Electronic Supplementary Material (ESI) for Chemical Communications.

Palladium-Catalyzed Synthesis of Polysubstituted Quinolines from 2-Amino Aromatic Ketones and Alkynes

Supporting Information

Wang Zhou,* Jianhua Lei

College of Chemical Engineering, Xiangtan University, Xiangtan 411105, China

E-mail: wzhou@xtu.edu.cn

Contents:

General Remarks.....S2

Typical Experimental Procedure…… …….S3

Analytical Data for Compounds **3**.....S4

References.....S19

Crystal Data and Structure Refinement for **3ka**.....S20

NMR and HRMS Spectra of Those Compounds S21

General Remarks

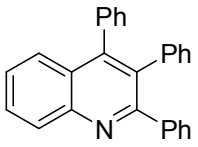
^{1}H-NMR spectra were recorded on a Bruker AVIII-400 spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ as an internal standard. ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and calibrated with $CDCl_3$ (δ = 77.0 ppm). Mass spectra were recorded using an Agilent 5975 GC-MS. A variety of 2-aminobenzophenones could be readily available *via* one-step synthesis from 2-cyano aniline and aromatic boronic acid.[1] Unless otherwise noted, materials obtained from commercial suppliers were used without further purification.

Typical Experimental Procedure

To a seal tube were added 2-amino aromatic ketone (**1,** 0.2 mmol), acetylene (**2**, 0.4 mmol), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH or AcOH (1.6 mmol), DCE (0.8 mL) and benzenenitrile (0.8 mL). The mixture was stirred and heated at 130 °C for 18 h until the substrate disappeared as monitored by TLC. The reaction mixture was neutralized with saturated $NaHCO_3$ and then extracted with ethyl acetate. The combined ethyl acetate solution was washed with brine, 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

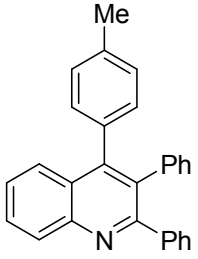
1) 2,3,4-triphenylquinoline (3aa)[2]



3aa

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 59 mg (83%) of **3aa** as white solid. m.p.: 203-204 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.31 (m, 1H), 7.75 (t, *J* = 7.47 Hz, 1H), 7.59 (d, *J* = 7.47 Hz, 1H), 7.47 (t, *J* = 7.47 Hz, 1H), 7.39-7.37 (m, 2H), 7.28-7.26 (m, 3H), 7.23-7.21 (m, 3H), 7.14-7.12 (m, 2H), 7.01-6.99 (m, 3H), 6.89-6.87 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.0, 147.7, 147.4, 141.2, 138.4, 137.0, 133.0, 131.4, 130.4, 130.0, 129.8, 129.4, 127.8, 127.7, 127.6, 127.4, 127.3, 126.72, 126.67, 126.6, 126.4 ppm; IR (KBr): ν_{max} = 3437, 3054, 3024, 2925, 1549, 1481, 1442, 1347, 1074, 1026, 774, 698, 630 cm^{-1}; MS (70 eV): m/z (%) 356.2 (M^+, 100).

2) 2,3-diphenyl-4-p-tolylquinoline (3ba)

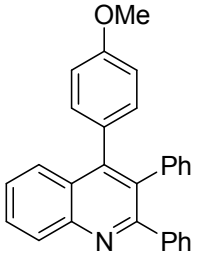


3ba

The reaction of (2-aminophenyl)(p-tolyl)methanone (**1b**, 0.2 mmol, 42.2 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 47 mg (64%) of **3ba** as white solid. m.p.: 153-154 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.26 (d, *J* = 7.9 Hz, 1H), 7.72 (t, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 1H), 7.40-7.34 (m, 2H), 7.23-7.16 (m, 3H), 7.11-7.05 (m, 2H),

7.05-6.98 (m, 5H), 6.92-6.86 (m, 2H), 2.32 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.0, 147.9, 147.3, 141.2, 138.5, 136.9, 133.9, 133.0, 131.4, 130.2, 129.9, 129.6, 129.4, 128.6, 127.7, 127.6, 127.4, 126.9, 126.8, 126.5, 126.3, 21.2 ppm; IR (KBr): ν_{max} = 3442, 3055, 3027, 2918, 1544, 1486, 1369, 1347, 1109, 1022, 831, 749, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{22}N$ $(M + H)^+$: 372.1747, found 372.1733.

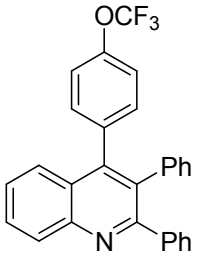
3) 4-(4-methoxyphenyl)-2,3-diphenylquinoline (3ca)



3ca

The reaction of (2-aminophenyl)(4-methoxyphenyl)methanone (**1c**, 0.2 mmol, 45.4 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 54 mg (70%) of **3ca** as white solid. m.p.: 170-171 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.25 (d, *J* = 8.1 Hz, 1H), 7.71 (t, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.45 (t, *J* = 8.1 Hz, 1H), 7.40-7.30 (m, 2H), 7.22-7.17 (m, 3H), 7.08-6.98 (m, 5H), 6.92-6.86 (m, 2H), 6.84-6.78 (m, 2H), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.1, 158.7, 147.5, 147.4, 141.3, 138.5, 133.2, 131.6, 131.4, 130.0., 129.7, 129.3, 129.1, 127.7, 127.6, 127.4, 127.1, 126.7, 126.5, 126.3, 131.3, 55.2 ppm; IR (KBr): ν_{max} = 3438, 3053, 3024, 2933, 1609, 1514, 1486, 1247, 1174, 1030, 853, 770, 696, 620 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{22}NO$ $(M + H)^+$: 388.1696, found 388.1690.

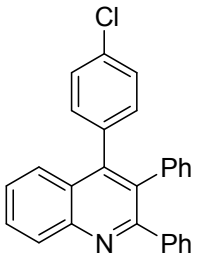
4) 2,3-diphenyl-4-(4-(trifluoromethoxy)phenyl)quinoline (3da)



3da

The reaction of (2-aminophenyl)(4-(trifluoromethoxy)phenyl)methanone (**1d**, 0.2 mmol, 56.2 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 64 mg (73%) of **3da** as white solid. m.p.: 130-131 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.19 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.8 (d, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.34-7.28 (m, 2H), 7.16-7.12 (m, 3H), 7.12-7.04 (m, 4H), 6.98-6.88 (m, 3H), 6.82-6.76 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.0, 148.4, 148.43, 148.41, 147.4, 146.2, 141.0, 138.0, 135.7, 133.2, 131.8, 131.3, 130.0, 129.5, 127.7, 127.5, 126.9, 126.6, 126.4, 126.2, 120.3, 119.2 ppm; IR (KBr): ν_{max} = 3422, 3063, 2924, 1486, 1349, 1283, 1255, 1212, 1159, 768, 701, 628 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{19}F_3NO$ $(M + H)^+$: 442.1413, found 442.1401.

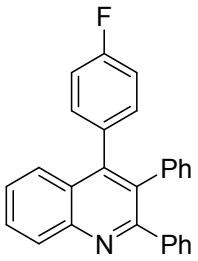
5) 4-(4-chlorophenyl)-2,3-diphenylquinoline (3ea)



3ea

The reaction of (2-aminophenyl)(4-chlorophenyl)methanone (**1e**, 0.2 mmol, 46.2 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 53 mg (68%) of **3ea** as white solid. m.p.: 173-174 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.26 (d, *J* = 7.9 Hz, 1H), 7.73 (t, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.46 (t, *J* = 7.9 Hz, 1H), 7.40-7.32 (m, 2H), 7.28-7.24 (m, 2H), 7.24-7.18 (m, 3H), 7.10-6.98 (m, 5H), 6.90-6.84 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.0, 153.9, 147.3, 146.3, 141.0, 138.1, 135.5, 133.4, 133.0, 131.7, 131.3, 129.9, 129.5, 128.2, 127.7, 127.6, 126.8, 126.6, 126.4, 126.2 ppm; IR (KBr): ν_{max} = 3432, 3058, 2923, 2852, 1548, 1482, 1348, 1086, 1015, 851, 793, 702, 628 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{19}ClN$ $(M + H)^+$: 392.1201, found 392.1207.

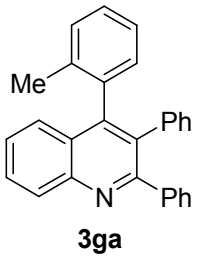
6) 4-(4-fluorophenyl)-2,3-diphenylquinoline (3fa)



3fa

The reaction of (2-aminophenyl)(4-fluorophenyl)methanone (**1f**, 0.2 mmol, 43.0 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 47 mg (63%) of **3fa** as white solid. m.p.: 168-169 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.26 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.40-7.34 (m, 2H), 7.22-7.16 (m, 3H), 7.14-7.06 (m, 2H), 7.04-6.94 (m, 5H), 6.90-6.86 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 162.0 (d, J_{C-F} = 250.0 Hz), 159.0, 147.4, 146.7, 141.0, 138.2, 133.2, 132.88 (d, J_{C-F} = 4.0 Hz), 132.01 (d, J_{C-F} = 8.0 Hz), 131.3, 130.0, 129.9, 129.5, 127.70, 127.68, 127.5, 126.74, 126.67, 126.5, 126.3, 115.0 (d, J_{C-F} = 20.0 Hz) ppm; IR (KBr): ν_{max} = 3439, 3058, 2923, 2856, 1603, 1510, 1486, 1347, 1222, 1155, 1092, 841, 765, 702, 693 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{19}FN$ $(M + H)^+$: 376.1496, found 376.1496.

7) 2,3-diphenyl-4-o-tolylquinoline (3ga)

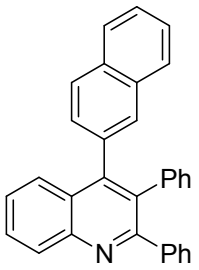


3ga

The reaction of (2-aminophenyl)(o-tolyl)methanone (**1g**, 0.2 mmol, 42.2 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 39 mg (53%) of **3ga** as white solid. m.p.: 149-150 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.26 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 7.46-7.34 (m, 4H), 7.24-7.16 (m, 4H), 7.16-7.08 (m, 2H), 7.08-6.82 (m, 6H), 1.92 (s, 3H); ^{13}C NMR ($CDCl_3$,

100 MHz): δ = 159.2, 147.5, 147.2, 141.1, 138.3, 136.5, 136.1, 133.0, 130.4, 130.0, 129.8, 129.7, 129.5, 127.8, 127.72, 127.65, 127.3, 126.7, 126.54, 126.47, 126.4, 125.2, 20.0 ppm; IR (KBr): ν_{max} = 3434, 3051, 3022, 1548, 1477, 1346, 1026, 763, 701, 629 cm^{-1}; HRMS m/z (ESI) calcd for $C_{28}H_{22}N$ $(M + H)^+$: 372.1747, found 372.1744.

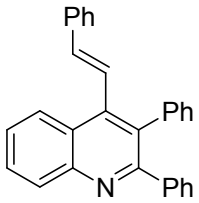
8) 4-(naphthalen-2-yl)-2,3-diphenylquinoline (3ha)



3ha

The reaction of (2-aminophenyl)(naphthalen-3-yl)methanone (**1h**, 0.2 mmol, 49.4mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and Benzenenitrile (0.8 mL) under **typical procedure** afforded 44 mg (54%) of **3ha** as white solid. m.p.: 104-105 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.28 (d, *J* = 8.6 Hz, 1H), 7.82-7.64 (m, 4H), 7.67 (s, 1H), 7.58 (d, *J* = 8.6 Hz, 1H), 7.50-7.36 (m, 5H), 7.22-7.18 (m, 4H), 6.98-6.88 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.1, 147.5, 147.4, 141.2, 138.3, 134.5, 133.2, 132.8, 132.3, 131.3, 130.0, 129.8, 129.6, 129.4, 128.2, 128.0, 127.8, 127.7, 127.6, 127.4, 126.7, 126.6, 126.4, 126.3, 126.25 ppm; IR (KBr): ν_{max} = 3439, 3054, 2924, 2853, 1730, 1236, 1041, 701 cm^{-1}; HRMS m/z (ESI) calcd for $C_{31}H_{22}N$ $(M + H)^+$: 408.1747, found 408.1752.

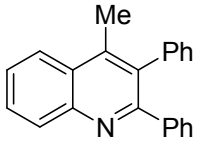
9) 2,3-diphenyl-4-styrylquinoline (3ia)



3ia

The reaction of (E)-1-(2-aminophenyl)-3-phenylprop-2-en-1-one (**1i**, 0.2 mmol, 44.6mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and Benzenenitrile (0.8 mL) under **typical procedure** afforded 57 mg (74%) of **3ia** as white solid. m.p.: 168-169 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.35 (d, *J* = 7.7 Hz, 1H), 8.26 (d, *J* = 7.7 Hz, 1H), 7.77 (t, *J* = 7.7 Hz, 1H), 7.58 (t, *J* = 7.7 Hz, 1H), 7.40-7.32 (m, 6H), 7.26-7.18 (m, 7H), 7.16-7.12 (m, 2H), 7.04 (d, *J* = 16.6 Hz, 1H), 6.85 (d, *J* = 16.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 158.7, 147.8, 143.3, 141.0, 138.3, 137.7, 136.8, 132.2, 131.4, 130.2, 129.9, 129.4, 128.8, 128.3, 127.9, 127.7, 127.6, 127.1, 126.7, 125.6, 125.8, 124.5, 124.4 ppm; IR (KBr): ν_{max} = 3433, 3055, 2922, 2852, 1486, 1447, 1398, 1348, 988, 975, 771, 746, 701, 688 cm^{-1}; HRMS m/z (ESI) calcd for $C_{29}H_{22}N$ $(M + H)^+$: 384.1747, found 384.1746.

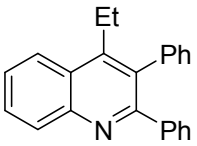
10) 4-methyl-2,3-diphenylquinoline (3ja)



3ja

The reaction of 1-(2-aminophenyl)ethanone (**1j**, 0.2 mmol, 27.0 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 37 mg (63%) of **3ja** as colorless liquid. ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.21 (d, *J* = 8.15 Hz, 1H), 8.08 (d, *J* = 8.15 Hz, 1H), 7.73 (t, *J* = 8.15 Hz, 1H), 7.60 (t, *J* = 8.15 Hz, 1H), 7.34-7.25 (m, 5H), 7.20-7.15 (m, 3H), 7.14-7.08 (m, 2H), 2.54 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 158.9, 146.8, 142.3, 141.4, 139.1, 134.0, 130.8, 130.3, 129.8, 129.1, 128.0 127.6, 127.4, 127.2, 127.0, 126.5, 124.2, 16.3 ppm; MS (70 eV): m/z (%) 294.1 (M^+, 100).

11) 4-ethyl-2,3-diphenylquinoline (3ka)[3]



3ka

The reaction of 1-(2-aminophenyl)propan-1-one (**1k**, 0.2 mmol, 29.8 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 34 mg (55%) of **3ka** as white solid. m.p.: 141-142 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.22 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.34-7.24 (m, 5H), 7.18-7.12 (m, 5H), 2.97 (q, *J* = 7.4 Hz, 2H), 1.21 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.1, 148.2, 147.4, 141.4, 138.9, 133.5, 130.6, 130.5, 129.7, 129.1, 128.0, 127.6, 127.4, 127.0, 126.6, 126.0, 124.2, 22.7, 15.3 ppm; IR (KBr): ν_{max} = 3434, 3051, 2971, 2932, 1566, 1491, 1443, 1346, 763, 697, 606 cm^{-1}; MS (70 eV): m/z (%) 308.2 (M^+, 100).

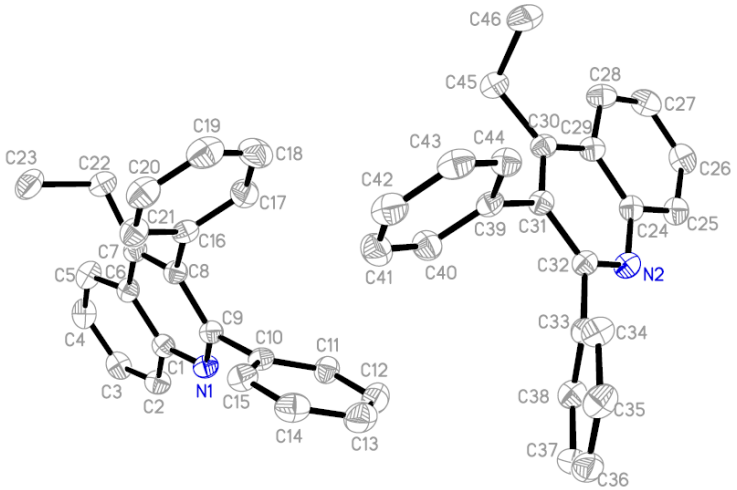
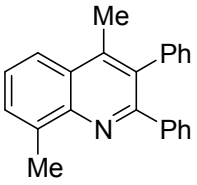


Figure S1. ORTEP drawing of **3ka**

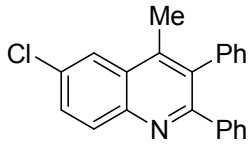
12) 4,8-dimethyl-2,3-diphenylquinoline (3la)



3la

The reaction of 1-(2-aino-3-methylphenyl)ethanone (**1l**, 0.2 mmol, 29.8 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 55 mg (89%) of **3la** as yellow solid. m.p.: 150-151 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.90 (d, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.42-7.36 (m, 2H), 7.32-7.24 (m, 3H), 7.20-7.14 (m, 3H), 7.12-7.08 (m, 2H), 2.87 (s, 3H), 2.51 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 156.9, 145.9, 142.3, 141.7, 139.6, 138.2, 133.5, 130.9, 130.3 129.3, 128.1, 127.4, 127.39, 127.0, 126.2, 122.1, 18.4, 16.5 ppm; IR (KBr): ν_{max} = 3436, 3059, 3021, 2918, 1560, 1483, 1440, 1347, 1073, 1015, 903, 756, 697, 615 cm^{-1}; HRMS m/z (ESI) calcd for $C_{23}H_{20}N$ $(M + H)^+$: 310.1590, found 310.1587.

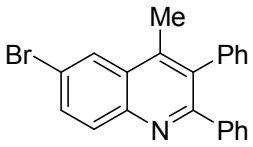
13) 6-chloro-4-methyl-2,3-diphenylquinoline (3ma)



3ma

The reaction of 1-(2-amino-5-chlorophenyl)ethanone (**1m**, 0.2 mmol, 33.8 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 40 mg (61%) of **3ma** as white solid. m.p.: 136-137^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.12 (d, *J* = 8.8 Hz, 1H), 8.04 (s, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.34-7.25 (m, 5H), 7.20-7.16 (m, 2H), 7.12-7.07 (m, 3H), 2.49 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.2, 145.2, 141.6, 141.0, 138.7, 134.8, 132.3, 131.9, 131.4 131.1, 130.7, 130.0, 129.7, 128.1, 127.7, 127.2, 123.4, 16.4 ppm; IR (KBr): ν_{max} = 3436, 3055, 2922, 1480, 1348, 765, 696 cm^{-1}; MS (70 eV): m/z (%) 328.1 (M^+, ^{35}Cl, 100), 330.1 (M^+, ^{37}Cl, 36).

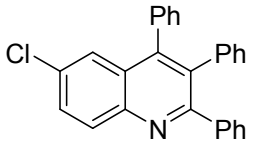
14) 6-bromo-4-methyl-2,3-diphenylquinoline (3na)



3na

The reaction of 1-(2-amino-5-bromophenyl)ethanone (**1n**, 0.2 mmol, 42.4 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 44 mg (59%) of **3na** as white solid. m.p.: 134-135 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.24 (s, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 9.0 Hz, 1H), 7.32-7.26 (m, 5H), 7.24-7.18 (m, 2H), 7.13-7.06 (m, 3H), 2.50 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.3, 145.4, 141.5, 141.0, 138.6, 132.6, 132.0, 131.4, 131.1 130.7, 129.7, 128.1, 127.9, 127.7, 127.2, 126.7, 120.6, 16.4 ppm; IR (KBr): ν_{max} = 3435, 3055, 2922, 1480, 1348, 1070, 828, 766, 696 cm^{-1}; MS (70 eV): m/z (%) 374.0 (M^+, ^{79}Br, 100), 376.0 (M^+, ^{81}Br, 100).

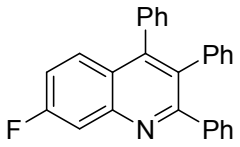
15) 6-chloro-2,3,4-triphenylquinoline (3oa)[4]



3oa

The reaction of (2-amino-5-chlorophenyl)(phenyl)methanone (**1o**, 0.2 mmol, 46.2 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 40 mg (51%) of **3oa** as white solid. m.p.: 193-194 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.19 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.55 (s, 1H), 7.40-7.26 (m, 5H), 7.24-7.18 (m, 3H), 7.14-7.08 (m, 2H), 7.04-6.98 (m, 3H), 6.90-6.86 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.3, 147.0, 145.7, 140.8, 138.0, 136.3, 133.8, 132.5, 131.4 131.3, 130.3, 130.2, 129.9, 128.1, 127.8, 127.76, 127.6, 127.5, 126.6, 125.4 ppm; IR (KBr): ν_{max} = 3443, 3060, 3025, 1471, 1443, 1367, 1080, 837, 699, 609 cm^{-1}; MS (70 eV): m/z (%) 390.1 (M^+, 100).

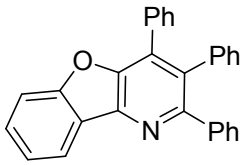
16) 7-fluoro-2,3,4-triphenylquinoline (3pa)



3pa

The reaction of (2-amino-4-fluorophenyl)(phenyl)methanone (**1p**, 0.2 mmol, 43.0 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 42 mg (56%) of **3pa** as yellow solid. m.p.: 195-196 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 7.87 (d, *J* = 9.6 Hz, 1H), 7.60-7.54 (m, 1H), 7.40-7.34 (m, 2H), 7.32-7.24 (m, 3H), 7.22-7.18 (m, 4H), 7.14-7.08 (m, 2H), 7.04-6.96 (m, 3H), 6.90-6.86 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 161.0 (d, J_{C-F} = 171.3 Hz), 147.9, 140.9, 138.1, 136.8, 133.4, 132.4 (d, J_{C-F} = 1.7 Hz), 131.4, 130.2 129.9, 129.5 (d, J_{C-F} = 9.8 Hz), 127.9, 127.8, 127.7, 127.5 127.4, 126.4, 123.8, 116.9 (d, J_{C-F} = 24.7 Hz), 113.1 (d, J_{C-F} = 20.1 Hz) ppm; IR (KBr): ν_{max} = 3440, 3057, 3026, 2924, 2855, 1617, 1481, 1444, 1149, 872, 752, 698, 614, 528 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{19}FN$ $(M + H)^+$: 376.1496, found 376.1501.

17) 2,3,4-triphenylbenzofuro[3,2-b]pyridine (3ra)

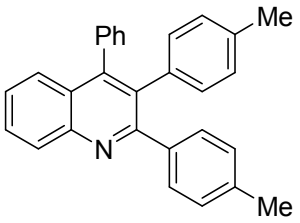


3ra

The reaction of (3-aminobenzofuran-2-yl)(phenyl)methanone (**1r**, 0.2 mmol, 47.4 mg), diphenylacetylene (**2a**, 0.4 mmol, 71.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 50 mg (63%) of **3ra** as yellow solid. m.p.: 178-179 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.27 (d, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.38-7.34 (m, 1H), 7.30-7.26 (m, 2H), 7.24-7.16 (m, 5H), 7.14-7.10 (m, 2H), 7.02-6.96 (m, 3H), 6.88-6.82 (m,

3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 158.1, 155.2, 147.2, 143.0, 141.3, 137.8, 133.3, 133.1, 133.0, 131.8, 131.0, 130.5, 130.2, 129.0, 128.0 127.7, 127.6, 127.2, 126.7, 123.8, 123.5, 121.6, 112.3 ppm; IR (KBr): ν_{max} = 3440, 3057, 3026, 2924, 1495, 1445, 1369, 1199, 872, 753, 699 cm^{-1}; HRMS m/z (ESI) calcd for $C_{29}H_{20}NO$ $(M + H)^+$: 398.1539, found 398.1540.

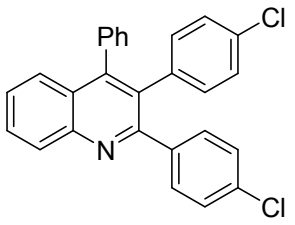
18) 4-phenyl-2,3-dip-tolylquinoline (3ab)



3ab

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), 1,2-dip-tolylethyne (**2b**, 0.4 mmol, 82.4 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 54 mg (70%) of **3ab** as white solid. m.p.: 199-200 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.23 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.32-7.24 (m, 5H), 7.16-7.08 (m, 2H), 7.14-6.98 (m, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 2.29 (s, 3H), 2.18 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.1, 147.6, 147.3, 138.5, 137.3, 135.7, 135.4, 132.9, 131.2, 130.3, 129.9, 129.7, 129.1, 128.4, 128.0, 127.8, 127.1, 126.7, 126.56, 126.3, 21.2, 21.1 ppm; IR (KBr): ν_{max} = 3435, 3058, 3021, 2918, 1548, 1479, 1346, 1188, 1069, 1020, 829, 763, 705, 612 cm^{-1}; HRMS m/z (ESI) calcd for $C_{29}H_{24}N$ $(M + H)^+$: 386.1903, found 386.1895.

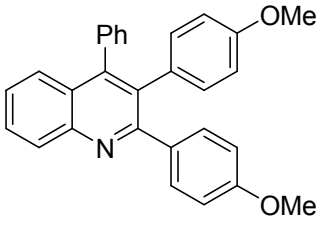
19) 2,3-bis(4-chlorophenyl)-4-phenylquinoline (3ac)



3ac

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), 1,2-bis(4-chlorophenyl)ethyne (**2c**, 0.4 mmol, 98.4 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 60 mg (70%) of **3ac** as yellow solid. m.p.: 241-242 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.23 (d, *J* = 7.7 Hz, 1H), 7.74 (t, *J* = 7.7 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H), 7.36-7.28 (m, 5H), 7.26-7.18 (m, 2H), 7.14-7.06 (m, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 157.4, 148.1, 147.4, 139.4, 136.7, 136.5, 134.1, 132.7, 132.6, 131.5, 131.3, 130.2, 129.8, 129.7, 128.1, 128.09, 127.9, 127.6, 127.0, 126.7, 126.6 ppm; IR (KBr): ν_{max} = 3433, 3059, 2924, 2853, 1571, 1489, 1342, 1125, 1013, 829, 767, 710 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{18}Cl_2N$ $(M + H)^+$: 426.0811, found 426.0812.

