2013 8:24:20 PM
Sample	1	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3aa

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
374.16431	1	C 26 H 20 N 3	100.00	374.16517	0.9	2.3	1.5	18.5	even	ok

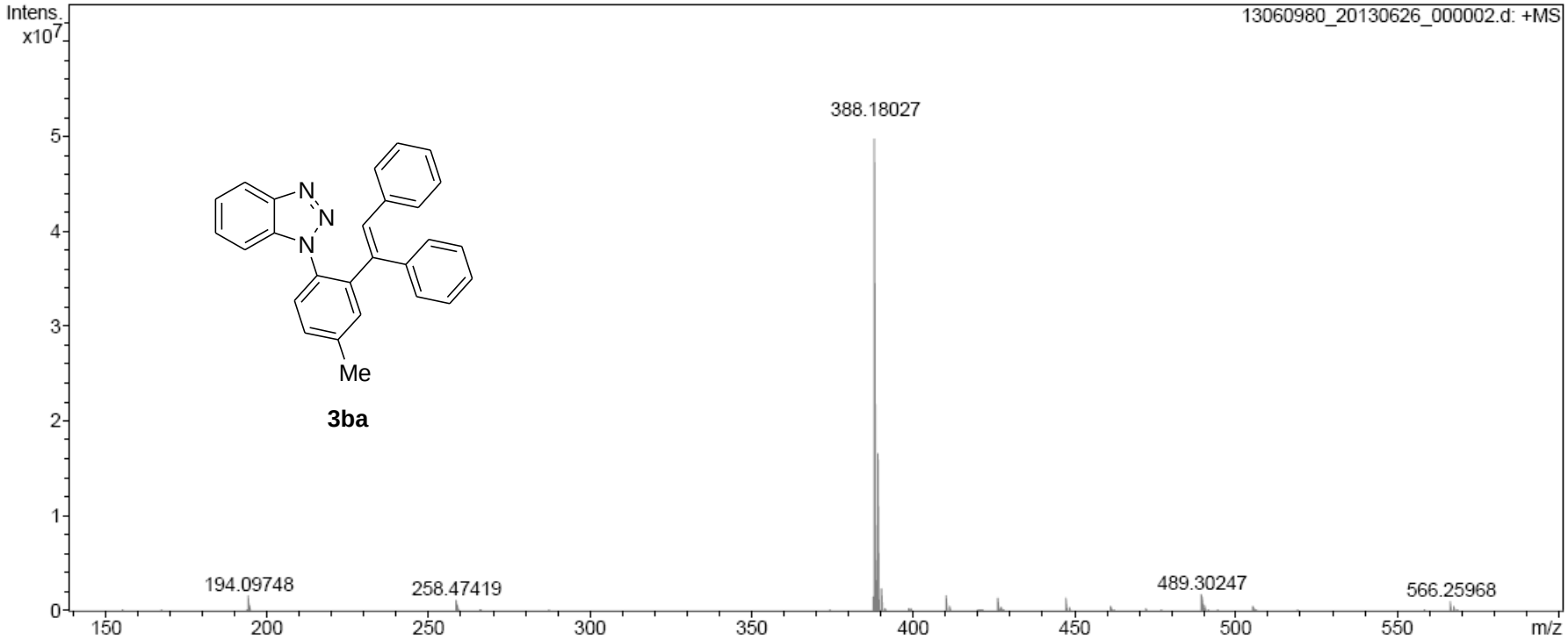




Peking University Mass Spectrometry Sample Analysis Report

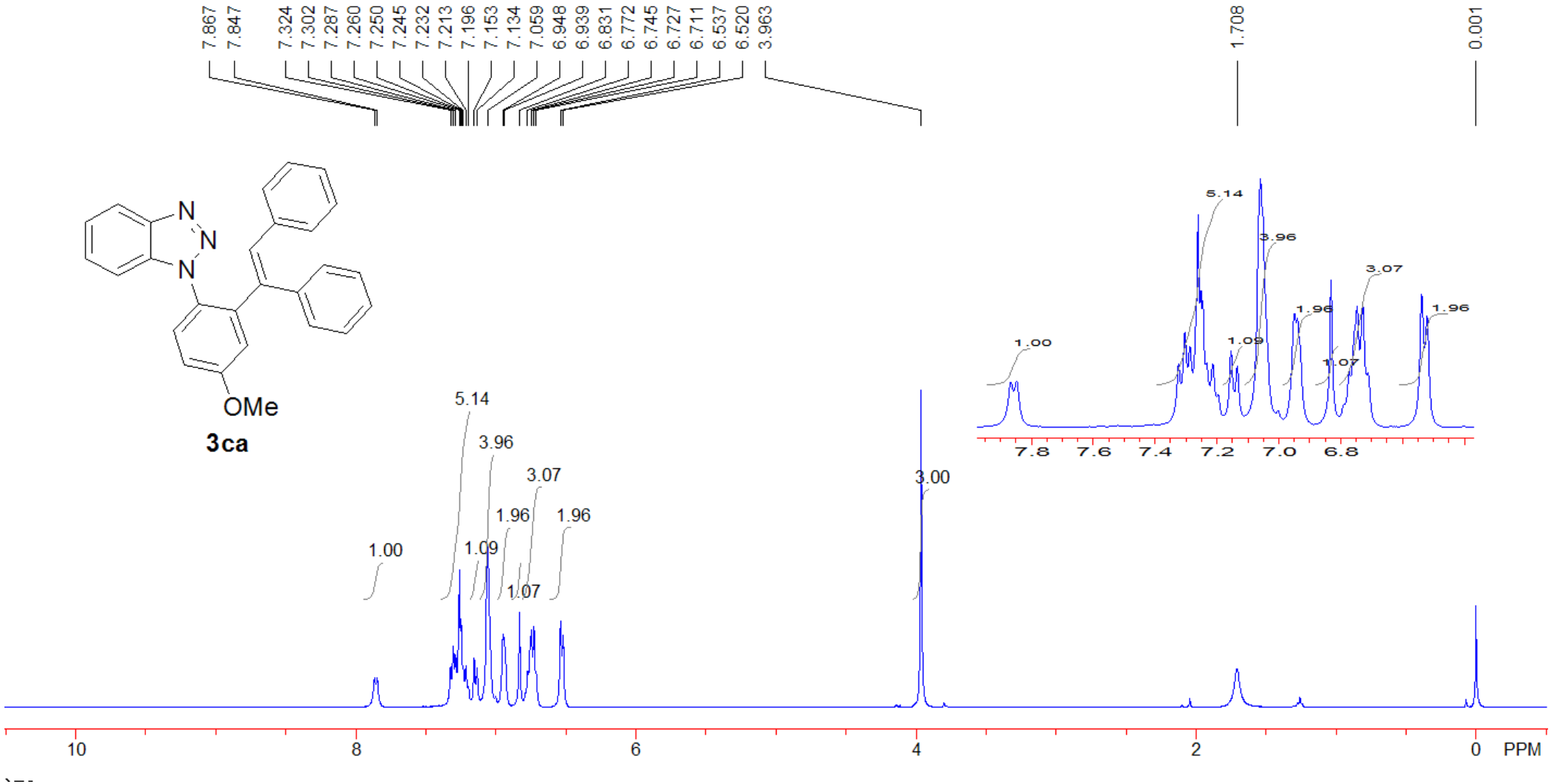
Analysis Info

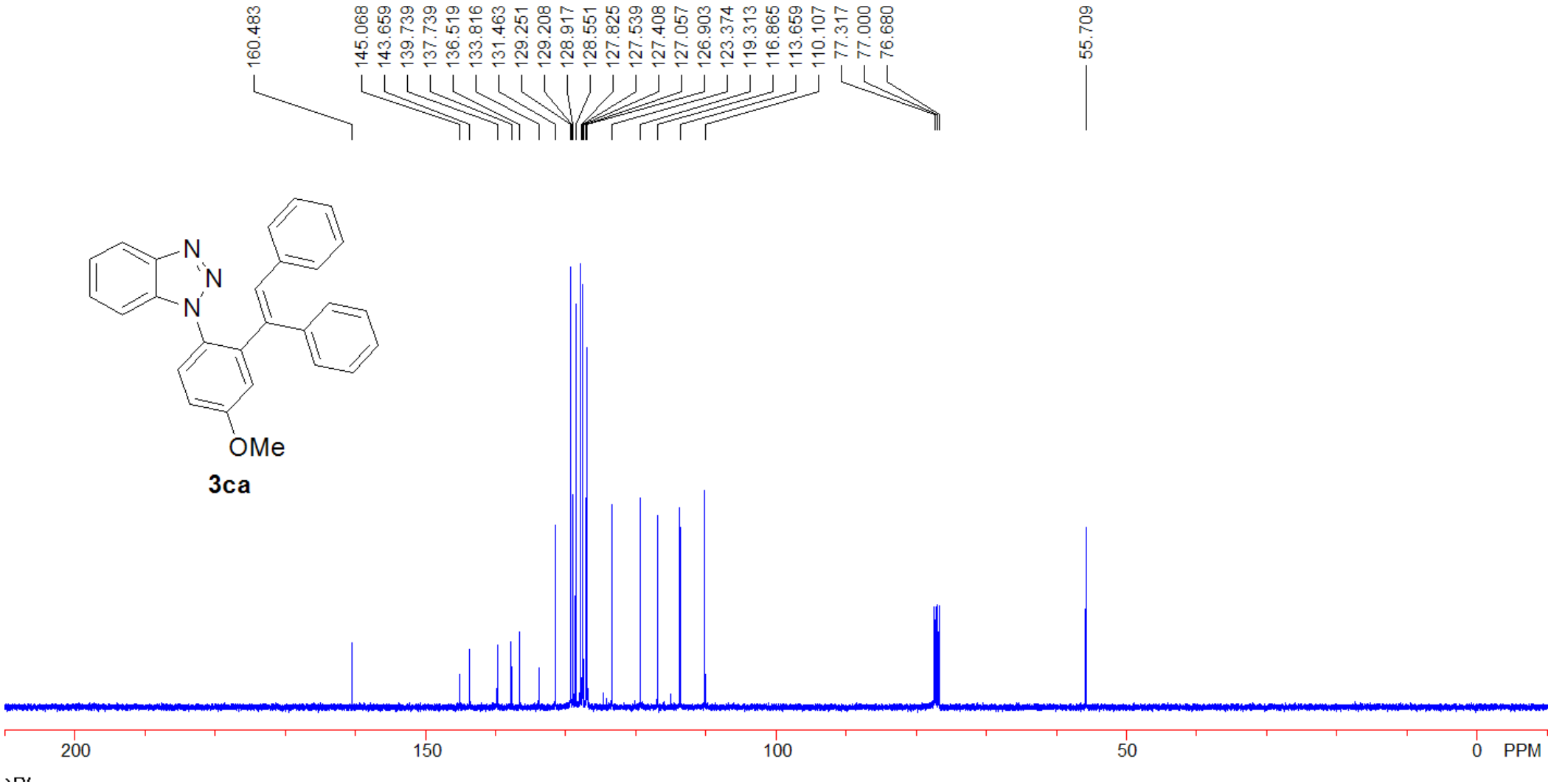
Analysis Name	13060980_20130626_000002.d	Acquisition Date	6/26/2013 8:26:28 PM
Sample	2	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ba

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
388.18027	1	C 27 H 22 N 3	100.00	388.18082	0.6	1.4	12.5	18.5	even	ok



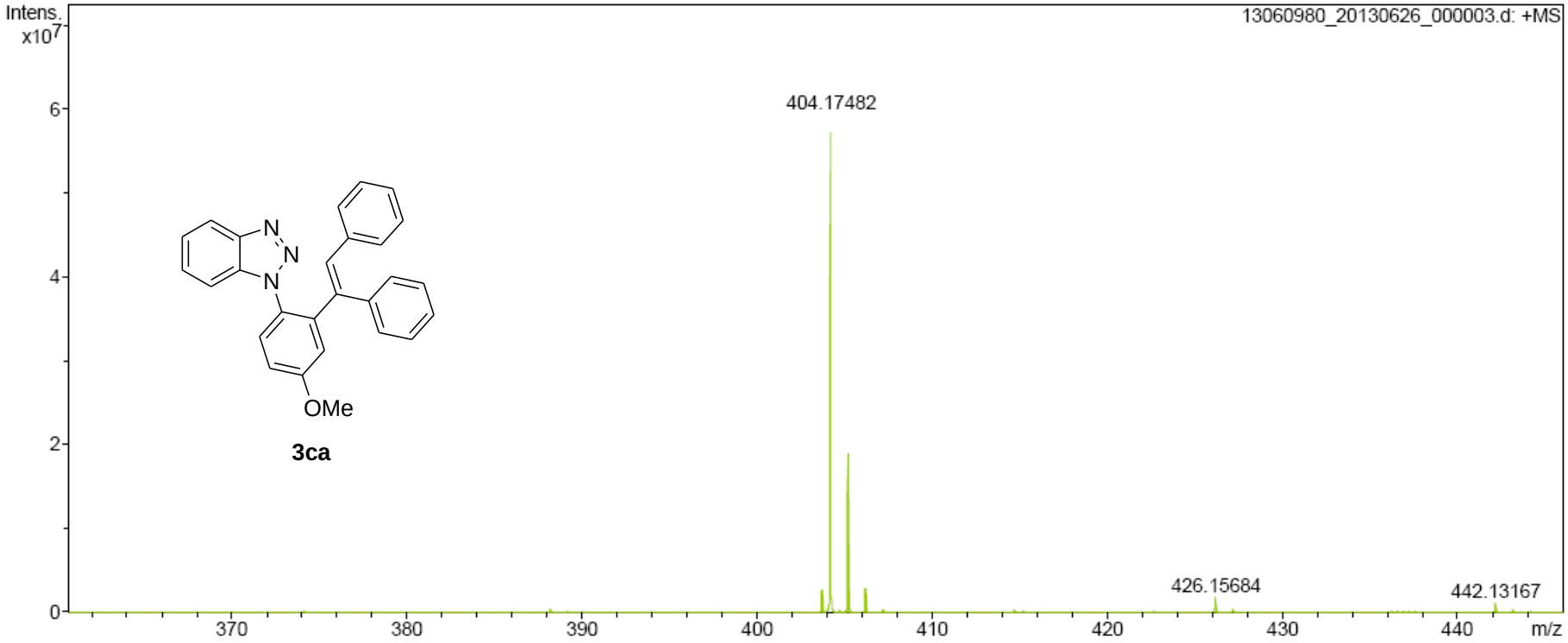


3ca

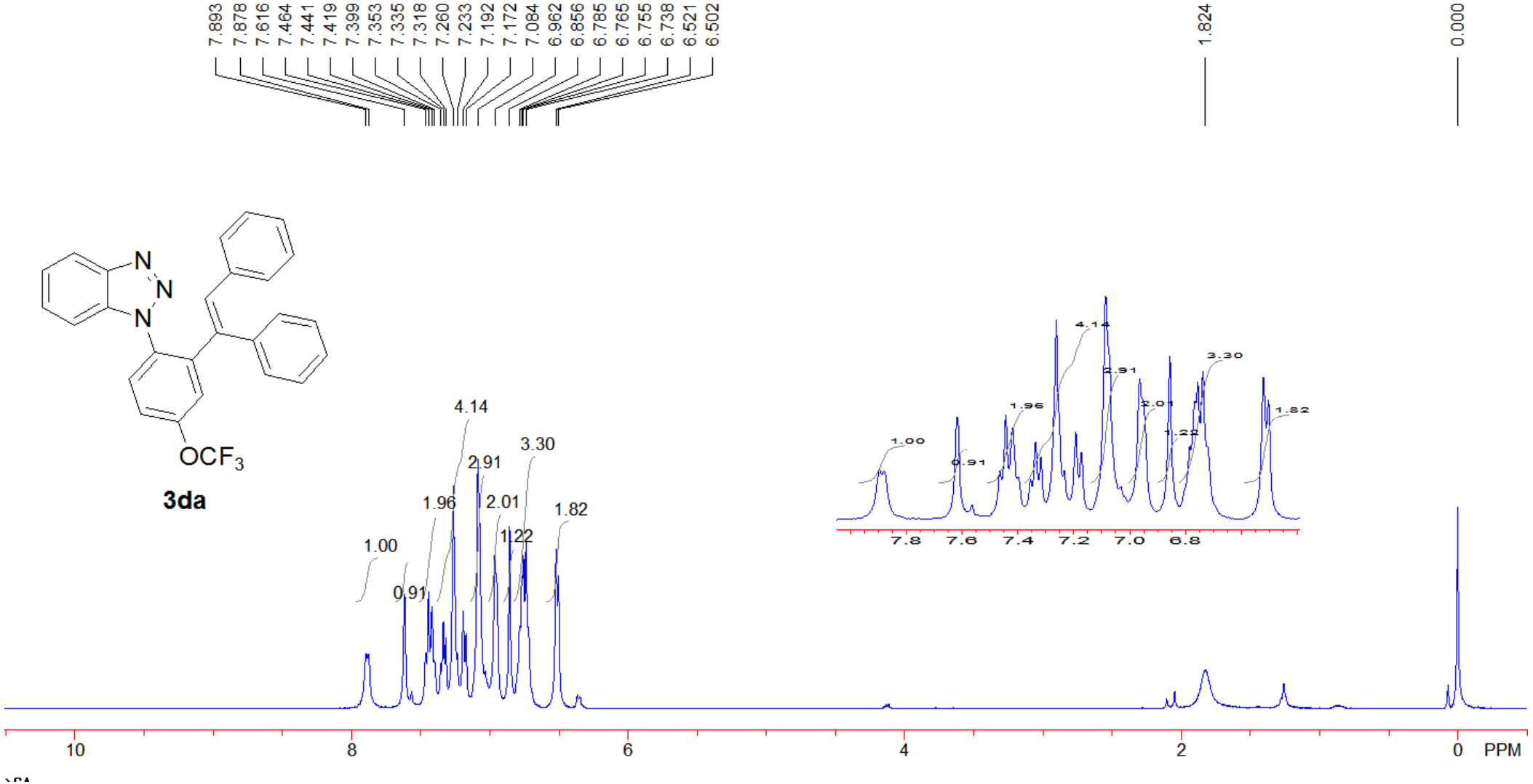
Peking University Mass Spectrometry Sample Analysis Report

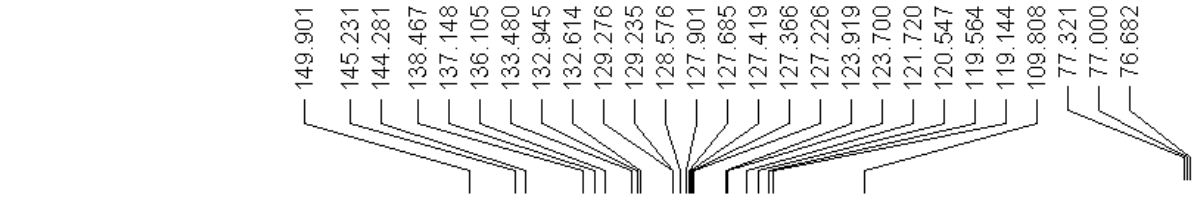
Analysis Info

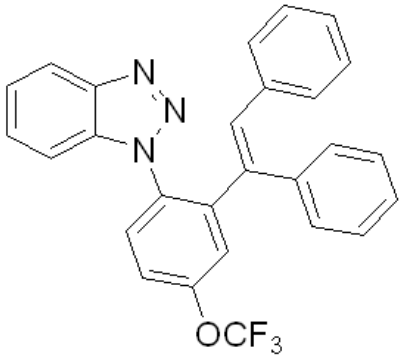
Analysis Name	13060980_20130626_000003.d	Acquisition Date	6/26/2013 8:29:56 PM
Sample	3	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



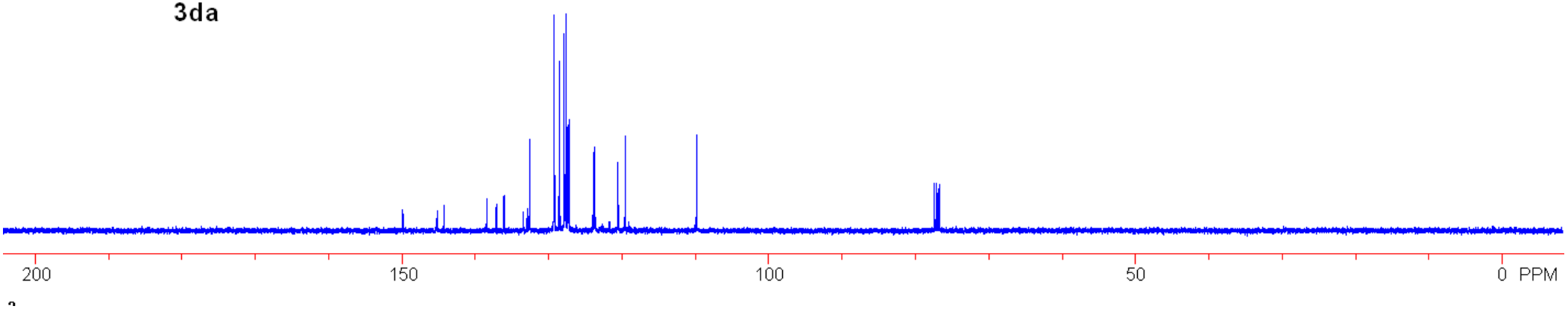
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
404.17482	1	C 27 H 22 N 3 O	100.00	404.17574	0.9	2.3	9.5	18.5	even	ok







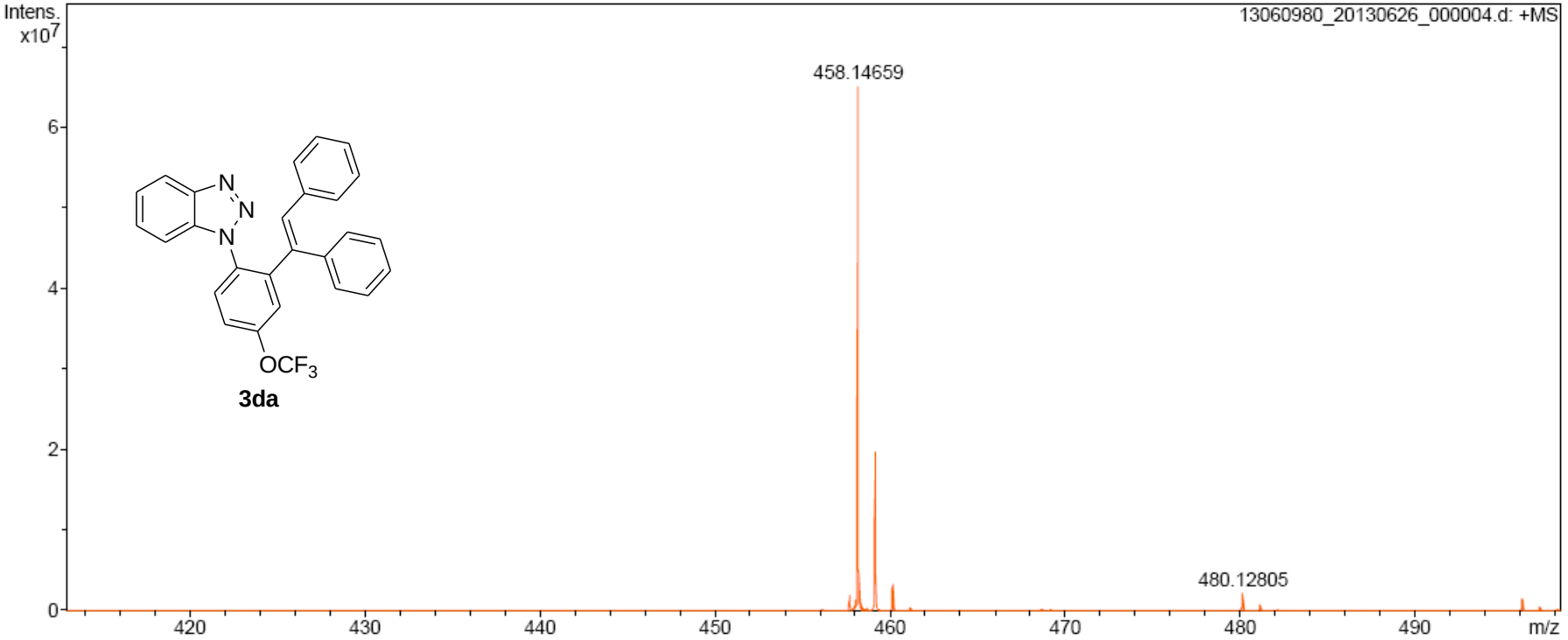
3da



Peking University Mass Spectrometry Sample Analysis Report

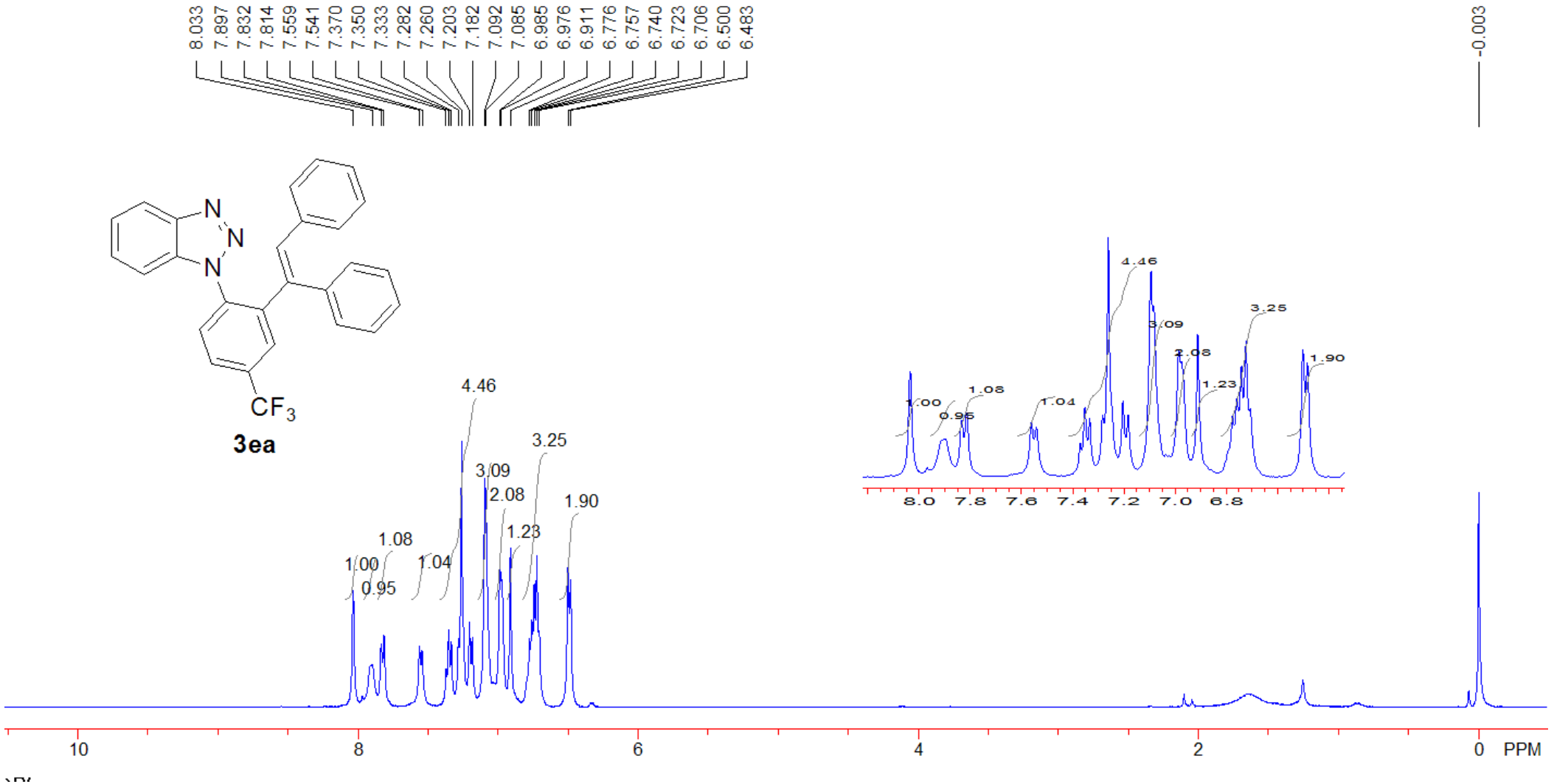
Analysis Info

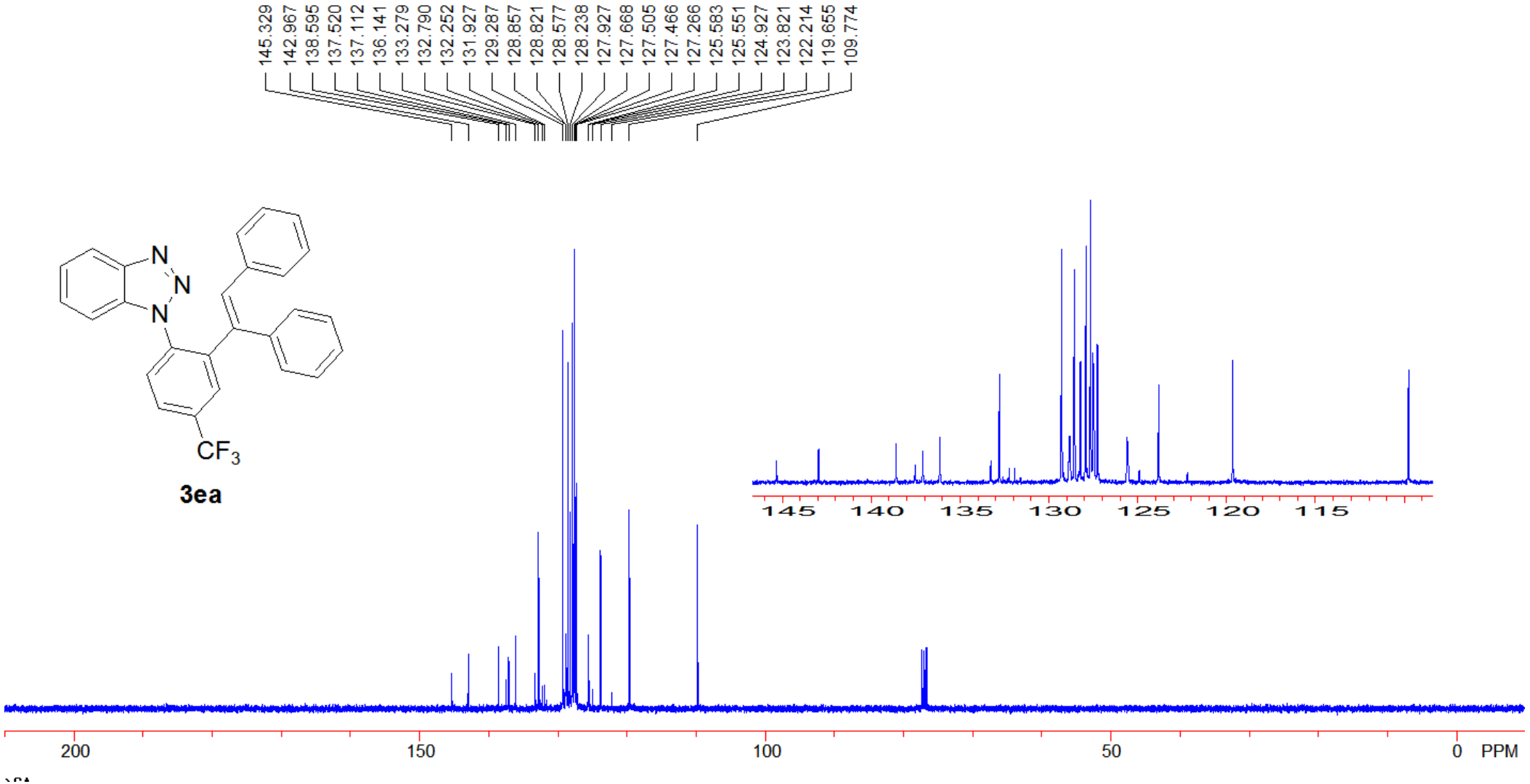
Analysis Name	13060980_20130626_000004.d	Acquisition Date	6/26/2013 8:32:32 PM
Sample	4	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3da

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
458.14659	1	C 27 H 19 F 3 N 3 O	100.00	458.14747	0.9	1.9	3.4	18.5	even	ok

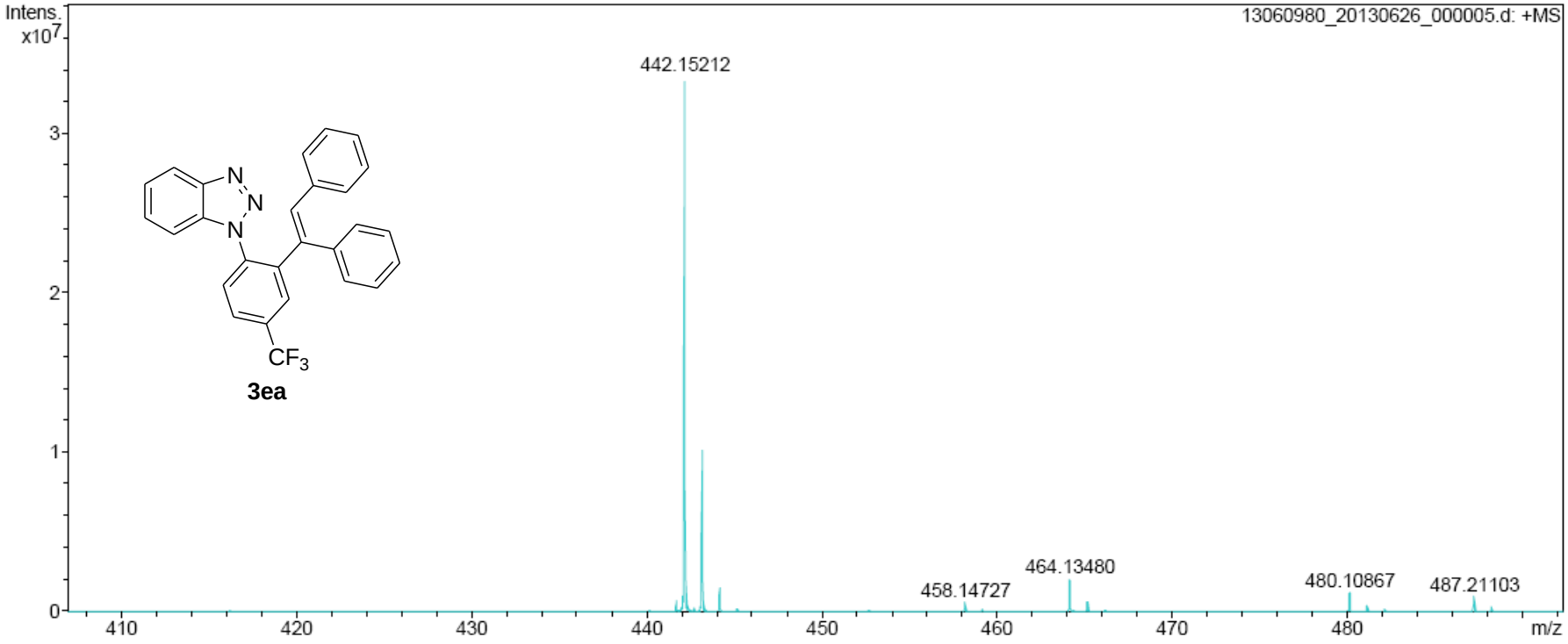




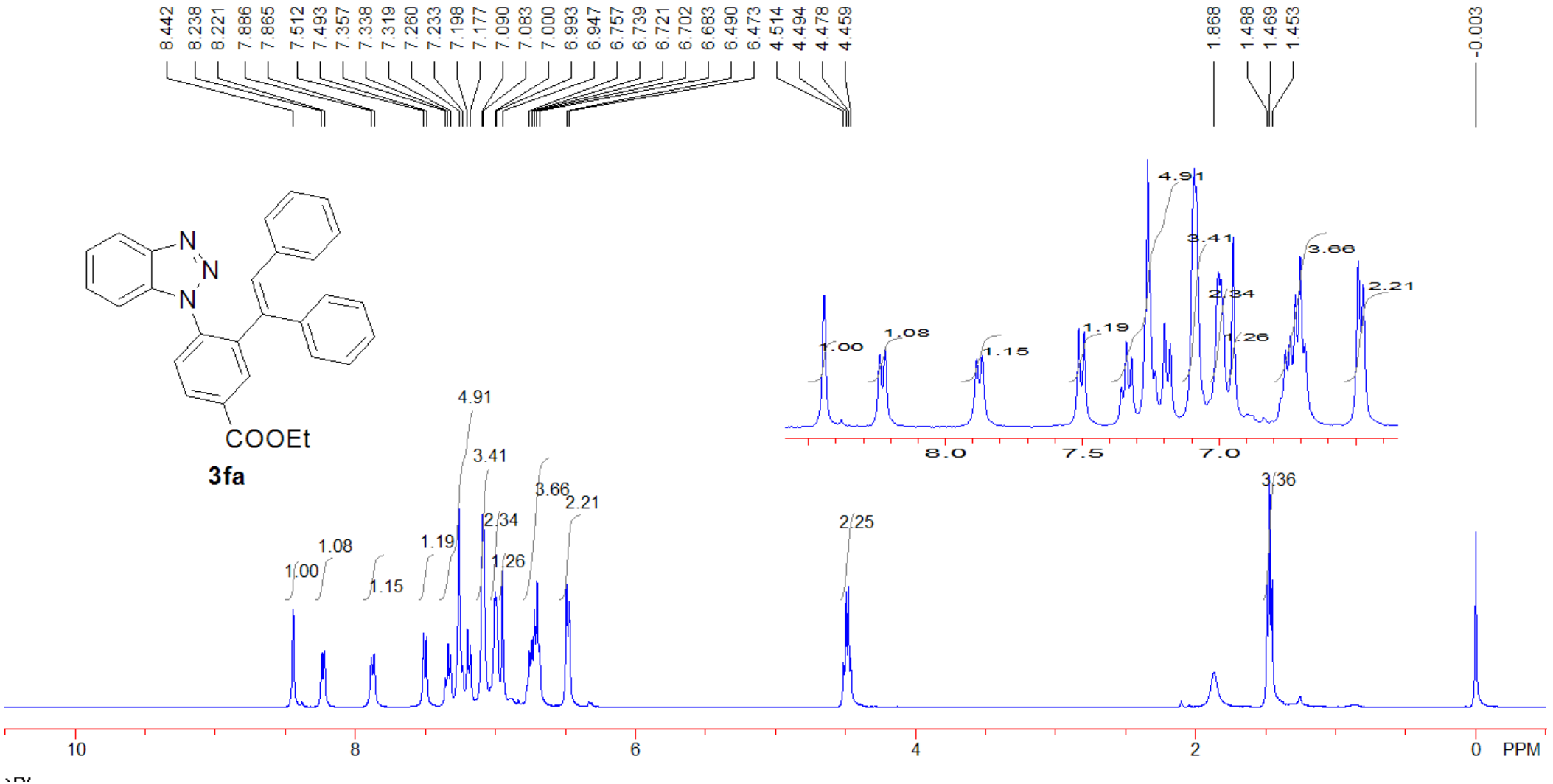
Peking University Mass Spectrometry Sample Analysis Report

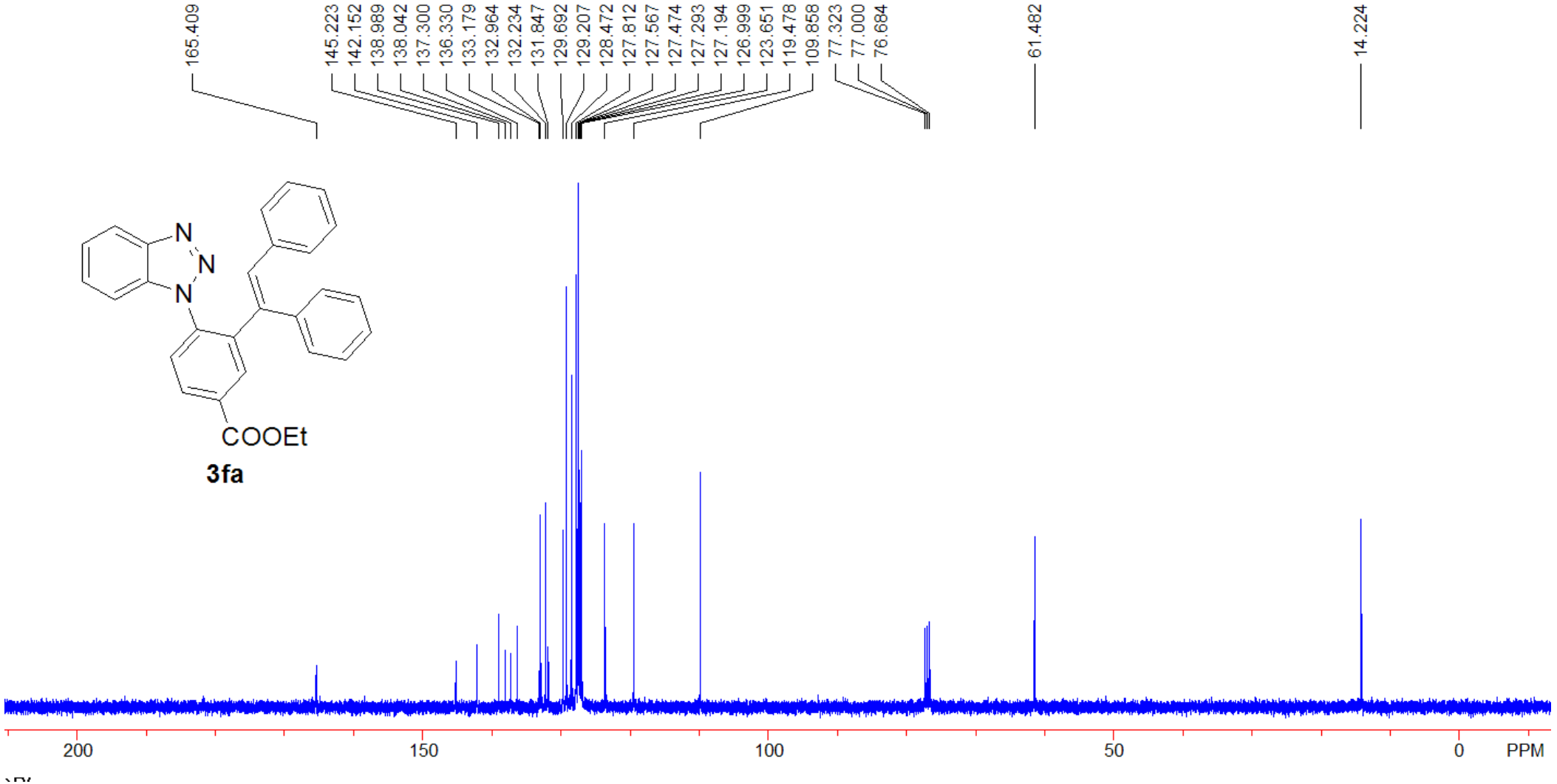
Analysis Info

Analysis Name	13060980_20130626_000005.d	Acquisition Date	6/26/2013 8:35:33 PM
Sample	5	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
442.15212	1	C 27 H 19 F 3 N 3	100.00	442.15256	0.4	1.0	1.9	18.5	even	ok



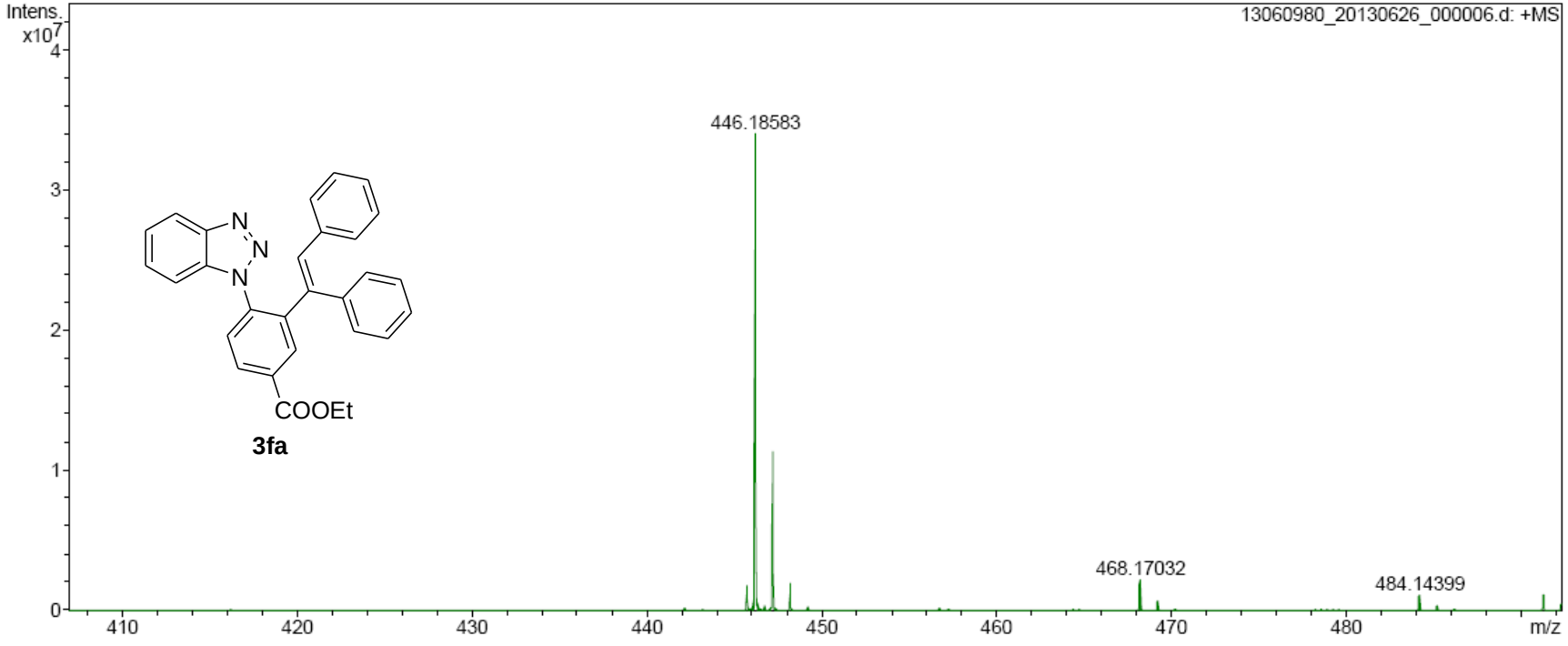


3fa

Peking University Mass Spectrometry Sample Analysis Report

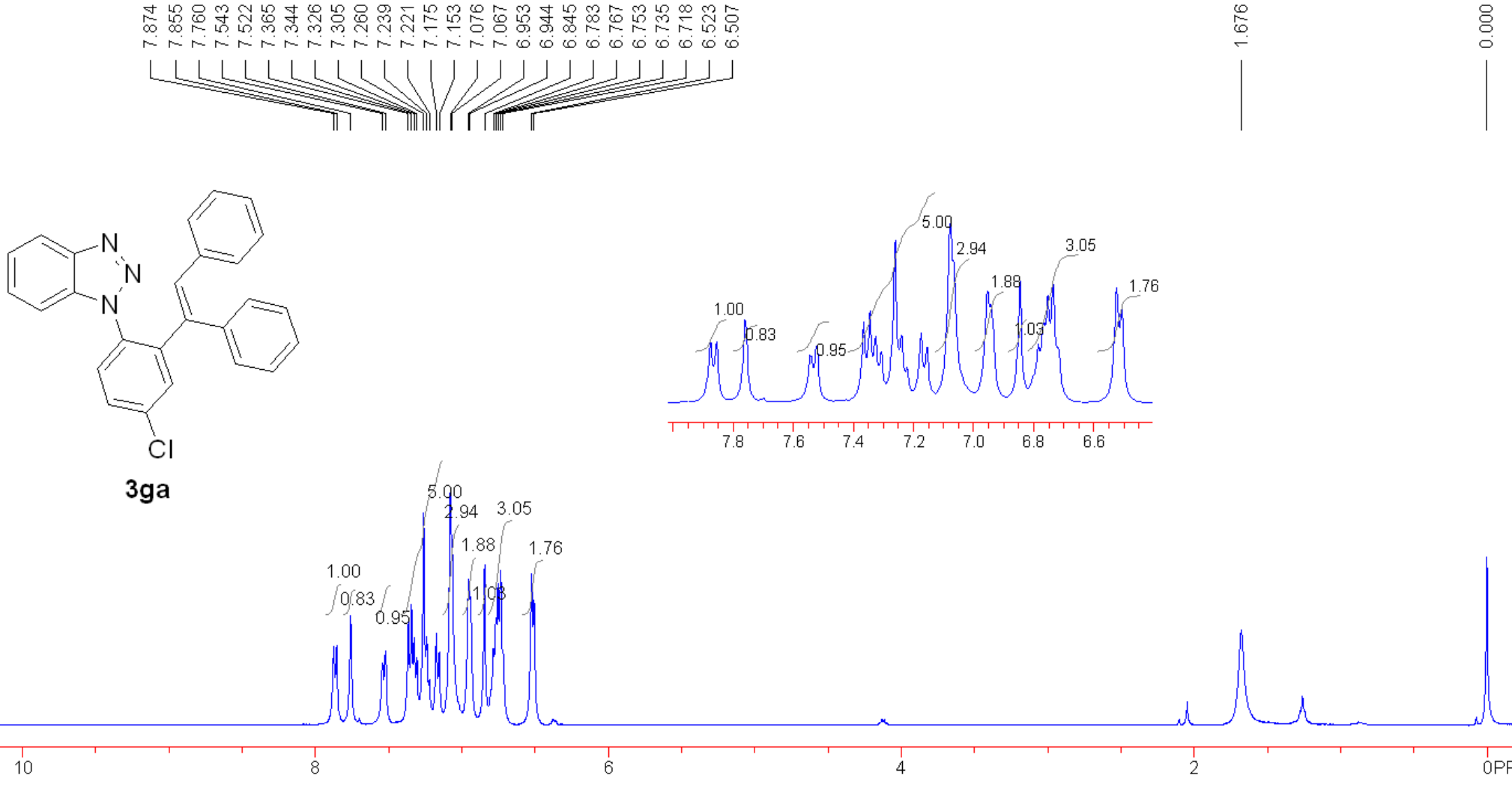
Analysis Info

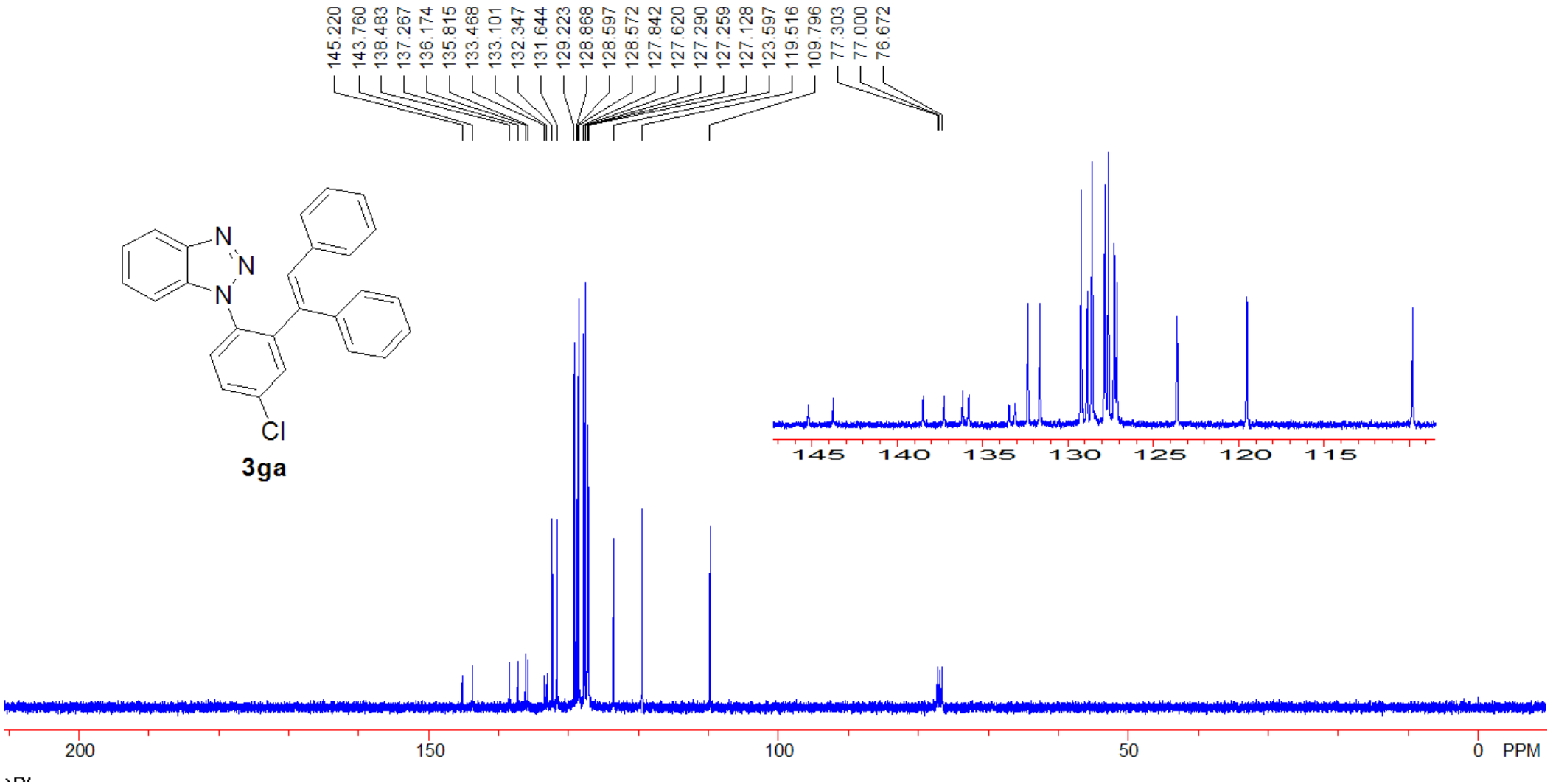
Analysis Name	13060980_20130626_000006.d	Acquisition Date	6/26/2013 8:37:42 PM
Sample	6	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3fa

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
446.18583	1	C 29 H 24 N 3 O 2	100.00	446.18630	0.5	1.1	4.9	19.5	even	ok