20) 2,3-bis(4-methoxyphenyl)-4-phenylquinoline (3ad)

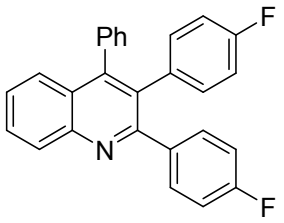


3ad

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), 1,2-bis(4-methoxyphenyl)ethyne (**2d**, 0.4 mmol, 95.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 57 mg (68%) of **3ad** as white solid. m.p.: 180-181 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.15 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 7.30-7.18 (m, 5H), 7.10-7.02 (m, 2H), 6.76-6.66 (m, 4H), 6.56-6.47 (m, 2H), 3.69 (s, 3H), 3.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 163.1,

159.2, 158.8, 158.0, 157.9, 137.3, 133.8, 132.5, 132.4, 131.4, 130.8, 130.3, 129.5, 129.2, 127.9, 127.2, 126.6, 126.3, 113.2, 113.0, 55.2, 55.0 ppm; IR (KBr): ν_{max} = 3433, 2926, 2837, 1607, 1511, 1247, 1180, 1027, 833, 765, 704, 617 cm^{-1}; HRMS m/z (ESI) calcd for $C_{29}H_{24}NO_2$ $(M + H)^+$: 418.1802, found 418.1810.

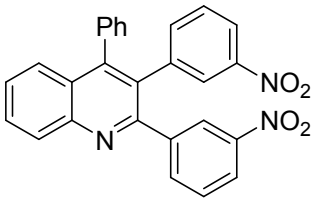
21) 2,3-bis(4-fluorophenyl)-4-phenylquinoline (3ae)



3ae

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), 1,2-bis(4-fluorophenyl)ethyne (**2e**, 0.4 mmol, 85.6 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), AcOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 53 mg (68%) of **3ae** as white solid. m.p.: 186-188 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.15 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.30-7.18 (m, 5H), 7.06-6.98 (m, 2H), 6.88-6.80 (m, 2H), 6.78-6.72 (m, 2H), 6.68-6.60 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 162.5 (d, J_{C-F} = 247 Hz), 161.4 (d, J_{C-F} = 246 Hz), 157.8, 148.1, 147.4, 137.1 (d, J_{C-F} = 3.5 Hz), 136.7, 134.2 (d, J_{C-F} = 4.1 Hz), 132.9 (d, J_{C-F} = 7.9 Hz), 131.81, 131.8 (d, J_{C-F} = 8.3 Hz), 130.2, 129.7, 129.66, 128.0, 127.5, 126.8, 126.7, 126.66, 114.9 (d, J_{C-F} = 21 Hz), 114.7 (d, J_{C-F} = 21 Hz) ppm; IR (KBr): ν_{max} = 3436, 3058, 2923, 1602, 1511, 1479, 1344, 1225, 1155, 1094, 822, 769, 744 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{18}F_2N$ $(M + H)^+$: 394.1402, found 394.1391.

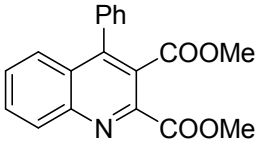
22) 2,3-bis(3-nitrophenyl)-4-phenylquinoline (3af)



3af

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), 1,2-bis(3-nitrophenyl)ethyne (**2f**, 0.4 mmol, 107.2 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 60 mg (67%) of **3af** as yellow solid. m.p.: 189-190 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.26 (s, 1H), 8.20 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.90-7.84 (m, 1H), 7.80-7.72 (m, 2H), 7.60-7.54 (m, 2H), 7.52-7.46 (m, 1H), 7.36-7.30 (m, 1H), 7.28-716 (m, 5H), 7.14-6.88 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 155.4, 149.1, 147.9, 147.7, 147.6, 142.0, 139.7, 137.2, 135.9, 135.6, 130.7, 130.2, 129.8, 129.1, 128.9, 128.2, 127.8, 126.9, 126.7, 126.0, 125.2, 123.0, 122.1 ppm; IR (KBr): ν_{max} = 3436, 3084, 2921, 1530, 1479, 1348, 1083, 765, 729, 701 cm^{-1}; HRMS m/z (ESI) calcd for $C_{27}H_{18}N_3O_4$ $(M + H)^+$: 448.1292, found 448.1293.

23) dimethyl 4-phenylquinoline-2,3-dicarboxylate (3ag)[4]

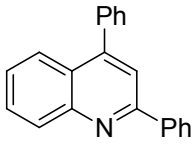


3ag

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), dimethyl but-2-ynedioate (**2g**, 0.4 mmol, 56.8 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 38 mg (59%) of **3ag** as white solid. m.p.: 124-126 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.33 (d, *J* = 8.4 Hz, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.65-7.56 (m, 2H), 7.51-7.49 (m, 3H), 7.38-7.35 (m, 2H), 4.07 (s, 3H), 3.63 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 167.6, 165.5, 148.1, 147.1, 144.9, 134.5, 131.0, 130.6, 129.3, 129.2, 128.8, 128.2, 127.6, 127.2, 126.6, 53.4, 52.4 ppm; IR (KBr): ν_{max} = 3436, 3051, 2951, 1731, 1726,

1560, 1443, 1312, 1250, 1234, 1205, 1129, 1050, 996, 865, 794, 769, 706, 606 cm^{-1}; MS (70 eV): m/z (%) 321.2 (M^+, 100).

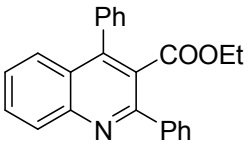
24) 2,4-diphenylquinoline (3ai)[5]



3ai

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), 1-ethynylbenzene (**2i**, 0.4 mmol, 40.8 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 32 mg (57%) of **3ai** as red liquid. ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.16 (d, *J* = 8.8 Hz, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.73 (s, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.48-7.34 (m, 10H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 156.9, 149.2, 148.8, 139.7, 138.4, 130.1, 129.5, 129.5, 129.3, 128.8, 128.6, 128.4, 127.6, 126.3, 125.8, 125.6, 119.3 ppm; MS (70 eV): m/z (%) 280.1 (M^+, 100).

25) Ethyl 2,4-diphenylquinoline-3-carboxylate (3aj)[6]

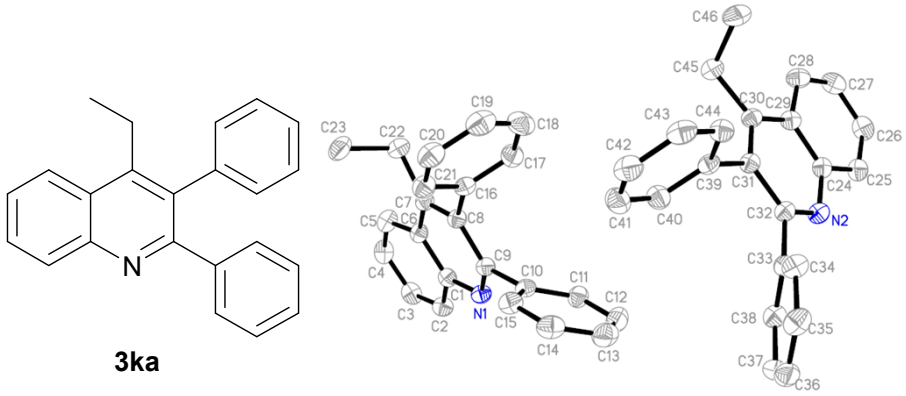


3aj

The reaction of 2-aminobenzophenone (**1a**, 0.2 mmol, 39.4 mg), ethyl 3-phenylpropiolate (**2j**, 0.4 mmol, 69.7 mg), $PdBr_2$ (2.7 mg, 0.01 mmol), PivOH (1.6 mmol), in DCE (0.8 mL) and benzenenitrile (0.8 mL) under **typical procedure** afforded 62 mg (88%) of **3aj** as white solid. ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.26 (d, *J* = 7.6 Hz, 1H), 7.82-7.44 (m, 3H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.52-7.40 (m, 9H)，7.63 (q, *J* = 7.2 Hz, 2H)，0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 168.1, 156.0, 147.9 147.1, 140.3, 135.6, 130.5, 129.9, 129.5, 128.9, 128.6, 128.4, 128.2, 127.2, 127.0, 126.6, 125.6, 61.3, 13.4 ppm; IR (KBr): ν_{max} = 3436, 3061, 2975, 1731, 1550, 1481, 1404, 1227, 1103, 775, 695 cm^{-1}; MS (70 eV): m/z (%) 353.0 (M^+, 100).

References

1. B. Zhao, X. Lu, *Tetrahedron Lett.,* 2006, **47**, 6765.
2. T. Mitamura, A. Ogawa, *J. Org. Chem.,* 2011, **76**, 1163.
3. T. Meng, W.-X. Zhang, H.-J. Zhang, Y. Liang, Z. Xi, *Synthesis,* 2012, **44**, 2754.
4. T. Chanda, M. Singh, R. Verma, *Chem. Asian J.,* 2012, **7***,* 778.
5. R. Martínez, D. Ramón, M. Yus, *J. Org. Chem.,* 2008, **73**, 9778.
6. S. Cai, J. Zeng, Y. Bai, X.-W. Liu, *J. Org. Chem.*, 2012, **77**, 801.

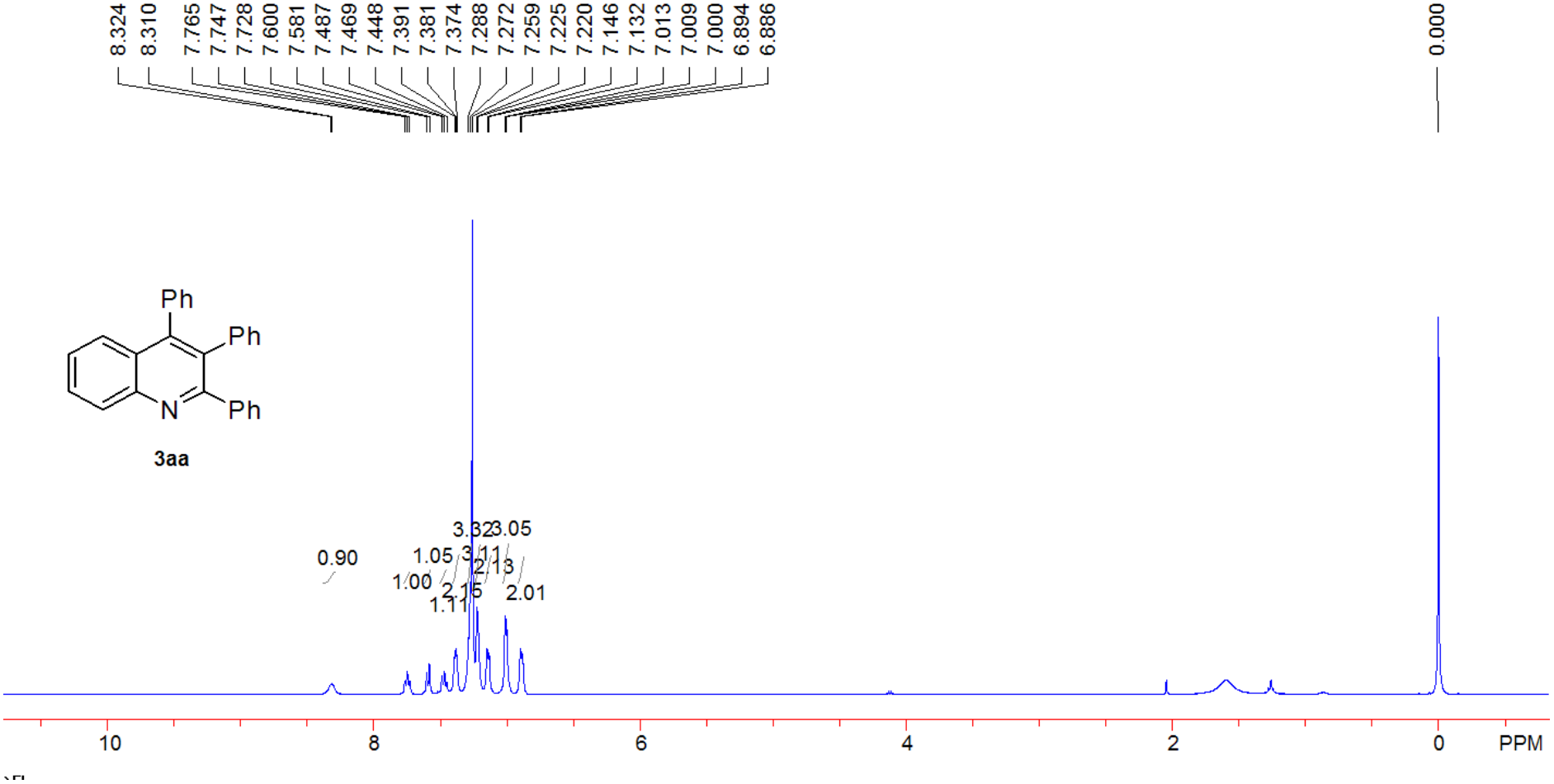


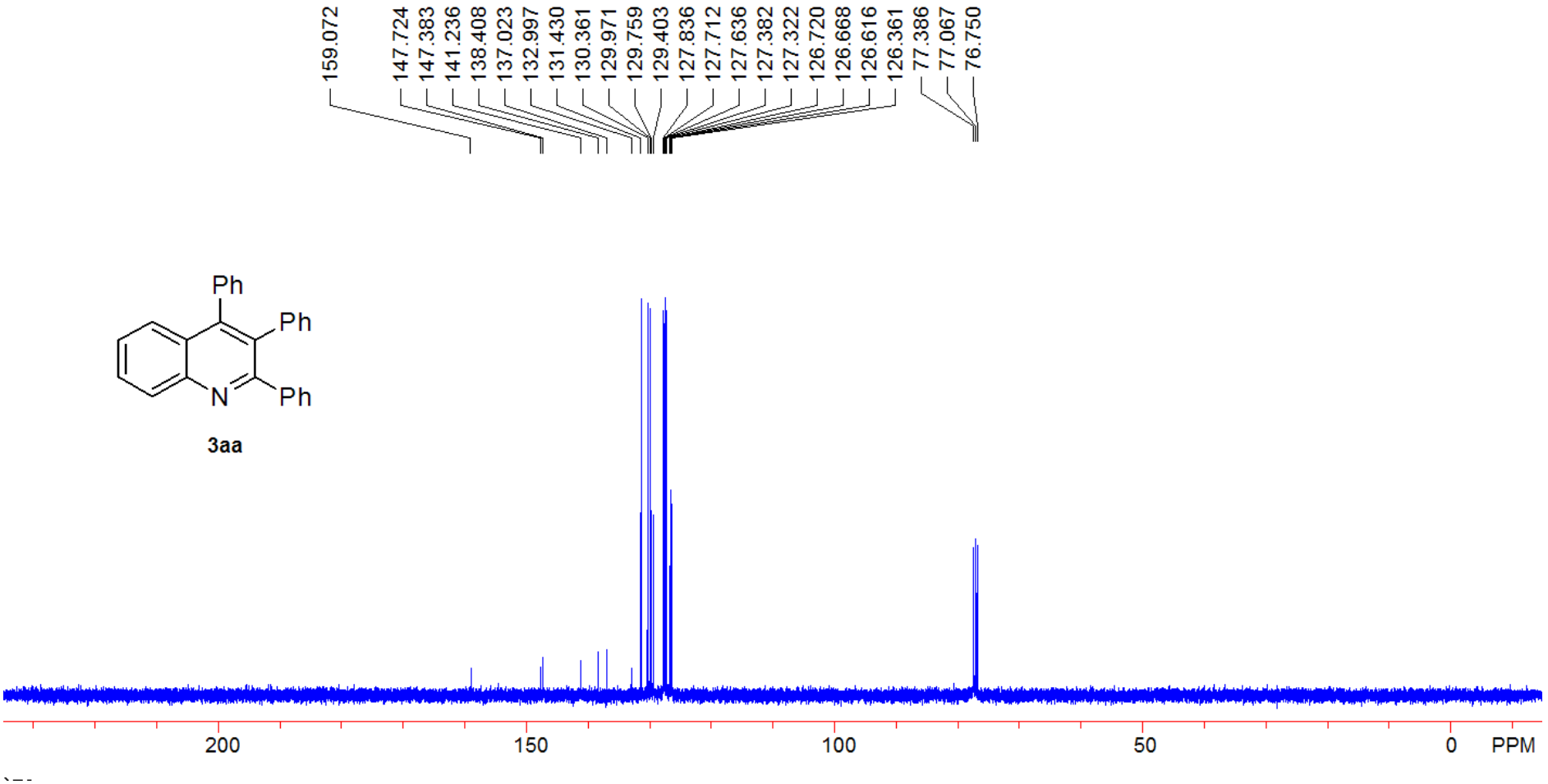
3ka

Table S1. Crystal data and structure refinement for **3ka** (CCDC 993171).

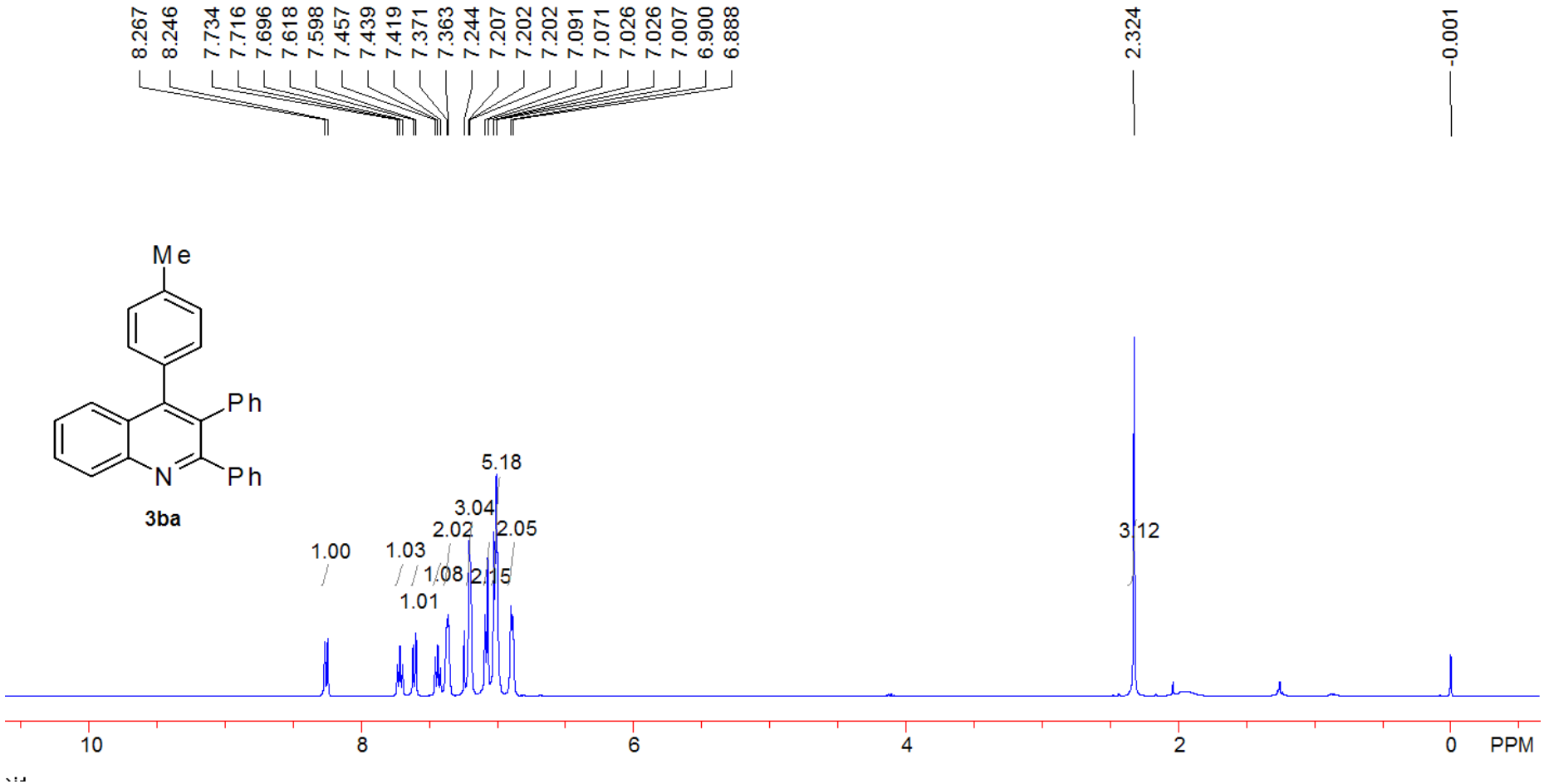
Identification code	3
Empirical formula	C23 H19 N
Formula weight	309.39
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P n a 21
Unit cell dimensions	a = 13.6312(15) A alpha = 90 deg.
	b = 9.0492(10) A beta = 90 deg.
	c = 27.107(3) A gamma = 90 deg.
Volume	3343.6(6) A^3
Z, Calculated density	8, 1.229 Mg/m^3
Absorption coefficient	0.071 mm^-1
F(000)	1312
Crystal size	0.32 x 0.25 x 0.20 mm
Theta range for data collection	2.37 to 26.00 deg.
Limiting indices	-16<=h<=16, -11<=k<=11, -31<=l<=33
Reflections collected / unique	25483 / 6411 [R(int) = 0.0257]
Completeness to theta = 26.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9860 and 0.9777
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6411 / 1 / 436
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0949
R indices (all data)	R1 = 0.0402, wR2 = 0.0990
Absolute structure parameter	0(3)
Extinction coefficient	0.0064(6)
Largest diff. peak and hole	0.145 and -0.114 e.A^-3

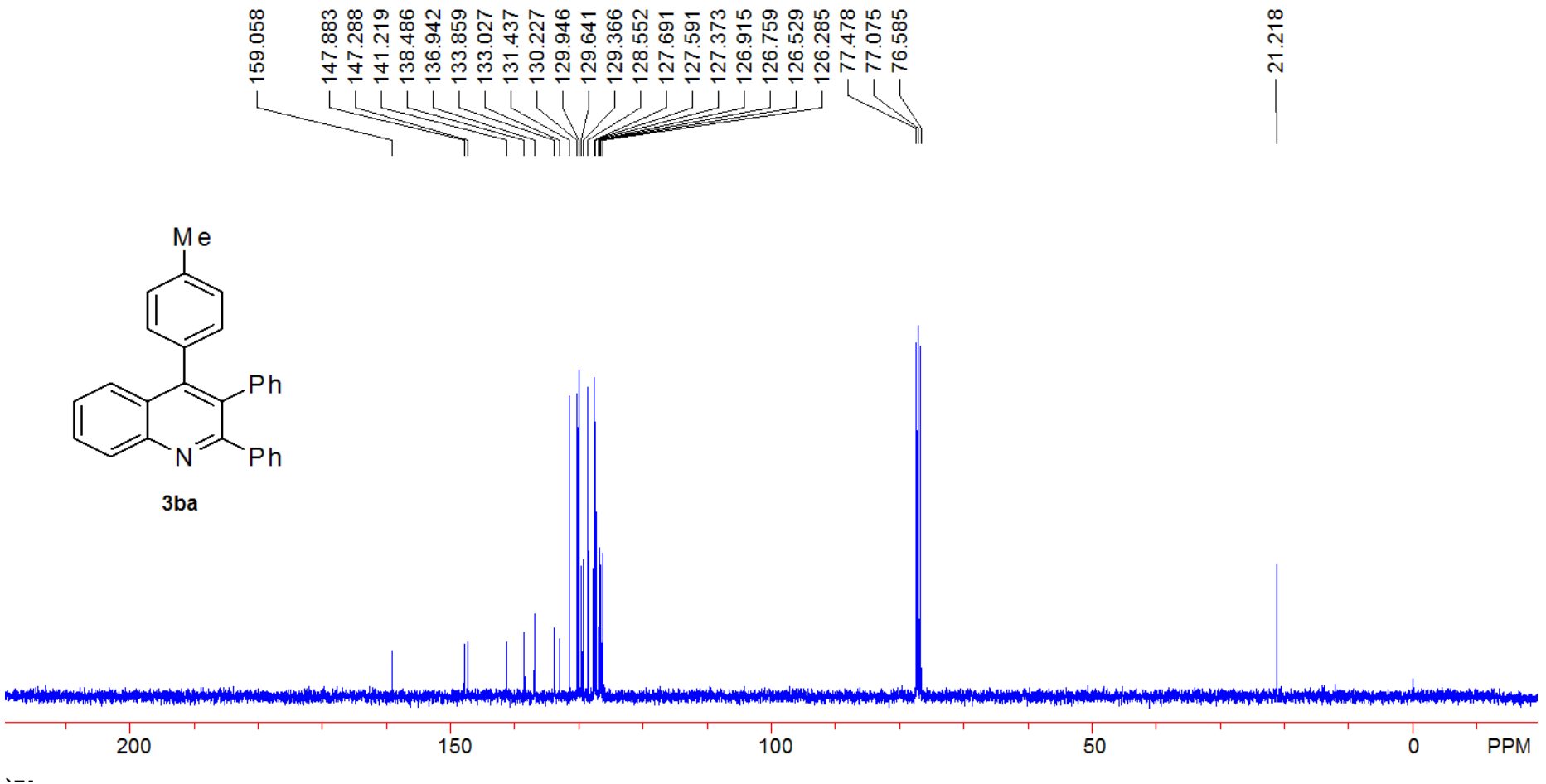
NMR and HRMS Spectra of Those Compounds




159.072
147.724
147.383
141.236
138.408
137.023
132.997
131.430
130.361
129.971
129.759
129.403
127.836
127.712
127.636
127.382
127.322
126.720
126.668
126.616
126.361
77.386
77.067
76.750
Ph
Ph
Ph
N
200
150
100
50
0
PPM