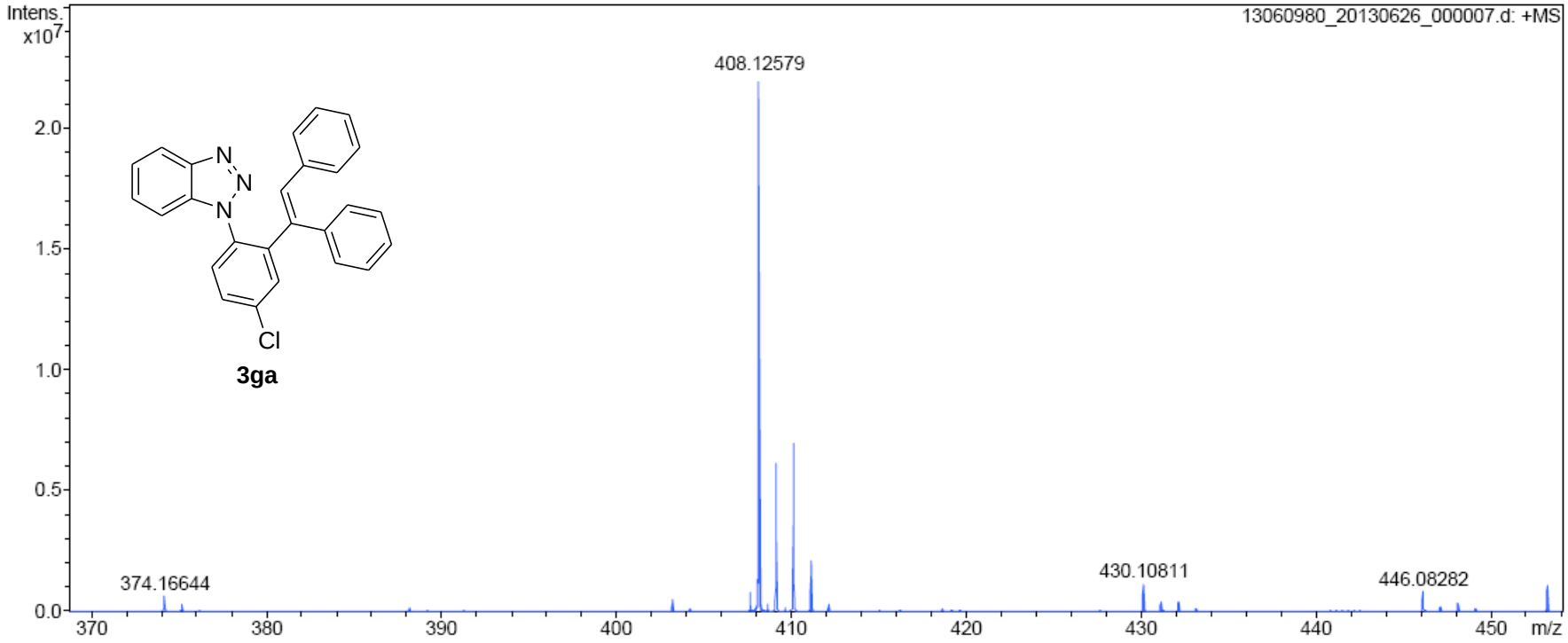




Peking University Mass Spectrometry Sample Analysis Report

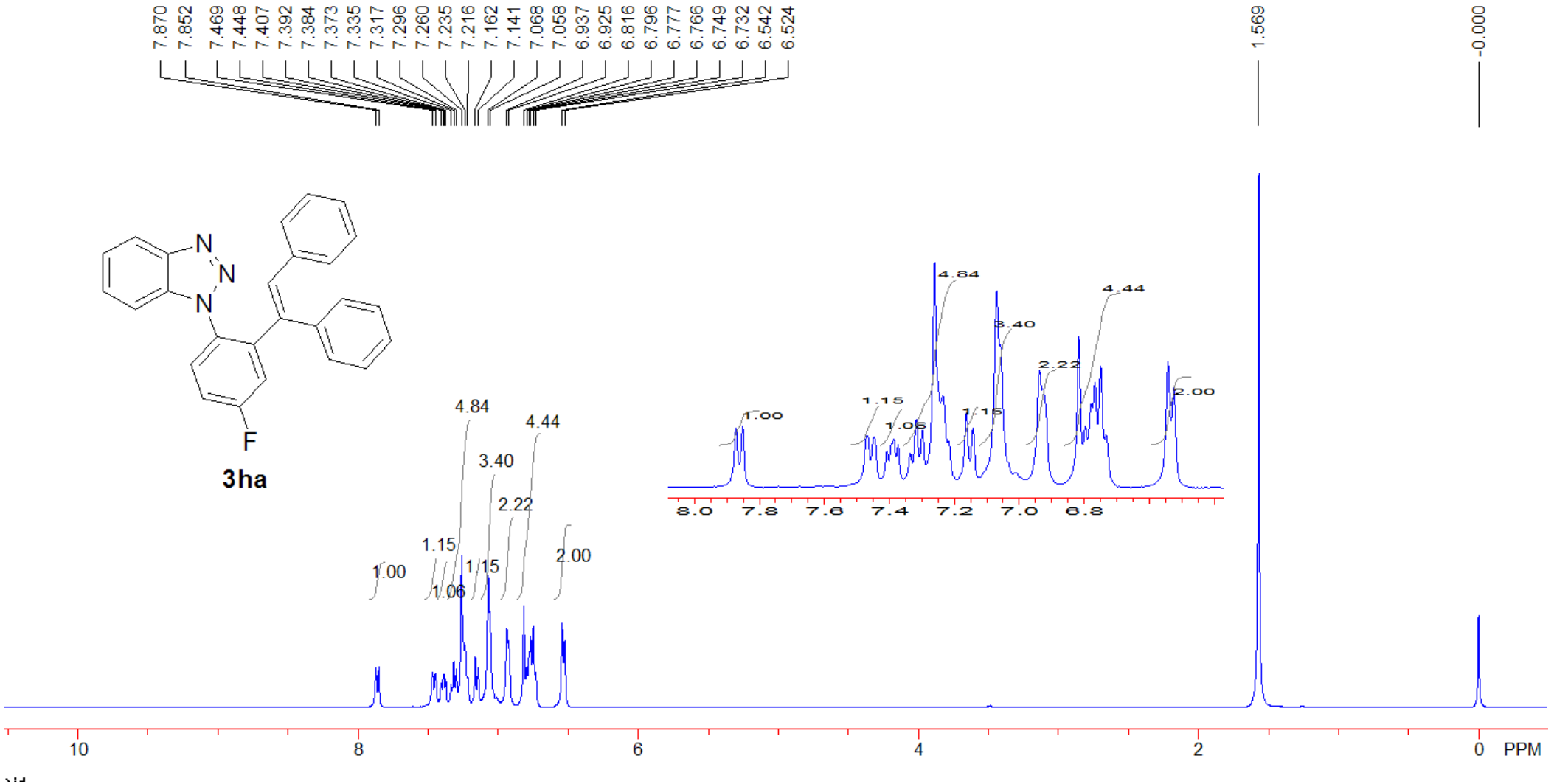
Analysis Info

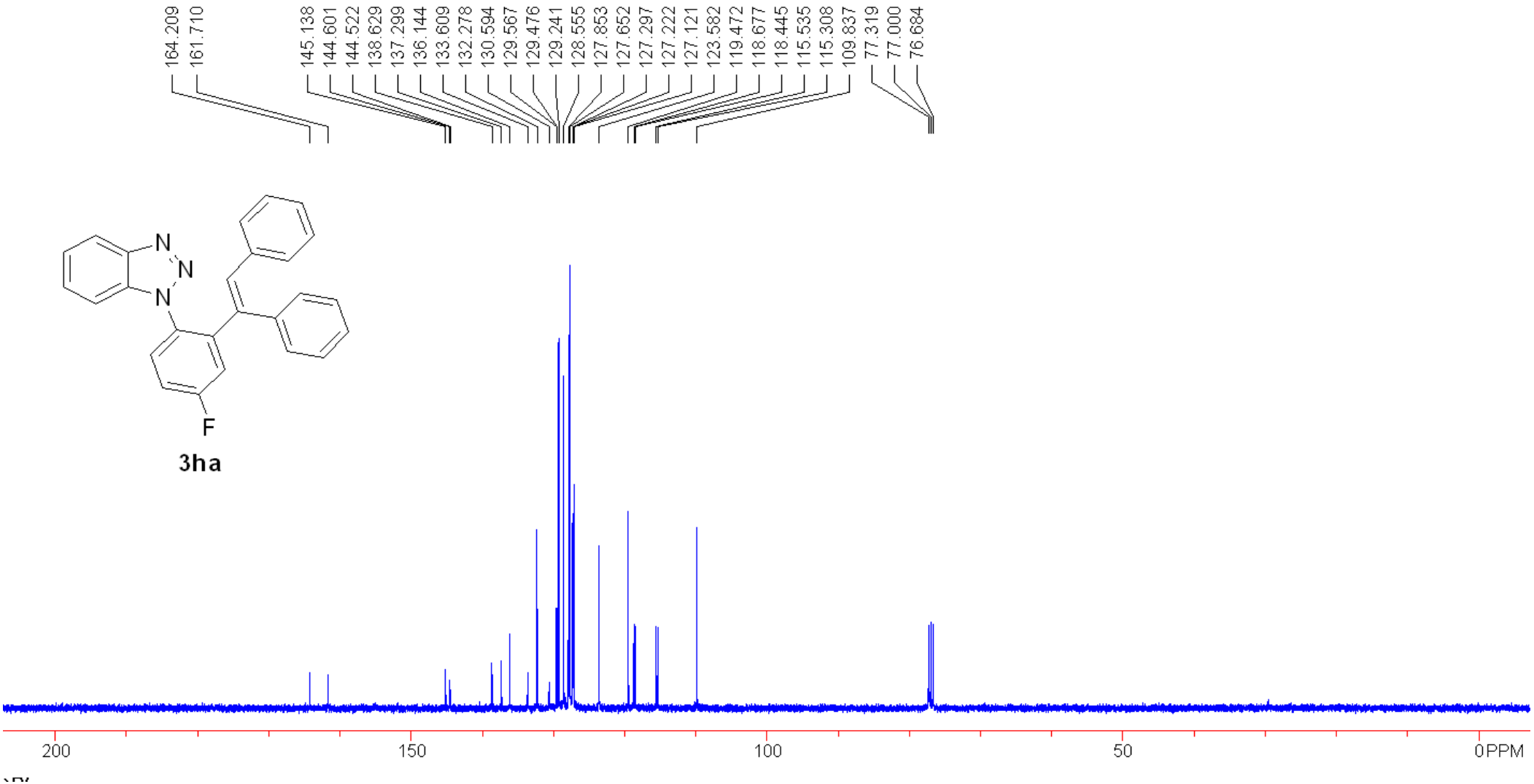
Analysis Name	13060980_20130626_000007.d	Acquisition Date	6/26/2013 8:39:43 PM
Sample	7	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ga

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
408.12579	1	C 26 H 19 Cl N 3	100.00	408.12620	0.4	1.0	15.9	18.5	even	ok



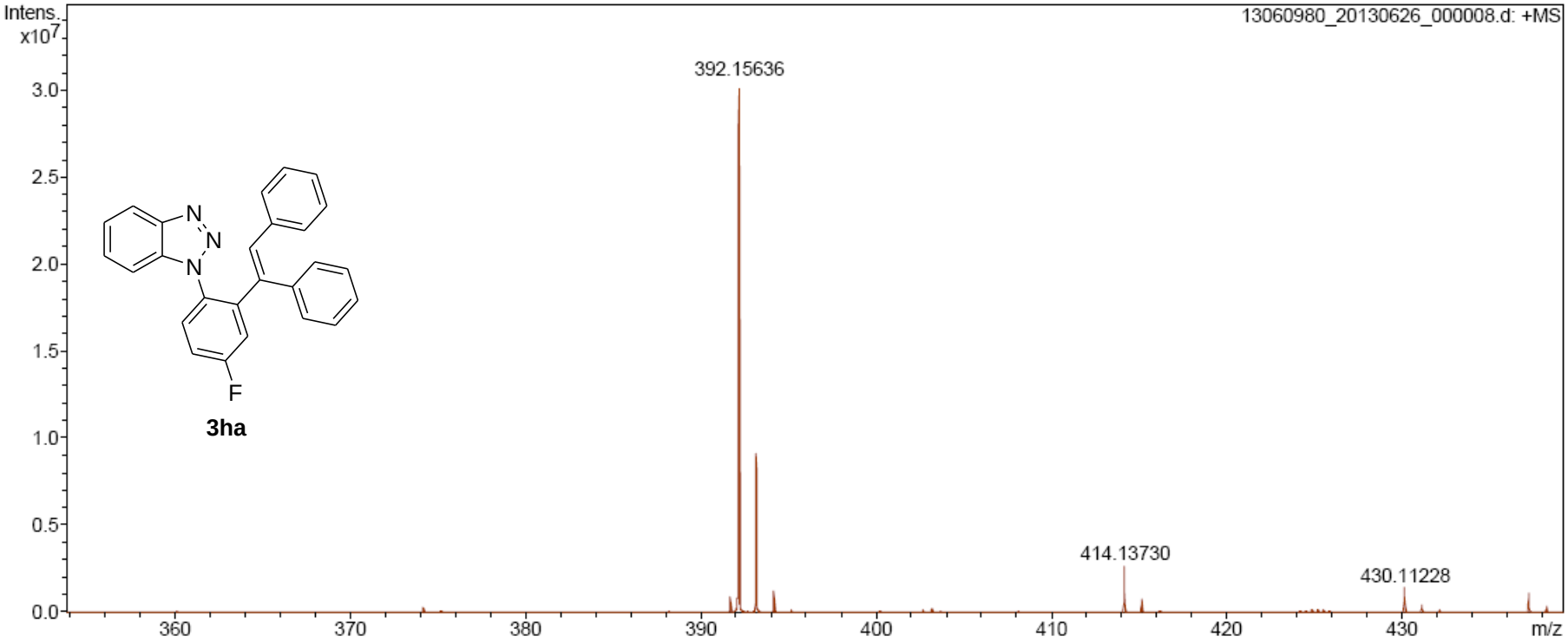


3ha

Peking University Mass Spectrometry Sample Analysis Report

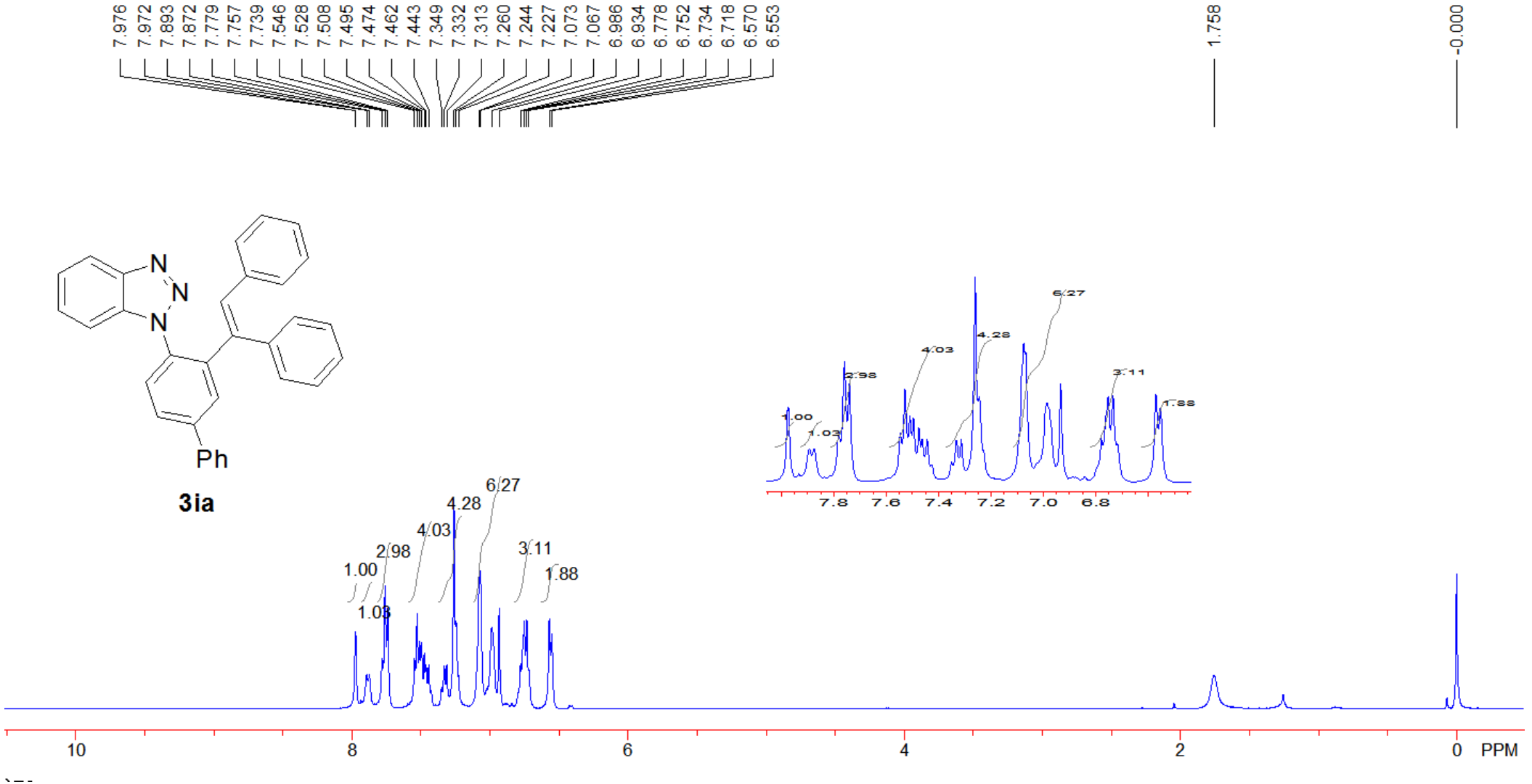
Analysis Info

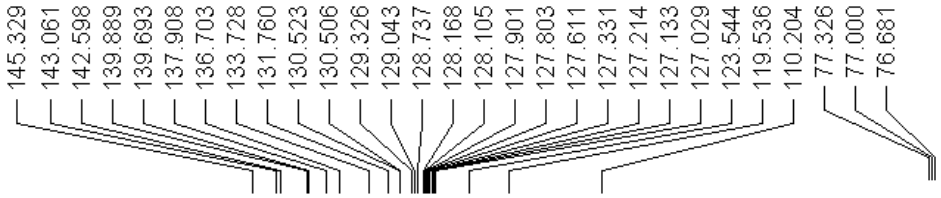
Analysis Name	13060980_20130626_000008.d	Acquisition Date	6/26/2013 8:41:39 PM
Sample	8	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University

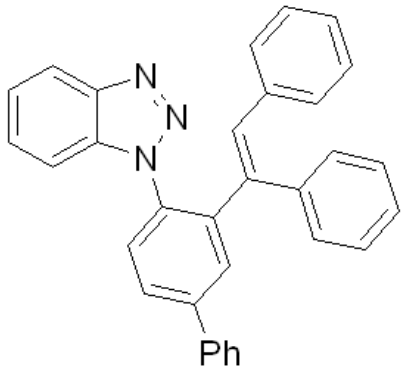


3ha

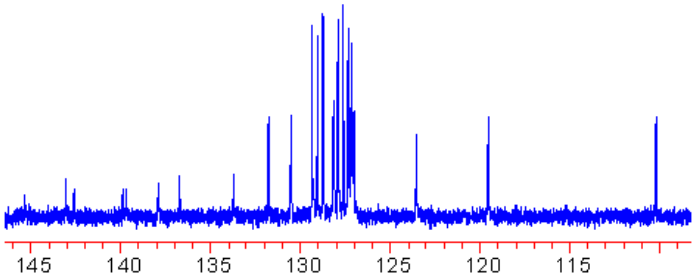
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
392.15636	1	C 26 H 19 F N 3	100.00	392.15575	-0.6	-1.5	5.7	18.5	even	ok

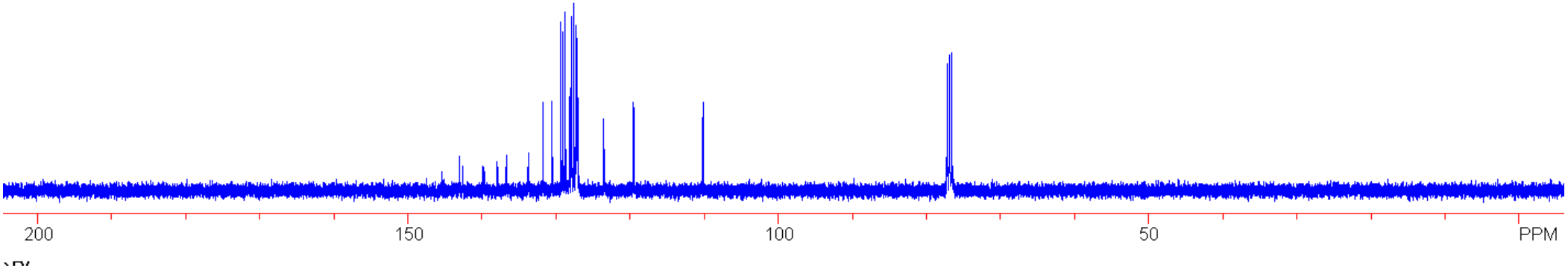






3ia

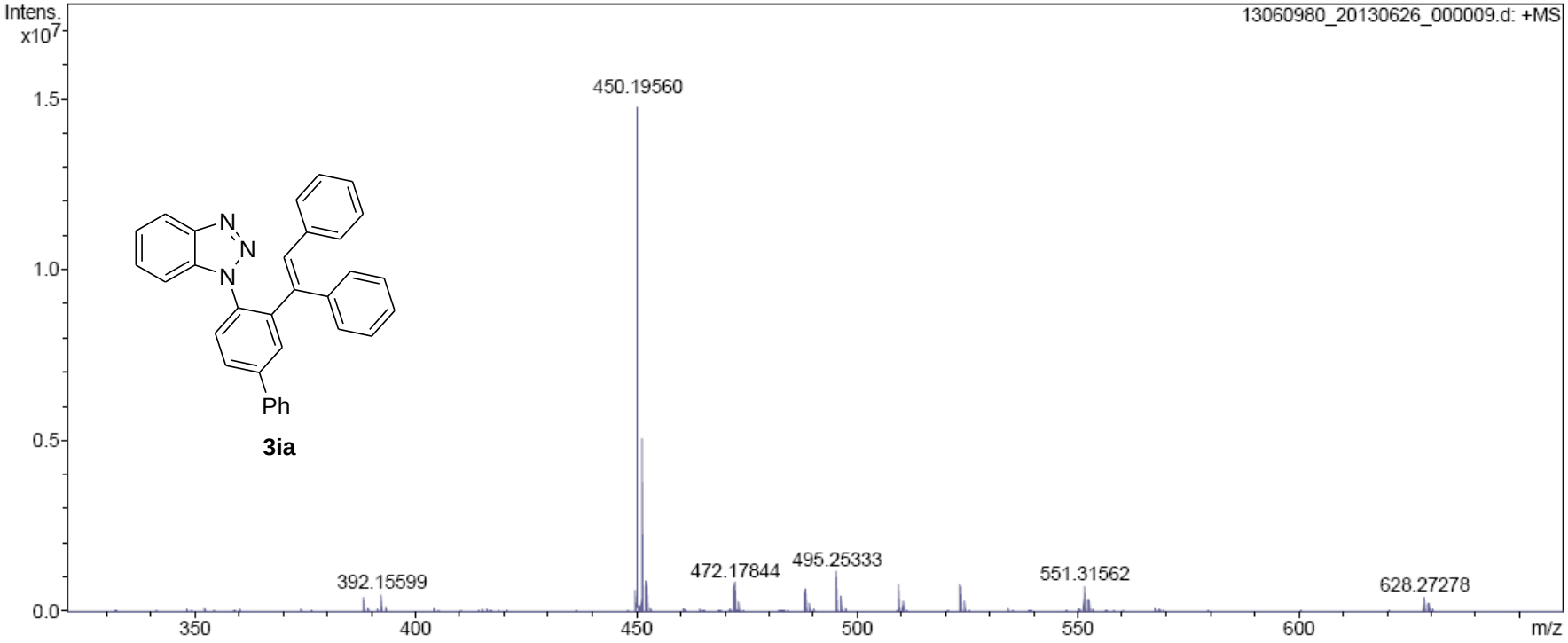




Peking University Mass Spectrometry Sample Analysis Report

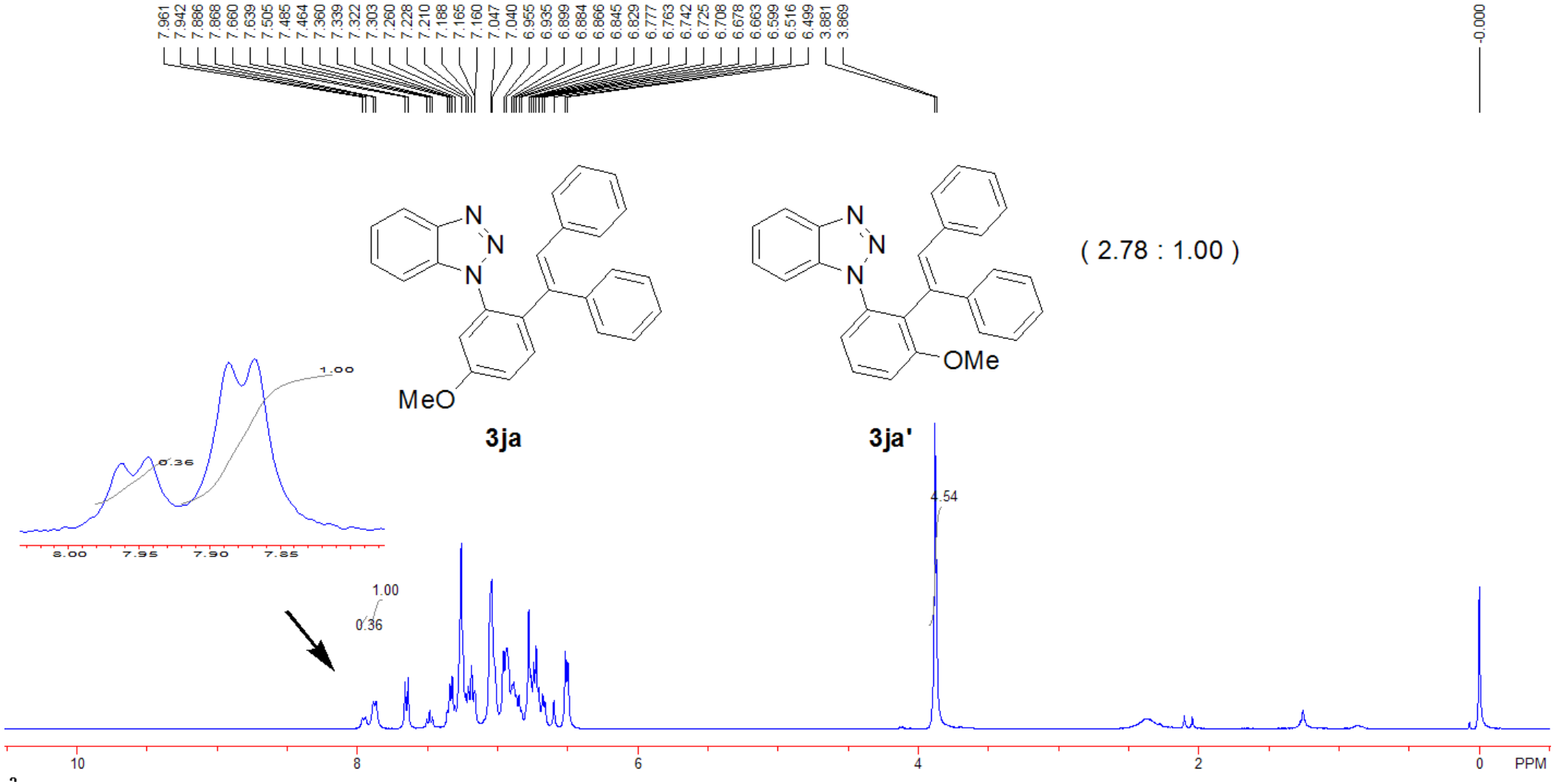
Analysis Info

Analysis Name	13060980_20130626_000009.d	Acquisition Date	6/26/2013 8:43:32 PM
Sample	9	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ia

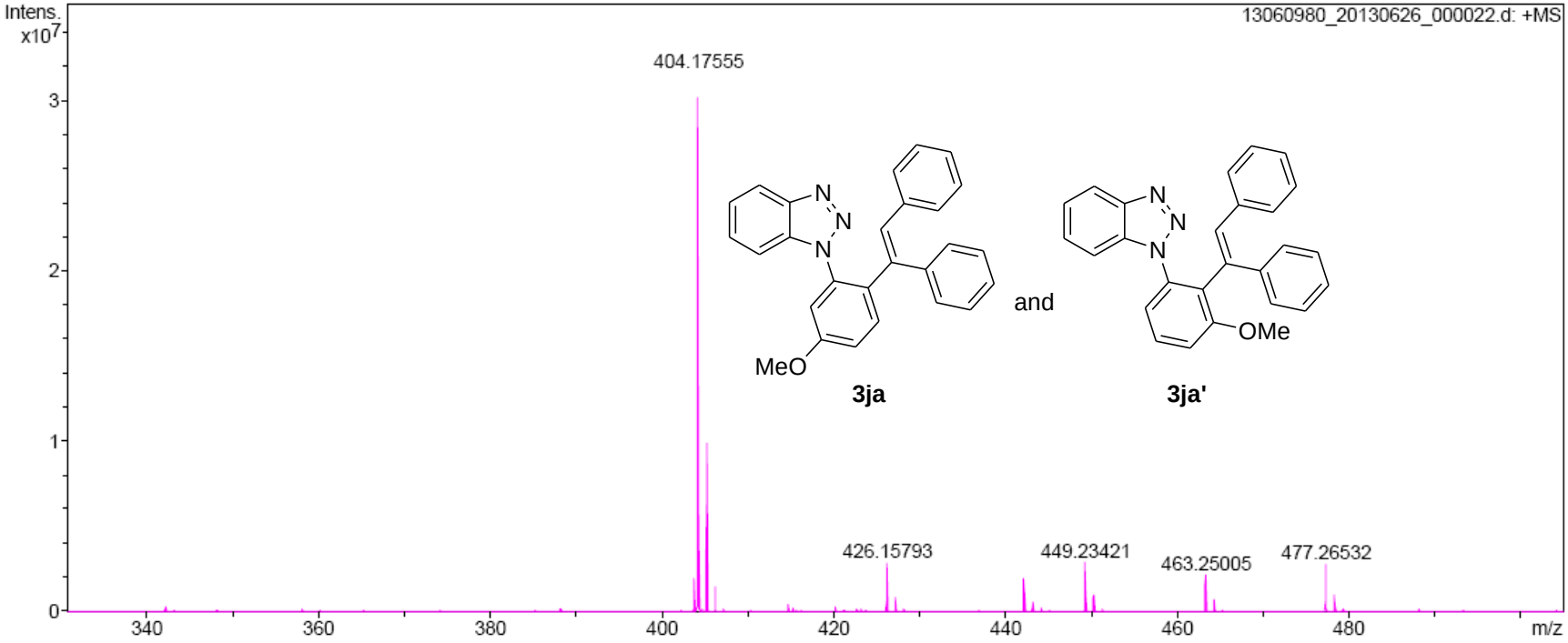
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
450.19560	1	C 32 H 24 N 3	100.00	450.19647	0.9	1.9	9.7	22.5	even	ok



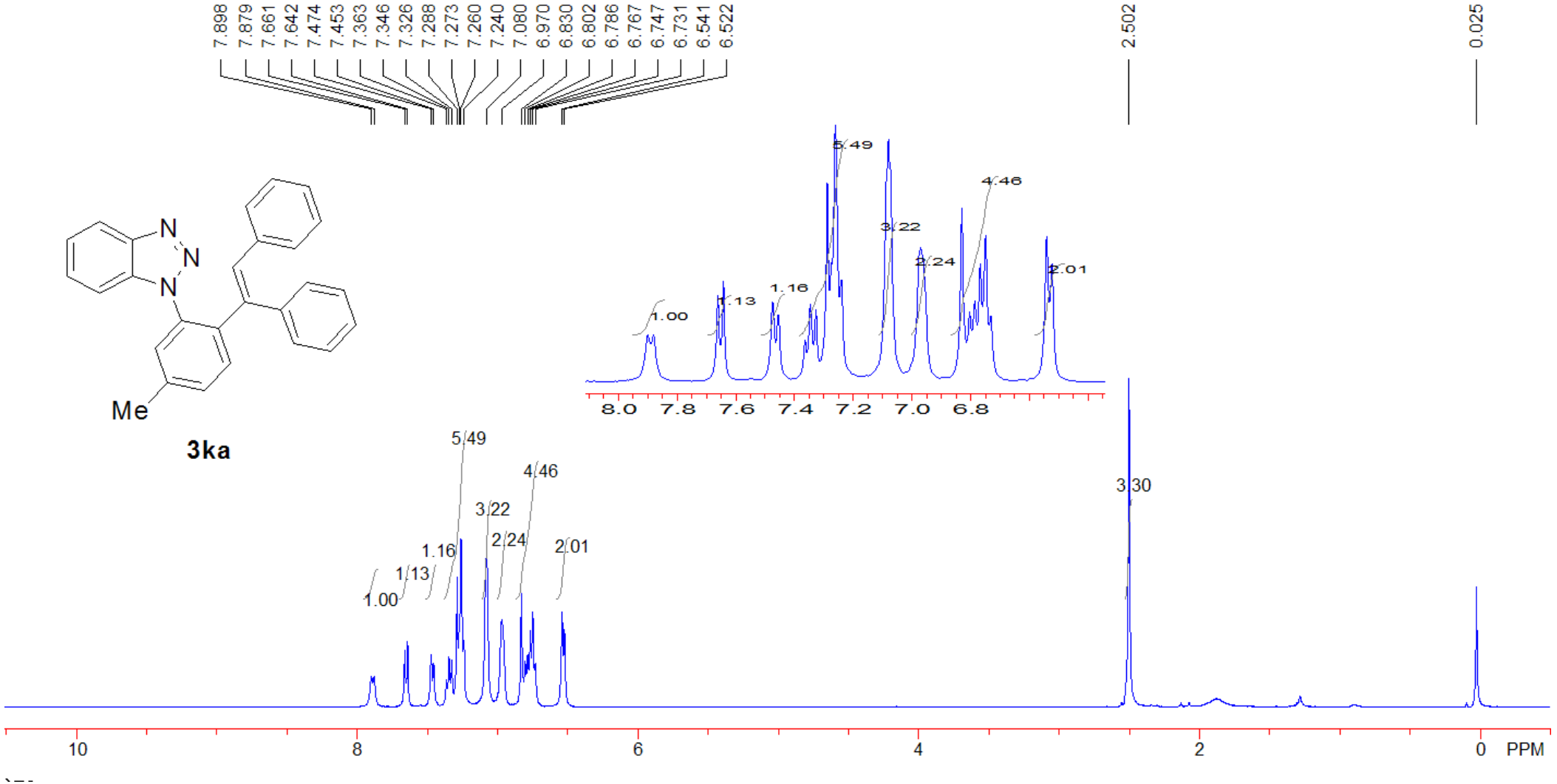
Peking University Mass Spectrometry Sample Analysis Report