3aa

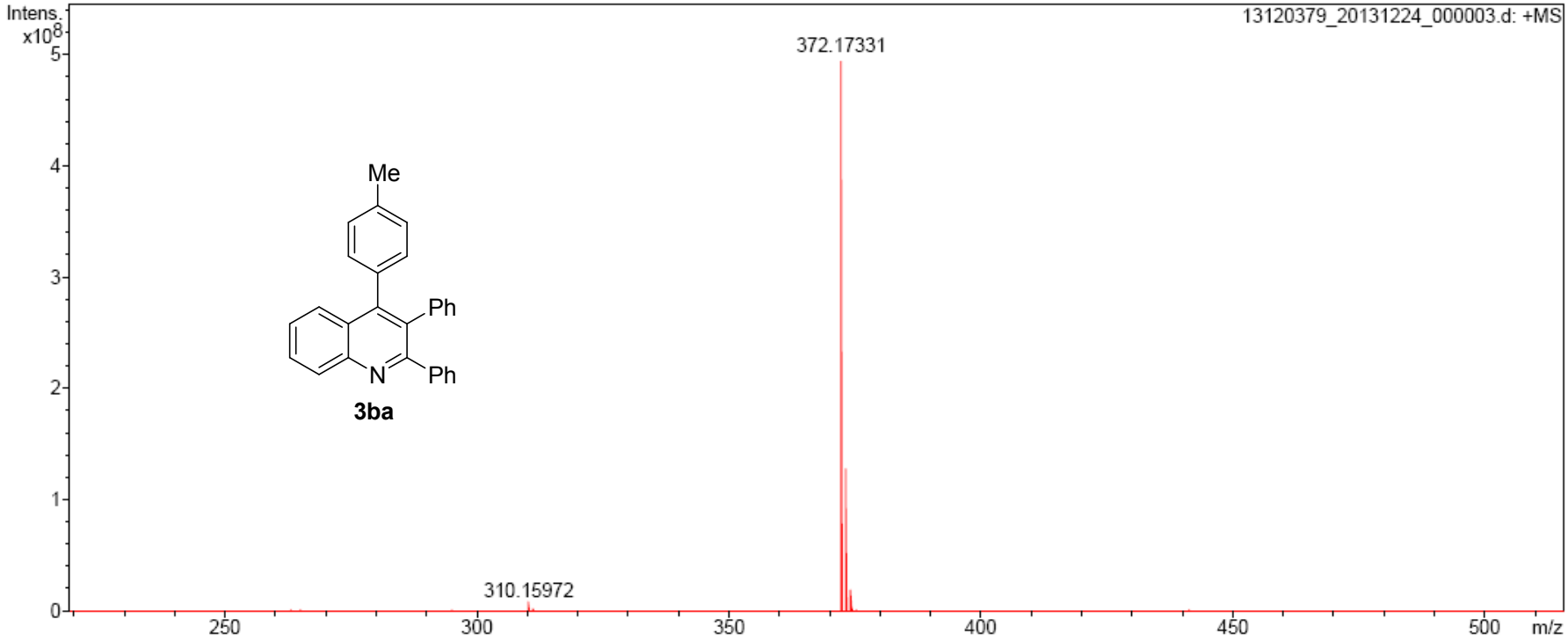

8.267
8.246
7.734
7.716
7.696
7.618
7.598
7.457
7.439
7.419
7.371
7.363
7.244
7.207
7.202
7.202
7.091
7.071
7.026
7.026
7.007
6.900
6.888
2.324
-0.001
Me
Ph
N
Ph
3ba
5.18
3.04
2.02
2.05
1.00
1.03
1.08
2.15
1.01
3.12
10
8
6
4
2
0
PPM


159.058
147.883
147.288
141.219
138.486
136.942
133.859
133.027
131.437
130.227
129.946
129.641
129.366
128.552
127.691
127.591
127.373
126.915
126.759
126.529
126.285
77.478
77.075
76.585
21.218
Me
Ph
Ph
N
3ba
200
150
100
50
0
PPM

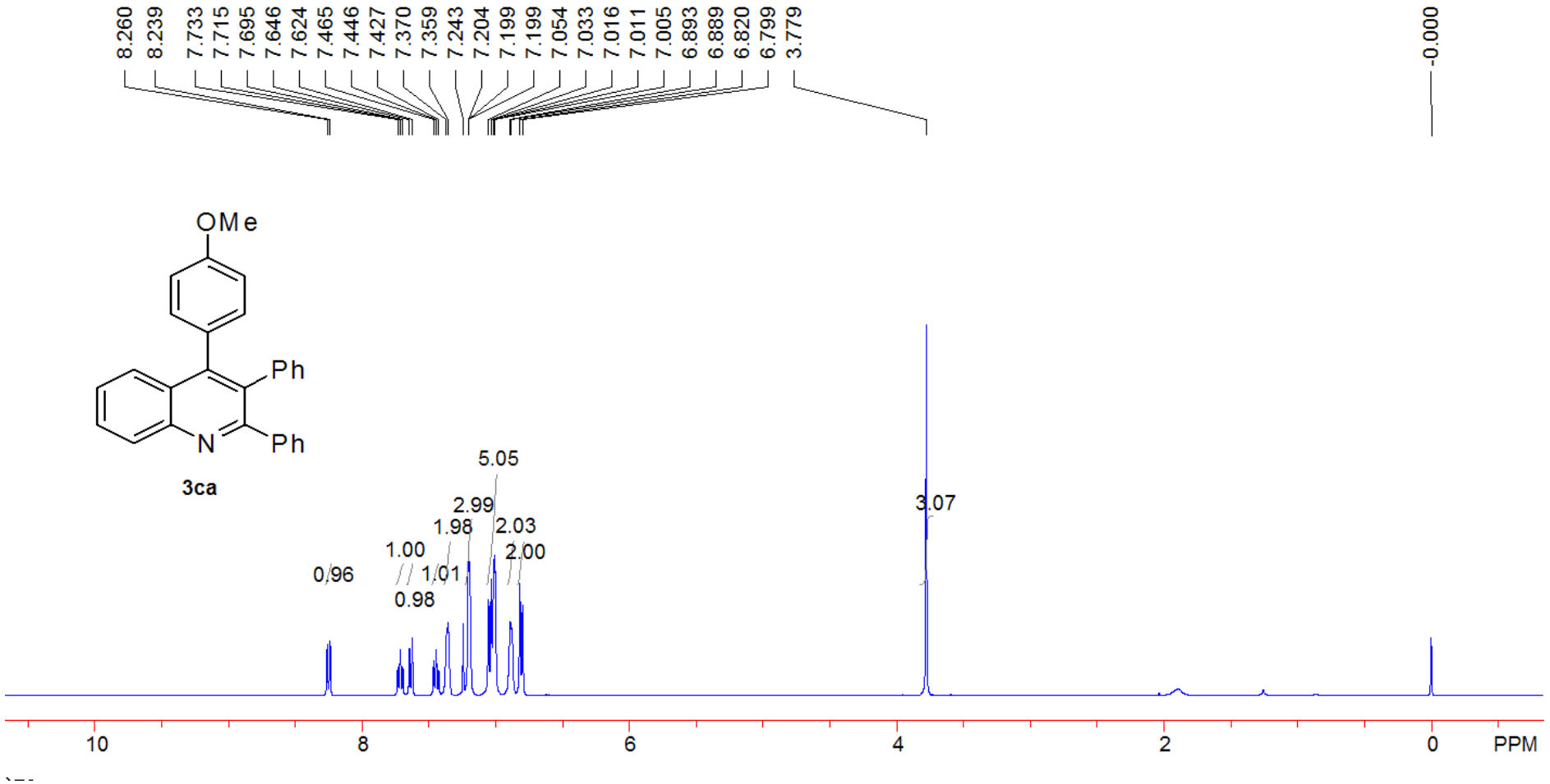
Peking University Mass Spectrometry Sample Analysis Report

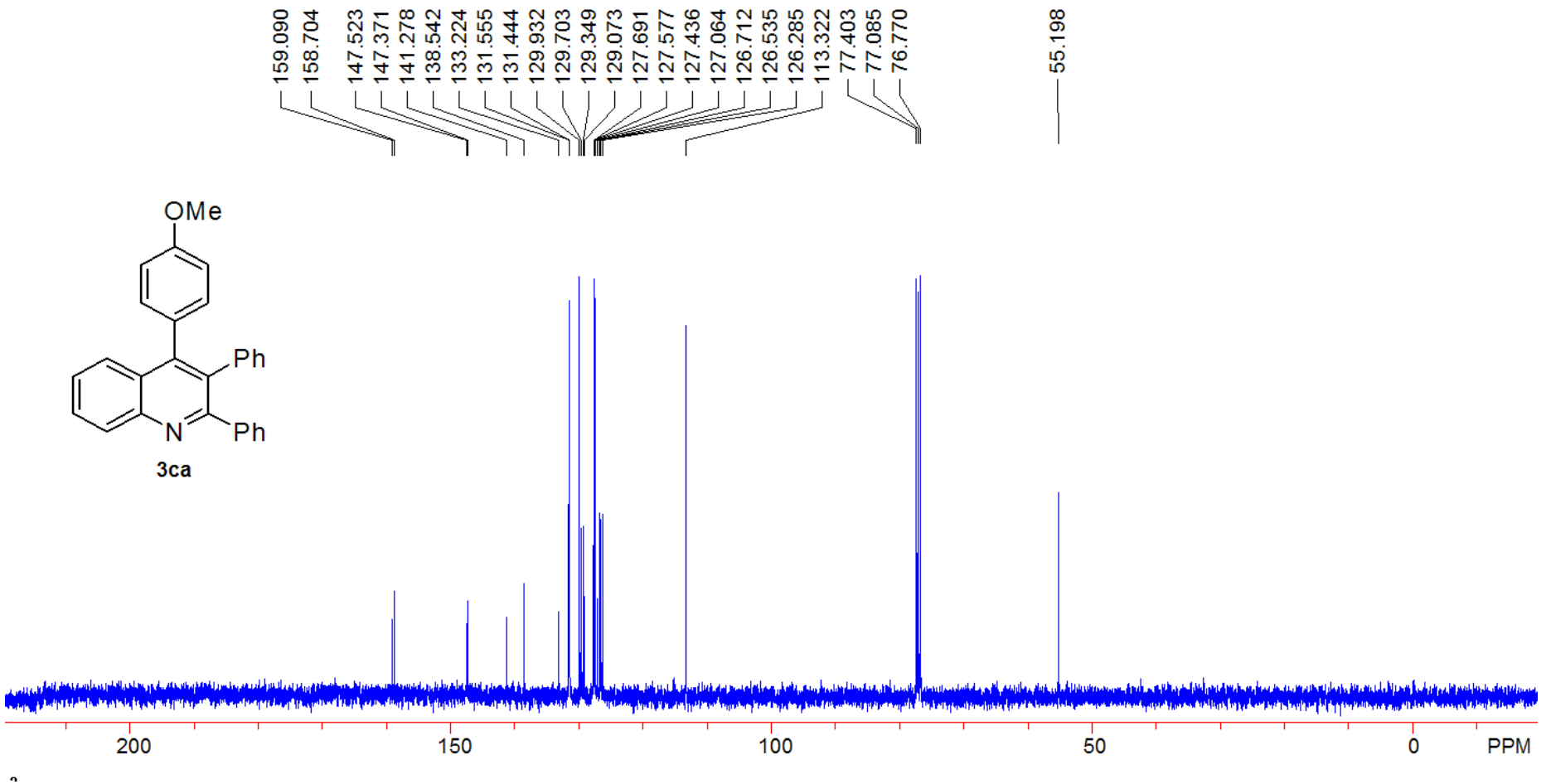
Analysis Info

Analysis Name	13120379_20131224_000003.d	Acquisition Date	12/24/2013 11:25:19 AM
Sample	B	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
372.17331	498028384	C 28 H 22 N	372.17468	1.4	3.7	23.9	18.5	even	ok

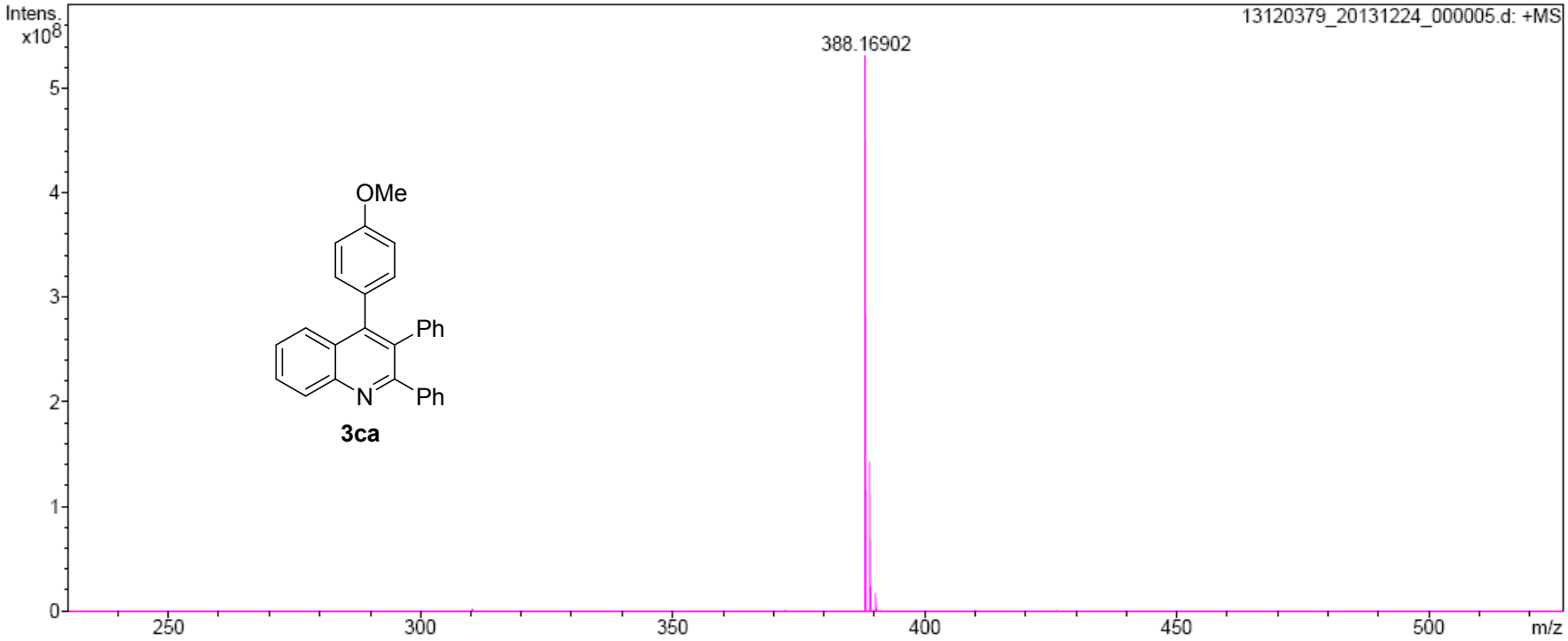

8.260
8.239
7.733
7.715
7.695
7.646
7.624
7.465
7.446
7.427
7.370
7.359
7.243
7.204
7.199
7.199
7.054
7.033
7.016
7.011
7.005
6.893
6.889
6.820
6.799
3.779
-0.000
OMe
Ph
N
Ph
3ca
5.05
2.99
1.98
2.03
2.00
1.00
1.01
0.96
0.98
3.07
10
8
6
4
2
0
PPM


159.090
158.704
147.523
147.371
141.278
138.542
133.224
131.555
131.444
129.932
129.703
129.349
129.073
127.691
127.577
127.436
127.064
126.712
126.535
126.285
113.322
77.403
77.085
76.770
55.198
OMe
Ph
Ph
N
3ca
200
150
100
50
0
PPM

Peking University Mass Spectrometry Sample Analysis Report

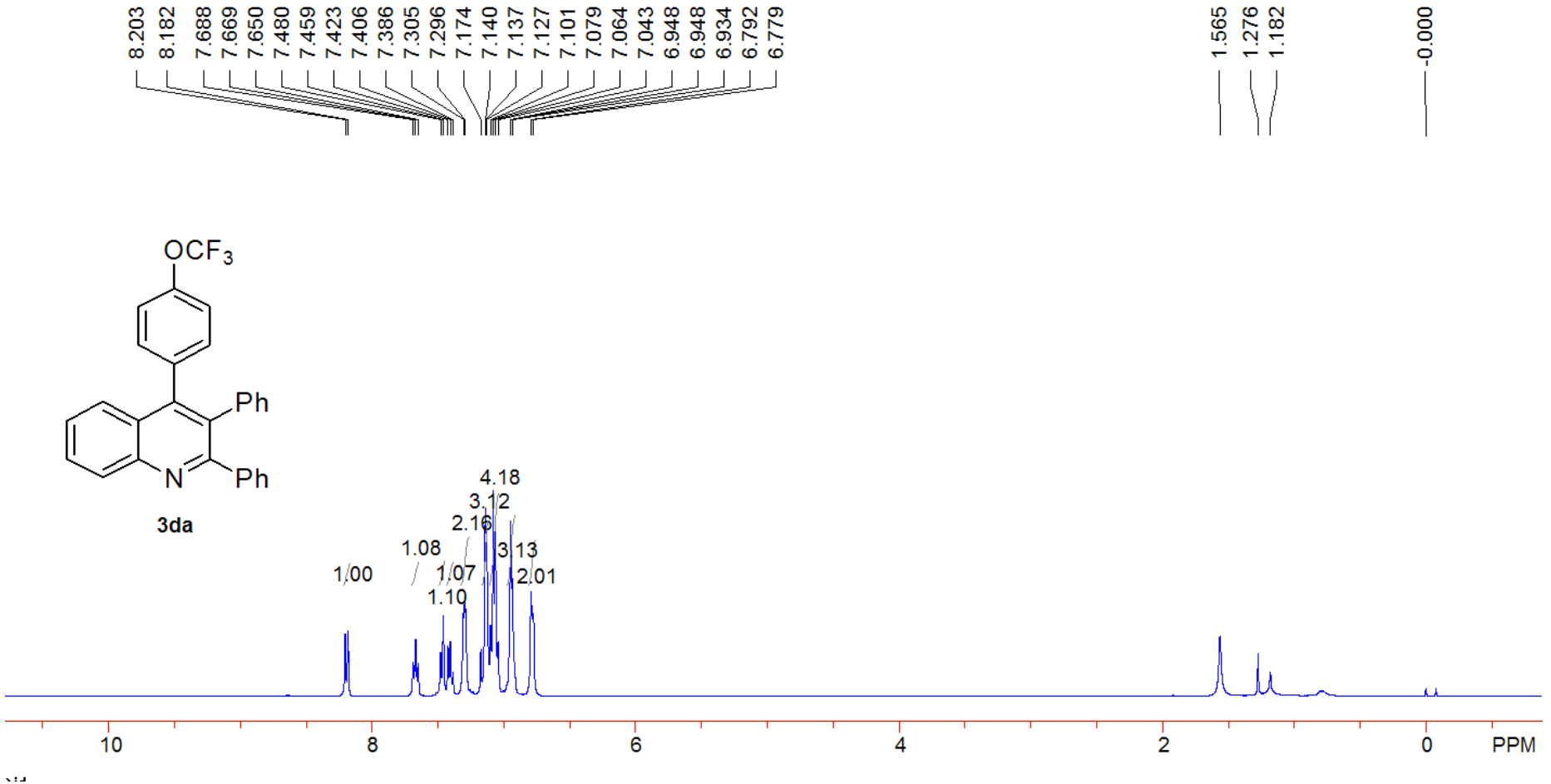
Analysis Info

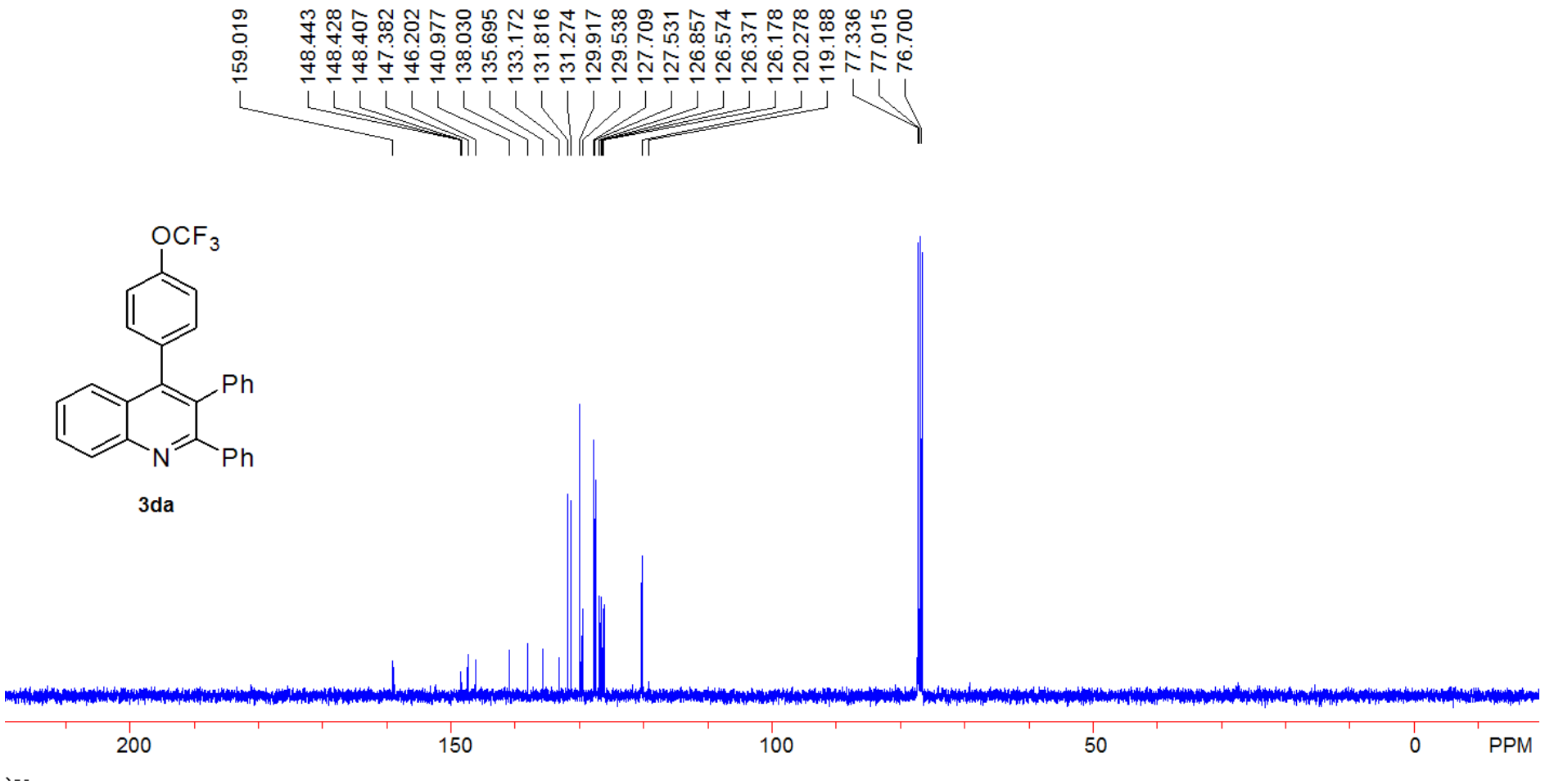
Analysis Name	13120379_20131224_000005.d	Acquisition Date	12/24/2013 11:29:20 AM
Sample	C	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ca

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
388.16902	531339008	C 28 H 22 N O	388.16959	0.6	1.5	18.9	18.5	even	ok

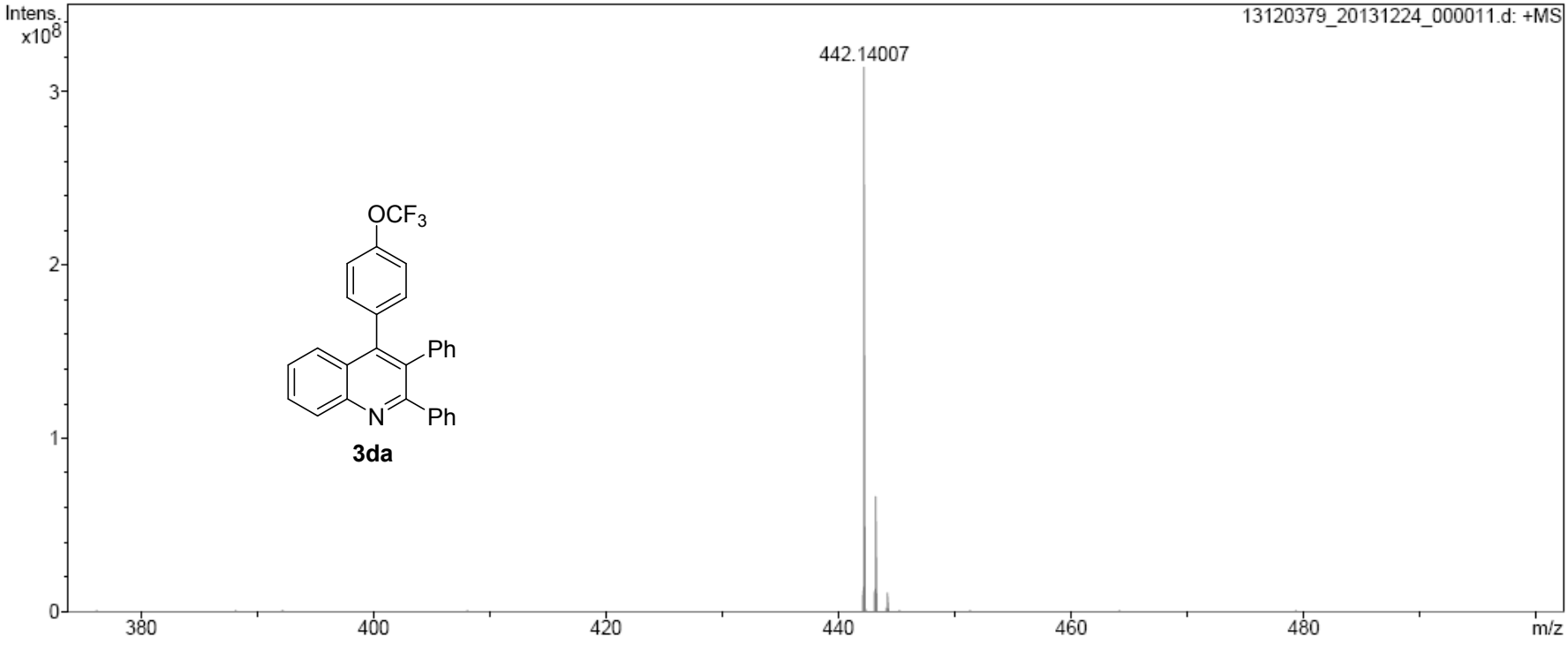

8.203
8.182
7.688
7.669
7.650
7.480
7.459
7.423
7.406
7.386
7.305
7.296
7.174
7.140
7.137
7.127
7.101
7.079
7.064
7.043
6.948
6.948
6.934
6.792
6.779
1.565
1.276
1.182
-0.000
OCF3
Ph
Ph
N
3da
4.18
3.12
2.16
1.08
3.13
1.00
1.07
2.01
1.10
10
8
6
4
2
0
PPM