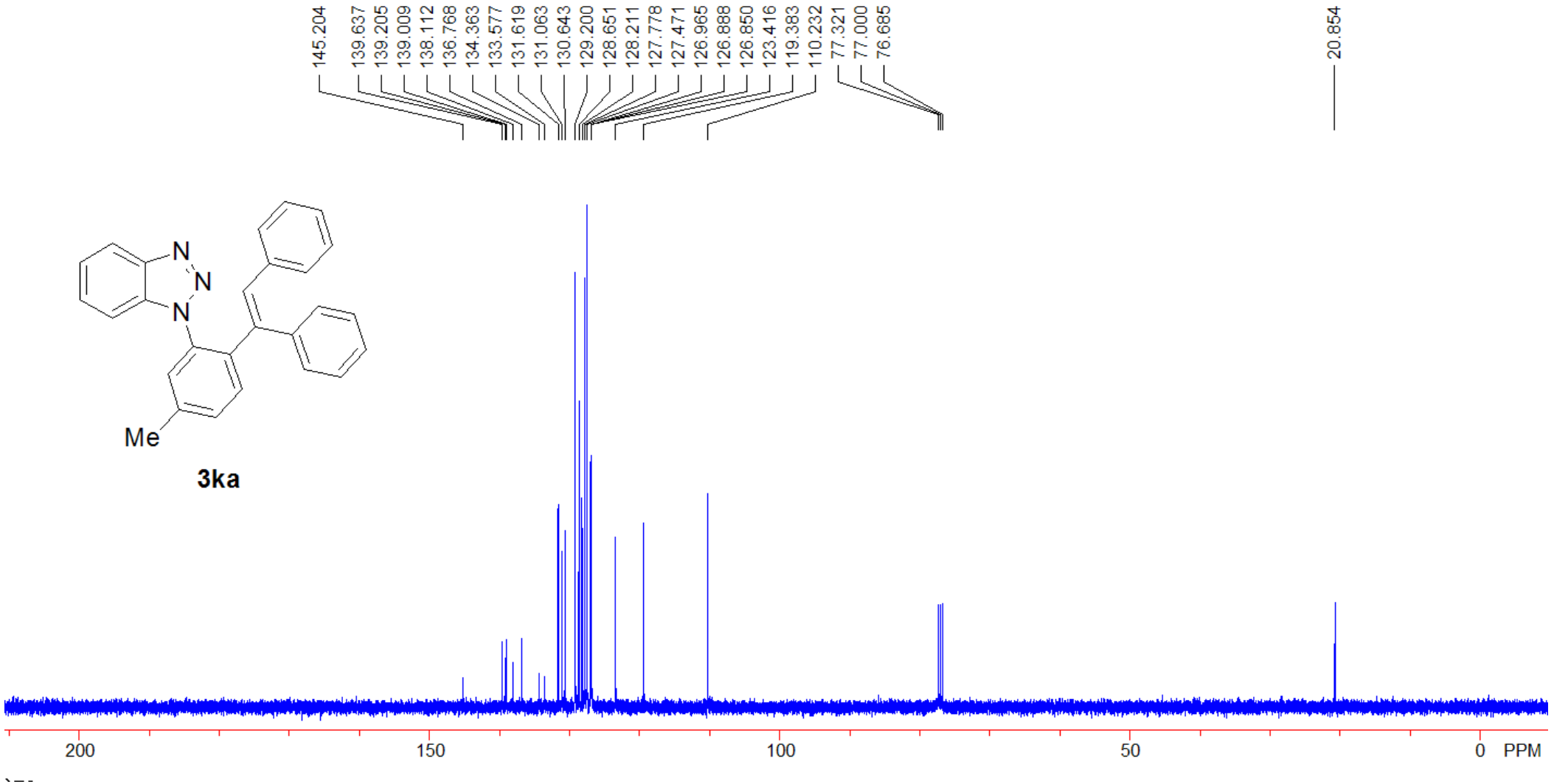
Analysis Info

Analysis Name	13060980_20130626_000022.d	Acquisition Date	6/26/2013 9:10:47 PM
Sample	21	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
404.17555	1	C 27 H 22 N 3 O	100.00	404.17574	0.2	0.5	6.3	18.5	even	ok



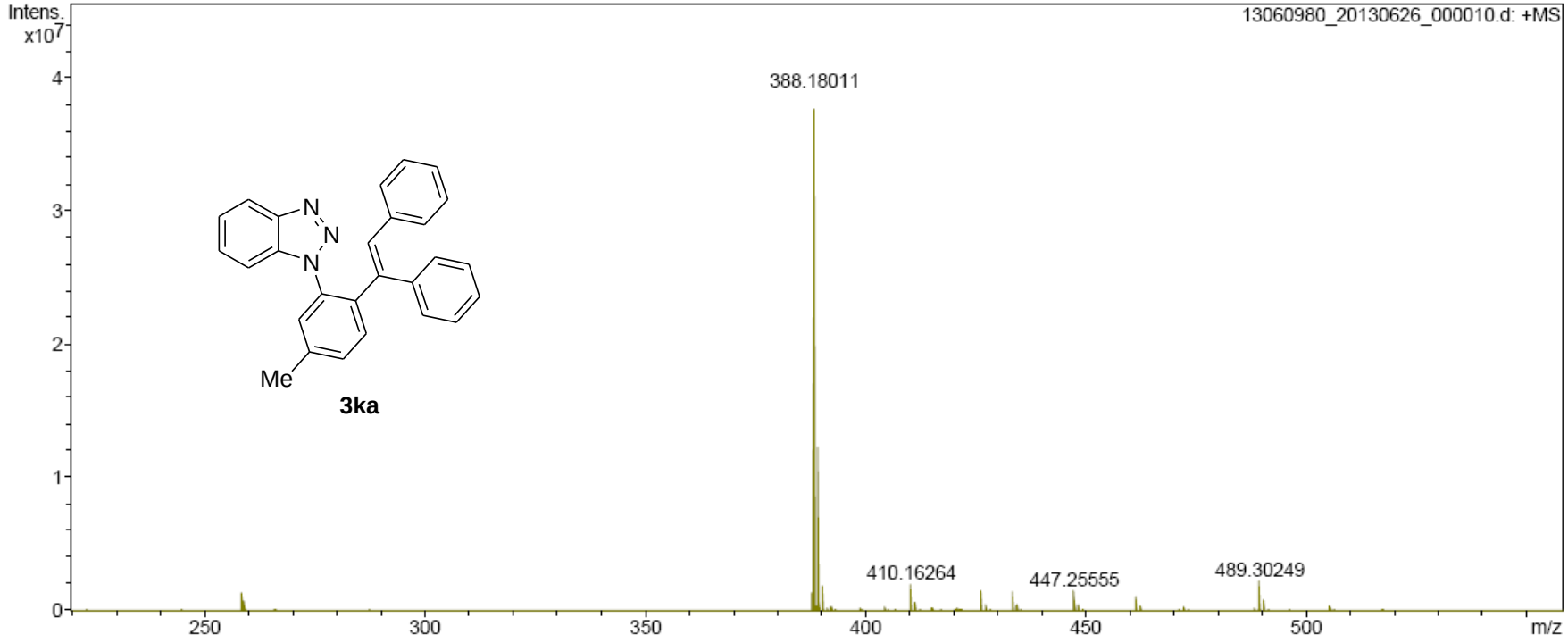


3ka

Peking University Mass Spectrometry Sample Analysis Report

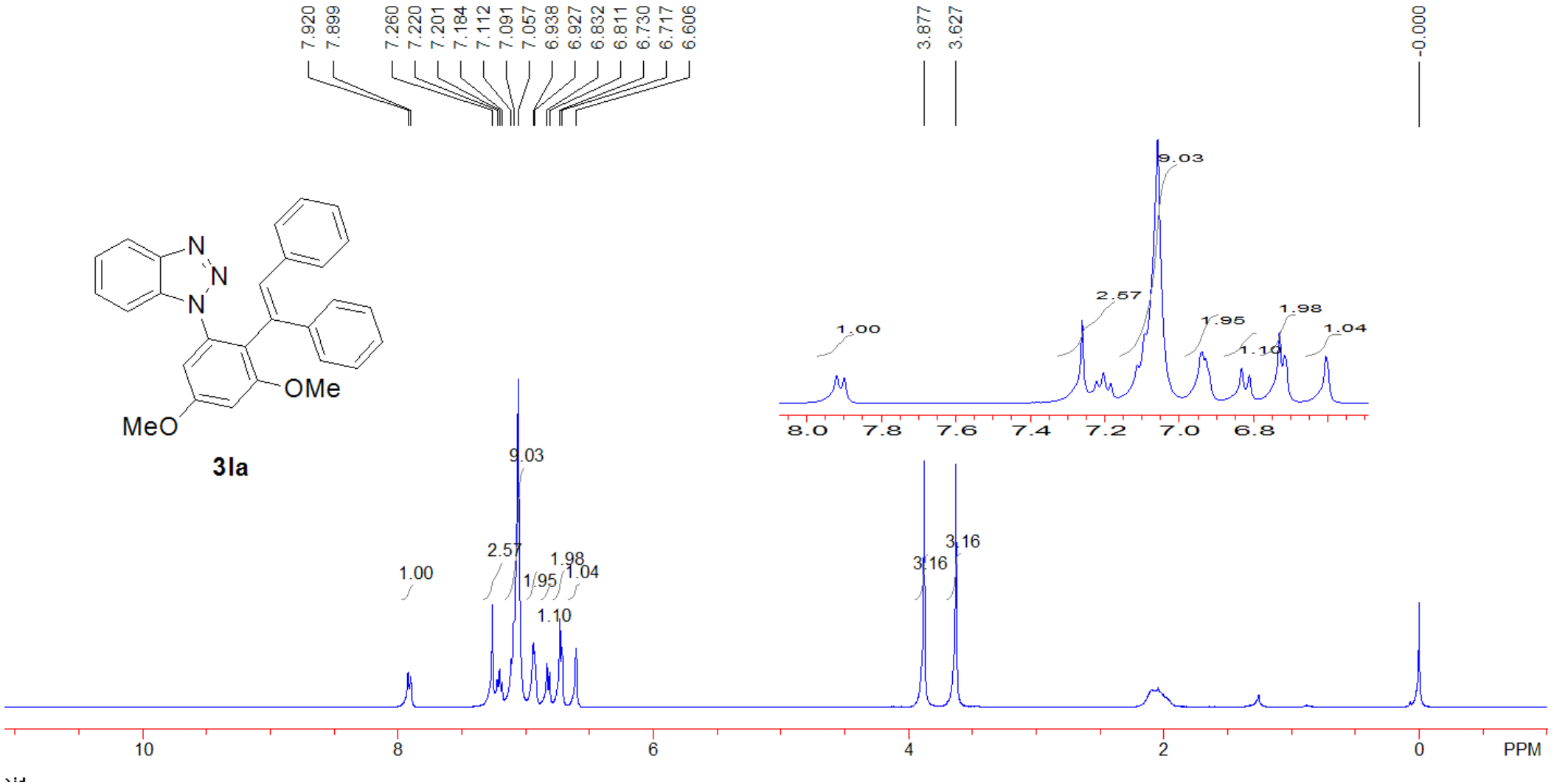
Analysis Info

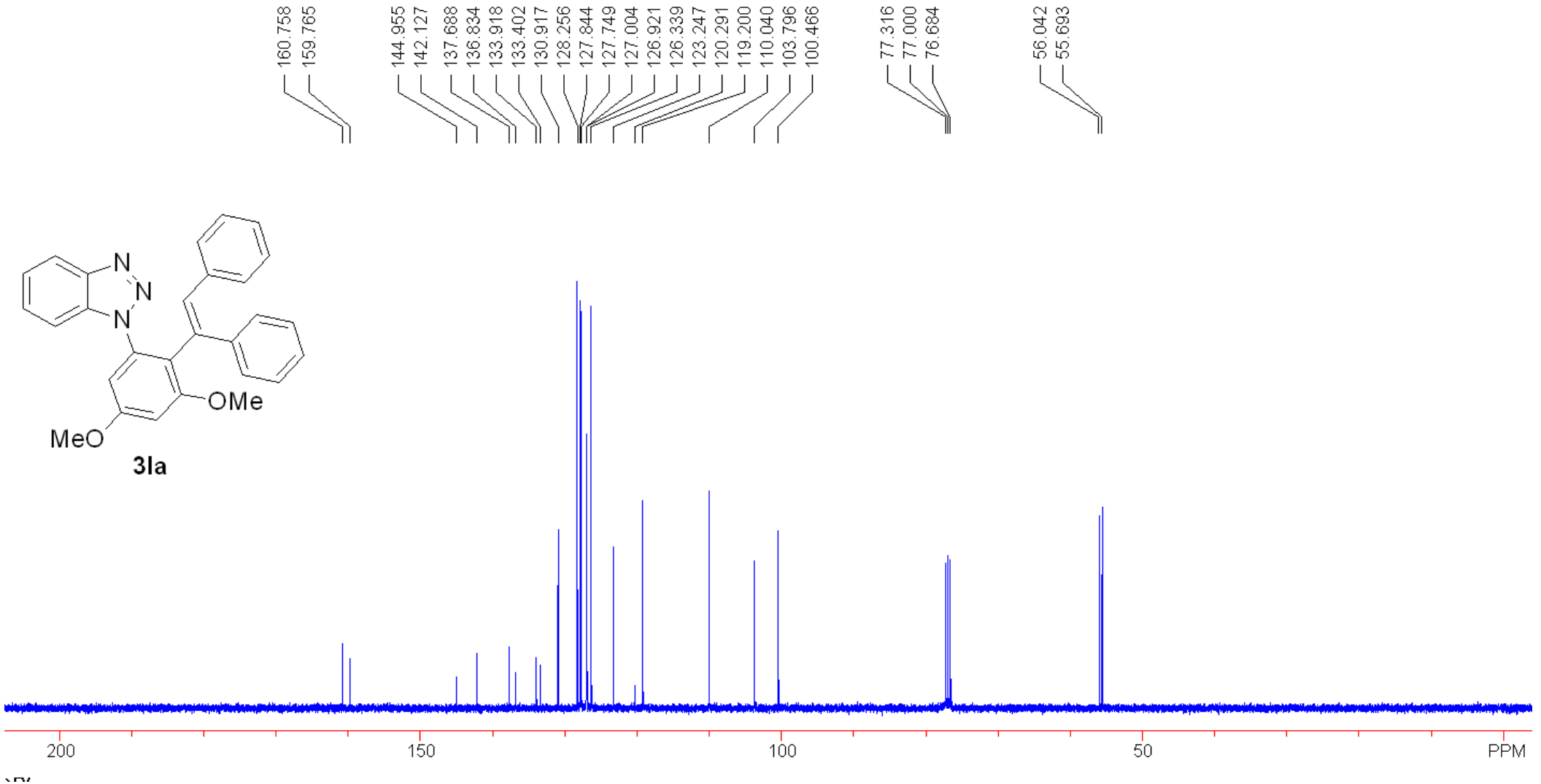
Analysis Name	13060980_20130626_000010.d	Acquisition Date	6/26/2013 8:45:30 PM
Sample	10	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ka

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
388.18011	1	C 27 H 22 N 3	100.00	388.18082	0.7	1.8	10.7	18.5	even	ok



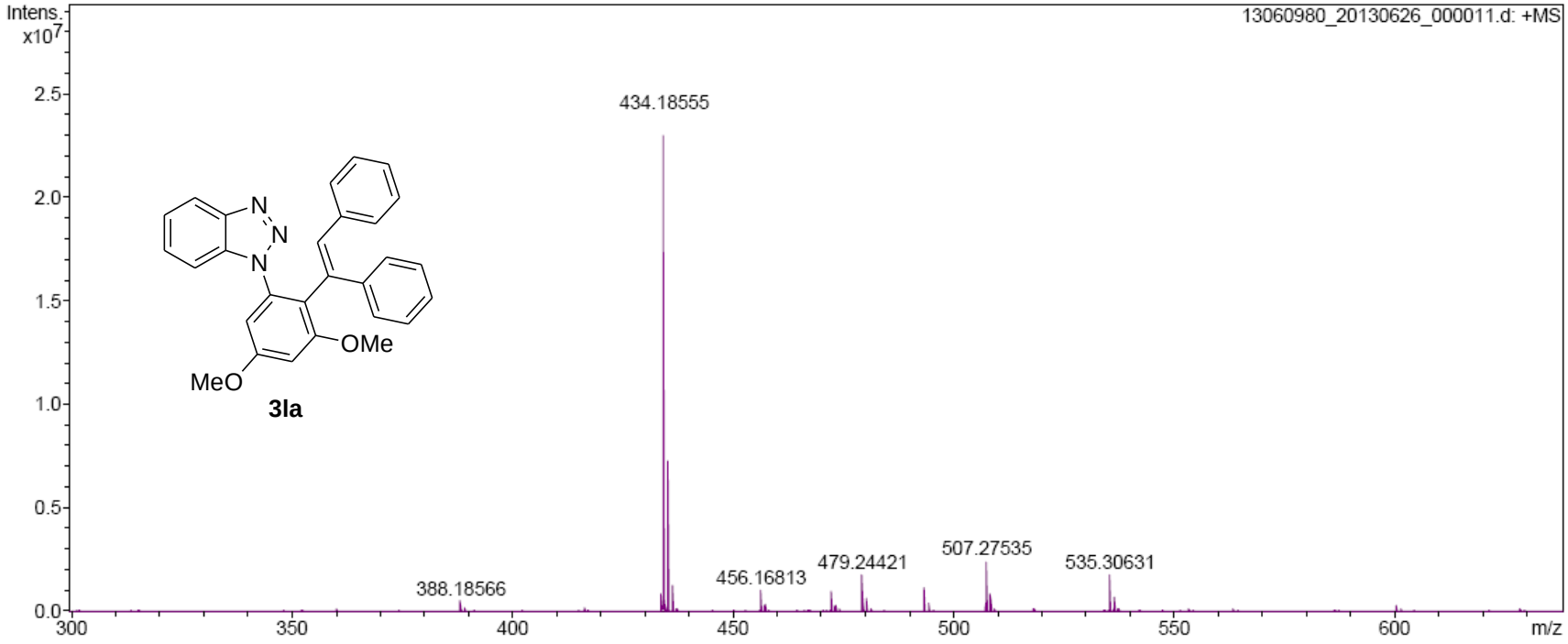


3la

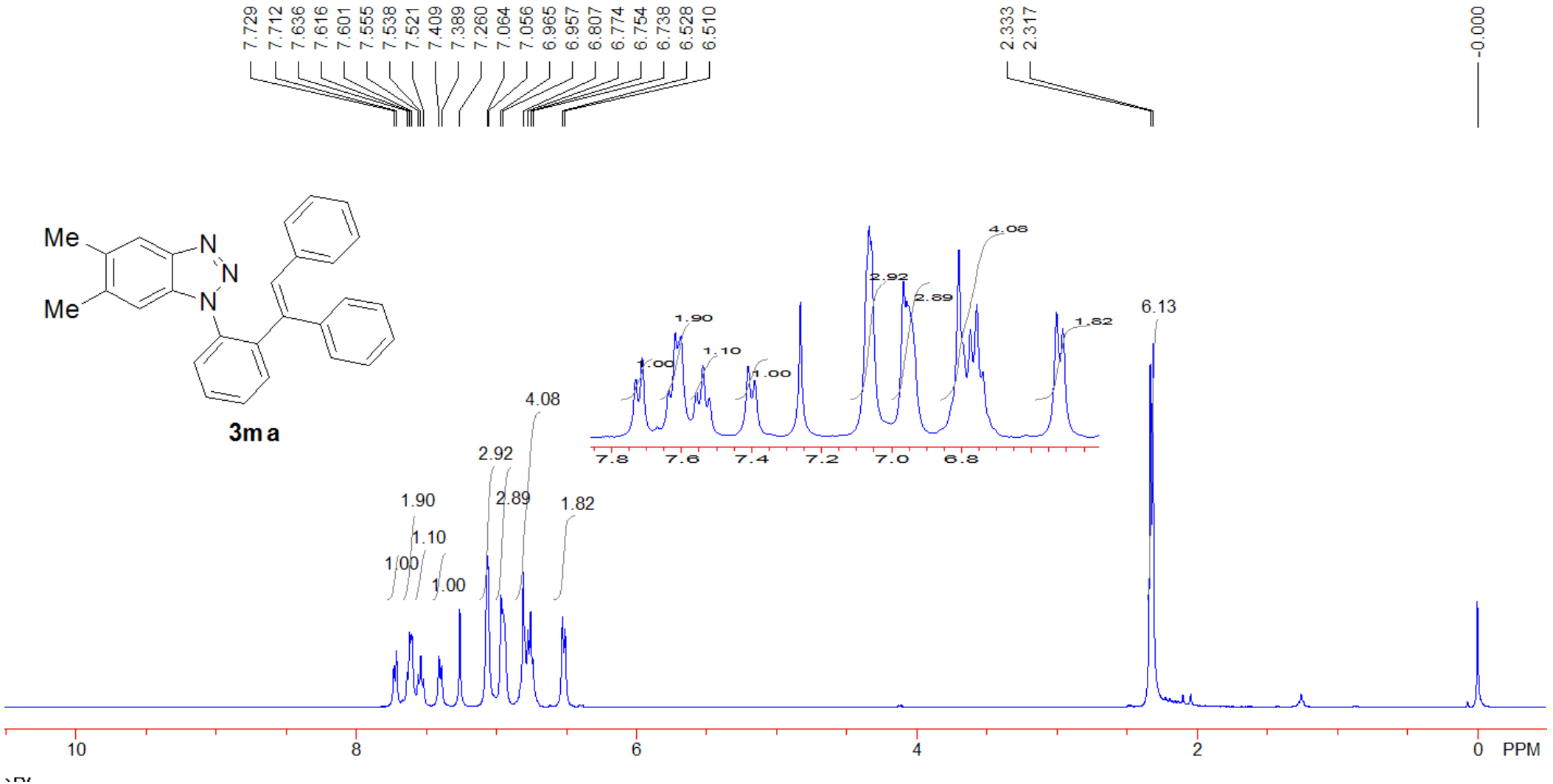
Peking University Mass Spectrometry Sample Analysis Report

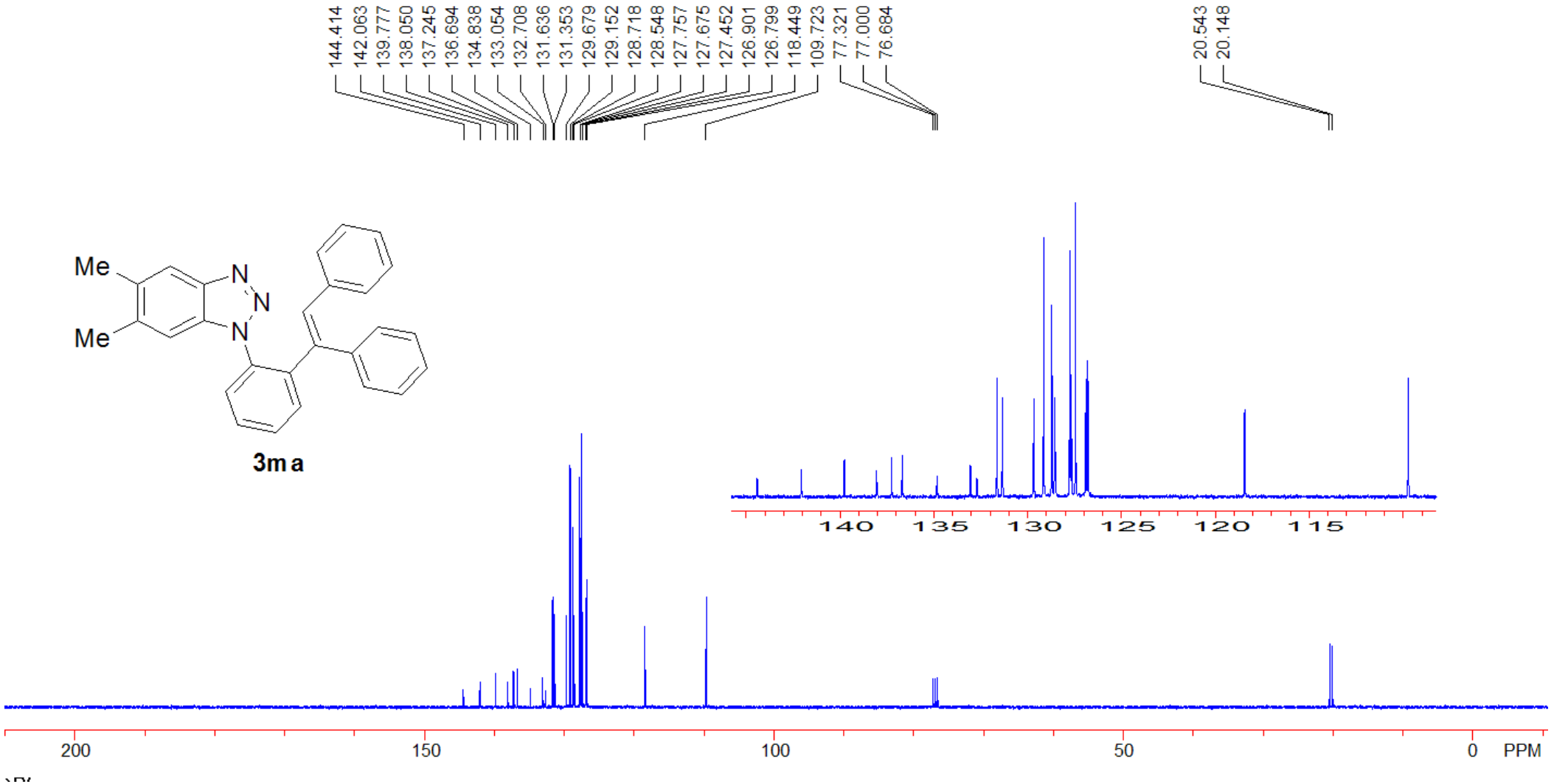
Analysis Info

Analysis Name	13060980_20130626_000011.d	Acquisition Date	6/26/2013 8:47:24 PM
Sample	11	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
434.18555	1	C 28 H 24 N 3 O 2	100.00	434.18630	0.8	1.7	4.6	18.5	even	ok