159.019
148.443
148.428
148.407
147.382
146.202
140.977
138.030
135.695
133.172
131.816
131.274
129.917
129.538
127.709
127.531
126.857
126.574
126.371
126.178
120.278
119.188
77.336
77.015
76.700
OCF3
Ph
Ph
N
3da
200
150
100
50
0
PPM

Peking University Mass Spectrometry Sample Analysis Report

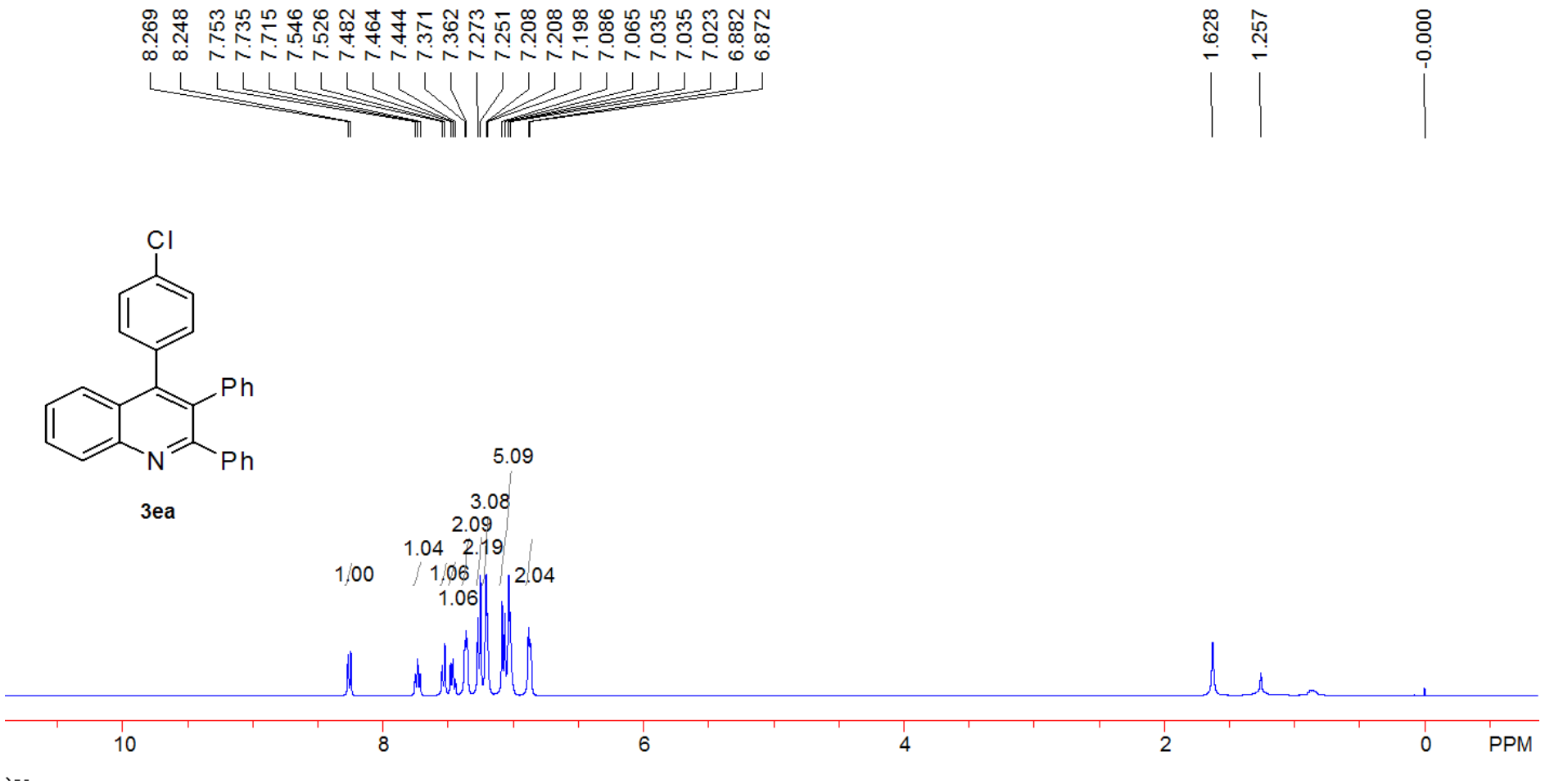
Analysis Info

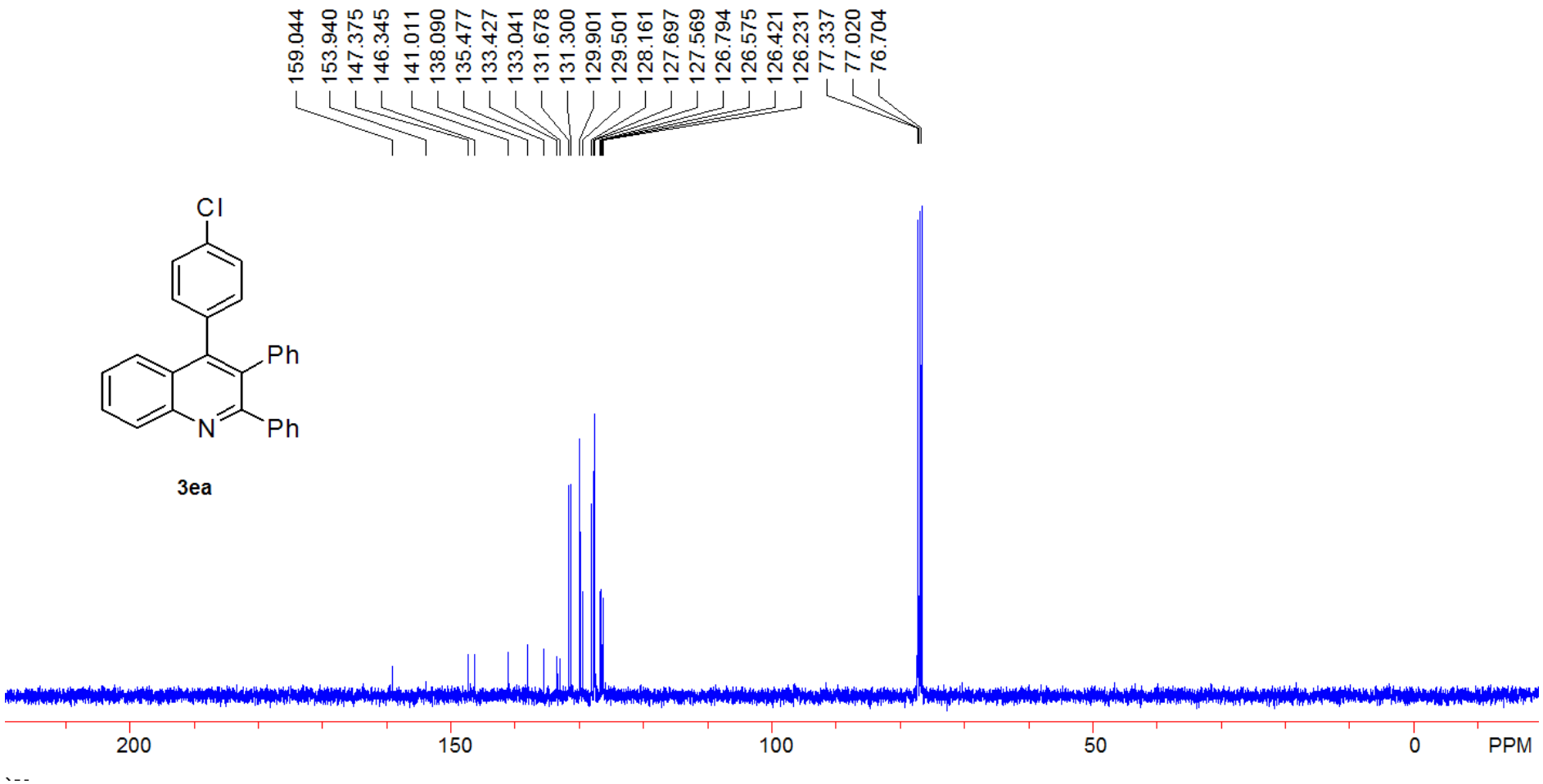
Analysis Name	13120379_20131224_000011.d	Acquisition Date	12/24/2013 11:37:21 AM
Sample	H	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3da

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
442.14007	314570080	C 28 H 19 F 3 N O	442.14133	1.3	2.8	46.3	18.5	even	ok


8.269
8.248
7.753
7.735
7.715
7.546
7.526
7.482
7.464
7.444
7.371
7.362
7.273
7.251
7.208
7.208
7.198
7.086
7.065
7.035
7.035
7.023
6.882
6.872
1.628
1.257
-0.000
Cl
Ph
Ph
N
3ea
5.09
3.08
2.09
2.19
1.04
1.00
1.06
1.06
2.04
10
8
6
4
2
0
PPM

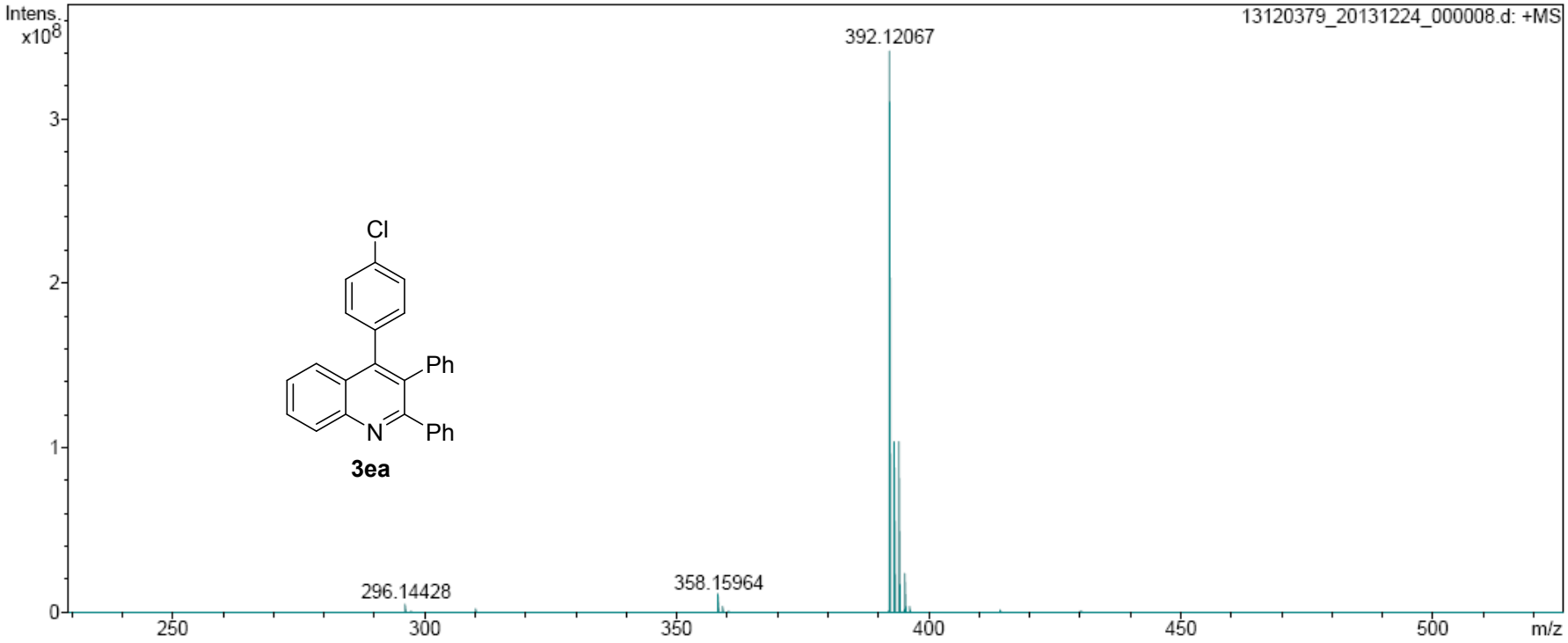

159.044
153.940
147.375
146.345
141.011
138.090
135.477
133.427
133.041
131.678
131.300
129.901
129.501
128.161
127.697
127.569
126.794
126.575
126.421
126.231
77.337
77.020
76.704
Cl
Ph
N
Ph
200
150
100
50
0
PPM

3ea

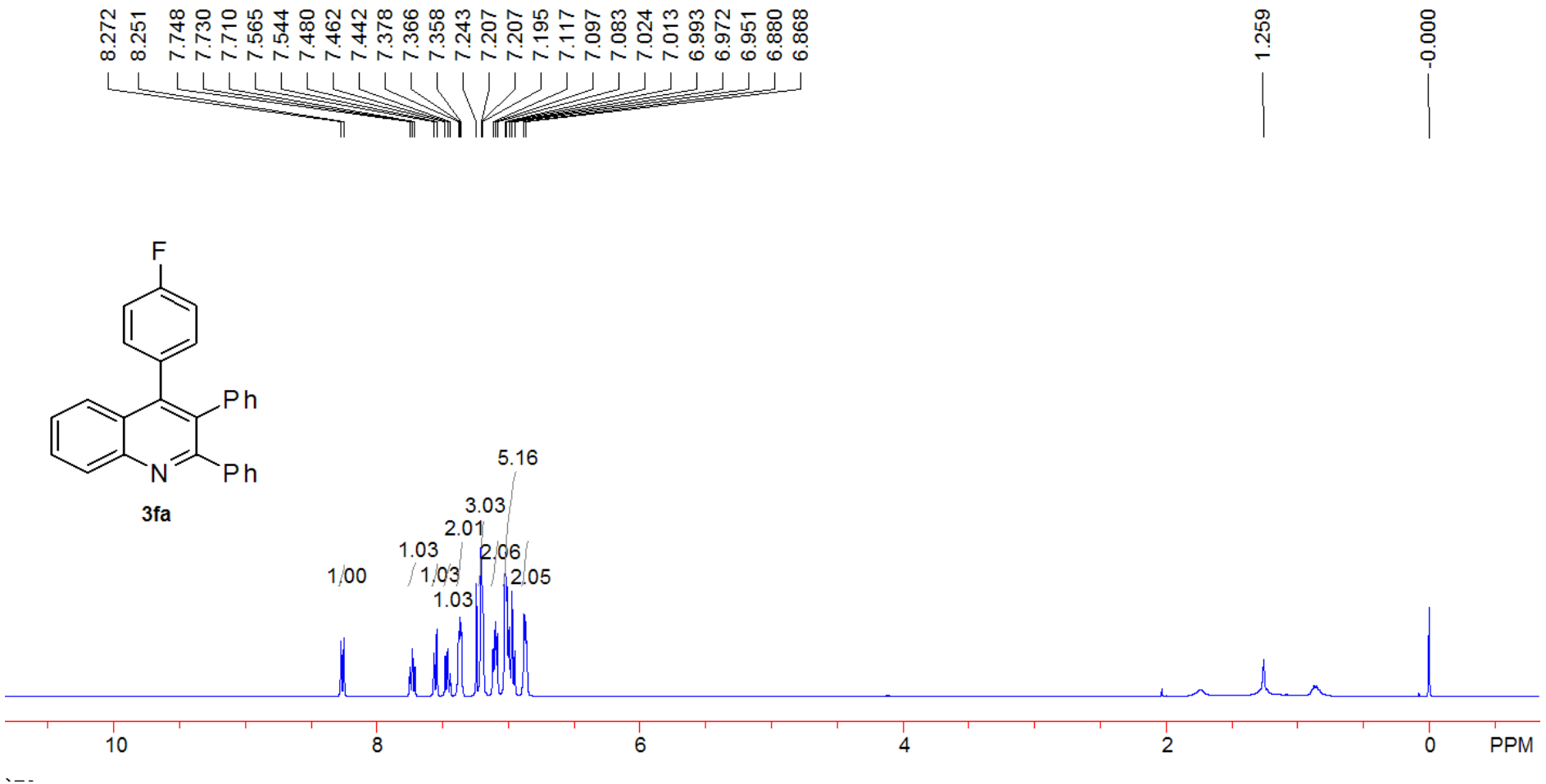
Peking University Mass Spectrometry Sample Analysis Report

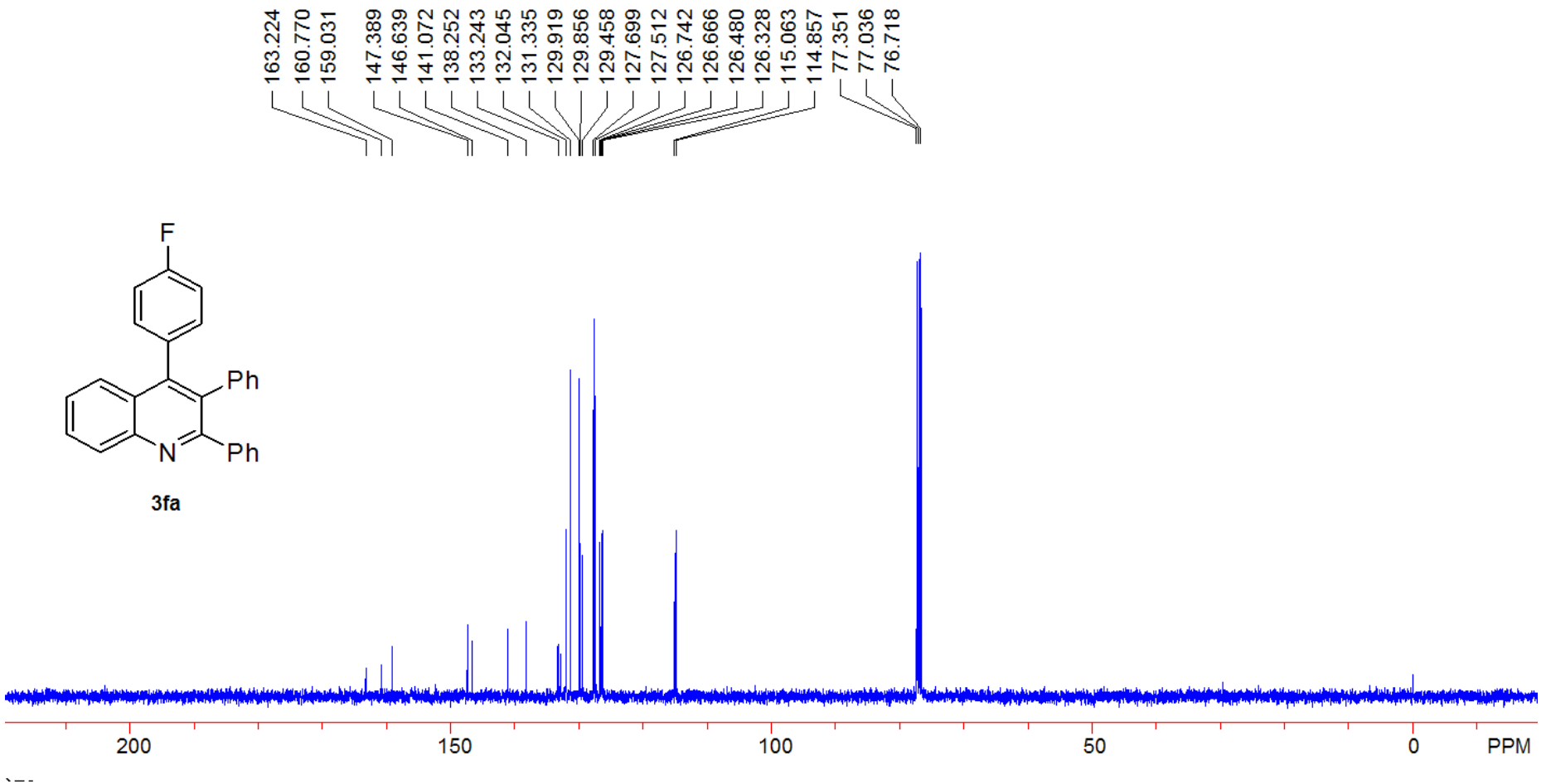
Analysis Info

Analysis Name	13120379_20131224_000008.d	Acquisition Date	12/24/2013 11:32:34 AM
Sample	E	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
392.12067	342384576	C 27 H 19 Cl N	392.12005	-0.6	-1.6	29.0	18.5	even	ok


8.272
8.251
7.748
7.730
7.710
7.565
7.544
7.480
7.462
7.442
7.378
7.366
7.358
7.243
7.207
7.207
7.195
7.117
7.097
7.083
7.024
7.013
6.993
6.972
6.951
6.880
6.868
1.259
-0.000
F
Ph
Ph
N
3fa
5.16
3.03
2.01
2.06
2.05
1.03
1.03
1.03
1.00
10
8
6
4
2
0
PPM

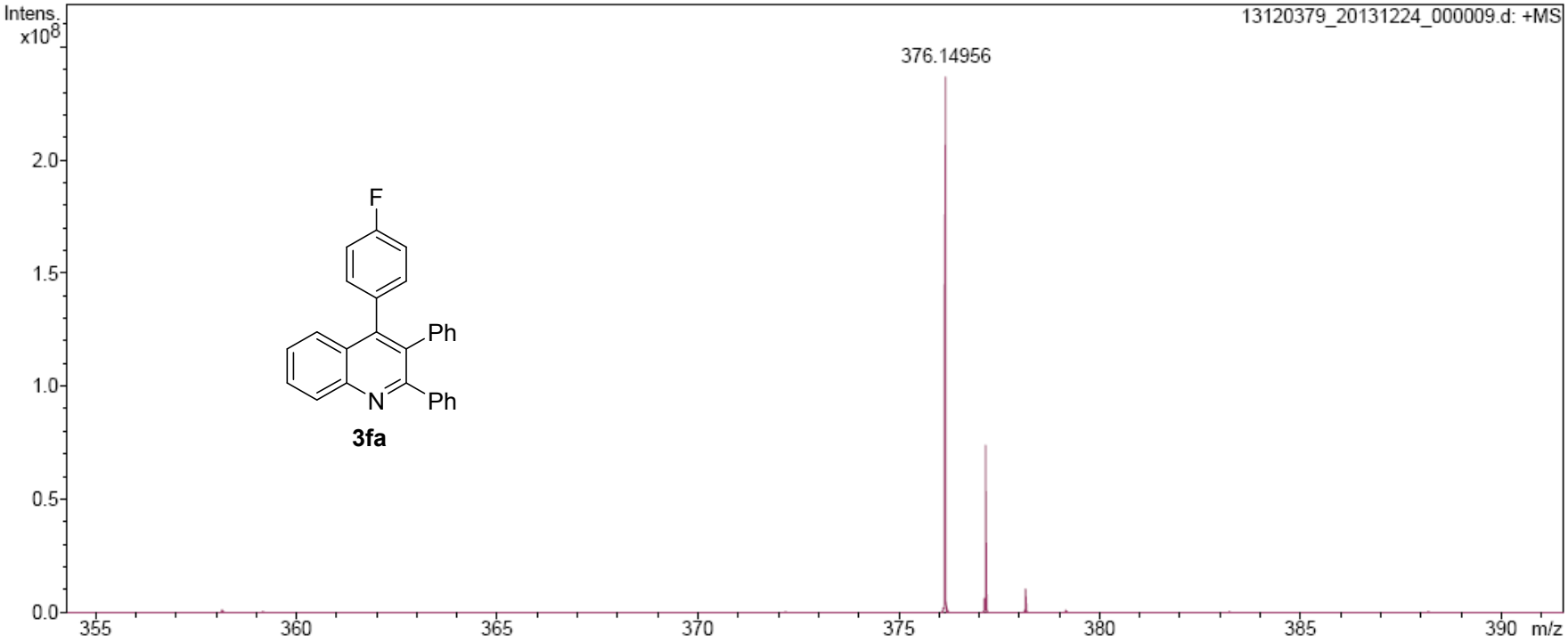

163.224
160.770
159.031
147.389
146.639
141.072
138.252
133.243
132.045
131.335
129.919
129.856
129.458
127.699
127.512
126.742
126.666
126.480
126.328
115.063
114.857
77.351
77.036
76.718
F
Ph
N
Ph
200
150
100
50
0
PPM