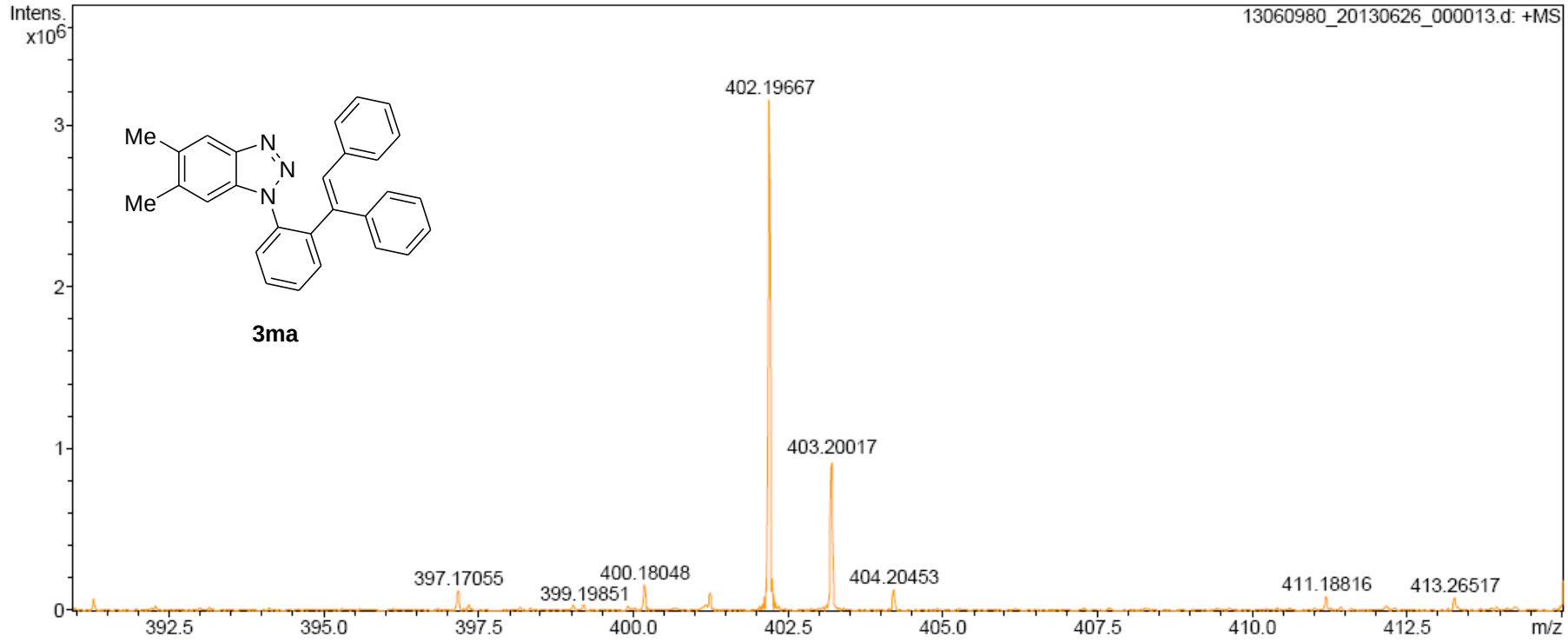




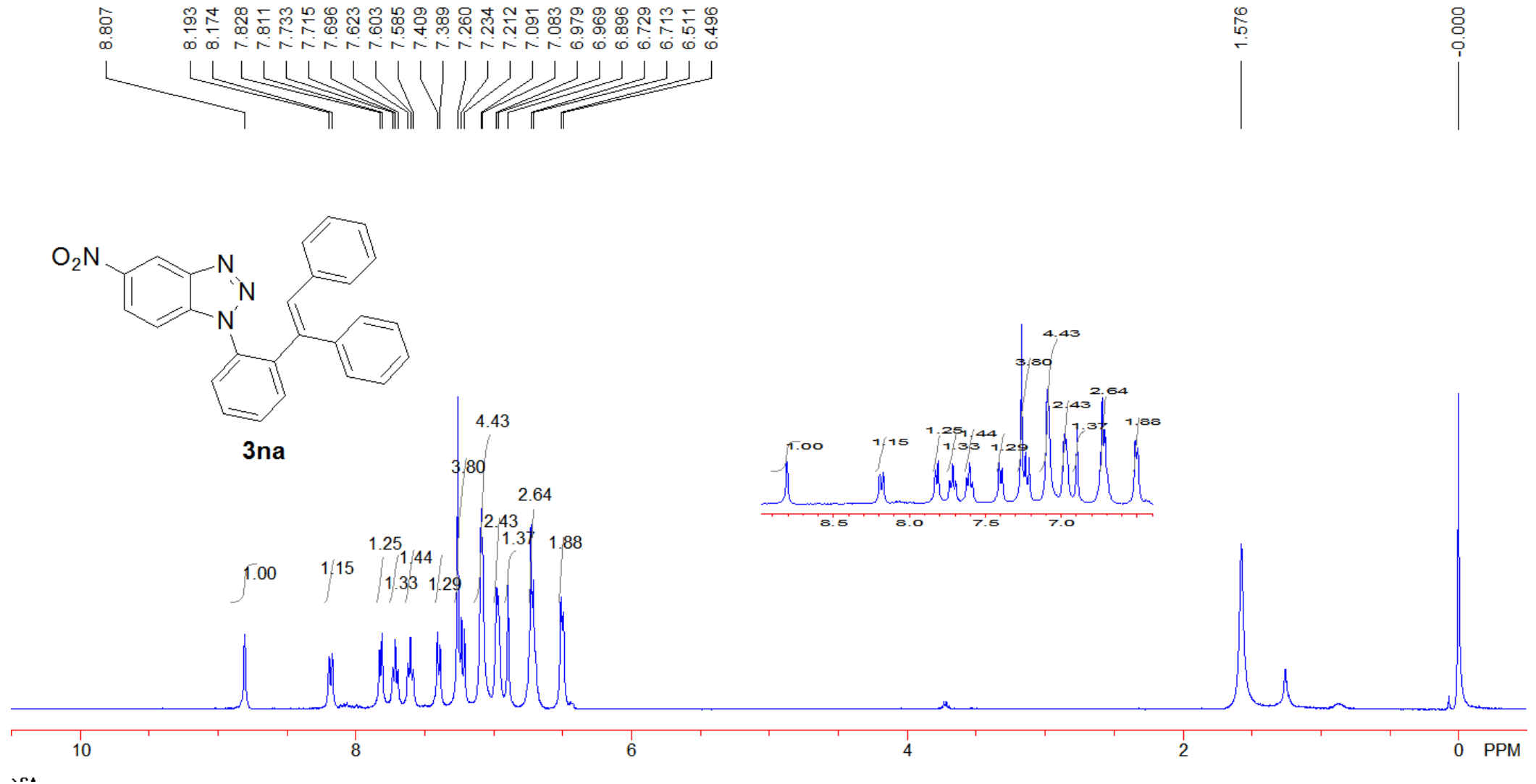
Peking University Mass Spectrometry Sample Analysis Report

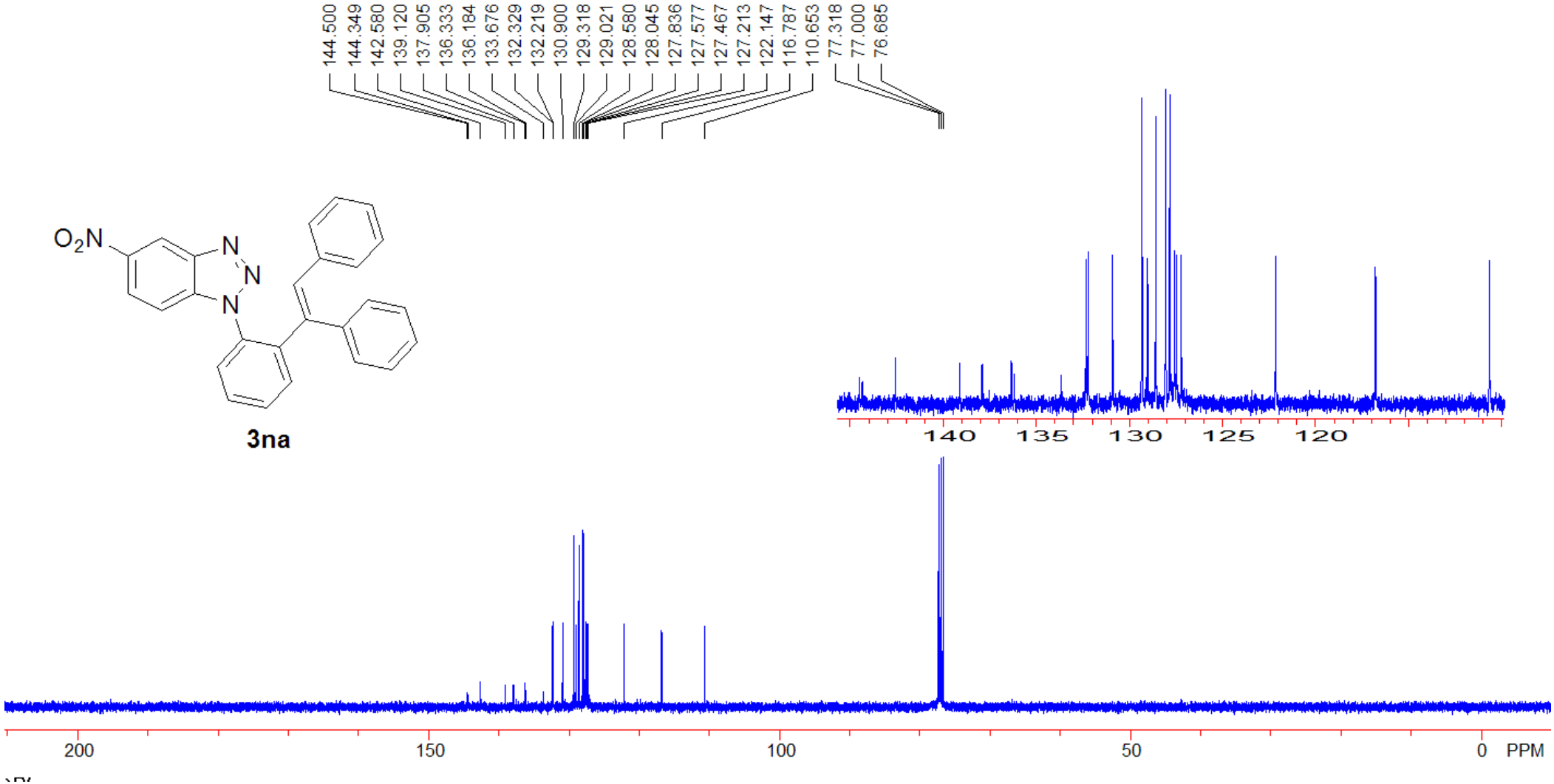
Analysis Info

Analysis Name	13060980_20130626_000013.d	Acquisition Date	6/26/2013 8:53:30 PM
Sample	12	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
402.19667	1	C 28 H 24 N 3	100.00	402.19647	-0.2	-0.5	8.6	18.5	even	ok

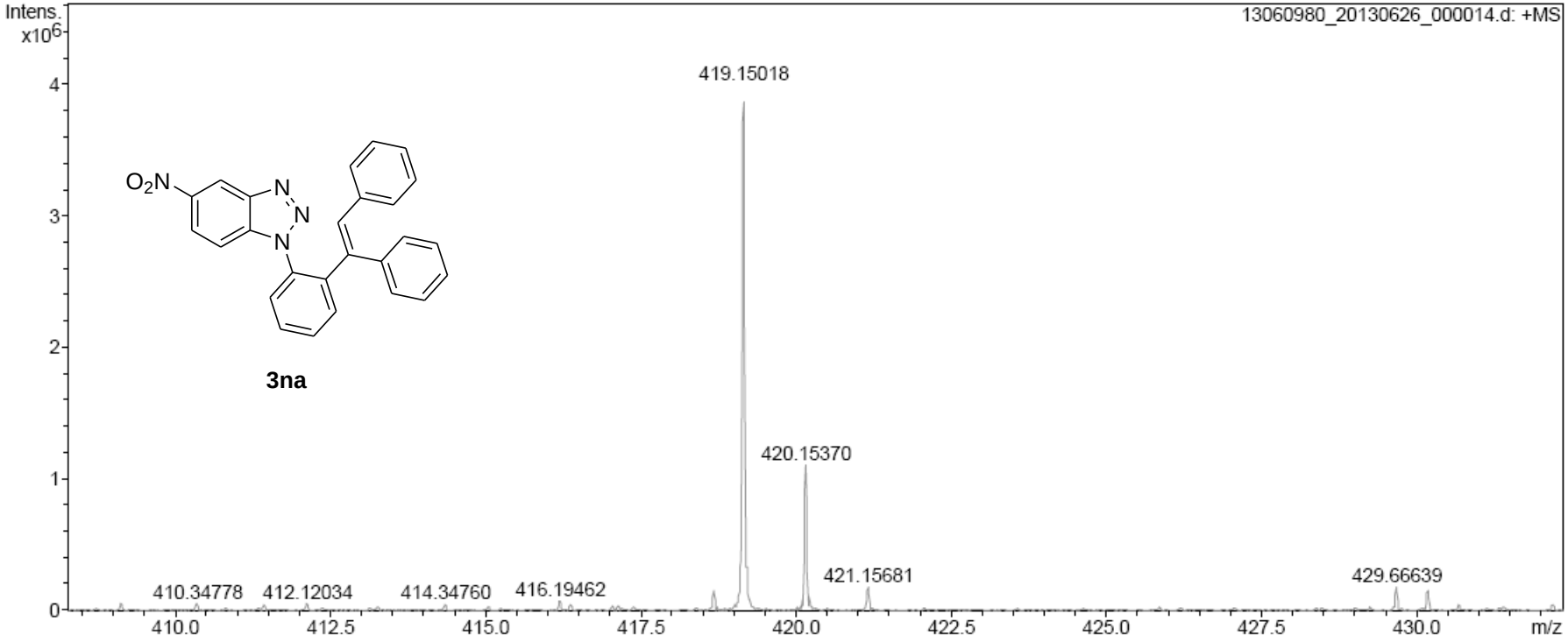




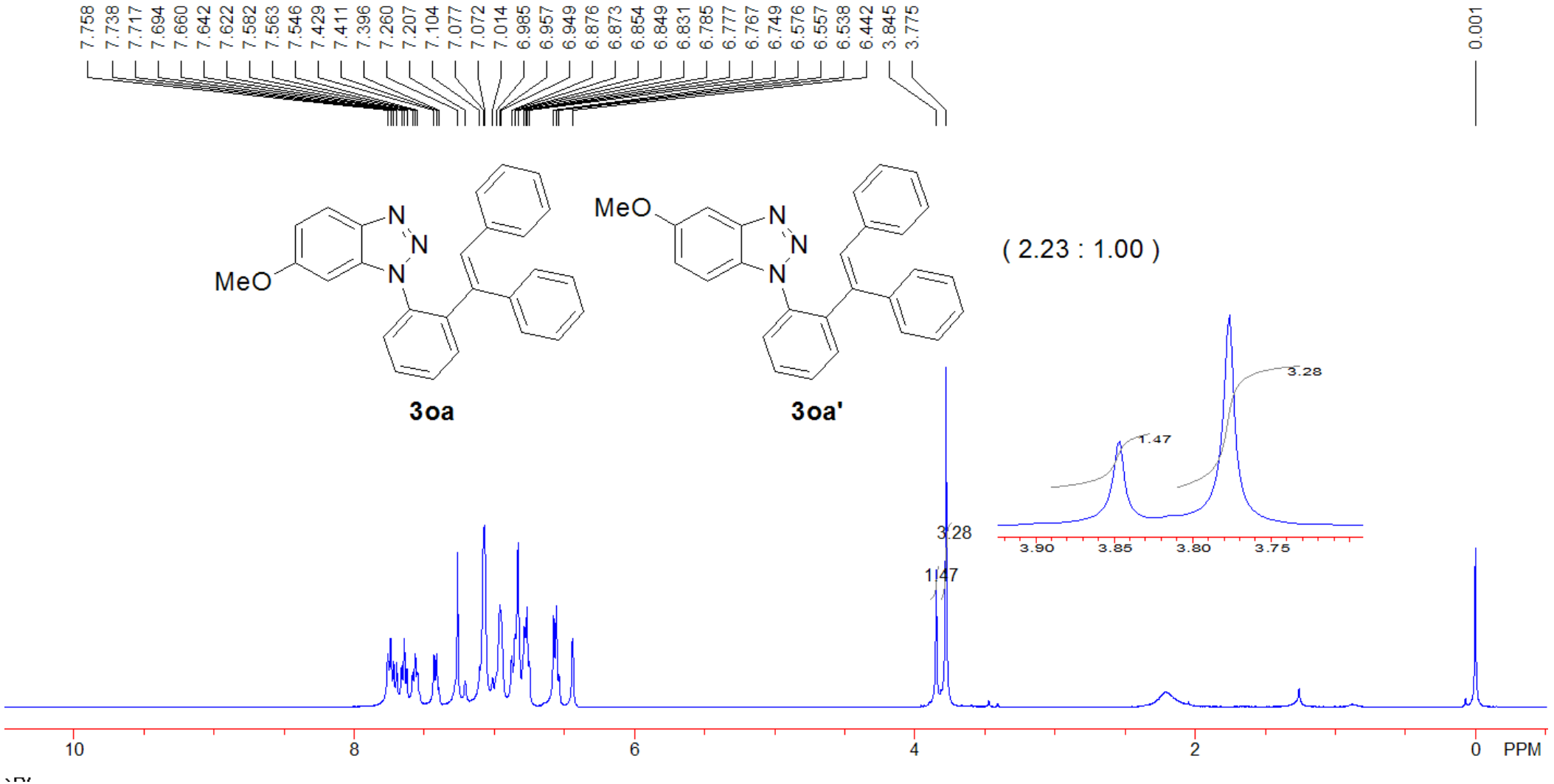
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	13060980_20130626_000014.d	Acquisition Date	6/26/2013 8:55:30 PM
Sample	13	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



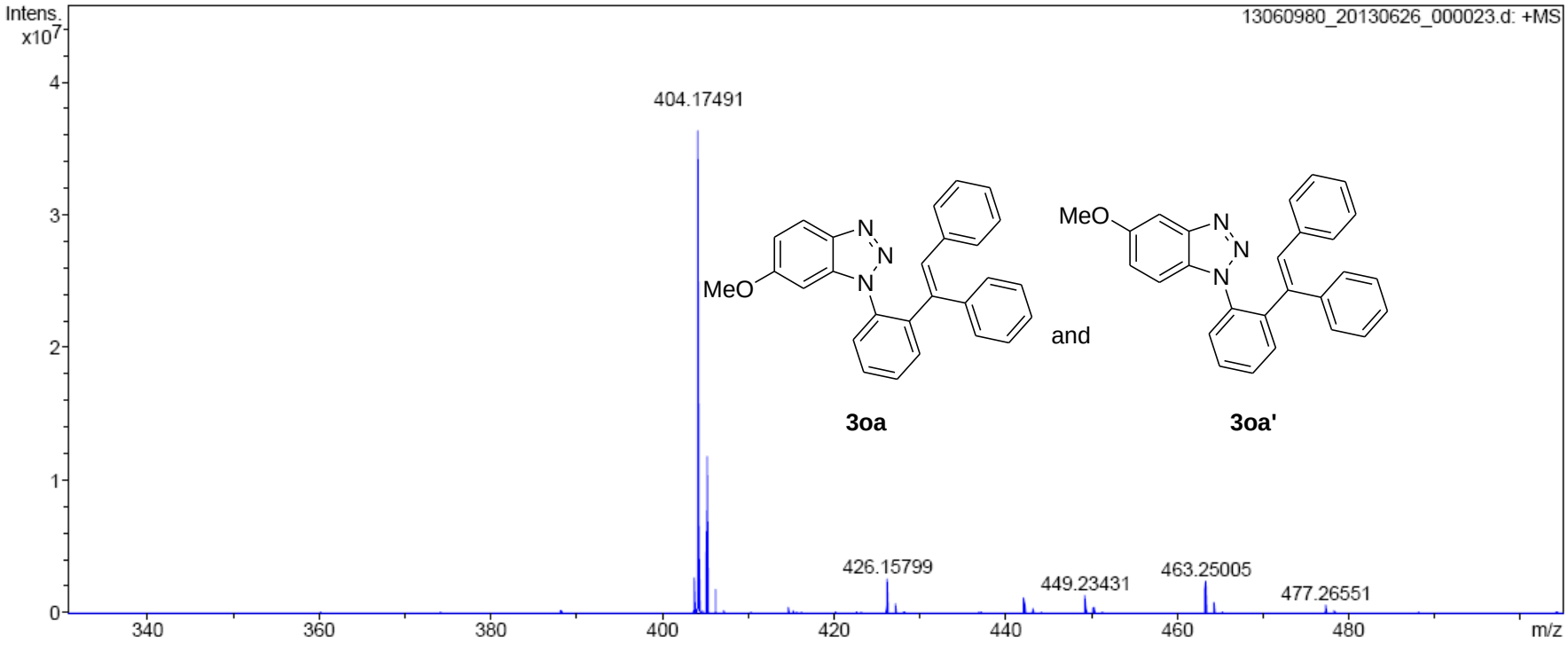
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
419.15018	1	C 26 H 19 N 4 O 2	100.00	419.15025	0.1	0.2	10.5	19.5	even	ok



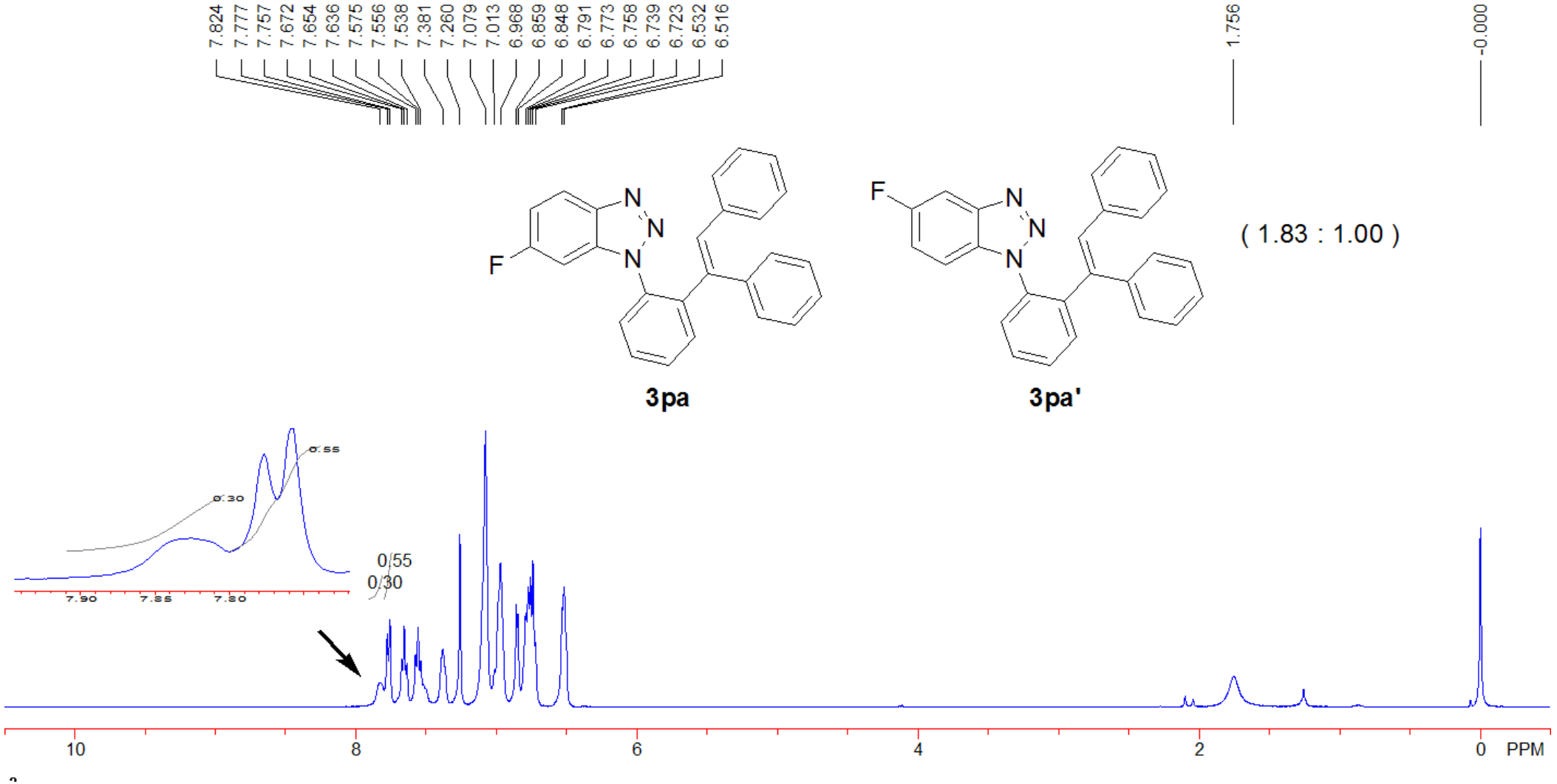
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	13060980_20130626_000023.d	Acquisition Date	6/26/2013 9:12:30 PM
Sample	22	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



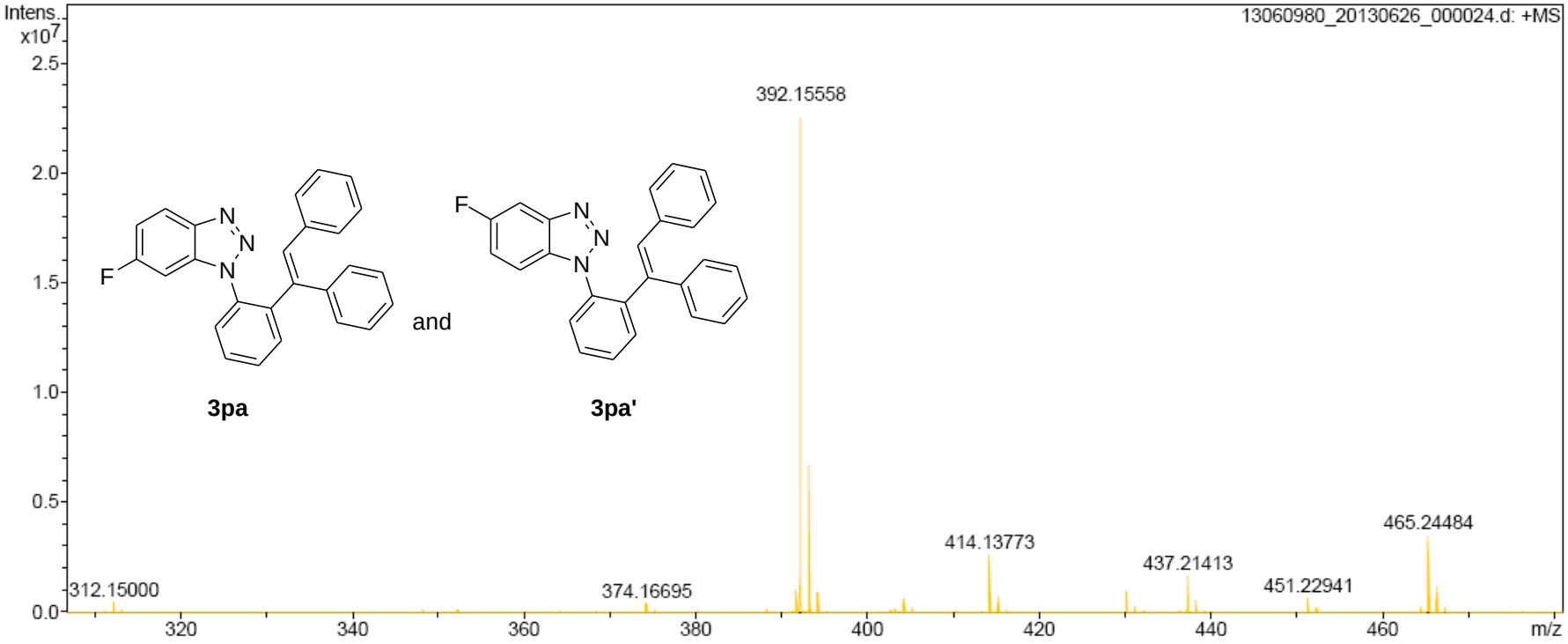
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
404.17491	1	C 27 H 22 N 3 O	100.00	404.17574	0.8	2.1	5.8	18.5	even	ok



Peking University Mass Spectrometry Sample Analysis Report

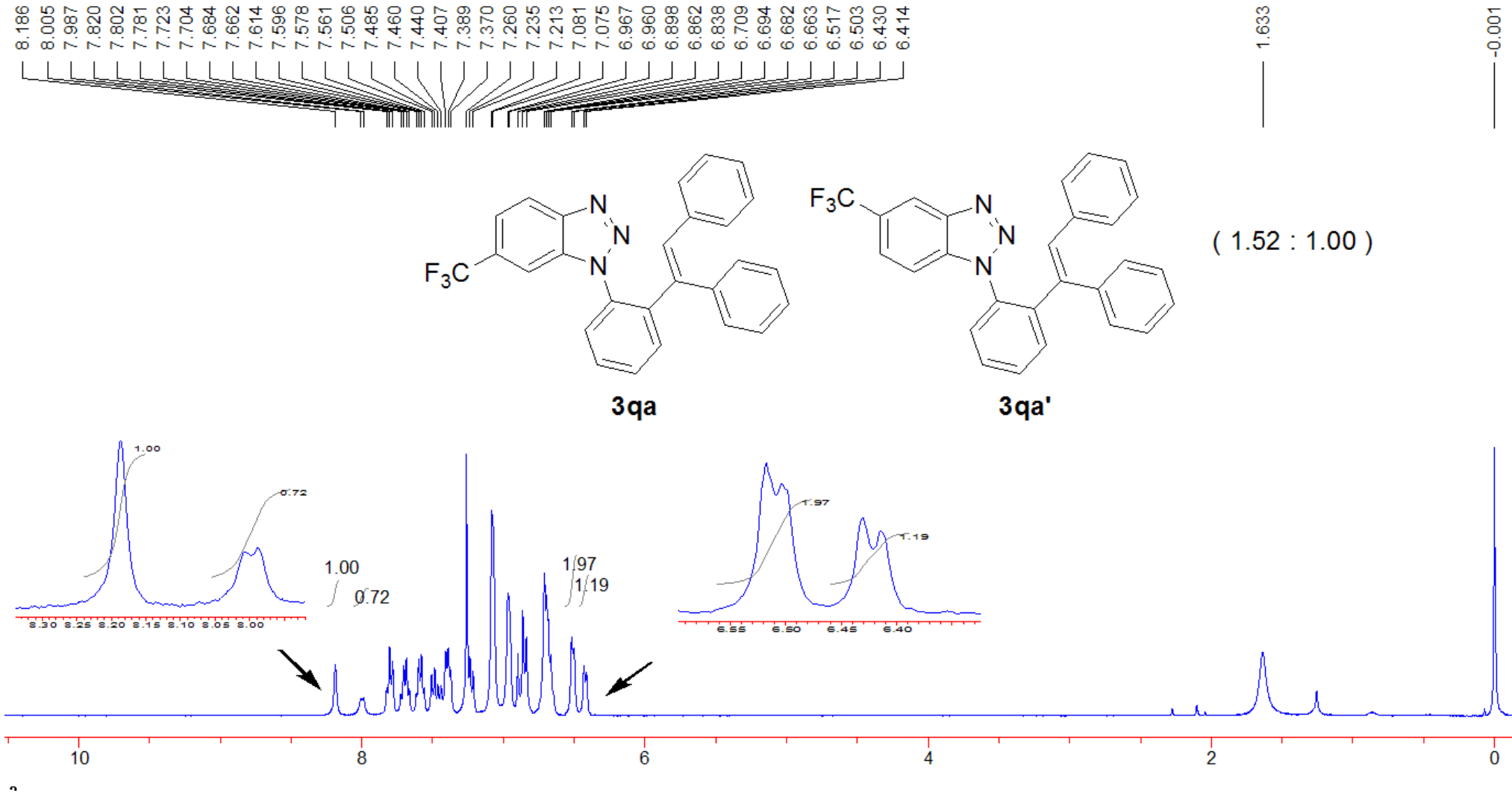
Analysis Info

Analysis Name	13060980_20130626_000024.d	Acquisition Date	6/26/2013 9:15:00 PM
Sample	23	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3pa and **3pa'**

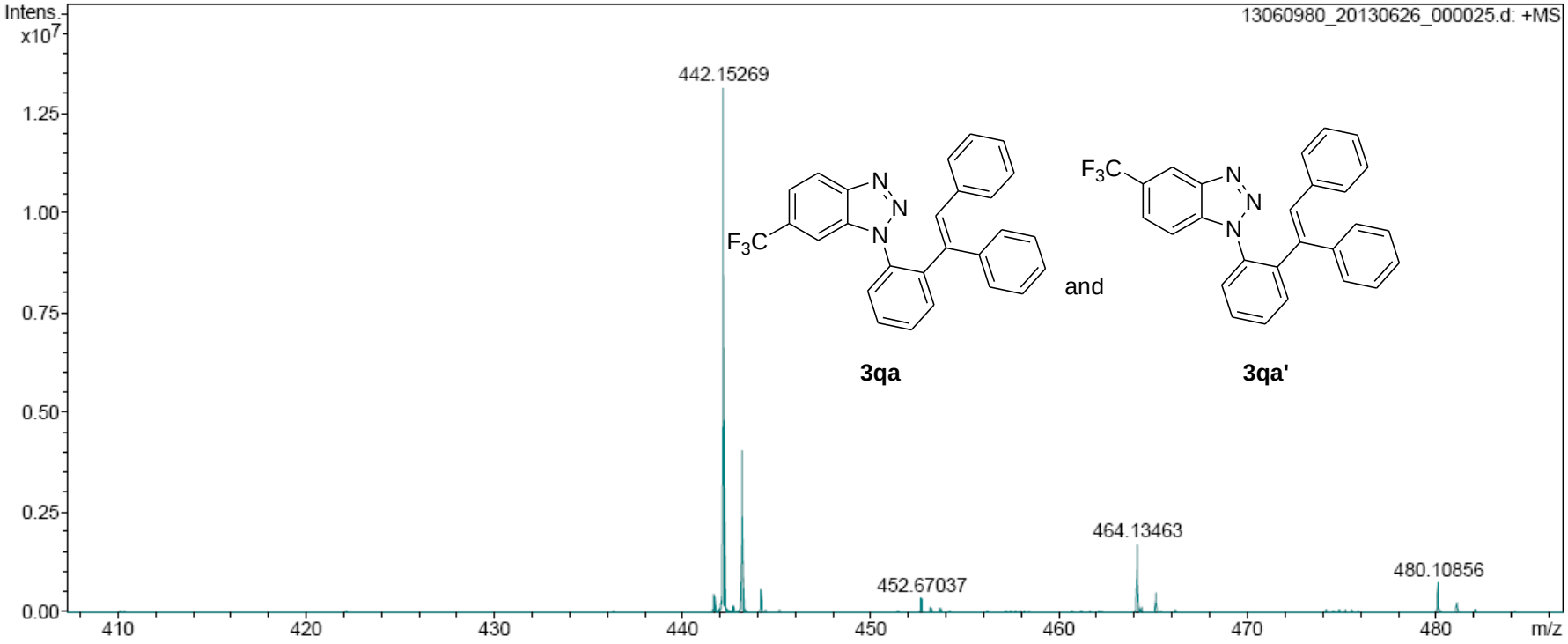
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
392.15558	1	C 26 H 19 F N 3	100.00	392.15575	0.2	0.4	0.2	18.5	even	ok



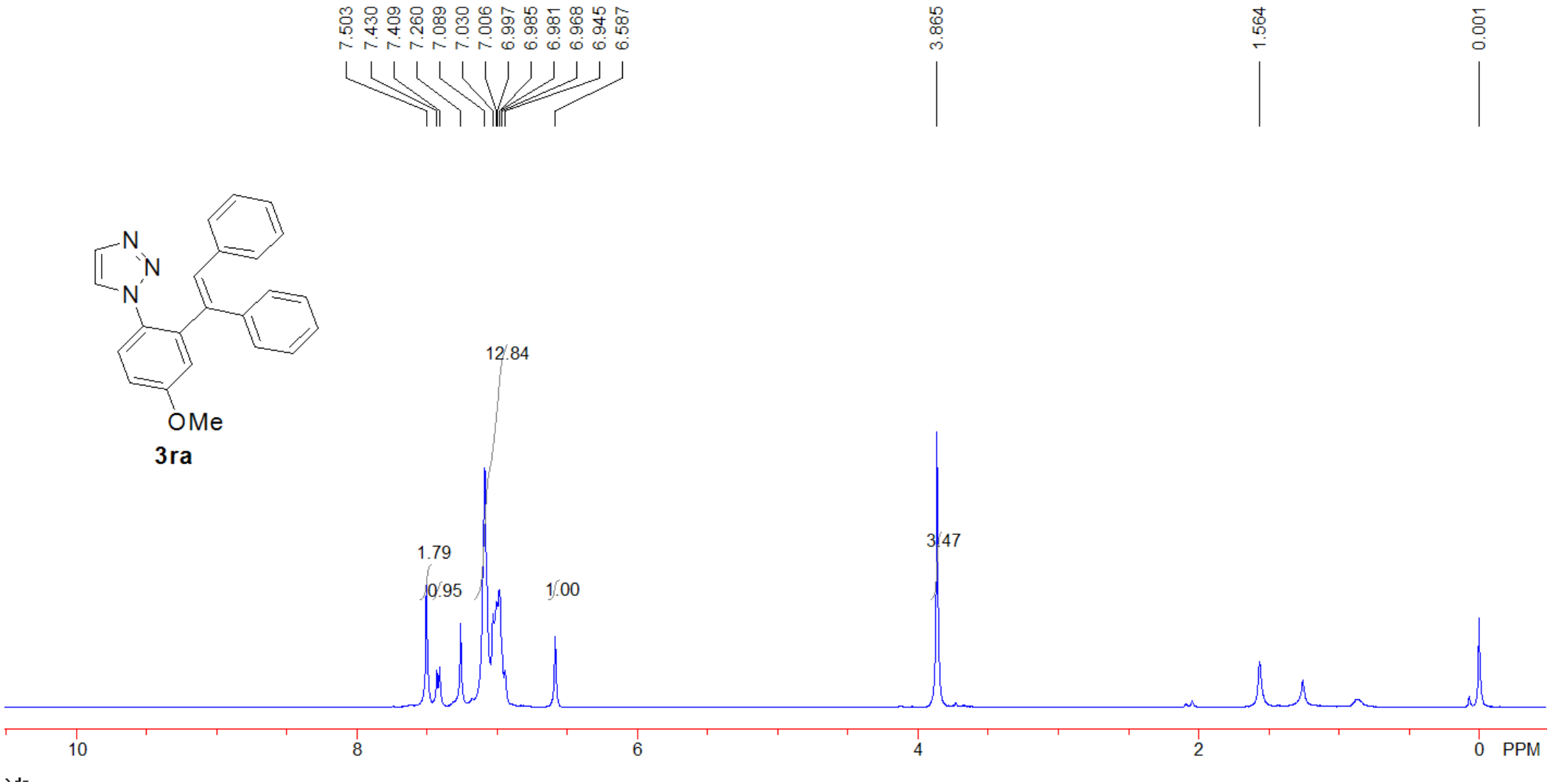
Peking University Mass Spectrometry Sample Analysis Report

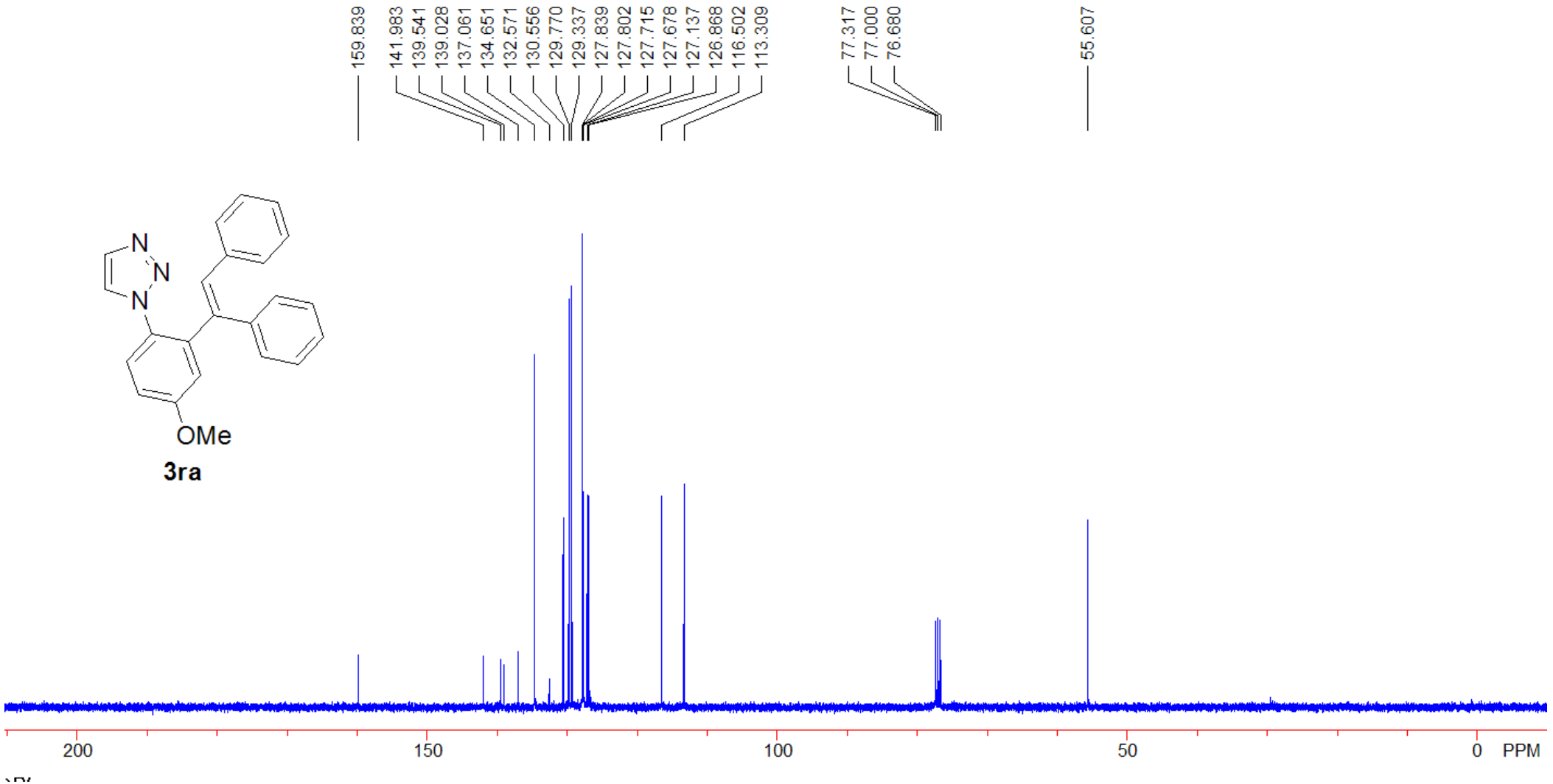
Analysis Info

Analysis Name	13060980_20130626_000025.d	Acquisition Date	6/26/2013 9:17:05 PM
Sample	24	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
442.15269	1	C 27 H 19 F 3 N 3	100.00	442.15256	-0.1	-0.3	3.4	18.5	even	ok



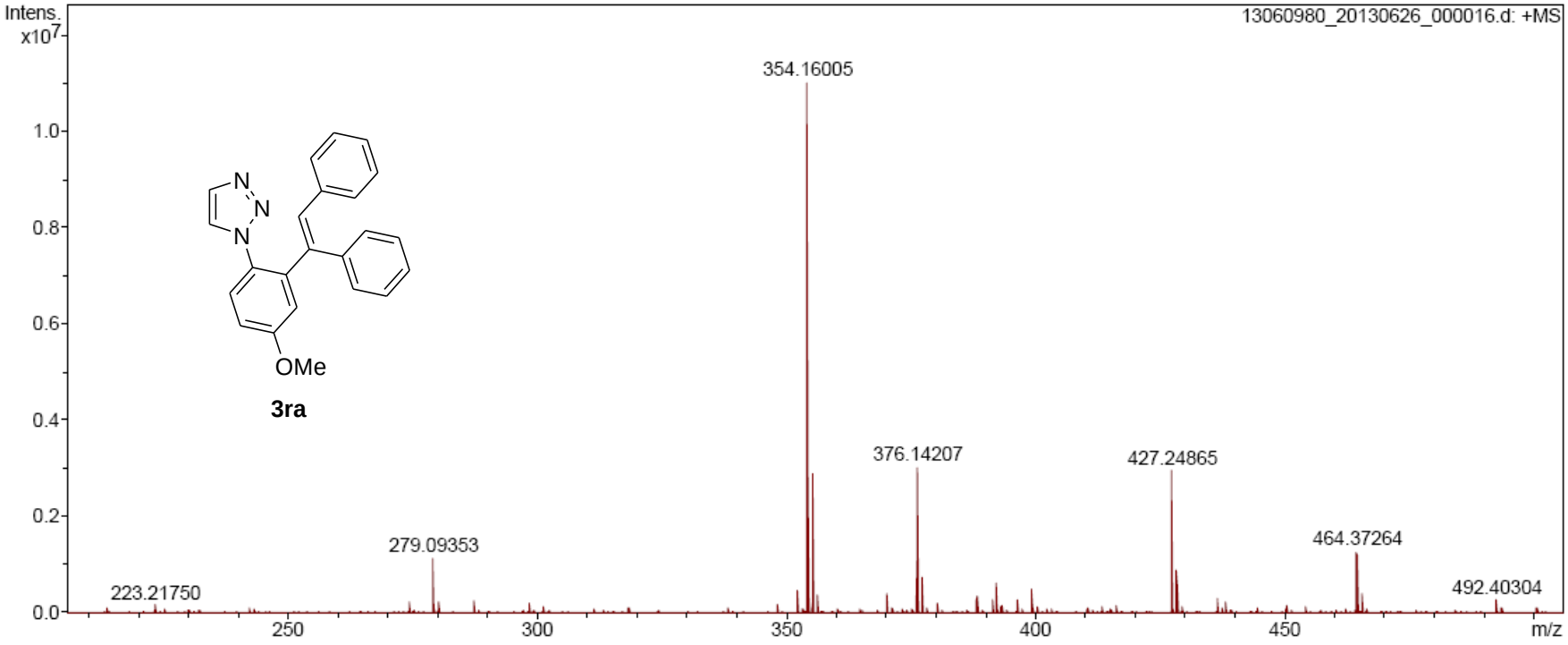


3ra

Peking University Mass Spectrometry Sample Analysis Report

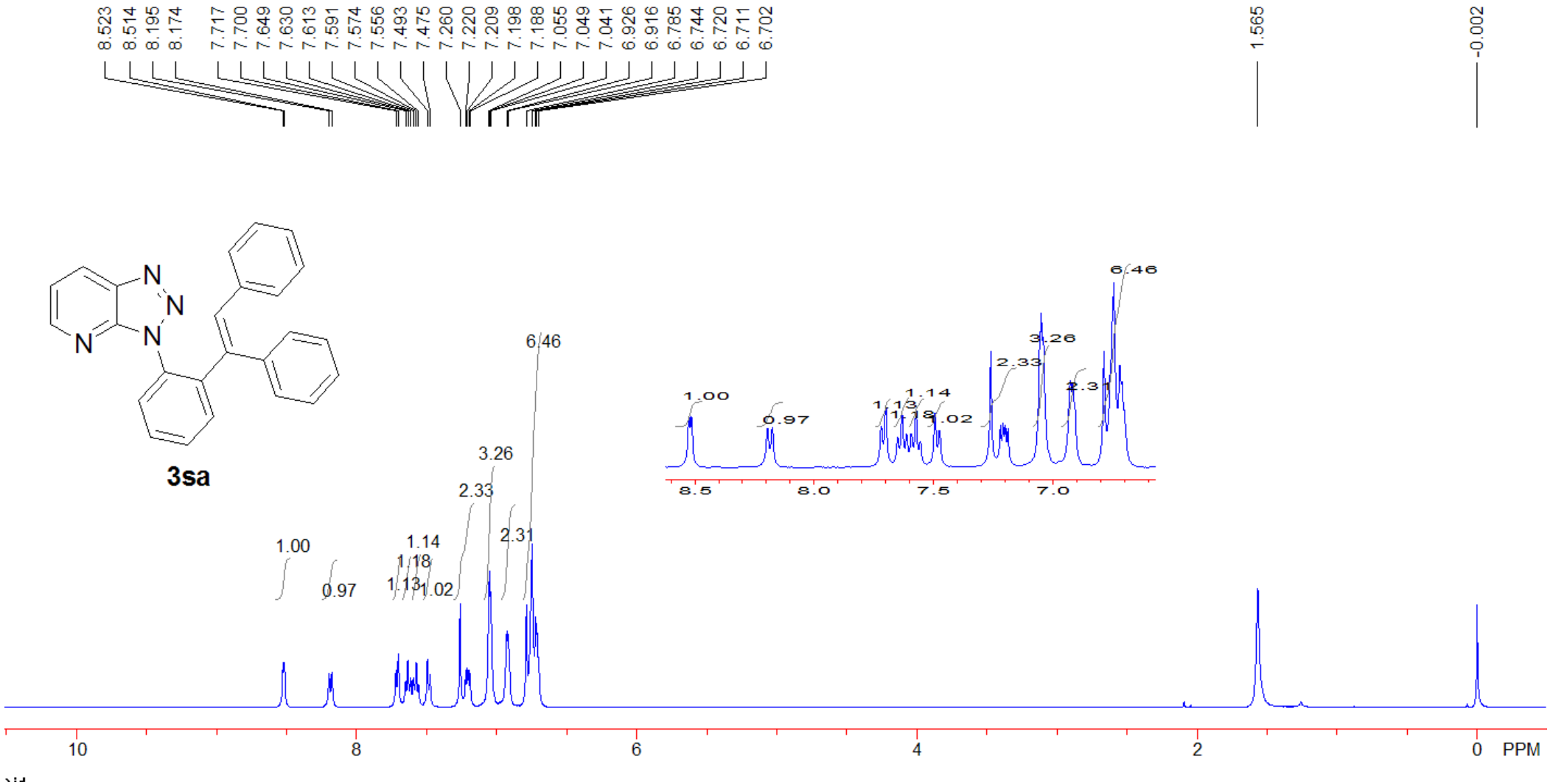
Analysis Info

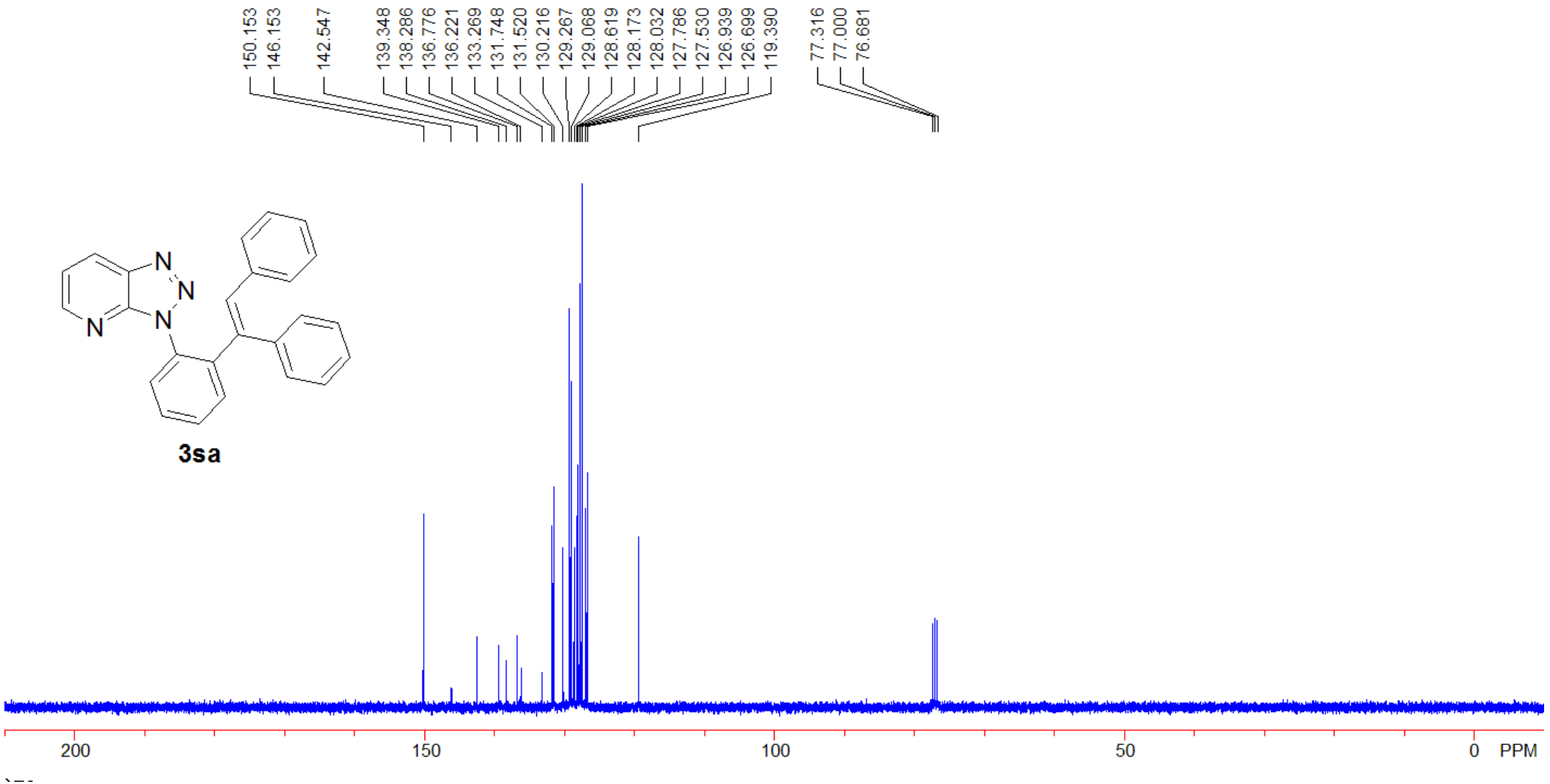
Analysis Name	13060980_20130626_000016.d	Acquisition Date	6/26/2013 8:59:14 PM
Sample	15	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ra

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
354.16005	1	C 23 H 20 N 3 O	100.00	354.16009	0.0	0.1	1.2	15.5	even	ok

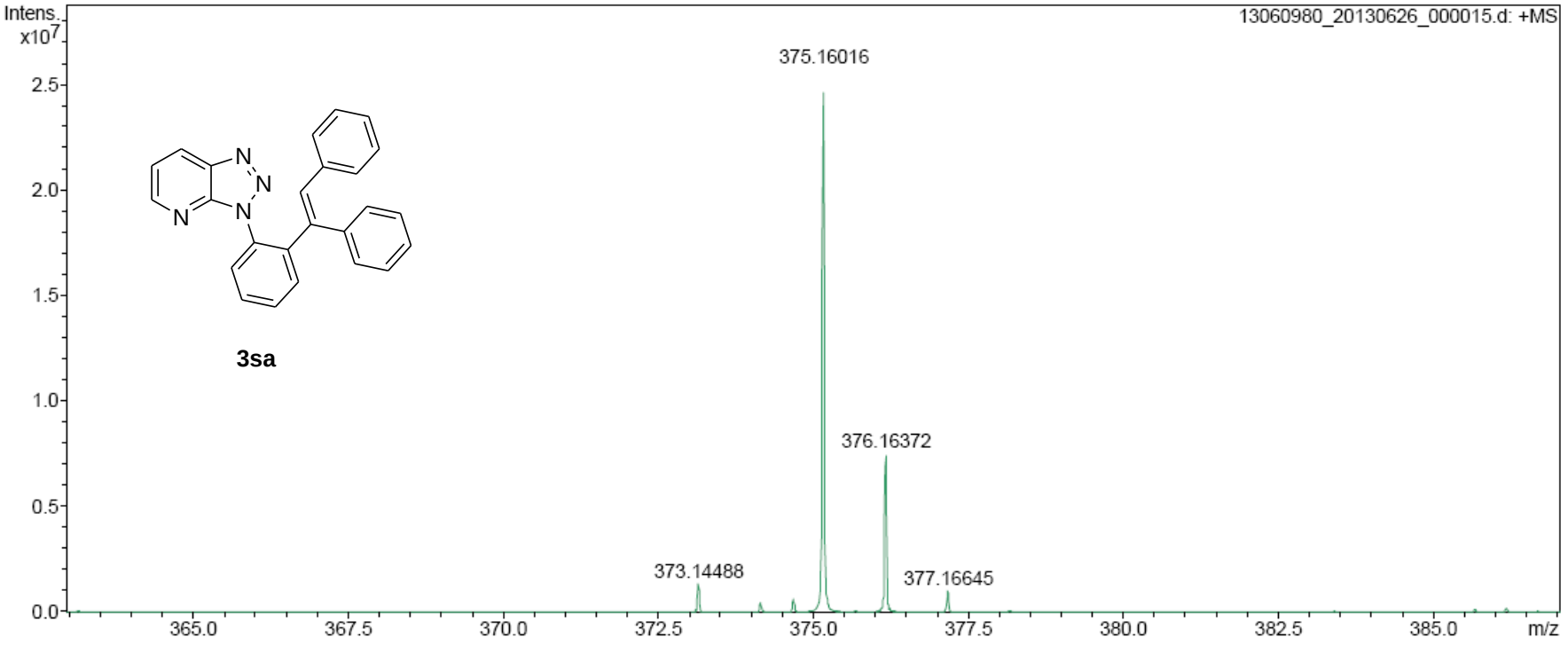




Peking University Mass Spectrometry Sample Analysis Report

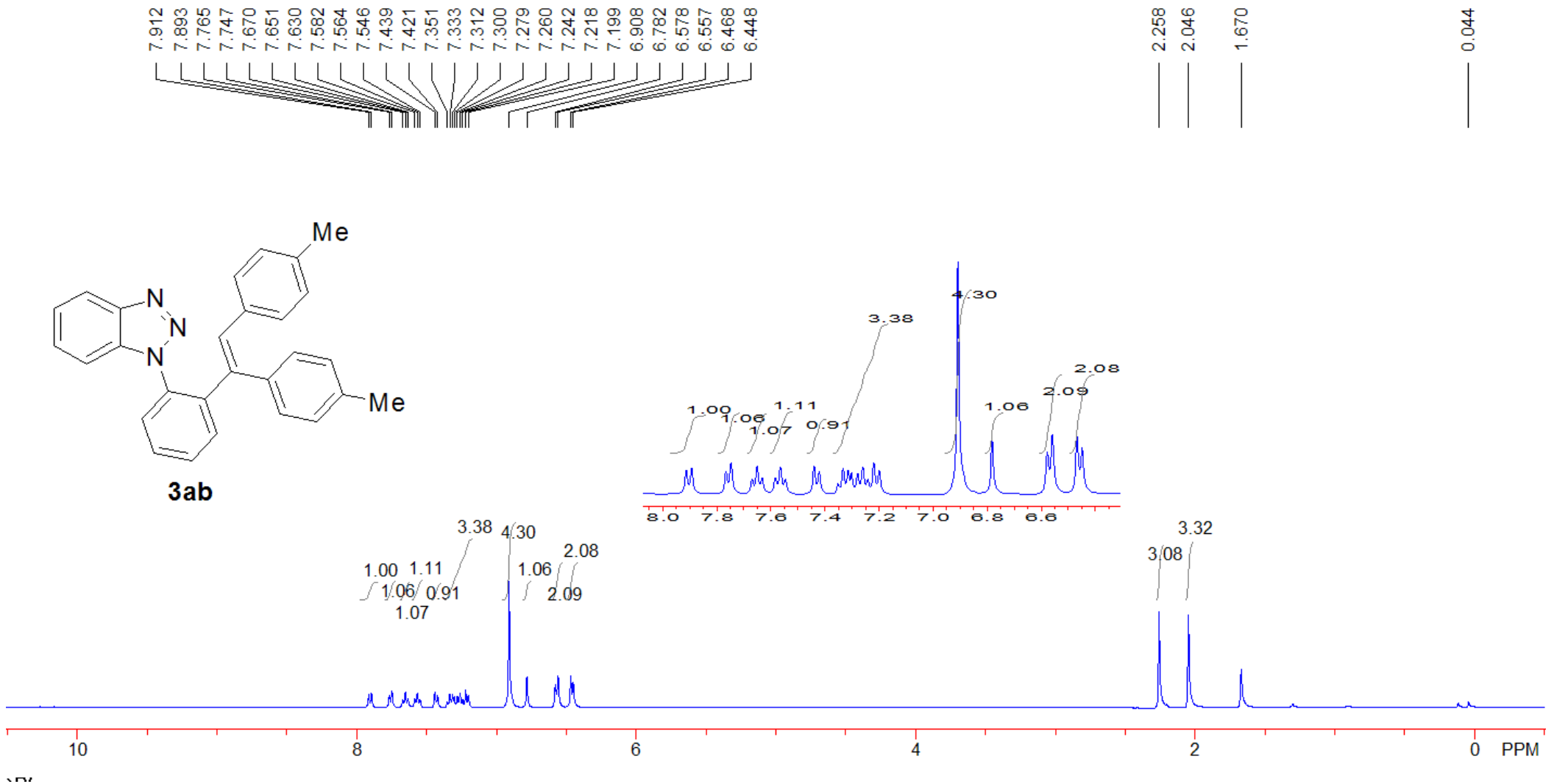
Analysis Info

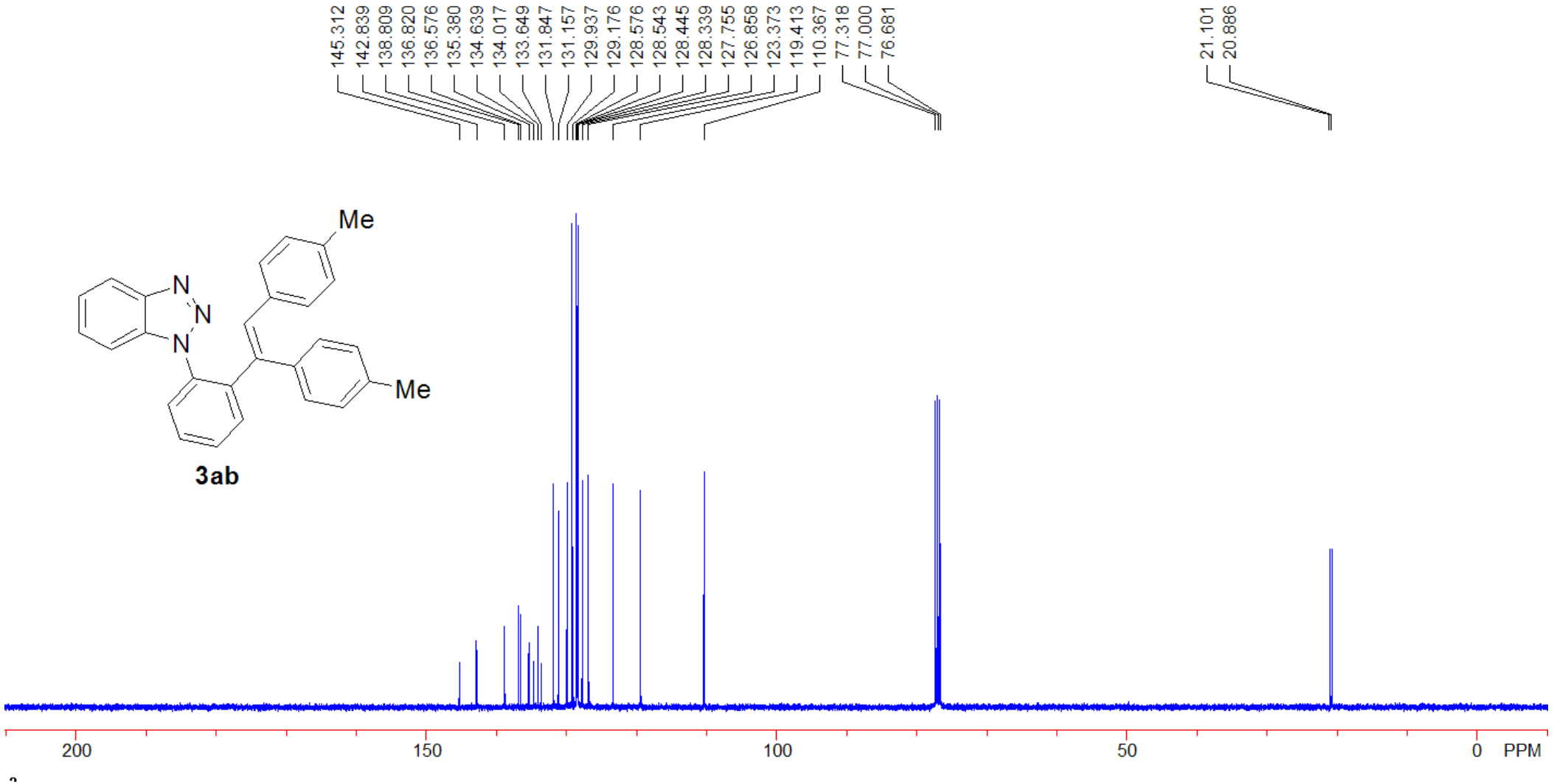
Analysis Name	13060980_20130626_000015.d	Acquisition Date	6/26/2013 8:57:15 PM
Sample	14	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3sa