3fa

Peking University Mass Spectrometry Sample Analysis Report

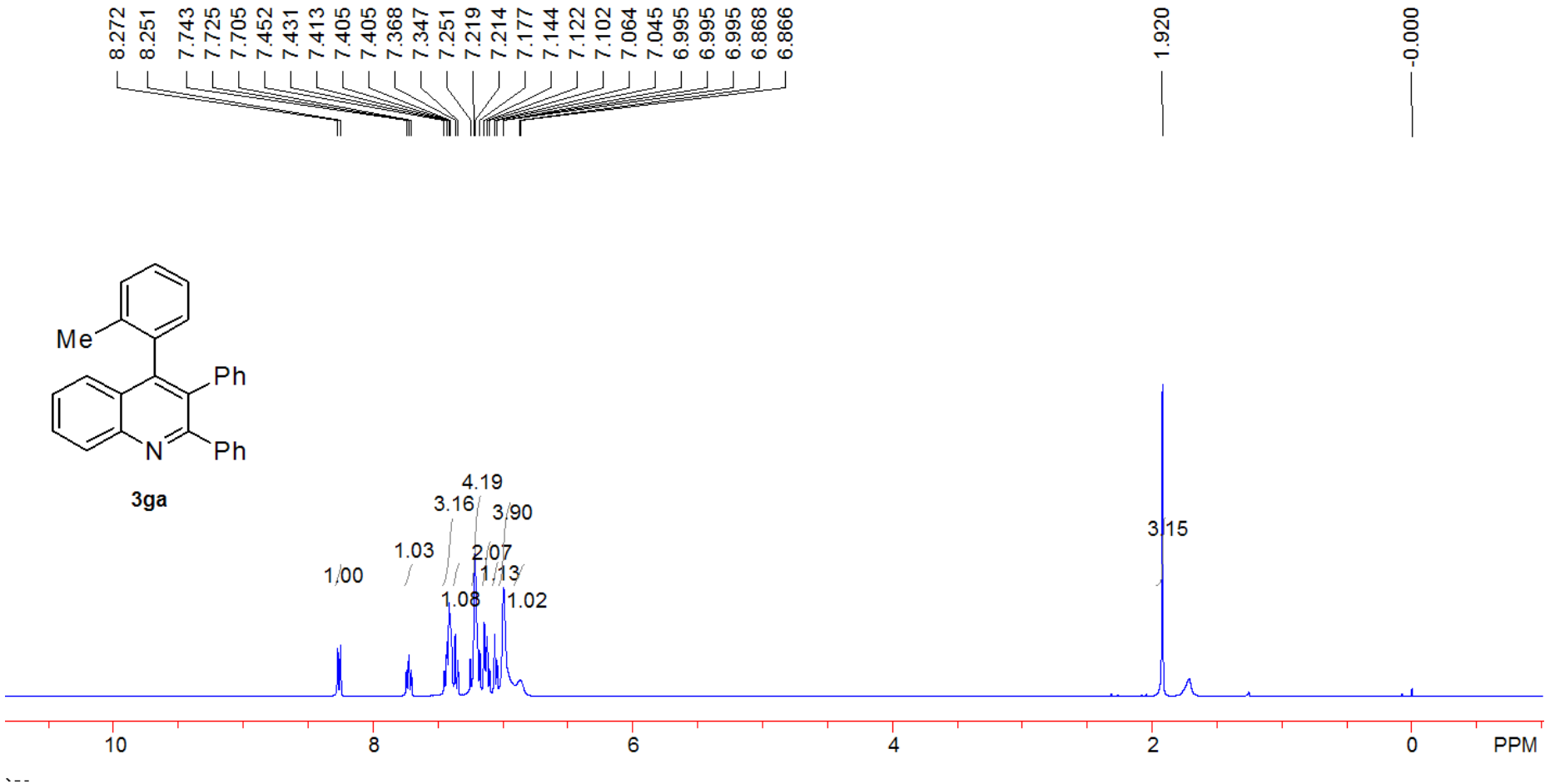
Analysis Info

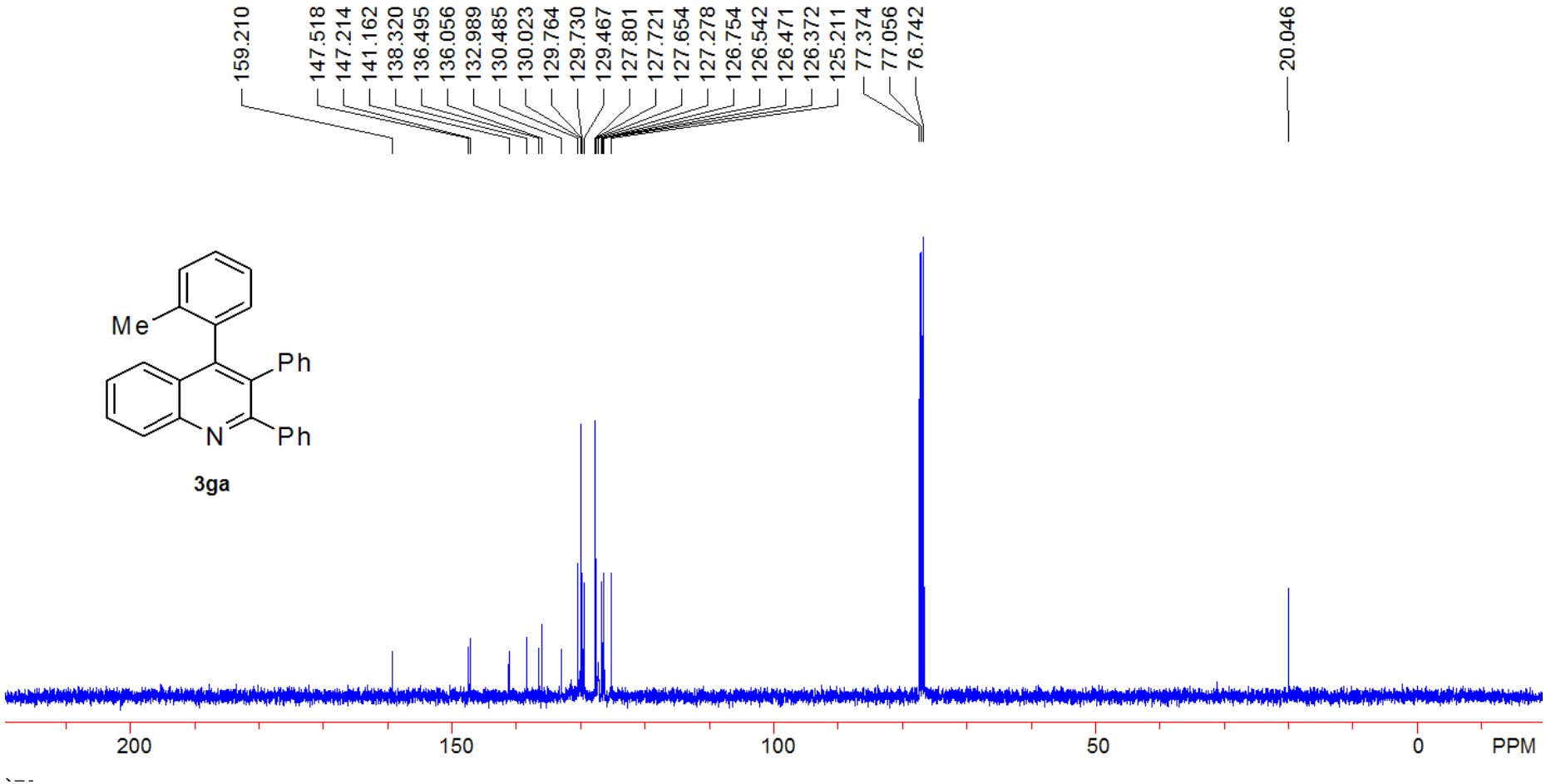
Analysis Name	13120379_20131224_000009.d	Acquisition Date	12/24/2013 11:33:55 AM
Sample	F	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3fa

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
376.14956	240869296	C 27 H 19 F N	376.14960	0.0	0.1	6.1	18.5	even	ok

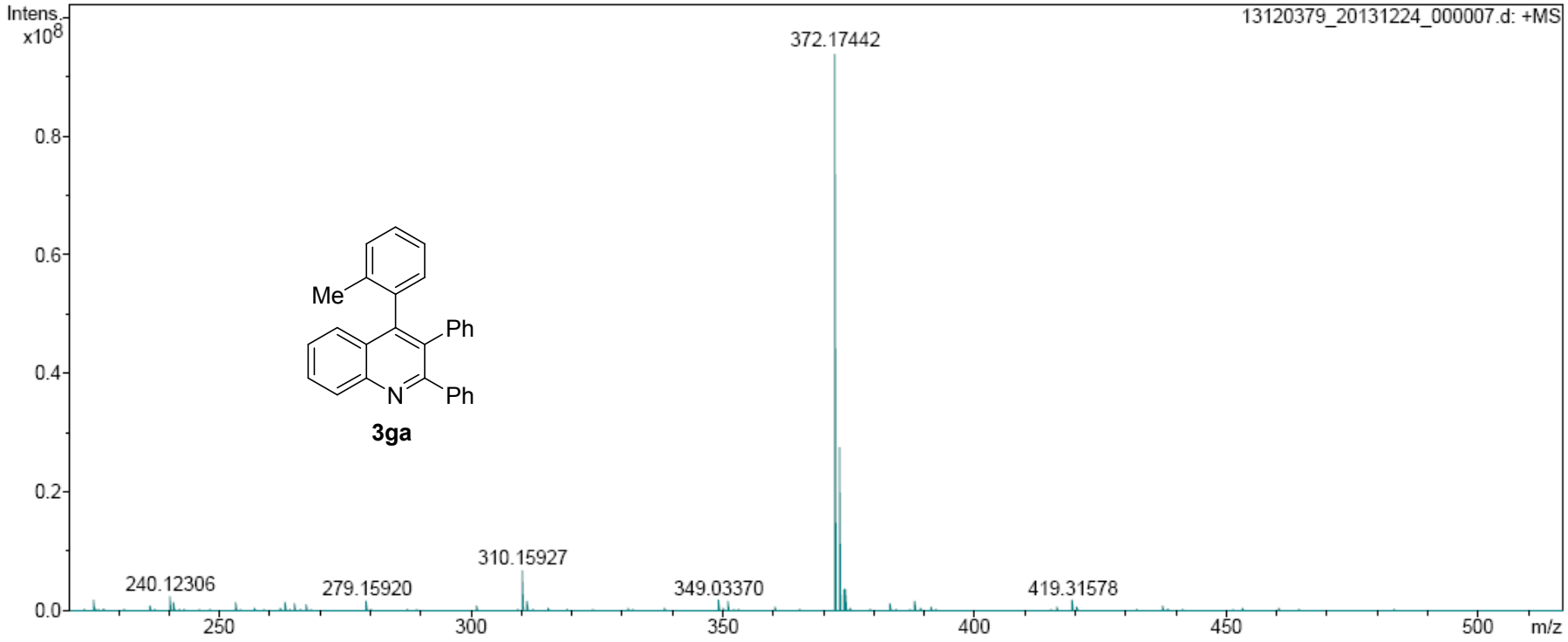

8.272
8.251
7.743
7.725
7.705
7.452
7.431
7.413
7.405
7.405
7.368
7.347
7.251
7.219
7.214
7.177
7.144
7.122
7.102
7.064
7.045
6.995
6.995
6.995
6.868
6.866
1.920
-0.000
Me
Ph
Ph
N
3ga
4.19
3.16
3.90
1.03
2.07
1.00
1.13
1.08
1.02
3.15
10
8
6
4
2
0
PPM


159.210
147.518
147.214
141.162
138.320
136.495
136.056
132.989
130.485
130.023
129.764
129.730
129.467
127.801
127.721
127.654
127.278
126.754
126.542
126.471
126.372
125.211
77.374
77.056
76.742
20.046
Me
Ph
Ph
N
3ga
200
150
100
50
0
PPM

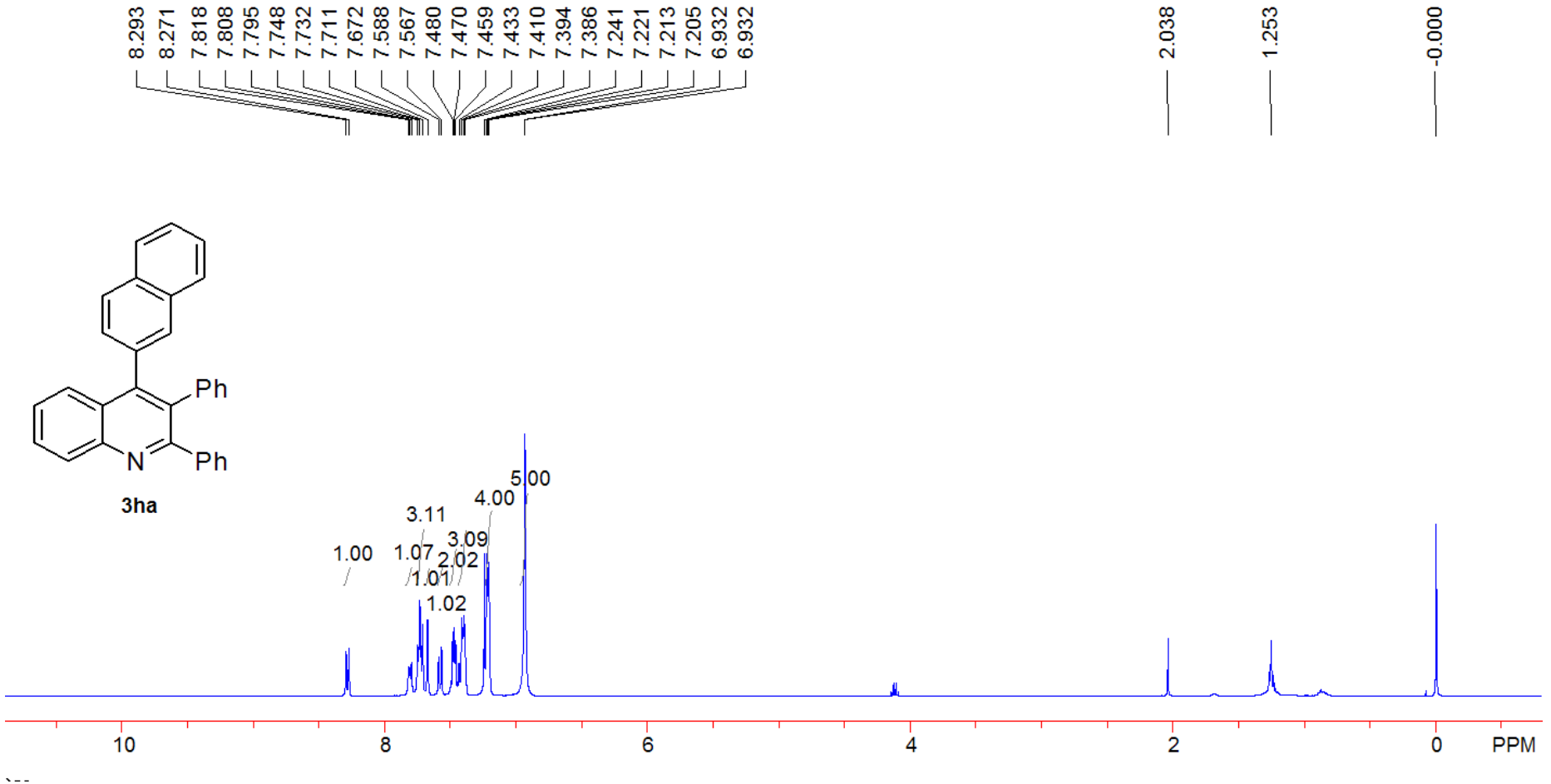
Peking University Mass Spectrometry Sample Analysis Report

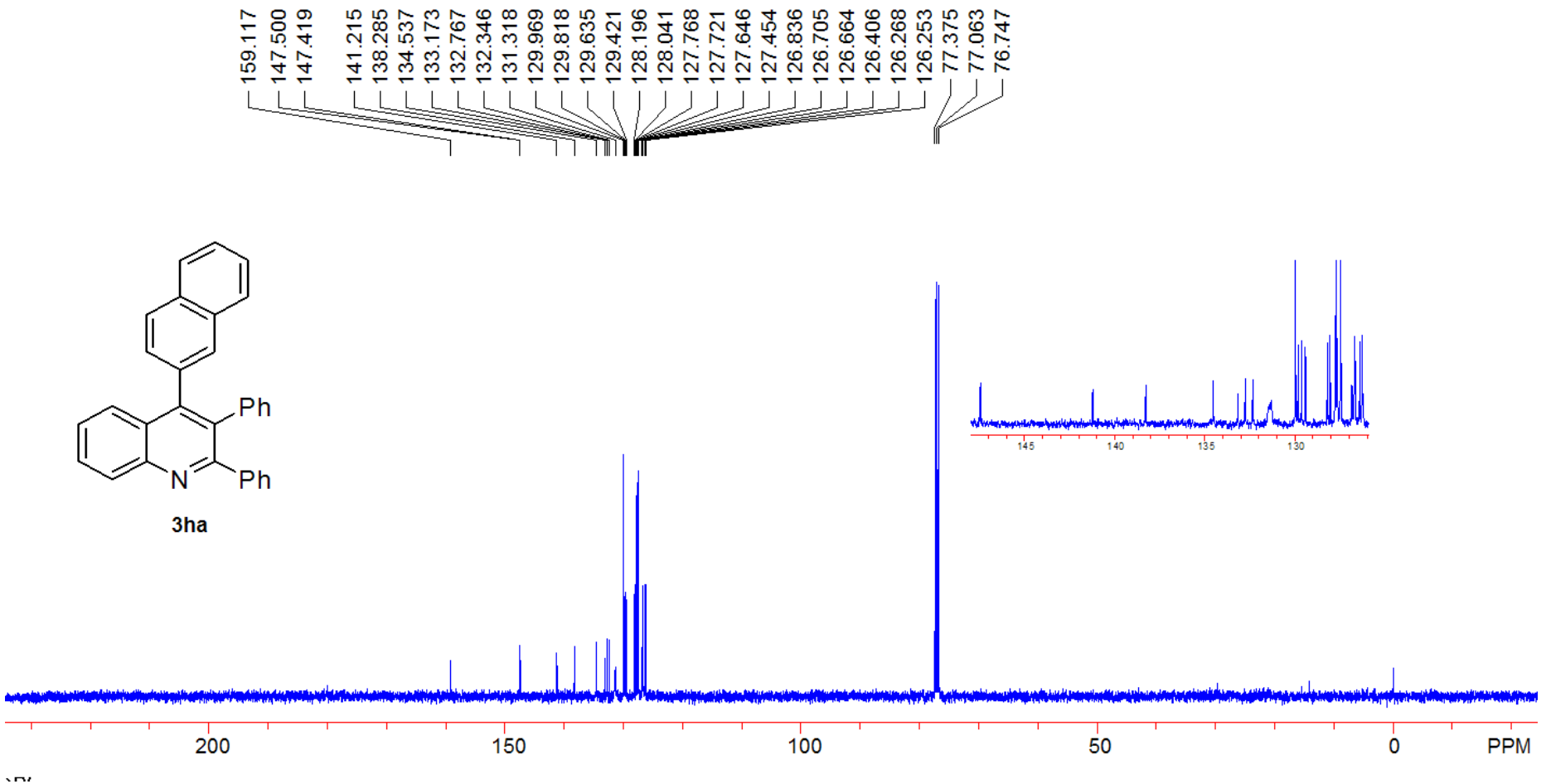
Analysis Info

Analysis Name	13120379_20131224_000007.d	Acquisition Date	12/24/2013 11:31:38 AM
Sample	D	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
372.17442	94272968	C 28 H 22 N	372.17468	0.3	0.7	6.7	18.5	even	ok

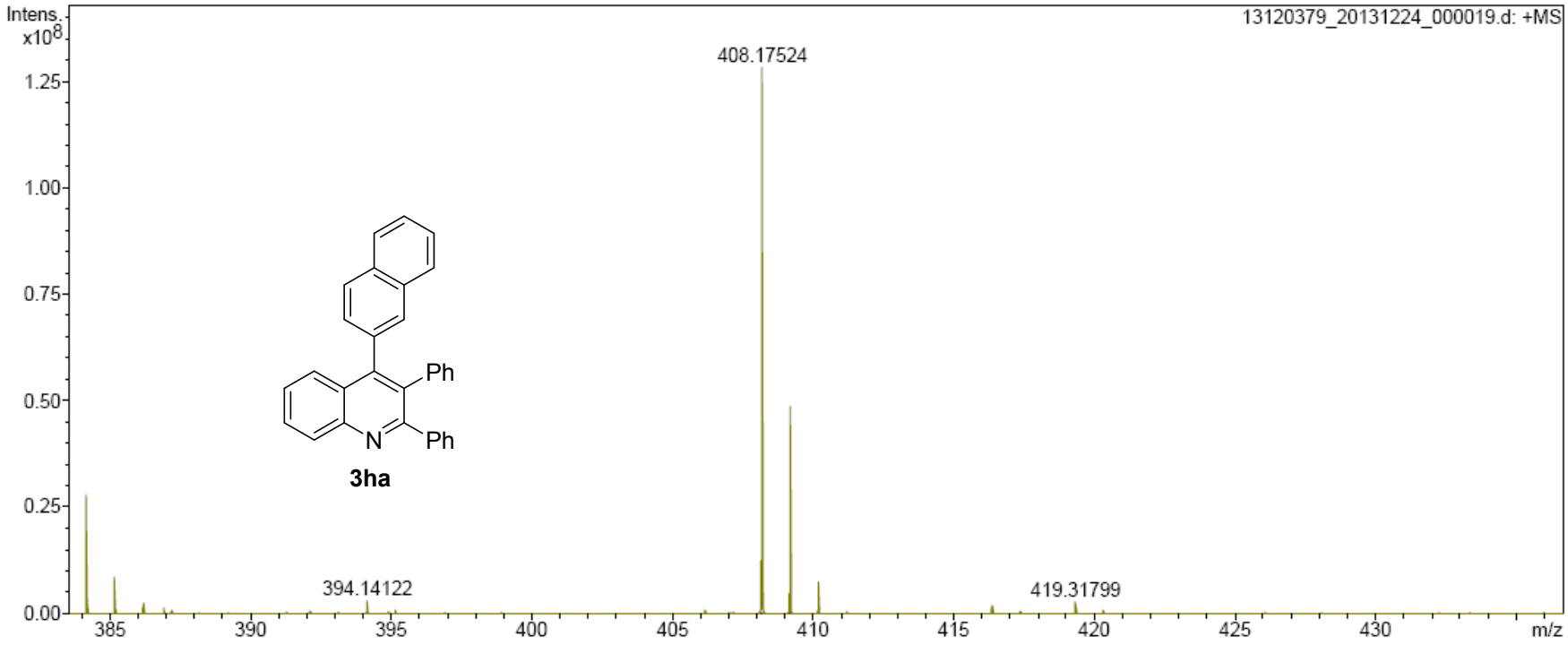

8.293
8.271
7.818
7.808
7.795
7.748
7.732
7.711
7.672
7.588
7.567
7.480
7.470
7.459
7.433
7.410
7.394
7.386
7.241
7.221
7.213
7.205
6.932
6.932
2.038
1.253
-0.000
Ph
Ph
N
3ha
1.00
1.07
3.11
1.01
2.02
3.09
1.02
4.00
5.00
10
8
6
4
2
0
PPM


159.117
147.500
147.419
141.215
138.285
134.537
133.173
132.767
132.346
131.318
129.969
129.818
129.635
129.421
128.196
128.041
127.768
127.721
127.646
127.454
126.836
126.705
126.664
126.406
126.268
126.253
77.375
77.063
76.747
Ph
Ph
N
3ha
145
140
135
130
200
150
100
50
0
PPM

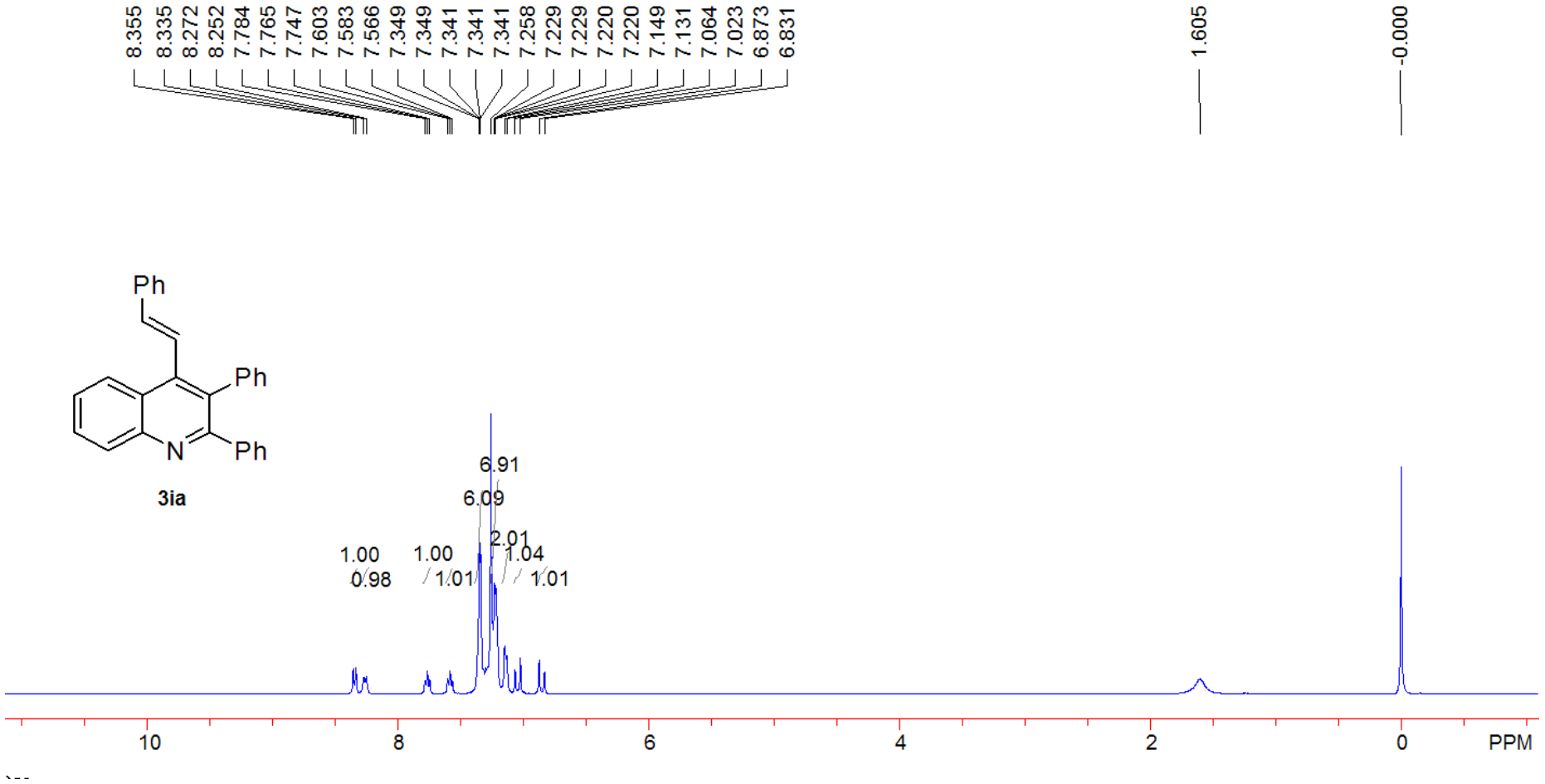
Peking University Mass Spectrometry Sample Analysis Report