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
375.16016	1	C 25 H 19 N 4	100.00	375.16042	0.3	0.7	5.1	18.5	even	ok

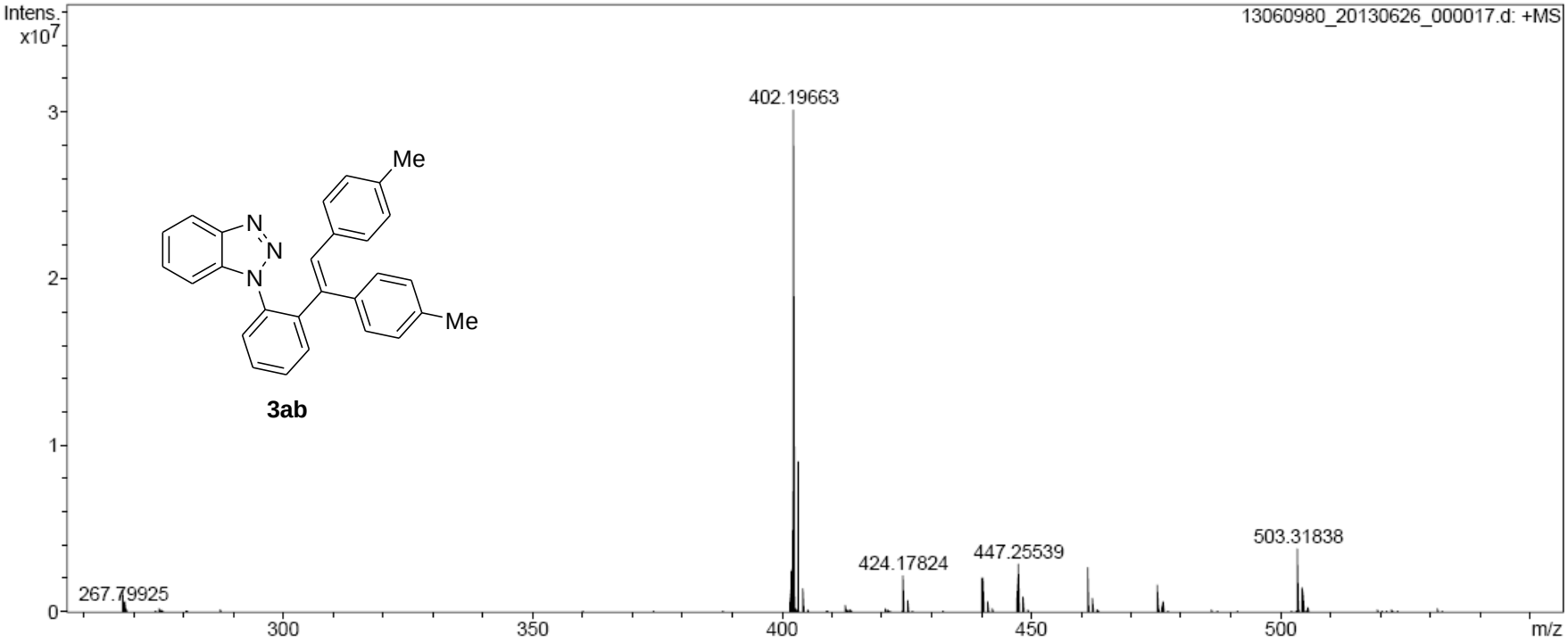




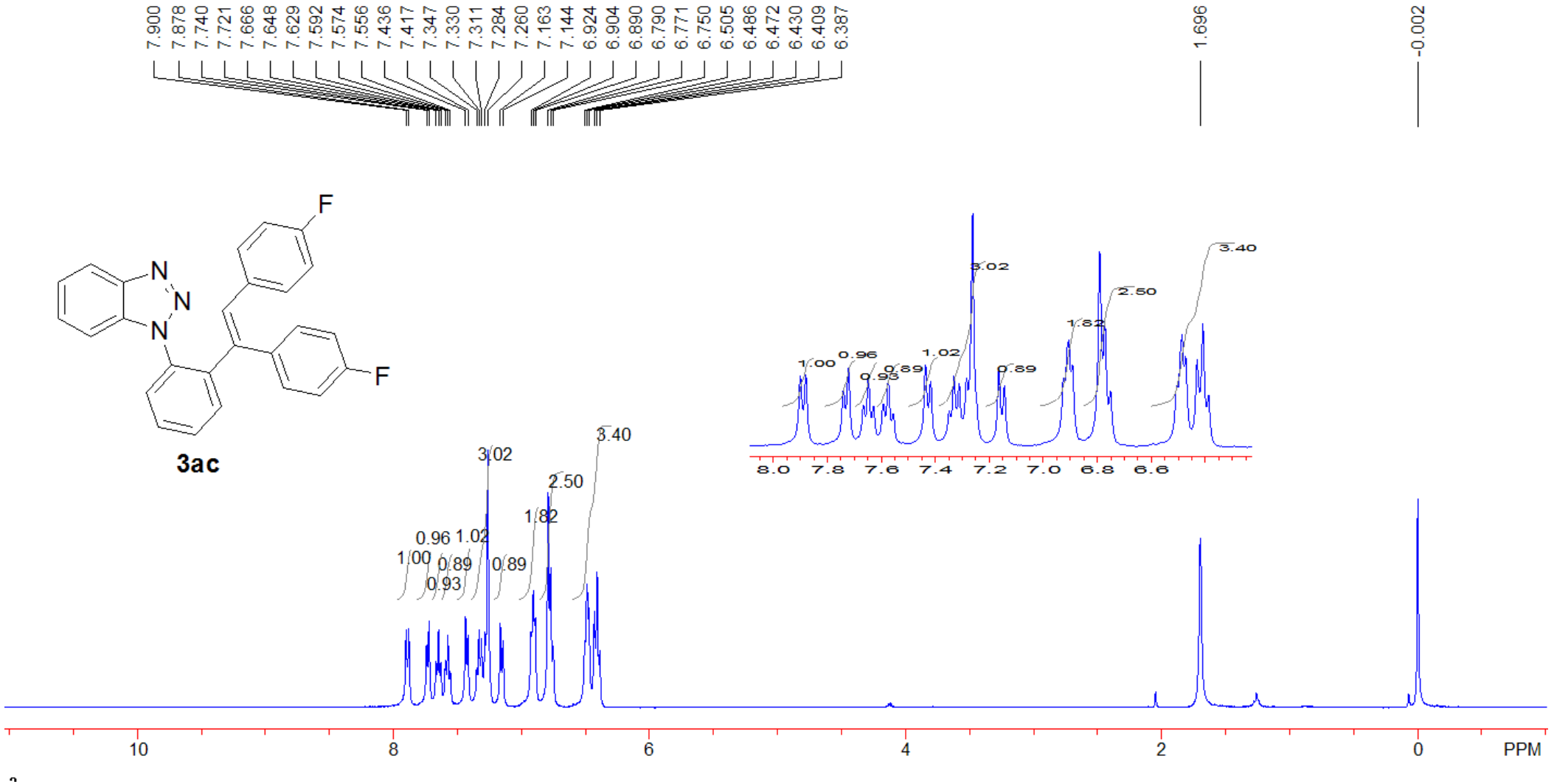
Peking University Mass Spectrometry Sample Analysis Report

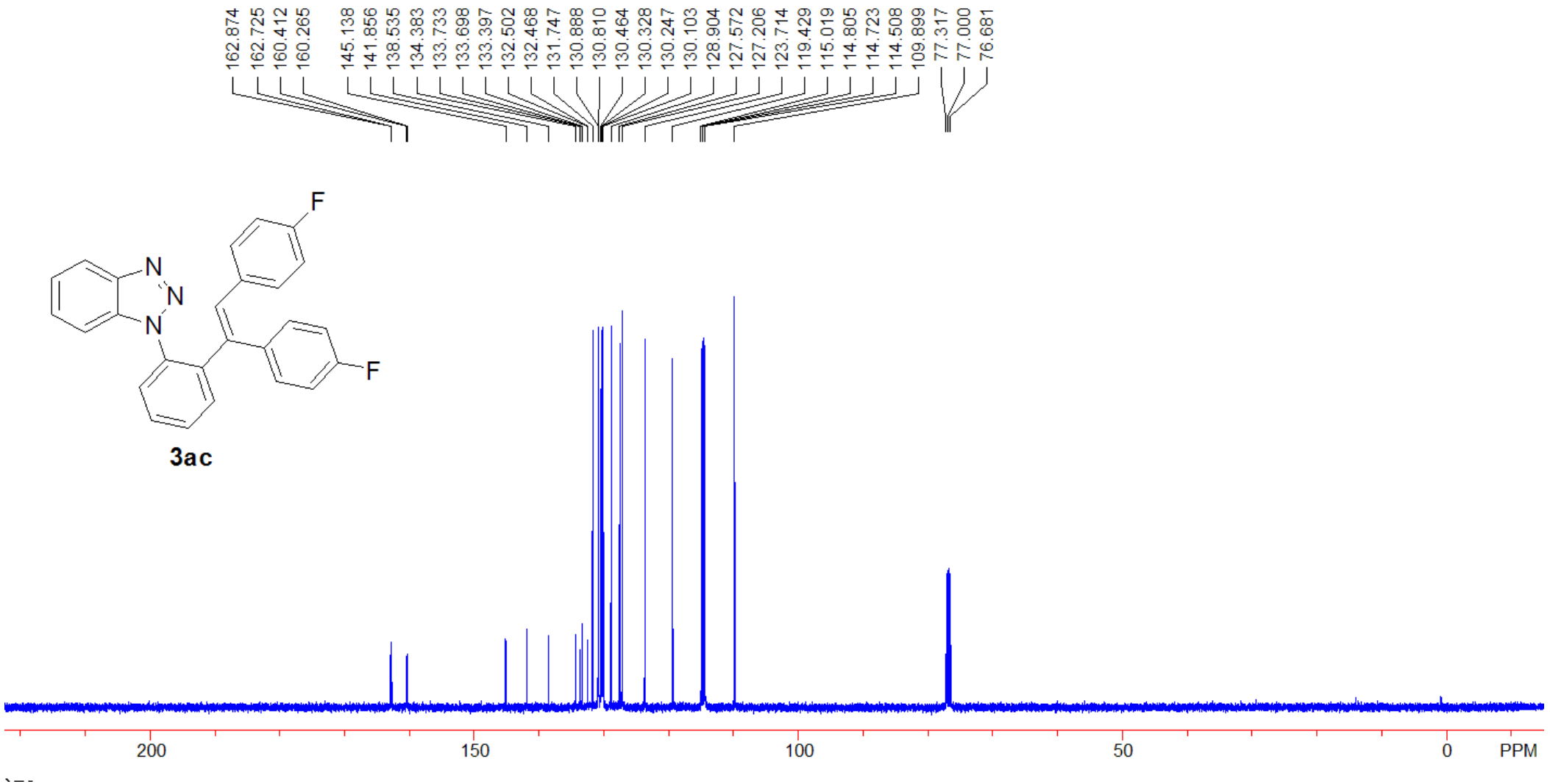
Analysis Info

Analysis Name	13060980_20130626_000017.d	Acquisition Date	6/26/2013 9:01:35 PM
Sample	16	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
402.19663	1	C 28 H 24 N 3	100.00	402.19647	-0.2	-0.4	1.3	18.5	even	ok

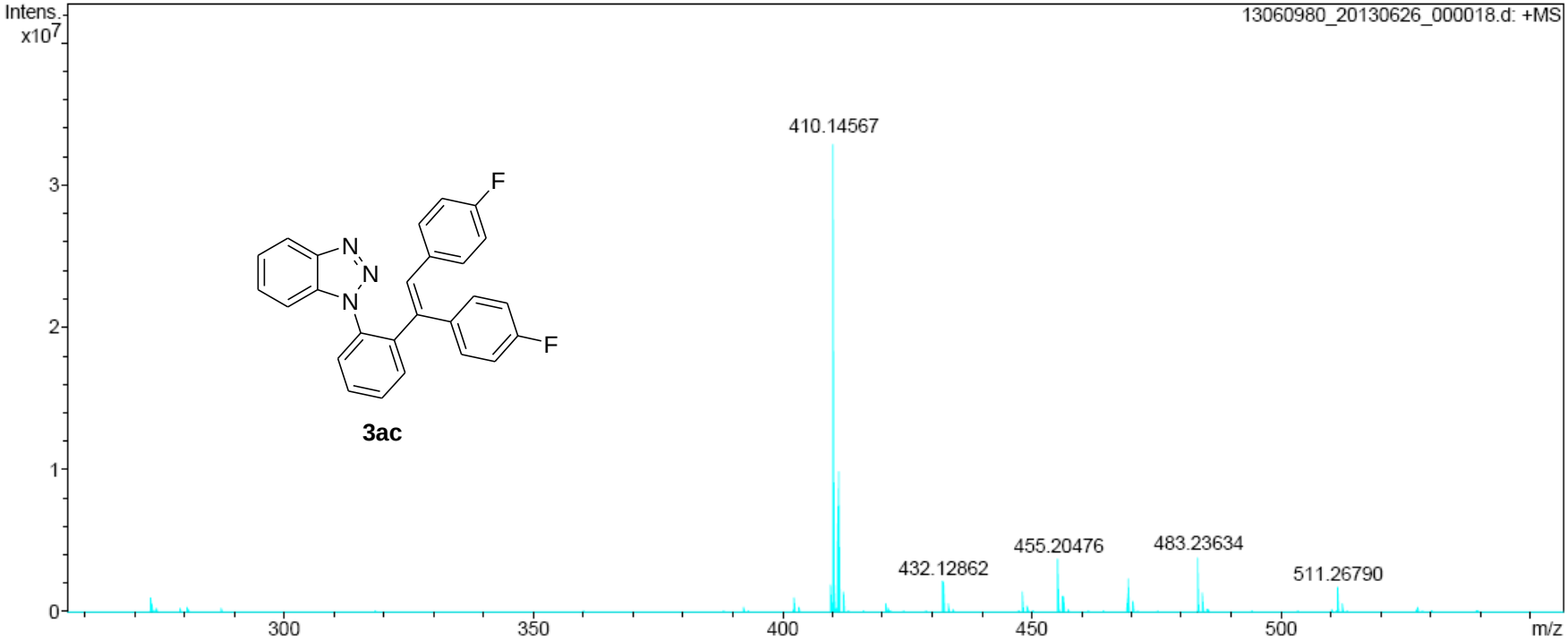




Peking University Mass Spectrometry Sample Analysis Report

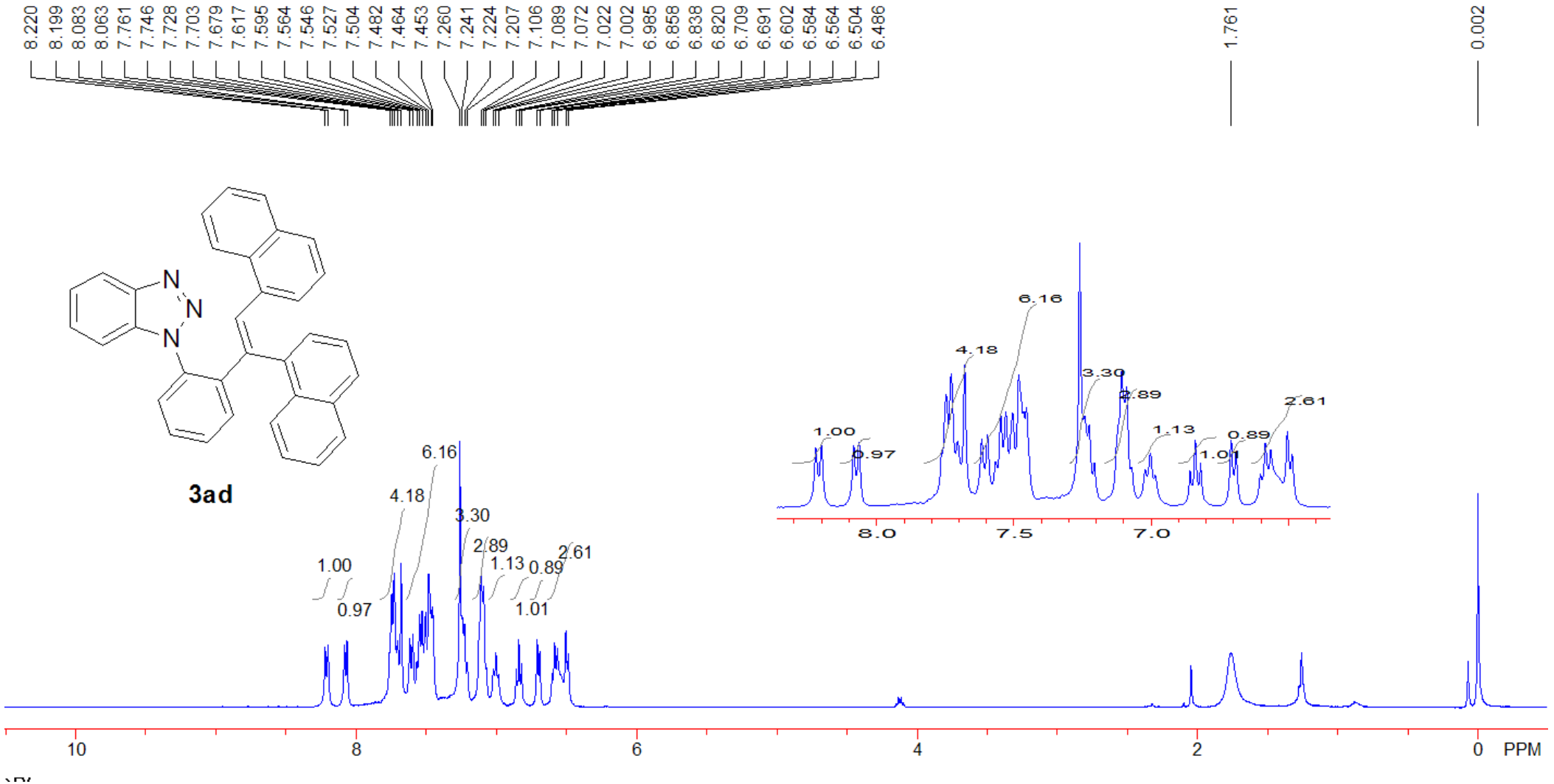
Analysis Info

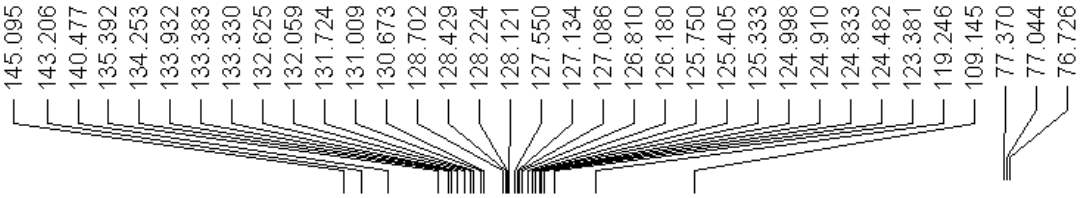
Analysis Name	13060980_20130626_000018.d	Acquisition Date	6/26/2013 9:03:25 PM
Sample	17	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University

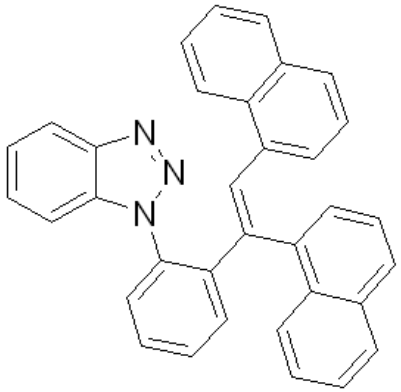


3ac

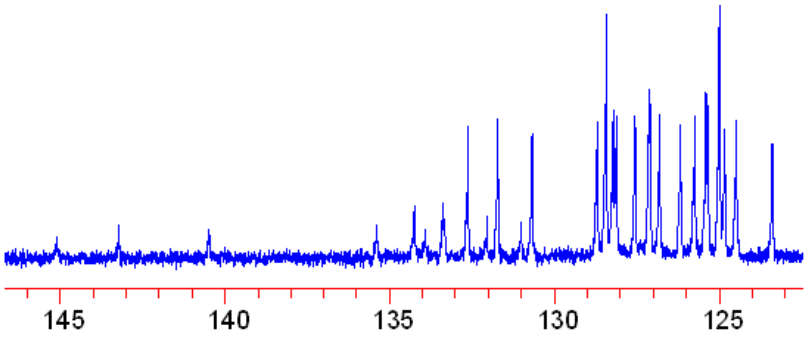
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
410.14567	1	C 26 H 18 F 2 N 3	100.00	410.14633	0.7	1.6	4.6	18.5	even	ok

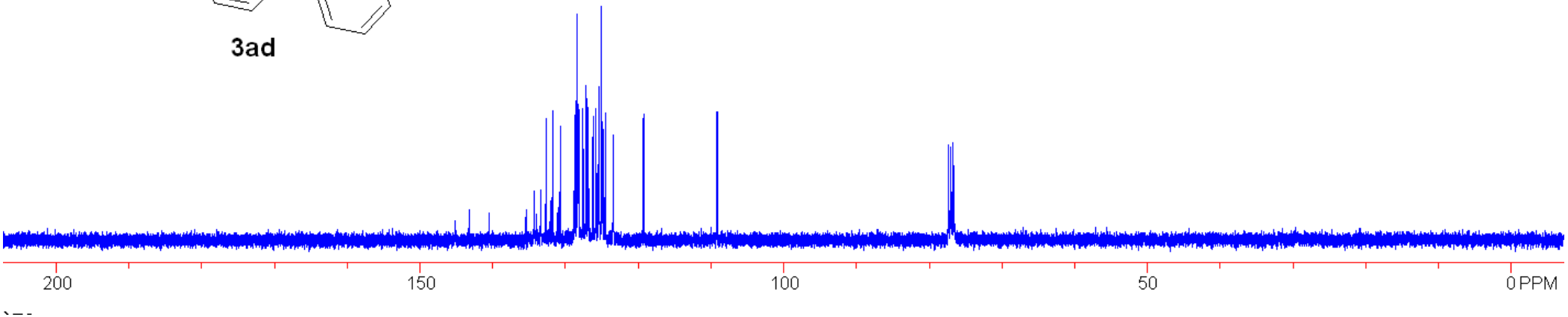






3ad

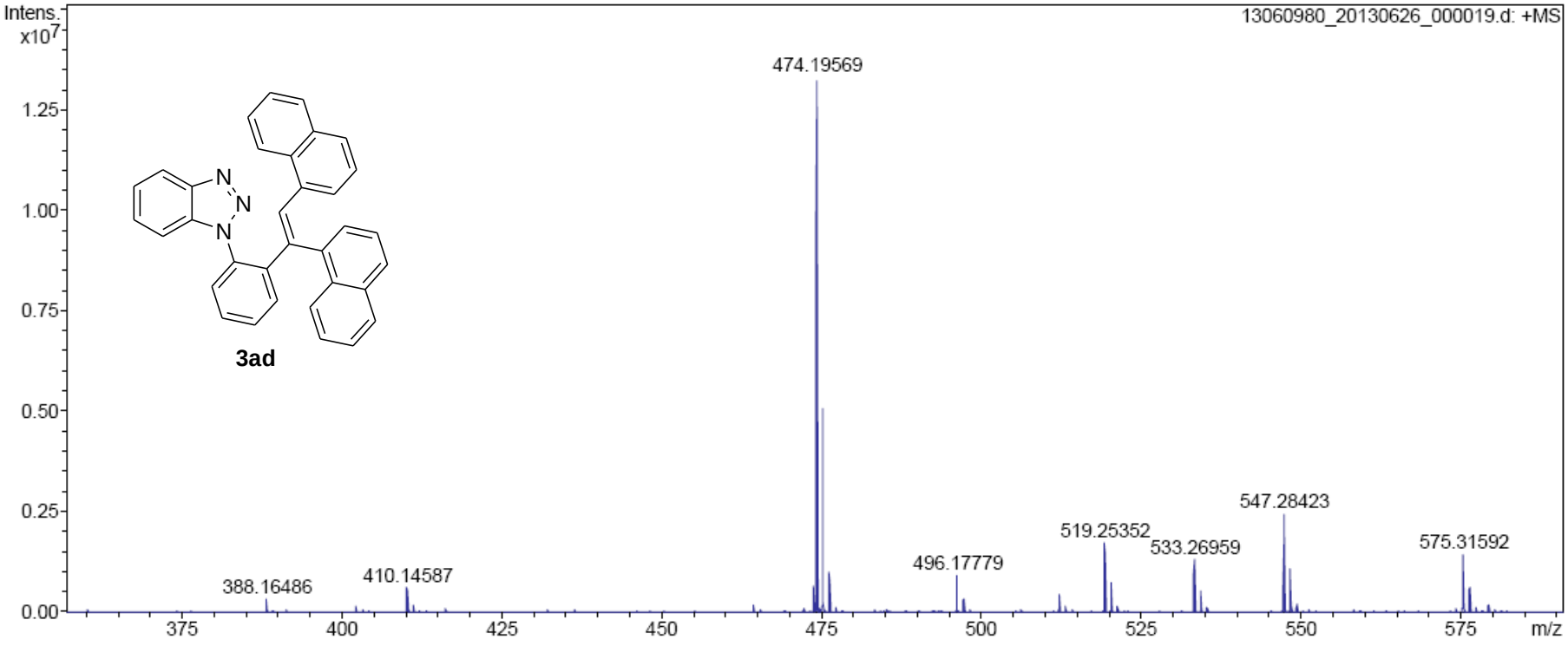




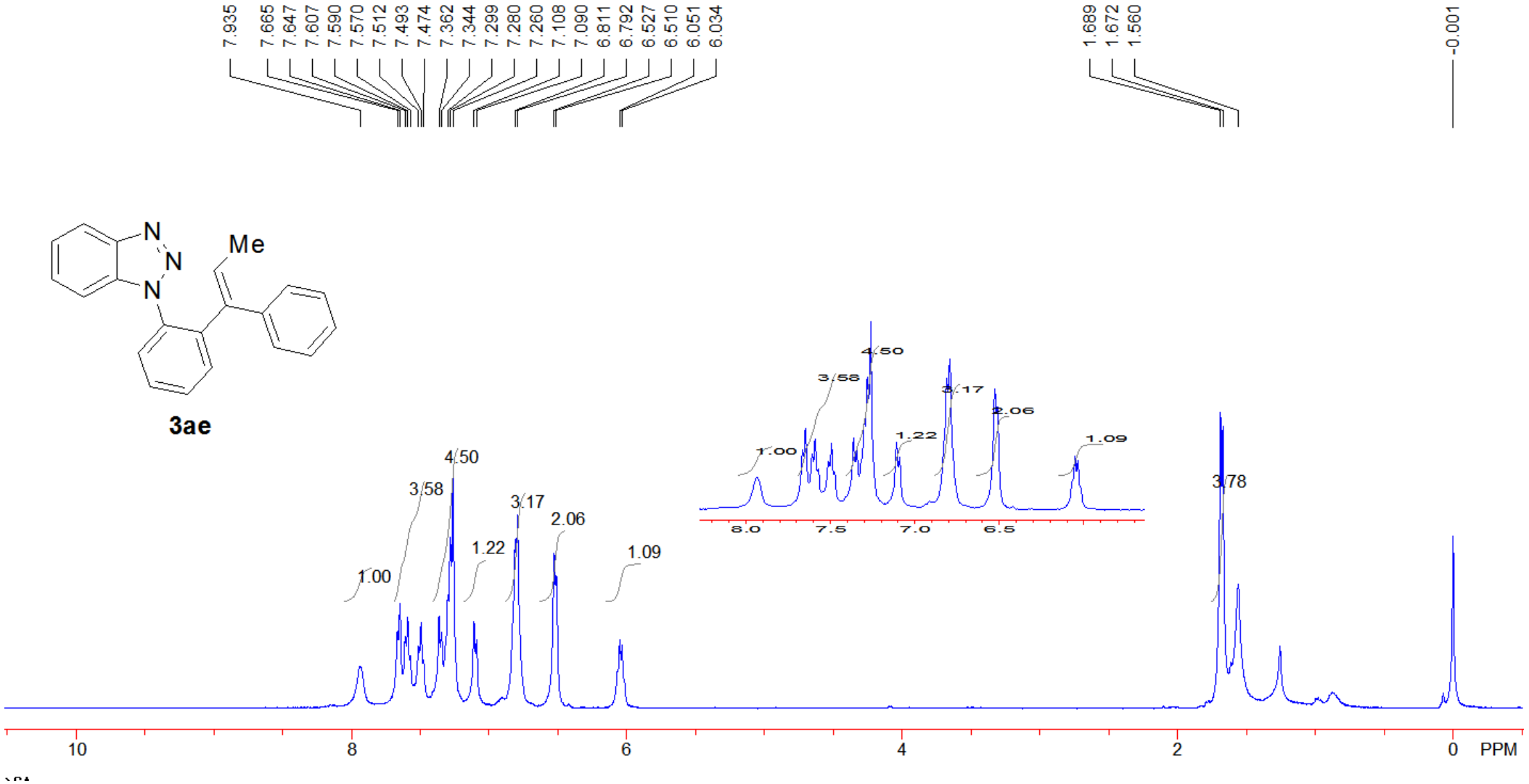
Peking University Mass Spectrometry Sample Analysis Report