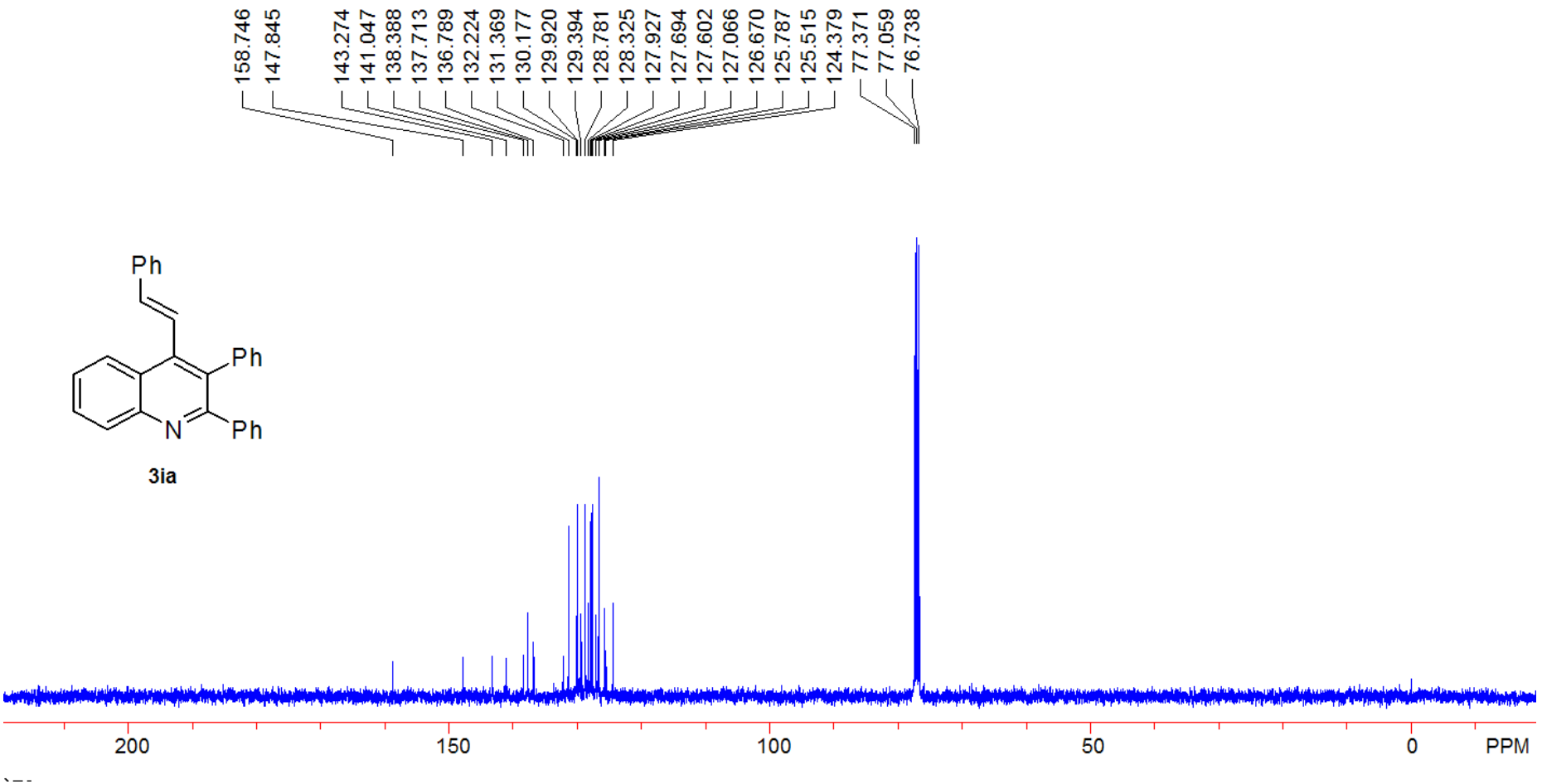
Analysis Info

Analysis Name	13120379_20131224_000019.d	Acquisition Date	12/24/2013 11:46:26 AM
Sample	P	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
408.17524	128222040	C 31 H 22 N	408.17468	-0.6	-1.4	20.4	21.5	even	ok

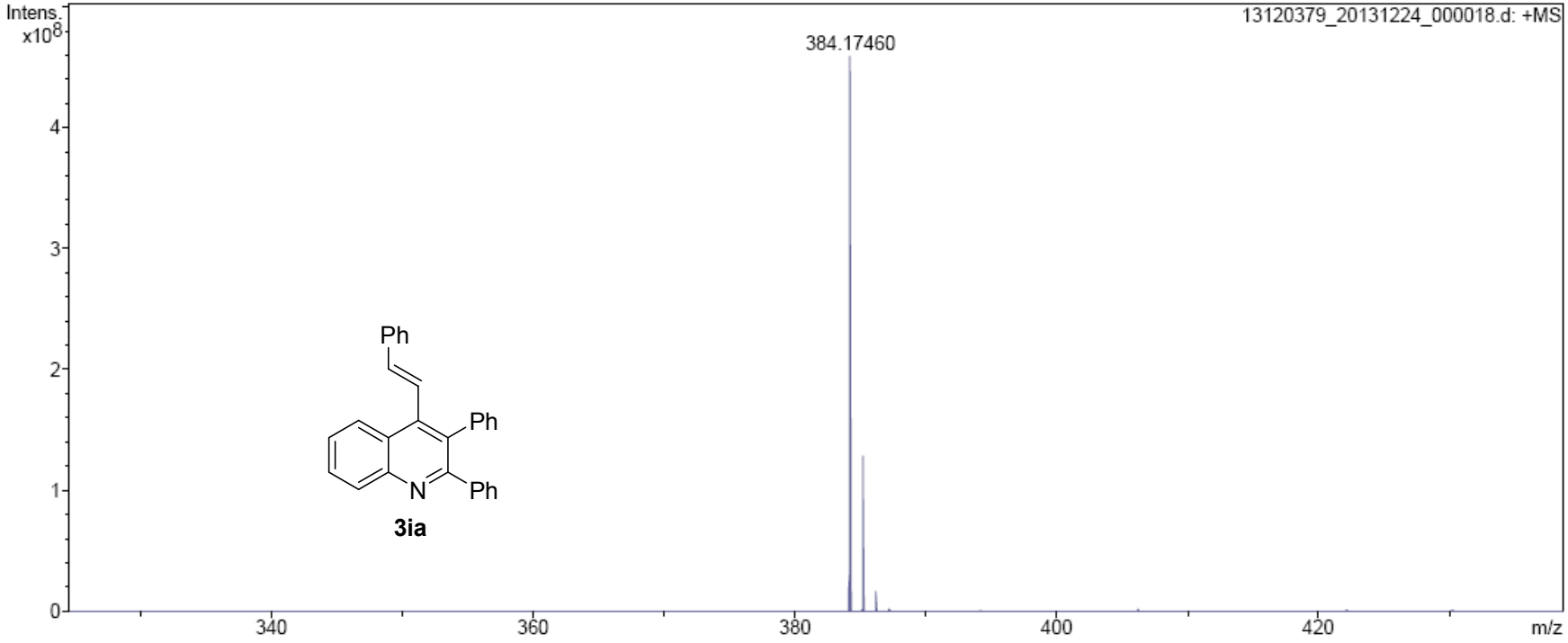

8.355
8.335
8.272
8.252
7.784
7.765
7.747
7.603
7.583
7.566
7.349
7.349
7.341
7.341
7.341
7.258
7.229
7.229
7.220
7.220
7.149
7.131
7.064
7.023
6.873
6.831
1.605
-0.000
Ph
Ph
Ph
N
3ia
6.91
6.09
2.01
1.04
1.00
0.98
1.00
1.01
1.01
10
8
6
4
2
0
PPM


158.746
147.845
143.274
141.047
138.388
137.713
136.789
132.224
131.369
130.177
129.920
129.394
128.781
128.325
127.927
127.694
127.602
127.066
126.670
125.787
125.515
124.379
77.371
77.059
76.738
Ph
Ph
Ph
N
3ia
200
150
100
50
0
PPM

Peking University Mass Spectrometry Sample Analysis Report

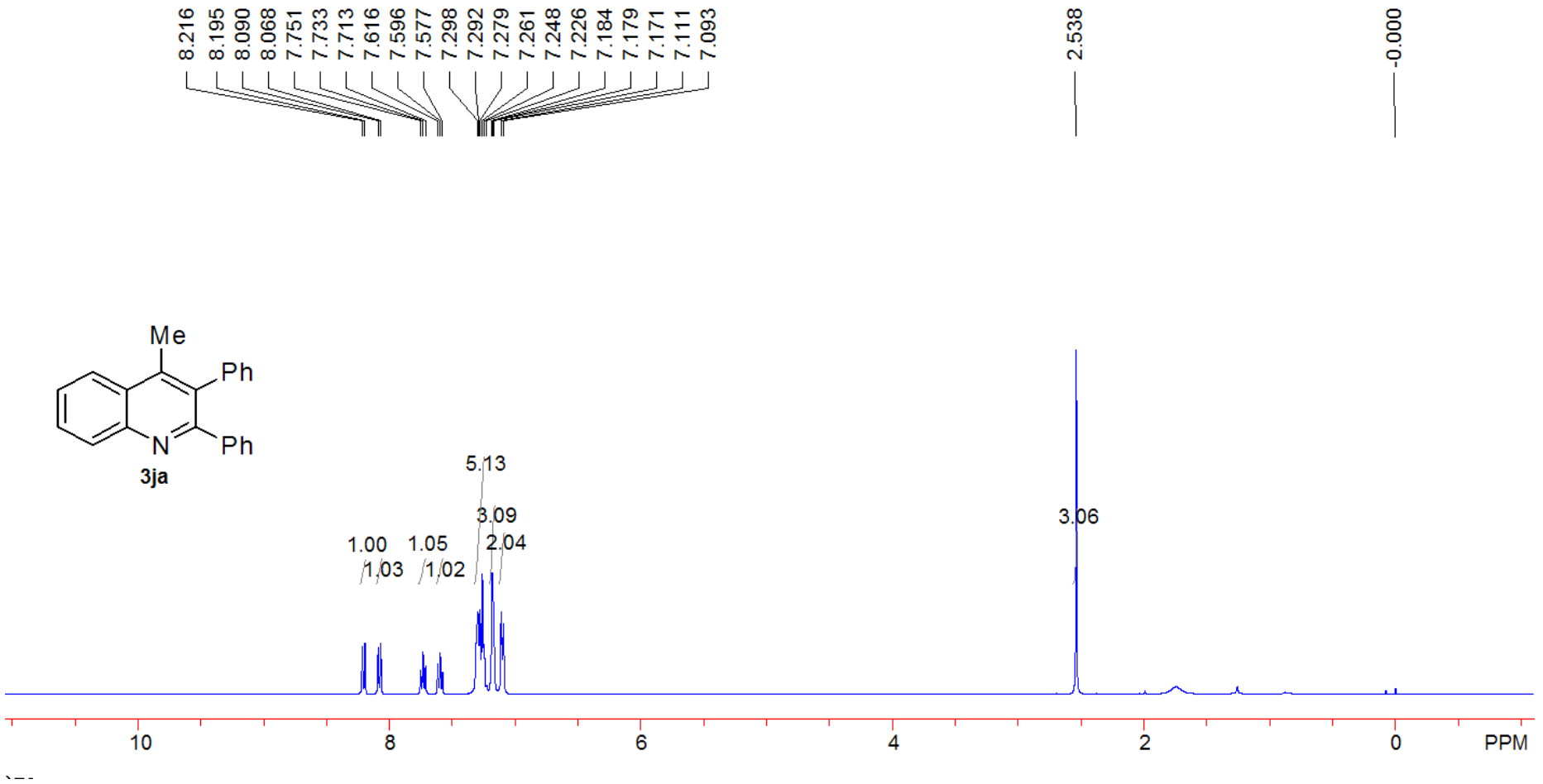
Analysis Info

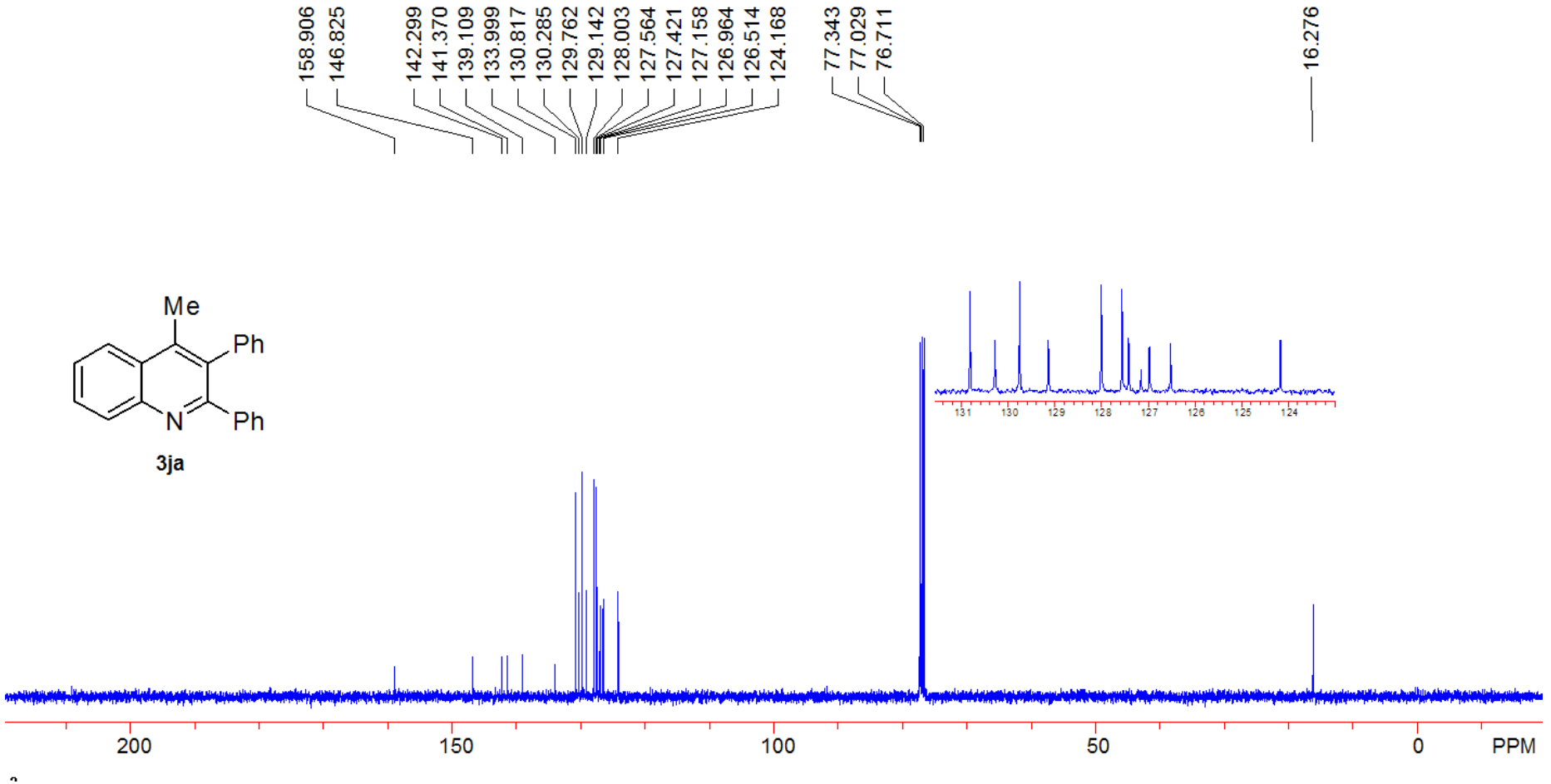
Analysis Name	13120379_20131224_000018.d	Acquisition Date	12/24/2013 11:45:27 AM
Sample	O	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University

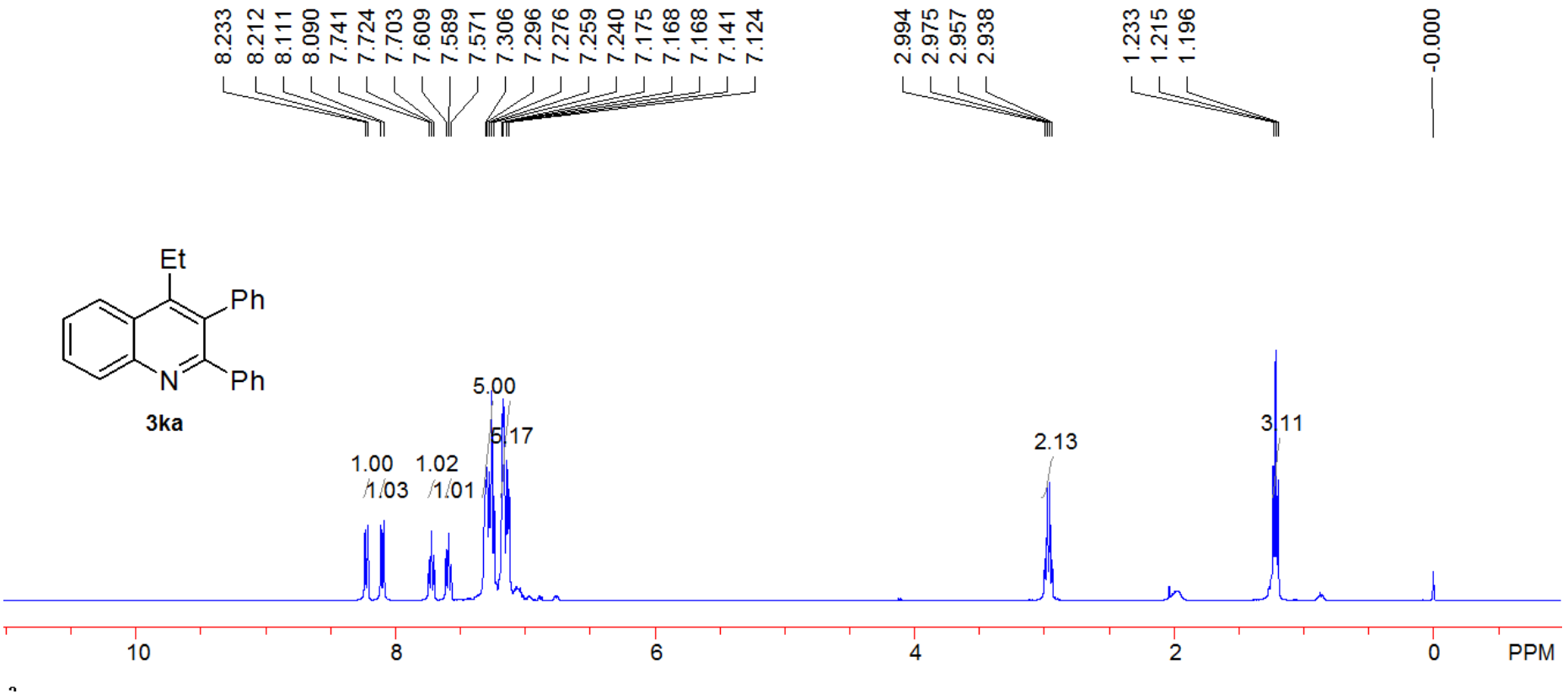


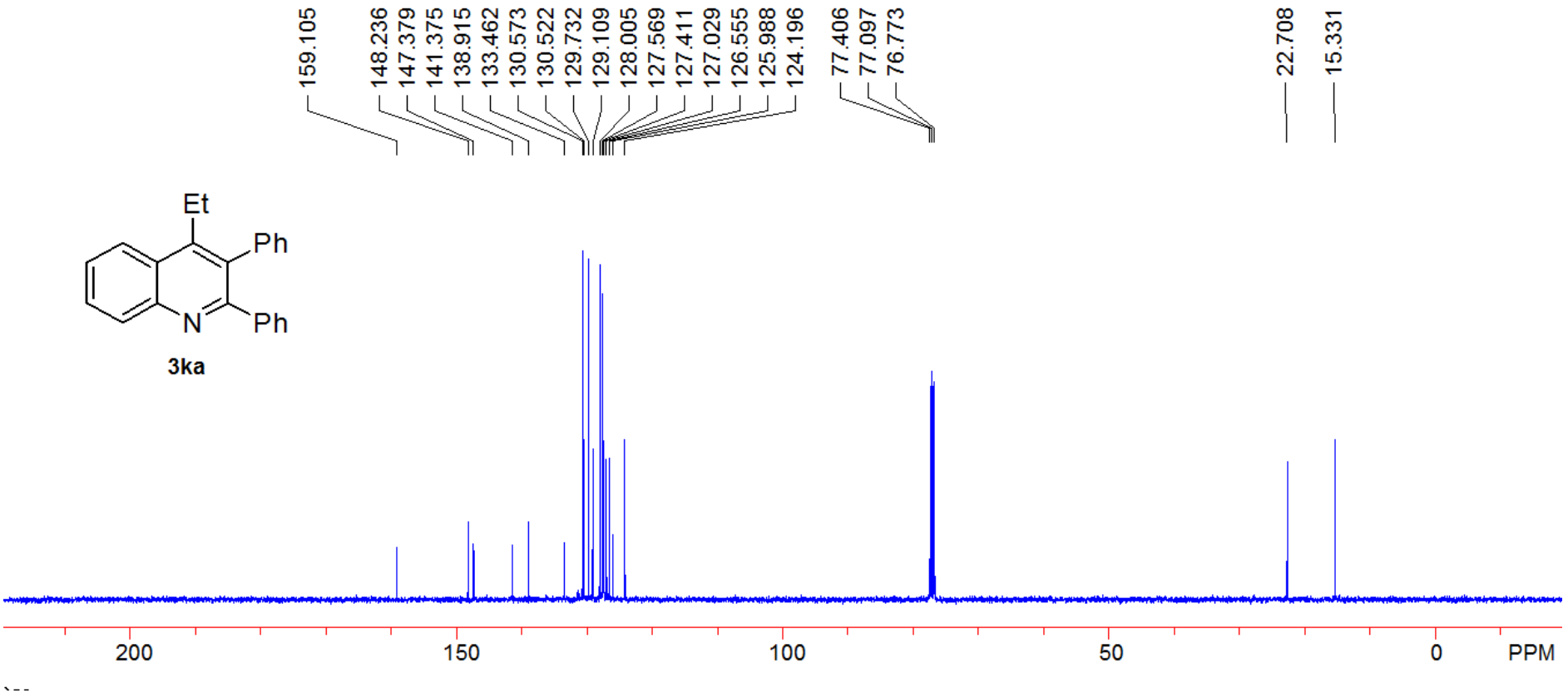
3ia

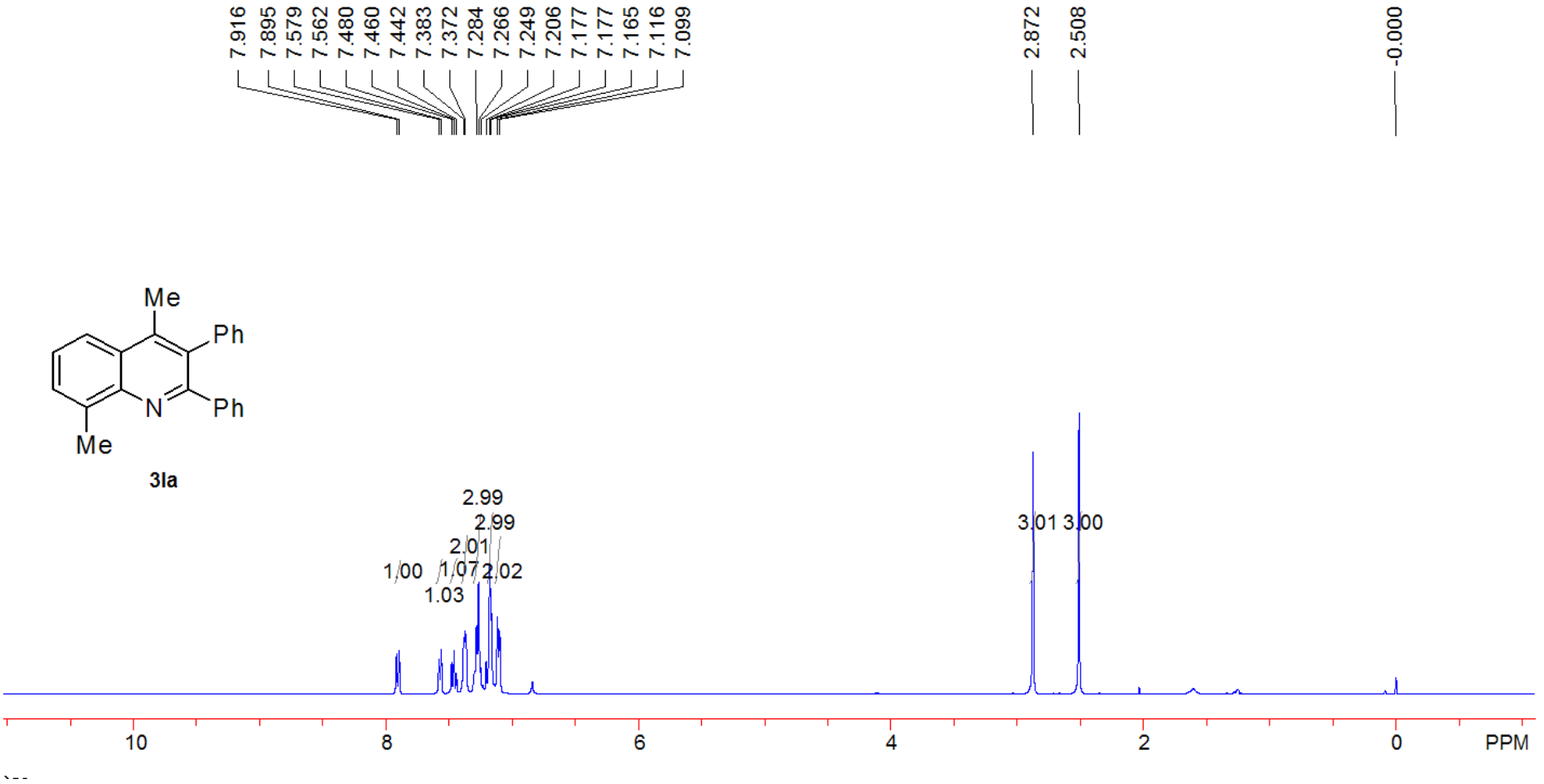
Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
384.17460	460019648	C 29 H 22 N	384.17468	0.1	0.2	17.4	19.5	even	ok

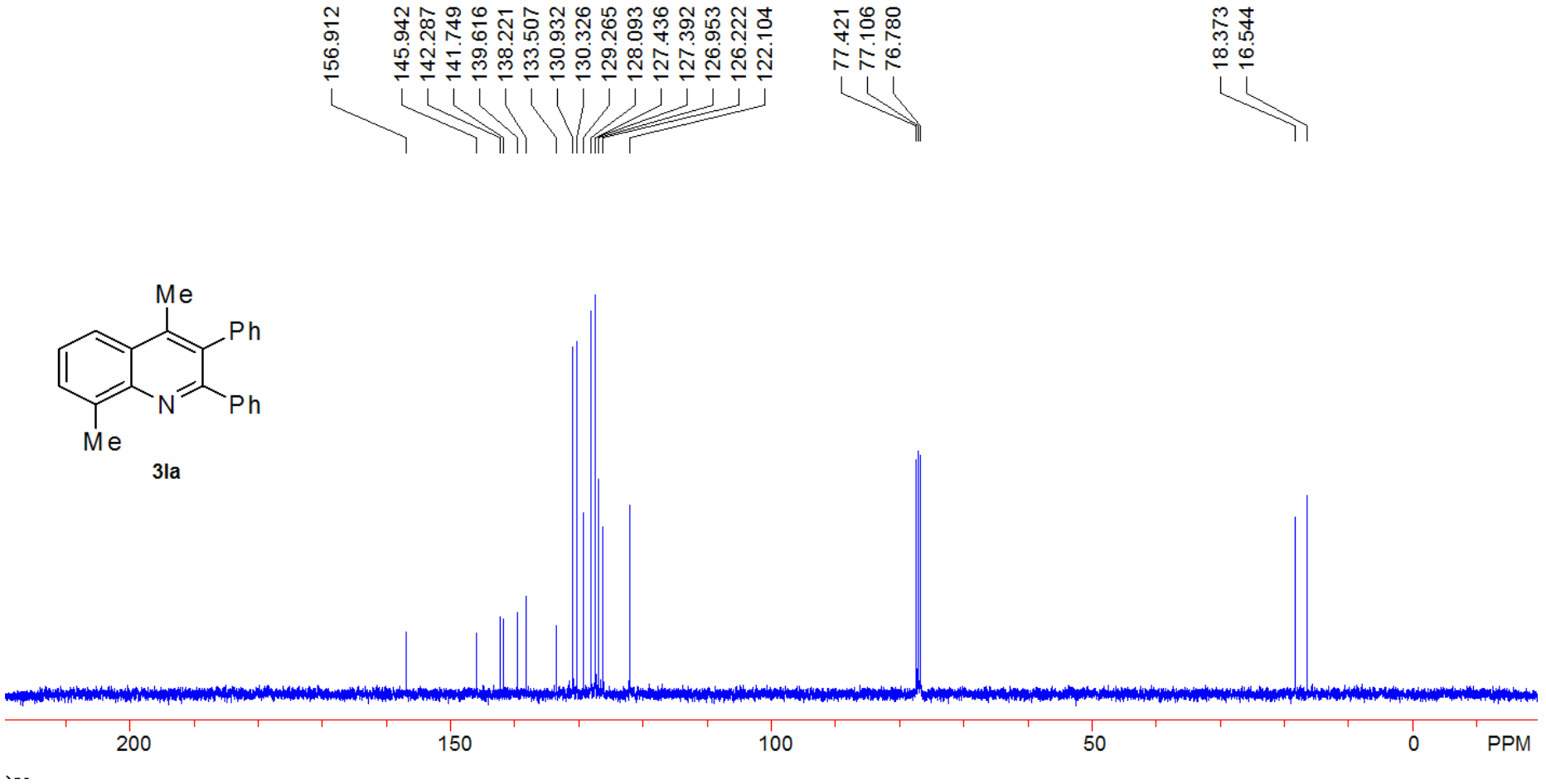

8.216
8.195
8.090
8.068
7.751
7.733
7.713
7.616
7.596
7.577
7.298
7.292
7.279
7.261
7.248
7.226
7.184
7.179
7.171
7.111
7.093
2.538
-0.000
Me
Ph
N
Ph
3ja
5.13
3.09
2.04
1.00
1.03
1.05
1.02
3.06
10
8
6
4
2
0
PPM


158.906
146.825
142.299
141.370
139.109
133.999
130.817
130.285
129.762
129.142
128.003
127.564
127.421
127.158
126.964
126.514
124.168
77.343
77.029
76.711
16.276
Me
Ph
Ph
N
3ja
131
130
129
128
127
126
125
124
200
150
100
50
0
PPM


8.233
8.212
8.111
8.090
7.741
7.724
7.703
7.609
7.589
7.571
7.306
7.296
7.276
7.259
7.240
7.175
7.168
7.168
7.141
7.124
2.994
2.975
2.957
2.938
1.233
1.215
1.196
-0.000
Et
Ph
Ph
N
3ka
1.00
1.03
1.02
1.01
5.00
5.17
2.13
3.11
10
8
6
4
2
0
PPM


159.105
148.236
147.379
141.375
138.915
133.462
130.573
130.522
129.732
129.109
128.005
127.569
127.411
127.029
126.555
125.988
124.196
77.406
77.097
76.773
22.708
15.331
Et
Ph
Ph
N
3ka
200
150
100
50
0
PPM


7.916
7.895
7.579
7.562
7.480
7.460
7.442
7.383
7.372
7.284
7.266
7.249
7.206
7.177
7.177
7.165
7.116
7.099
2.872
2.508
-0.000
Me
Ph
N
Ph
Me
3Ia
2.99
2.99
2.01
1.00
1.07
2.02
1.03
3.01
3.00
10
8
6
4
2
0
PPM

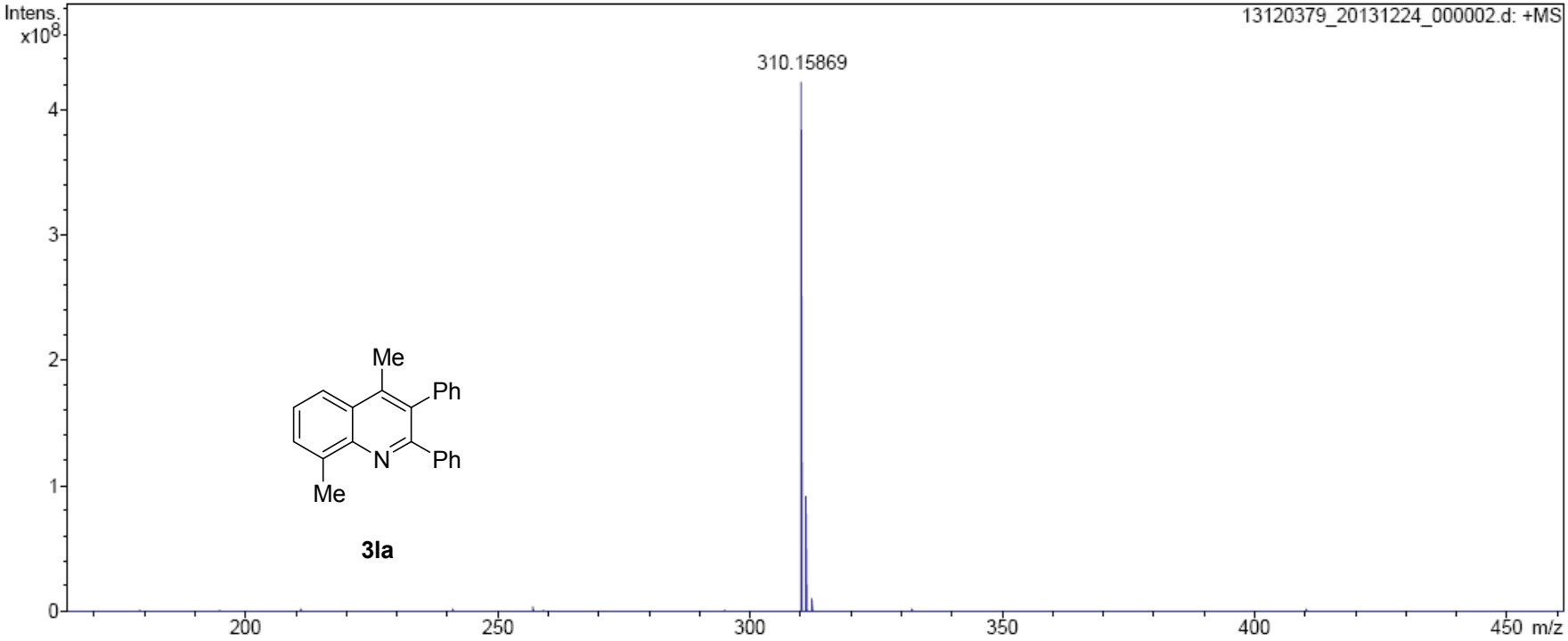

156.912
145.942
142.287
141.749
139.616
138.221
133.507
130.932
130.326
129.265
128.093
127.436
127.392
126.953
126.222
122.104
77.421
77.106
76.780
18.373
16.544
Me
Ph
N
Ph
Me
200
150
100
50
0
PPM

3la

Peking University Mass Spectrometry Sample Analysis Report

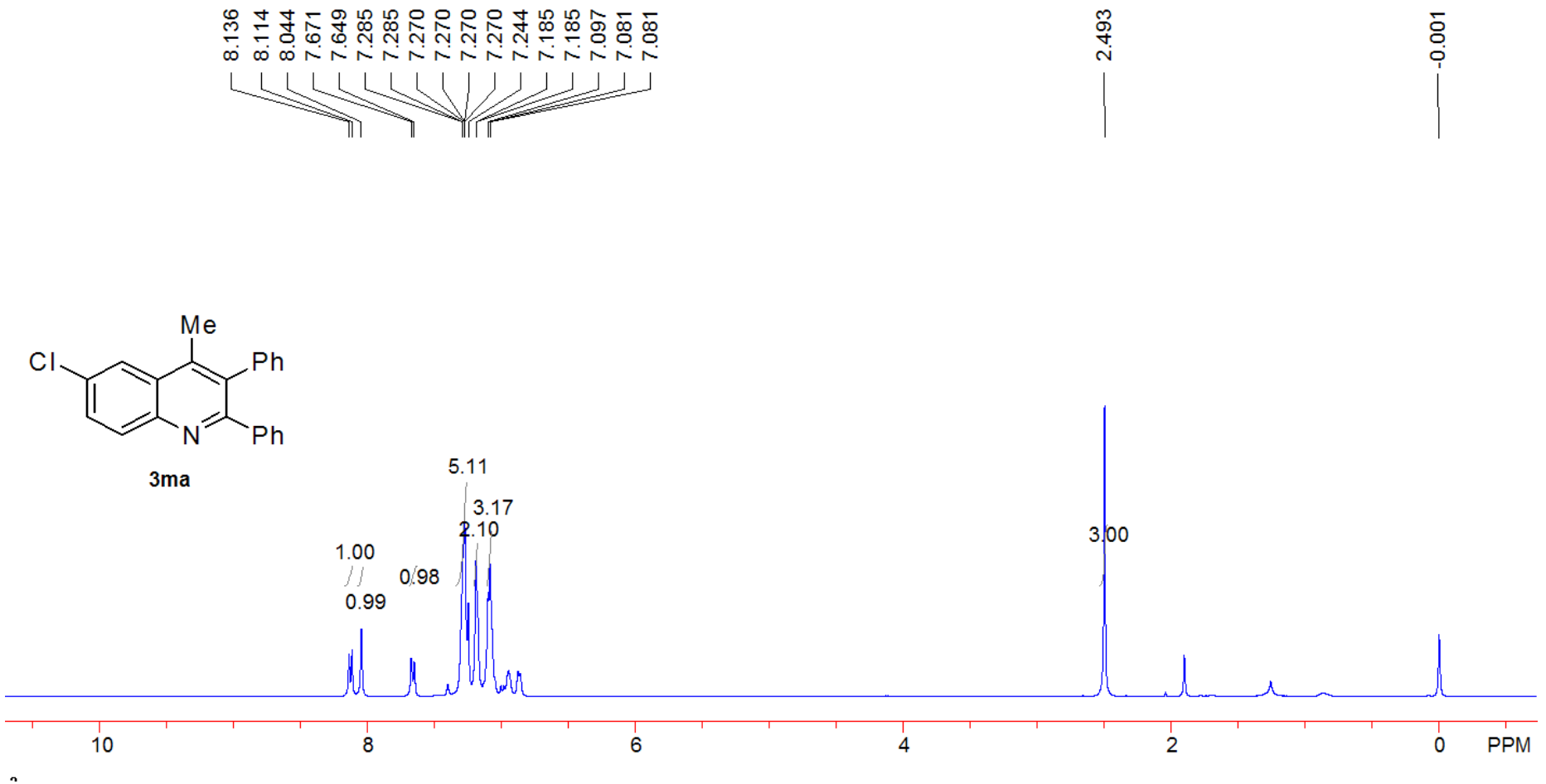
Analysis Info

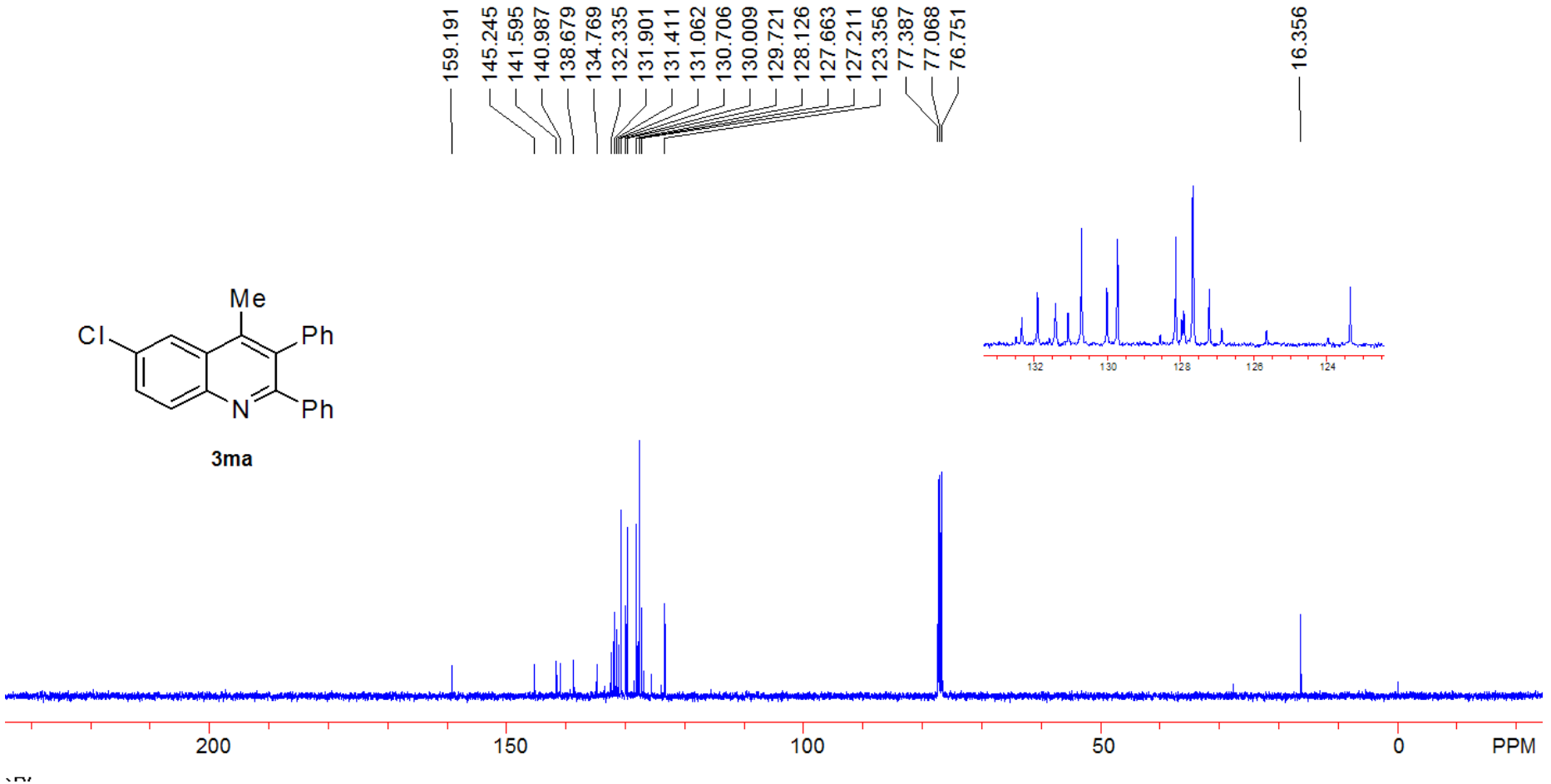
Analysis Name	13120379_20131224_000002.d	Acquisition Date	12/24/2013 11:23:13 AM
Sample	A	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University

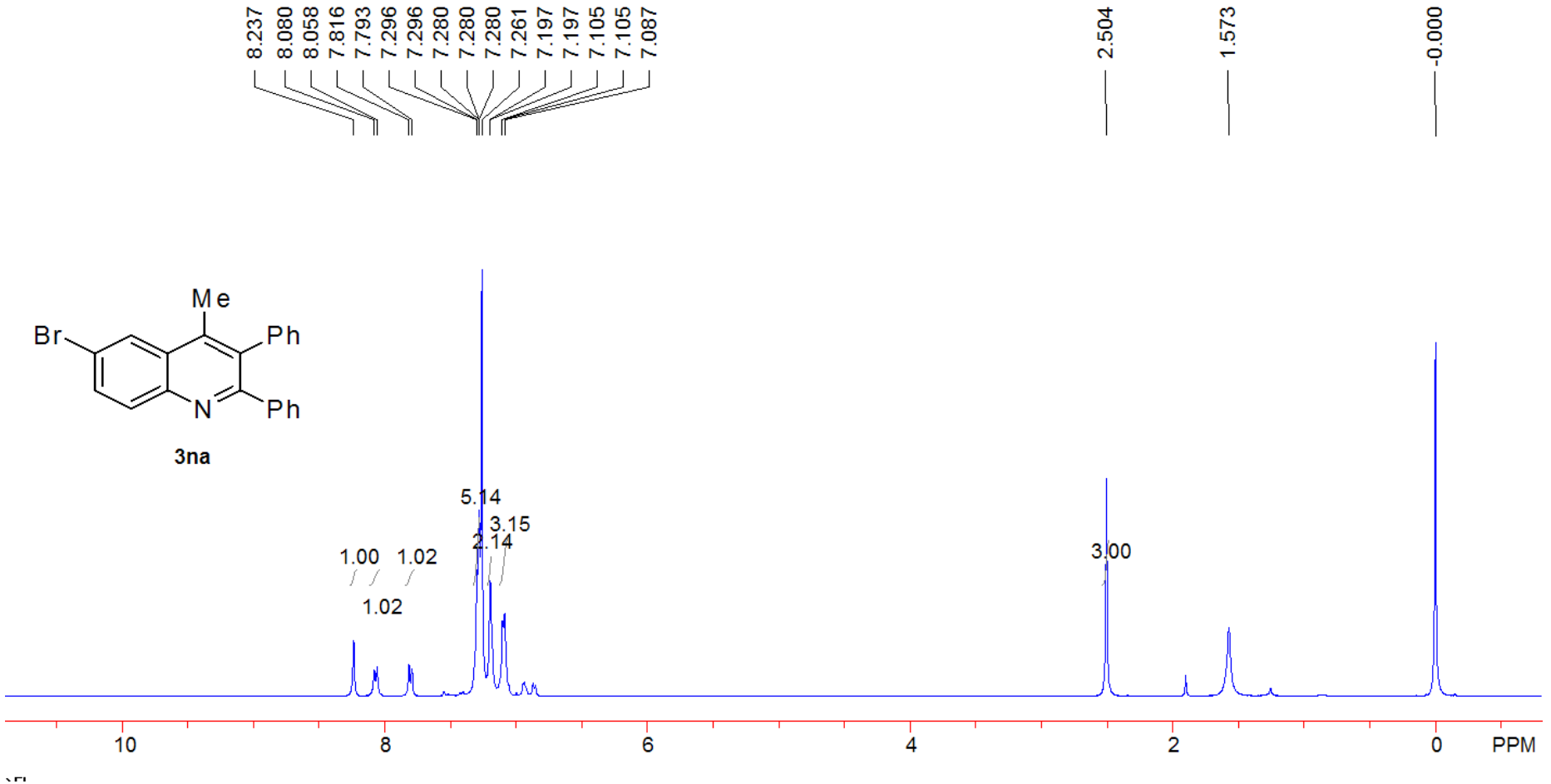


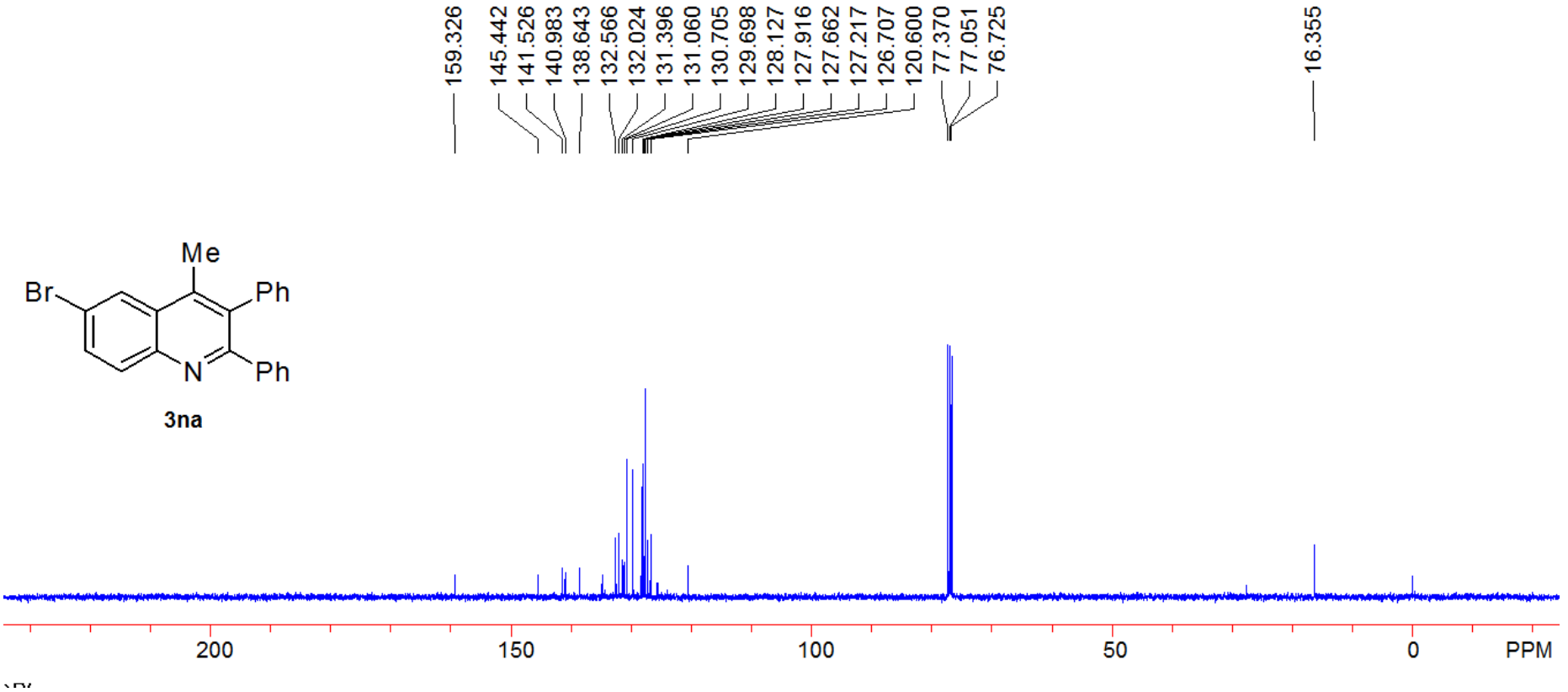
3la

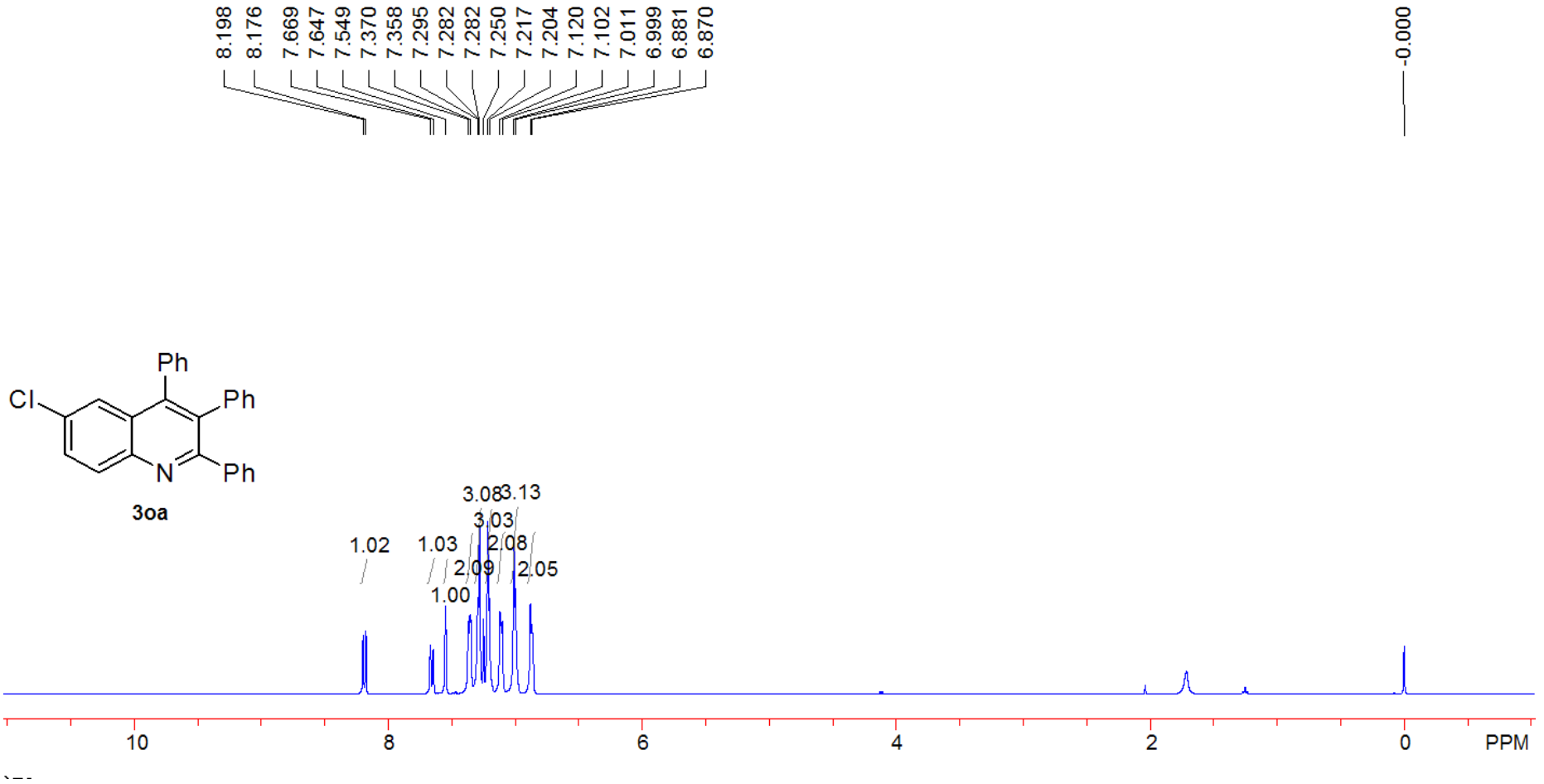
Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
310.15869	428252512	C 23 H 20 N	310.15903	0.3	1.1	20.3	14.5	even	ok