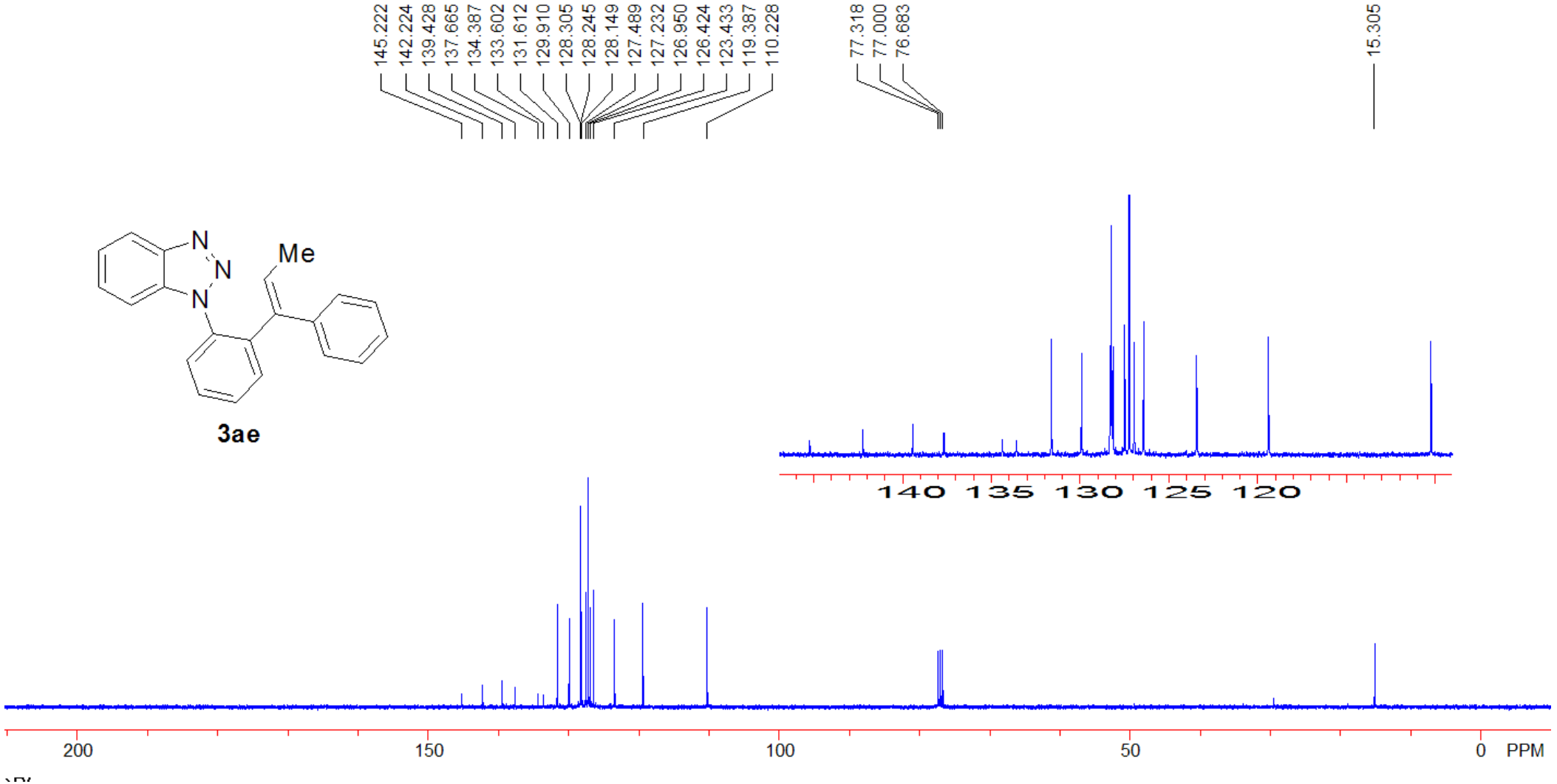
Analysis Info

Analysis Name	13060980_20130626_000019.d	Acquisition Date	6/26/2013 9:05:08 PM
Sample	18	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
474.19569	1	C 34 H 24 N 3	100.00	474.19647	0.8	1.7	5.5	24.5	even	ok

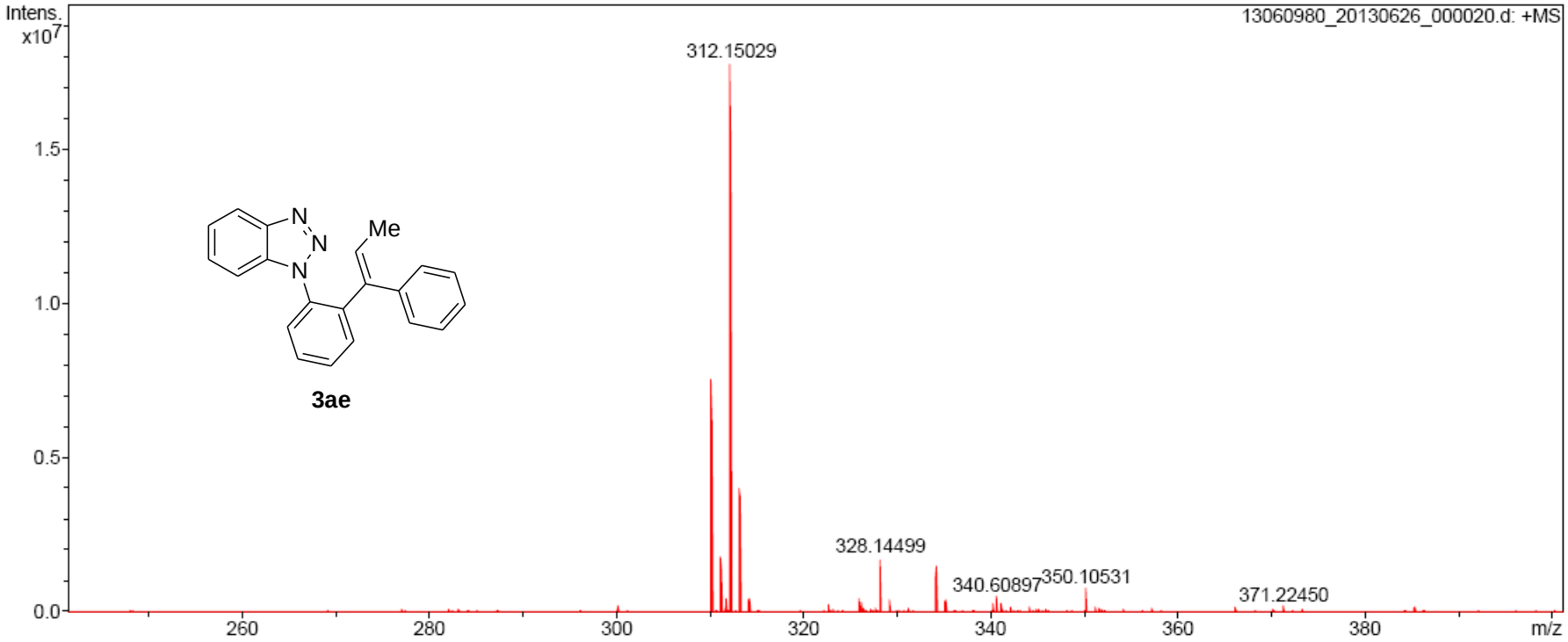




Peking University Mass Spectrometry Sample Analysis Report

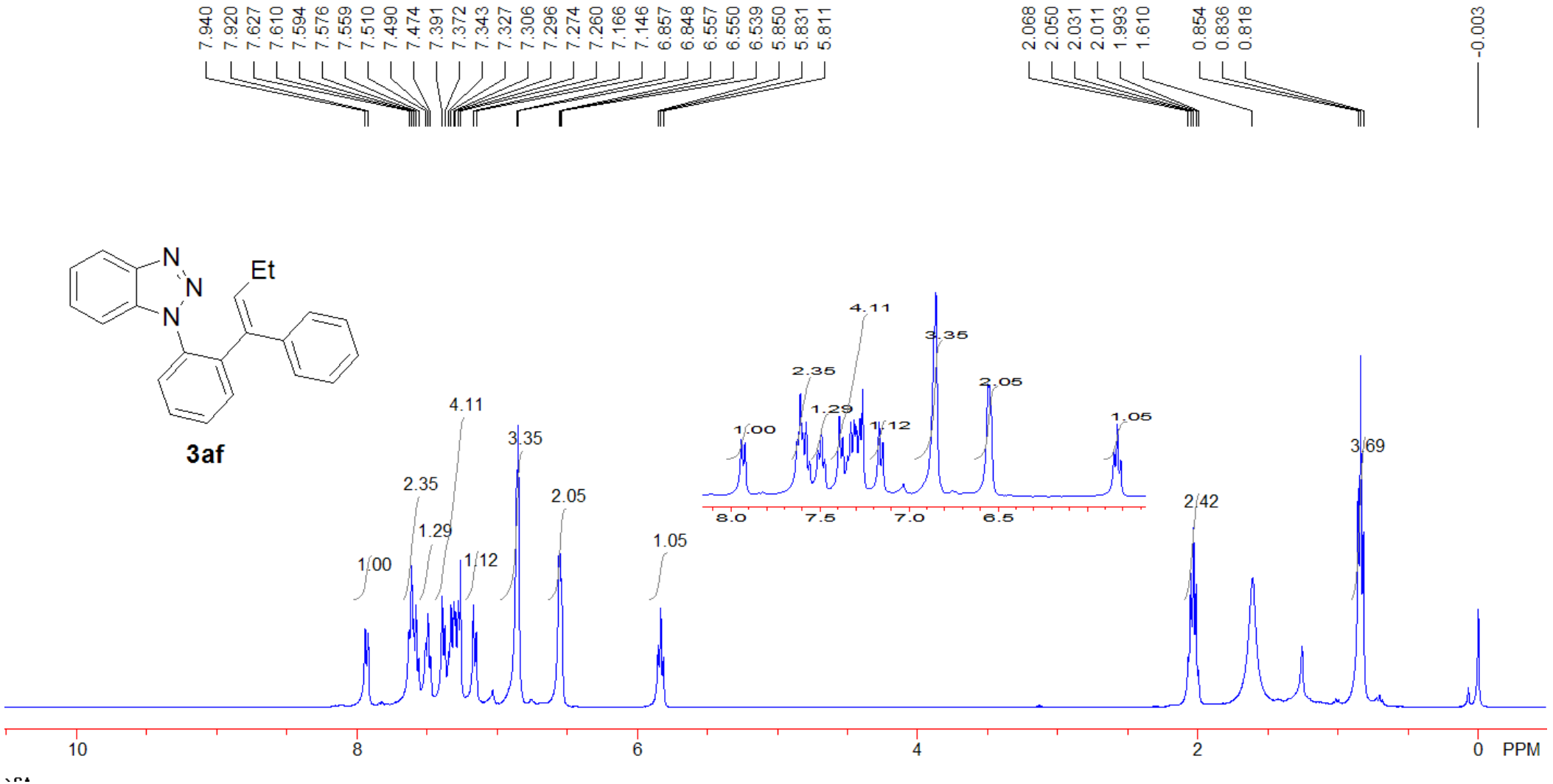
Analysis Info

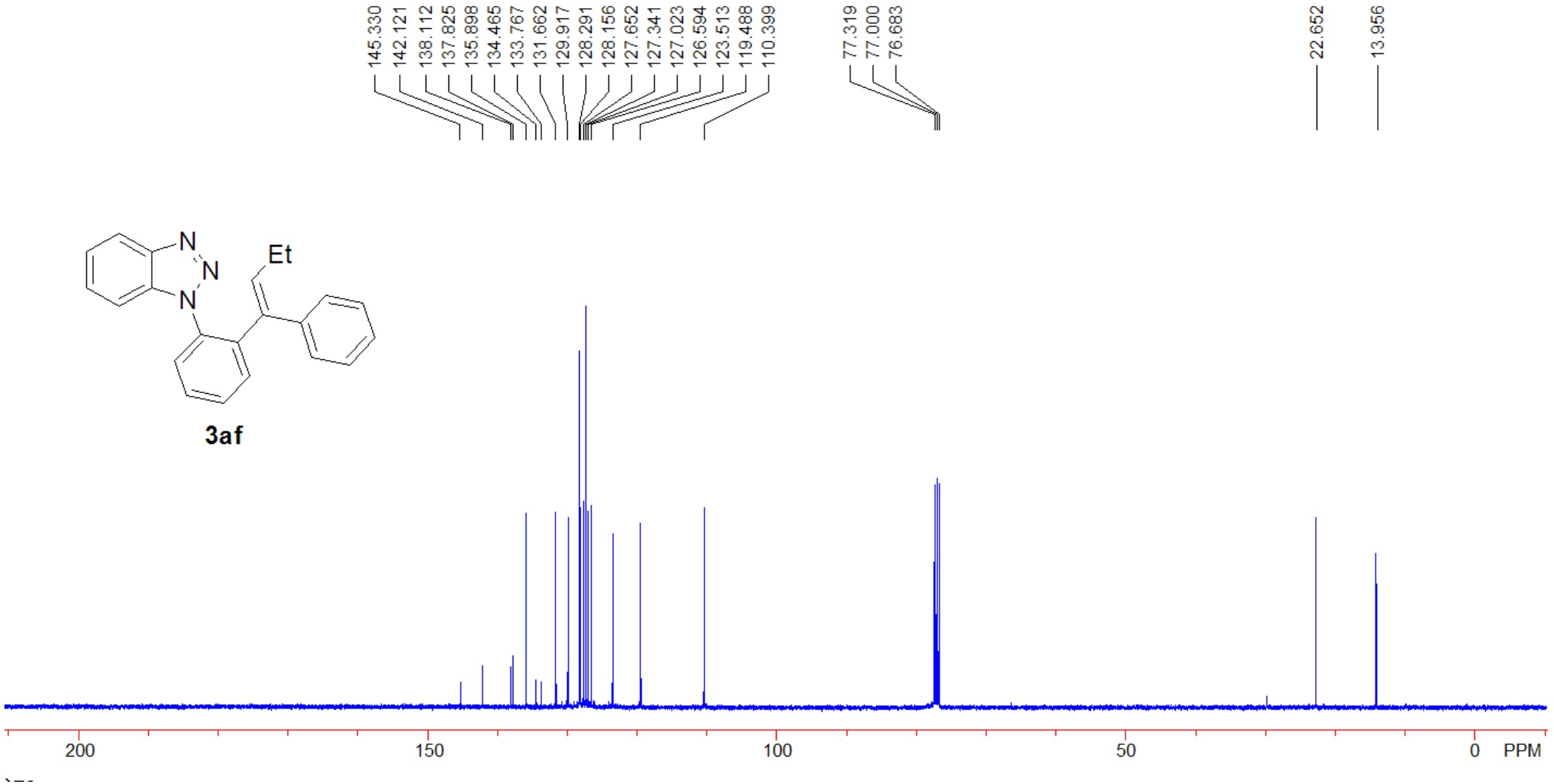
Analysis Name	13060980_20130626_000020.d	Acquisition Date	6/26/2013 9:07:10 PM
Sample	19	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ae

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
312.15029	1	C 21 H 18 N 3	100.00	312.14952	-0.8	-2.4	4.6	14.5	even	ok



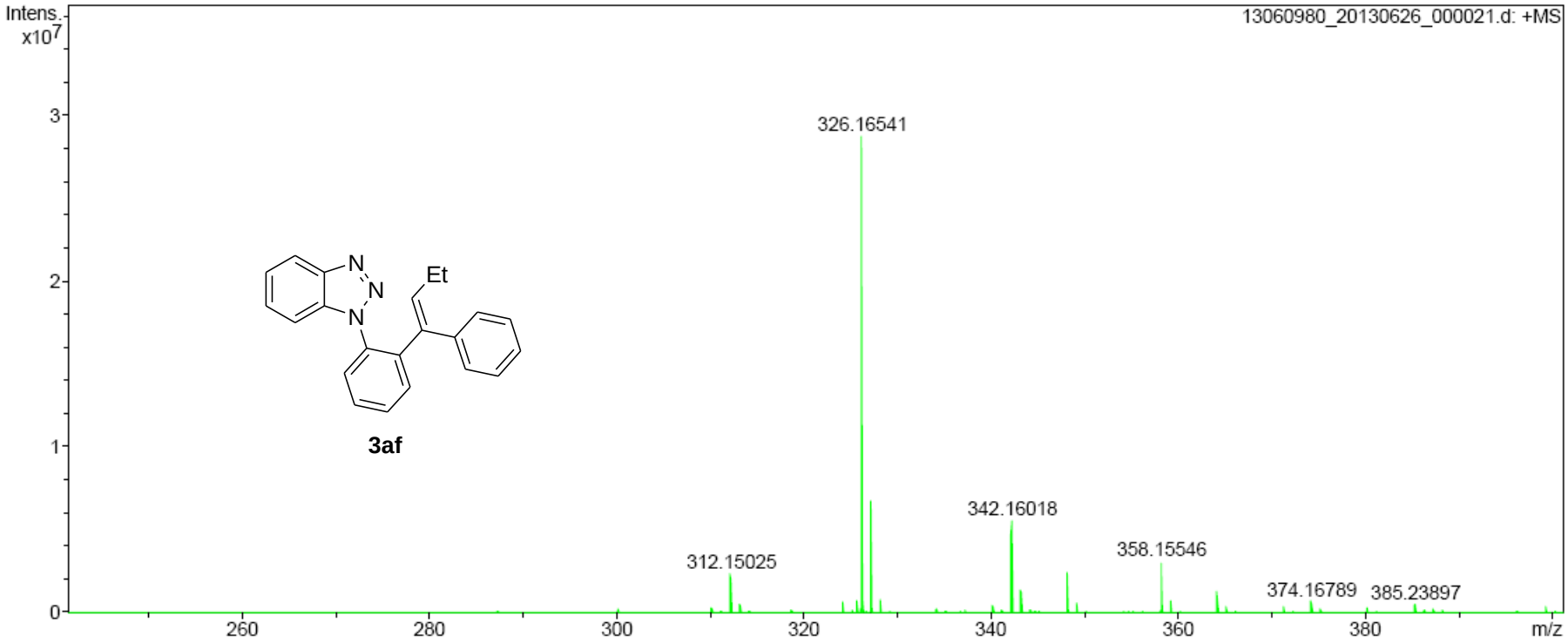


3af

Peking University Mass Spectrometry Sample Analysis Report

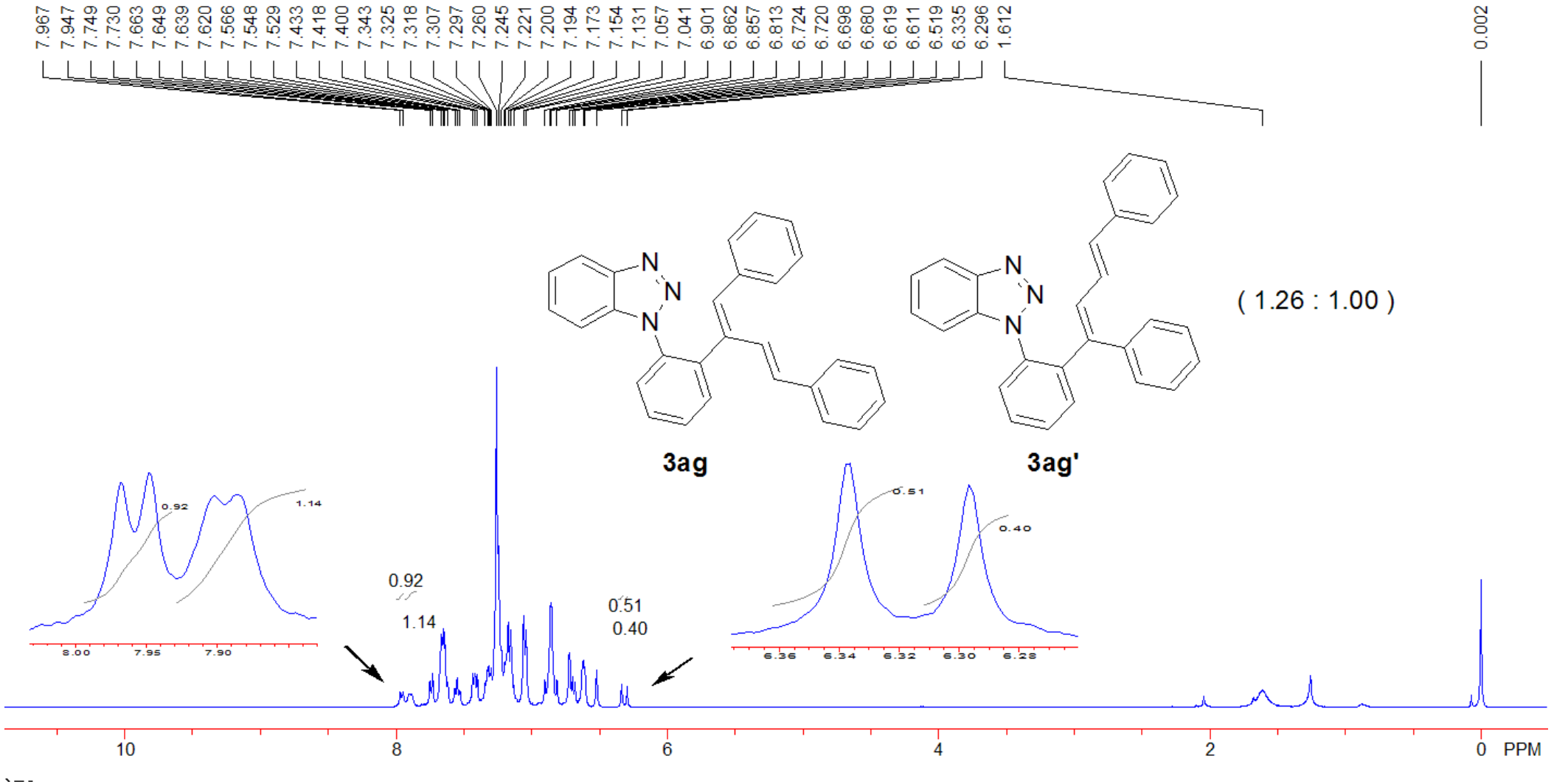
Analysis Info

Analysis Name	13060980_20130626_000021.d	Acquisition Date	6/26/2013 9:08:54 PM
Sample	20	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3af

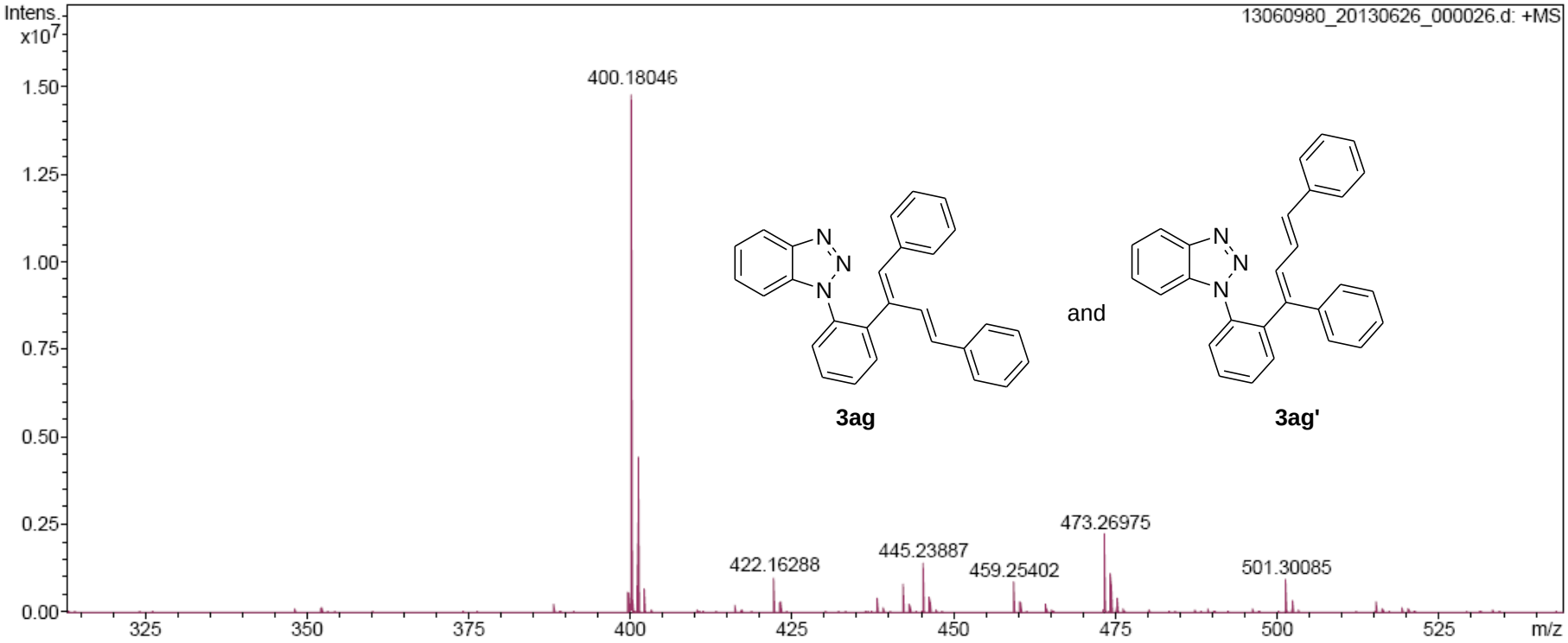
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
326.16541	1	C 22 H 20 N 3	100.00	326.16517	-0.2	-0.7	4.8	14.5	even	ok



Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	13060980_20130626_000026.d	Acquisition Date	6/26/2013 9:19:06 PM
Sample	25	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ag

and

3ag'

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
400.18046	1	C 28 H 22 N 3	100.00	400.18082	0.4	0.9	1.4	19.5	even	ok