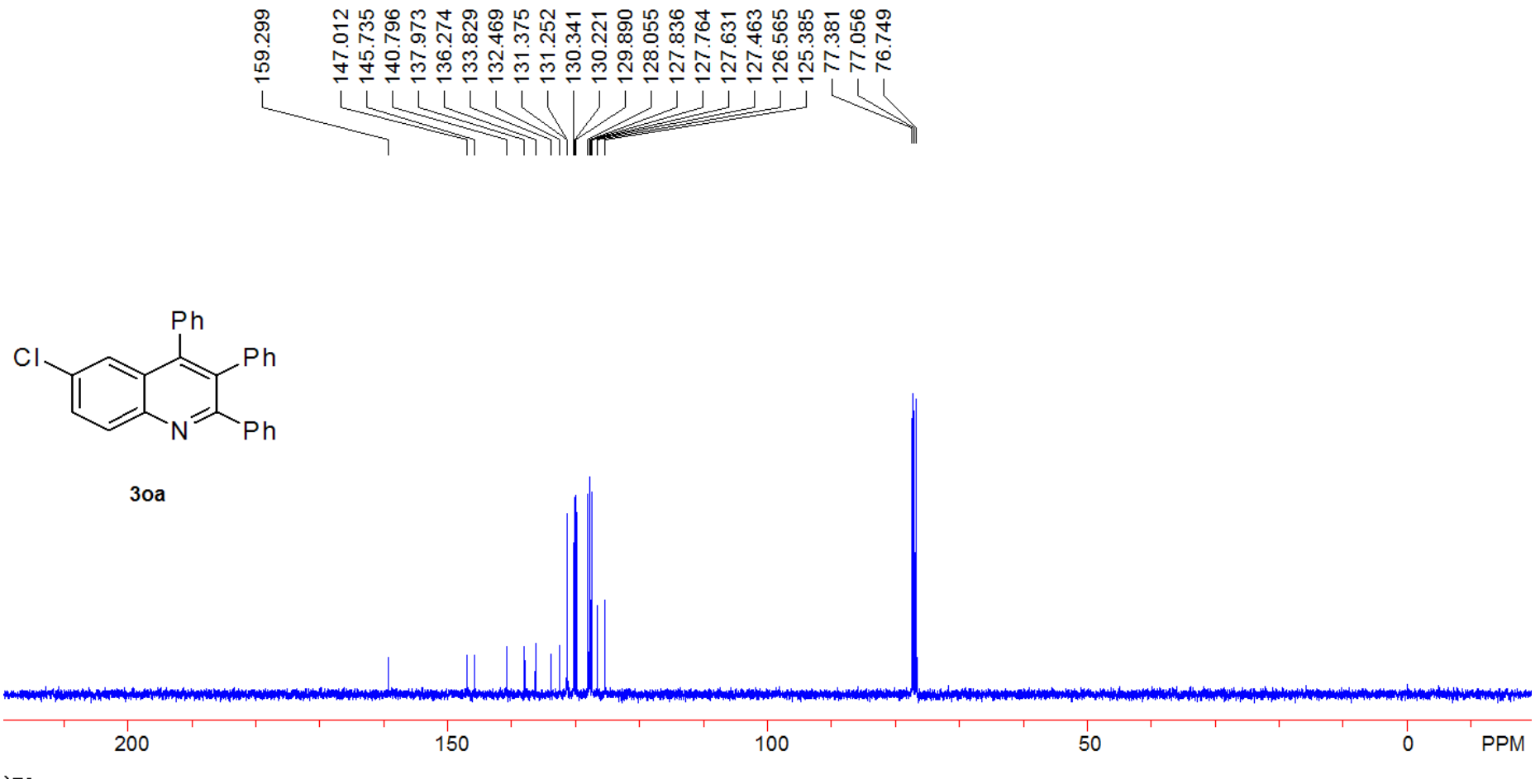

8.136
8.114
8.044
7.671
7.649
7.285
7.285
7.270
7.270
7.270
7.270
7.244
7.185
7.185
7.097
7.081
7.081
2.493
-0.001
Me
Cl
Ph
N
Ph
3ma
5.11
3.17
2.10
1.00
0.99
0.98
3.00
10
8
6
4
2
0
PPM


159.191
145.245
141.595
140.987
138.679
134.769
132.335
131.901
131.411
131.062
130.706
130.009
129.721
128.126
127.663
127.211
123.356
77.387
77.068
76.751
16.356
Me
Cl
Ph
Ph
N
3ma
132
130
128
126
124
200
150
100
50
0
PPM

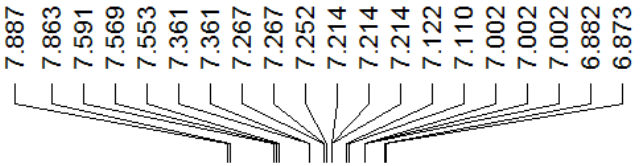

8.237
8.080
8.058
7.816
7.793
7.296
7.296
7.280
7.280
7.280
7.261
7.197
7.197
7.105
7.105
7.087
2.504
1.573
-0.000
Me
Br
Ph
N
Ph
3na
5.14
3.15
2.14
1.00
1.02
1.02
3.00
10
8
6
4
2
0
PPM

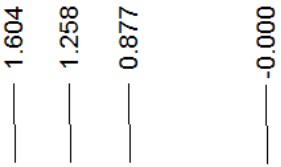

159.326
145.442
141.526
140.983
138.643
132.566
132.024
131.396
131.060
130.705
129.698
128.127
127.916
127.662
127.217
126.707
120.600
77.370
77.051
76.725
16.355
Me
Br
Ph
N
Ph
3na
200
150
100
50
0
PPM

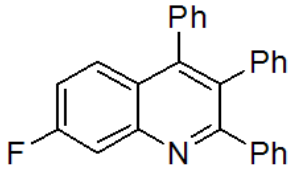

8.198
8.176
7.669
7.647
7.549
7.370
7.358
7.295
7.282
7.282
7.250
7.217
7.204
7.120
7.102
7.011
6.999
6.881
6.870
-0.000
Ph
Cl
Ph
N
Ph
3oa
1.02
1.03
2.09
1.00
3.08
3.13
3.03
2.08
2.05
10
8
6
4
2
0
PPM


159.299
147.012
145.735
140.796
137.973
136.274
133.829
132.469
131.375
131.252
130.341
130.221
129.890
128.055
127.836
127.764
127.631
127.463
126.565
125.385
77.381
77.056
76.749
Cl
Ph
Ph
Ph
N
200
150
100
50
0
PPM

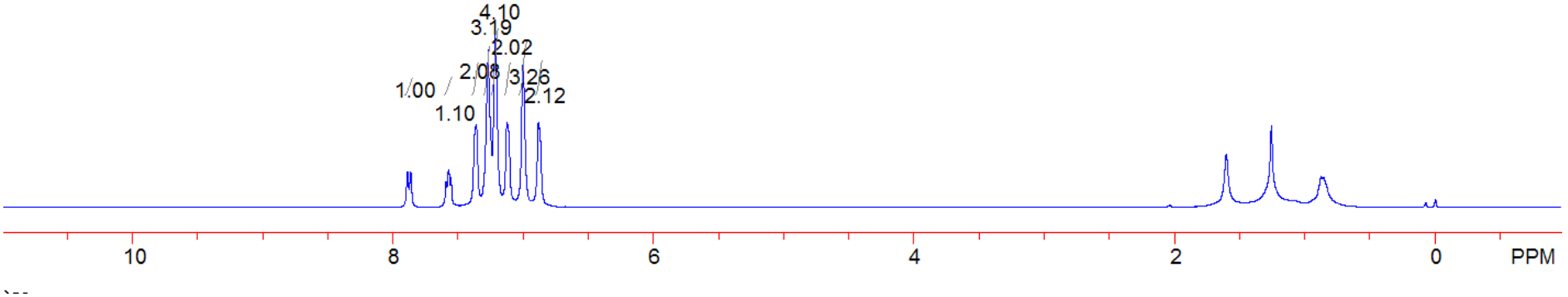
3oa

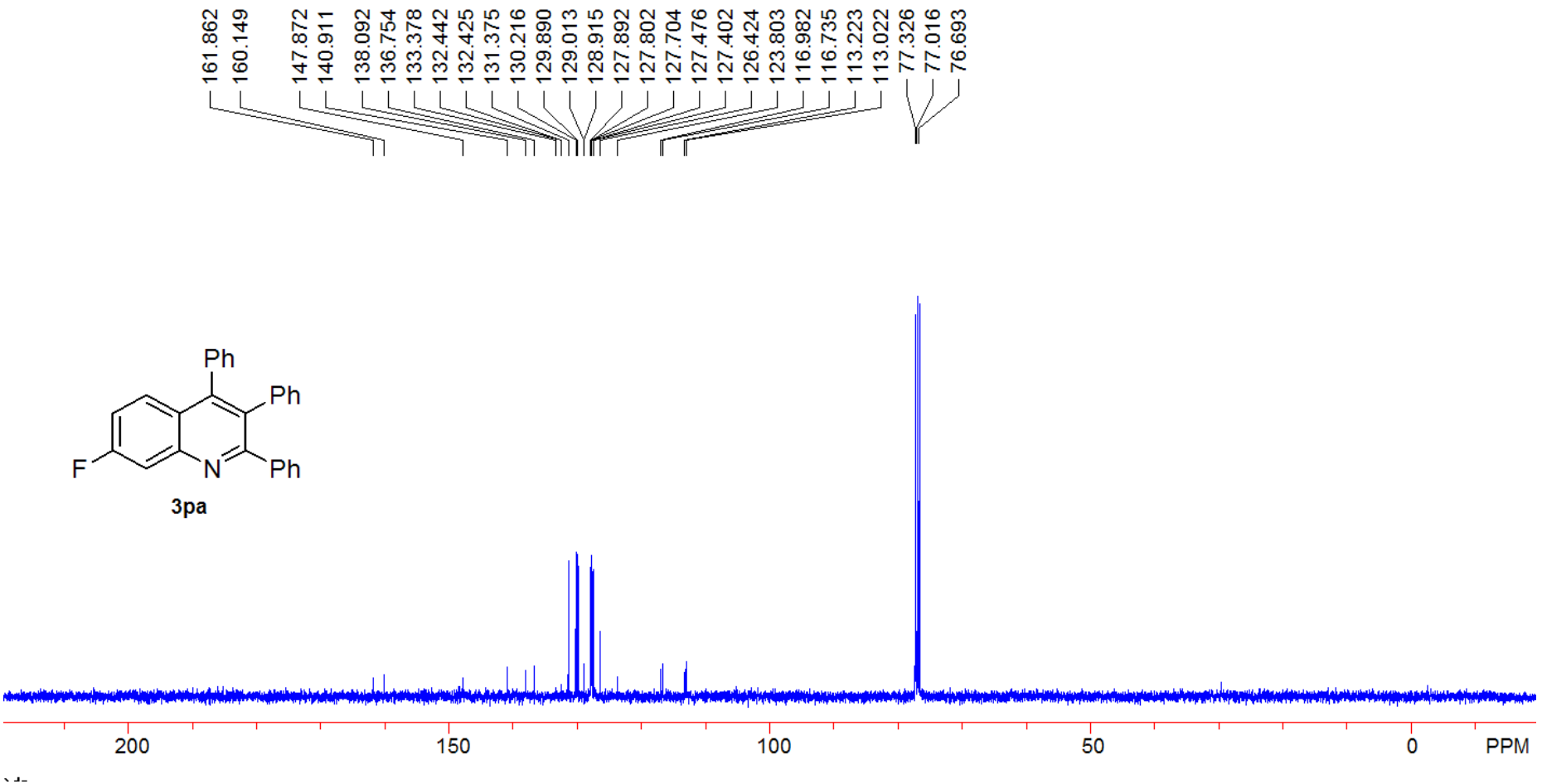

7.887
7.863
7.591
7.569
7.553
7.361
7.361
7.267
7.267
7.252
7.214
7.214
7.214
7.122
7.110
7.002
7.002
7.002
6.882
6.873


1.604
1.258
0.877
-0.000


Ph
Ph
F
N
Ph

3pa


4.10
3.19
2.02
2.08
3.26
2.12
1.00
1.10
10
8
6
4
2
0
PPM

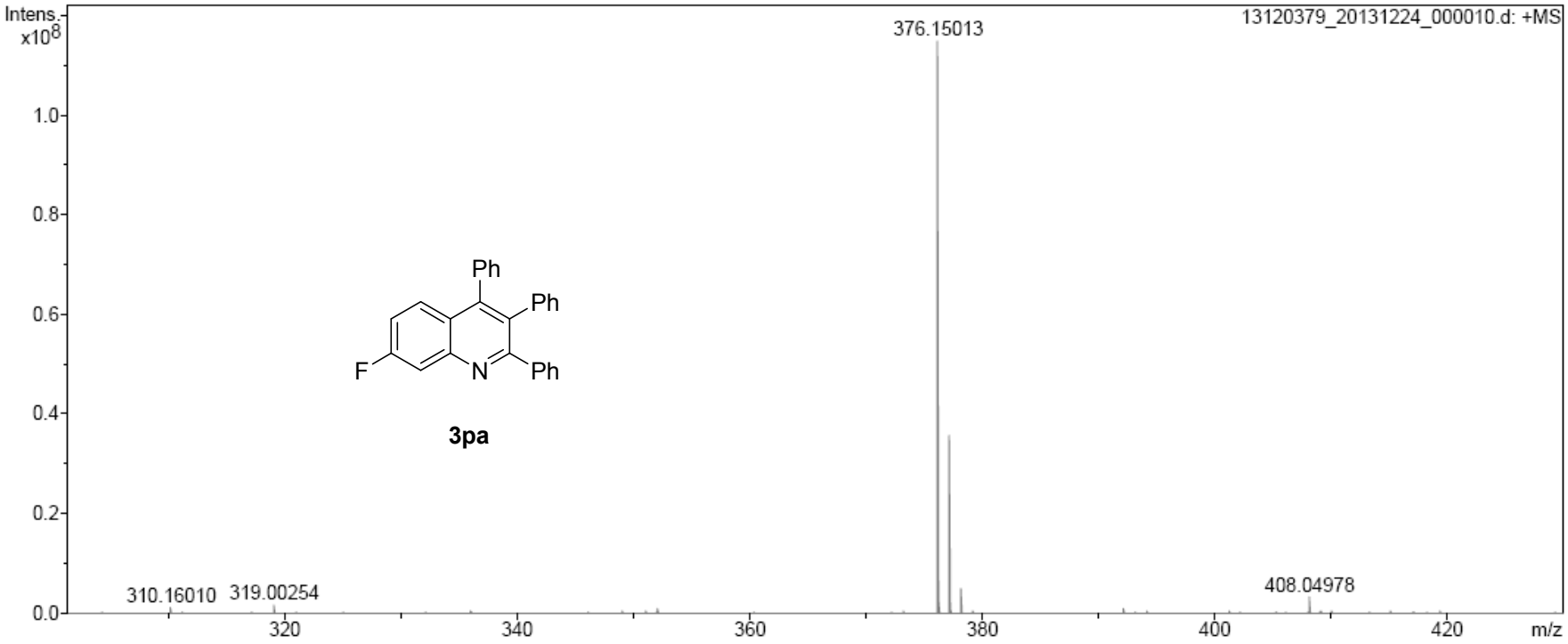

161.862
160.149
147.872
140.911
138.092
136.754
133.378
132.442
132.425
131.375
130.216
129.890
129.013
128.915
127.892
127.802
127.704
127.476
127.402
126.424
123.803
116.982
116.735
113.223
113.022
77.326
77.016
76.693
Ph
Ph
F
N
Ph
200
150
100
50
0
PPM

3pa

Peking University Mass Spectrometry Sample Analysis Report

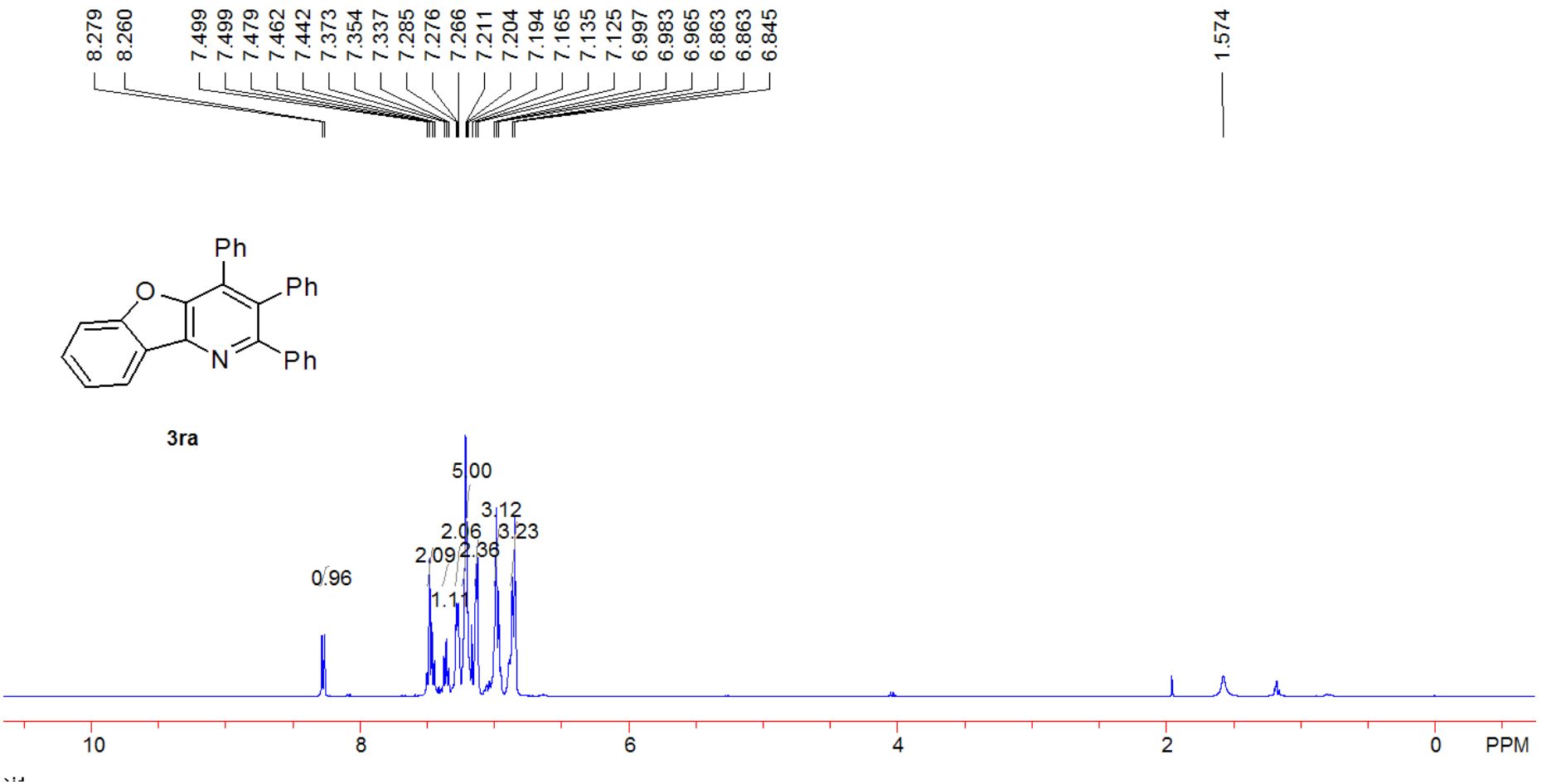
Analysis Info

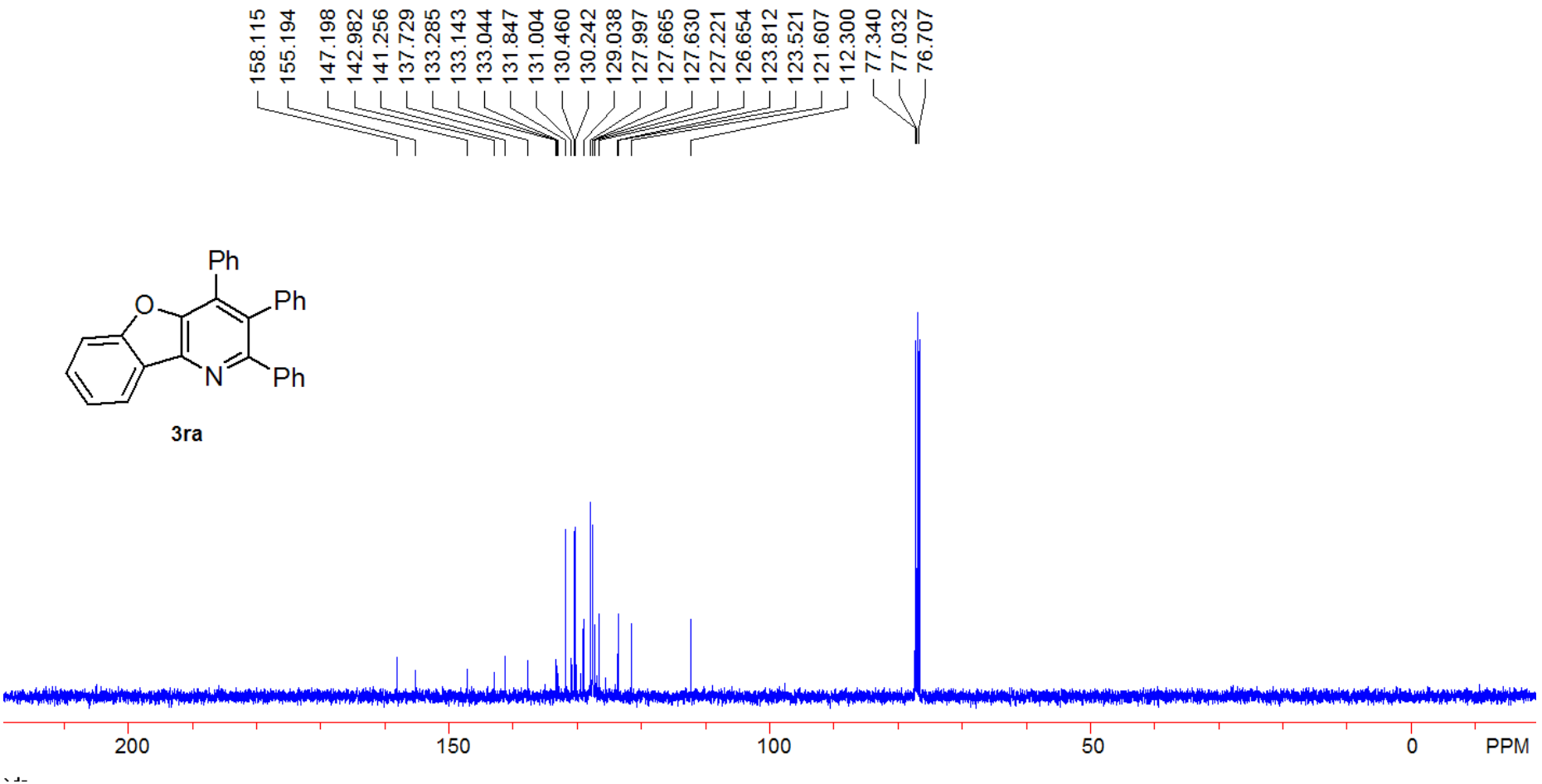
Analysis Name	13120379_20131224_000010.d	Acquisition Date	12/24/2013 11:36:18 AM
Sample	G	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3pa

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
376.15013	114950704	C 27 H 19 F N	376.14960	-0.5	-1.4	7.8	18.5	even	ok

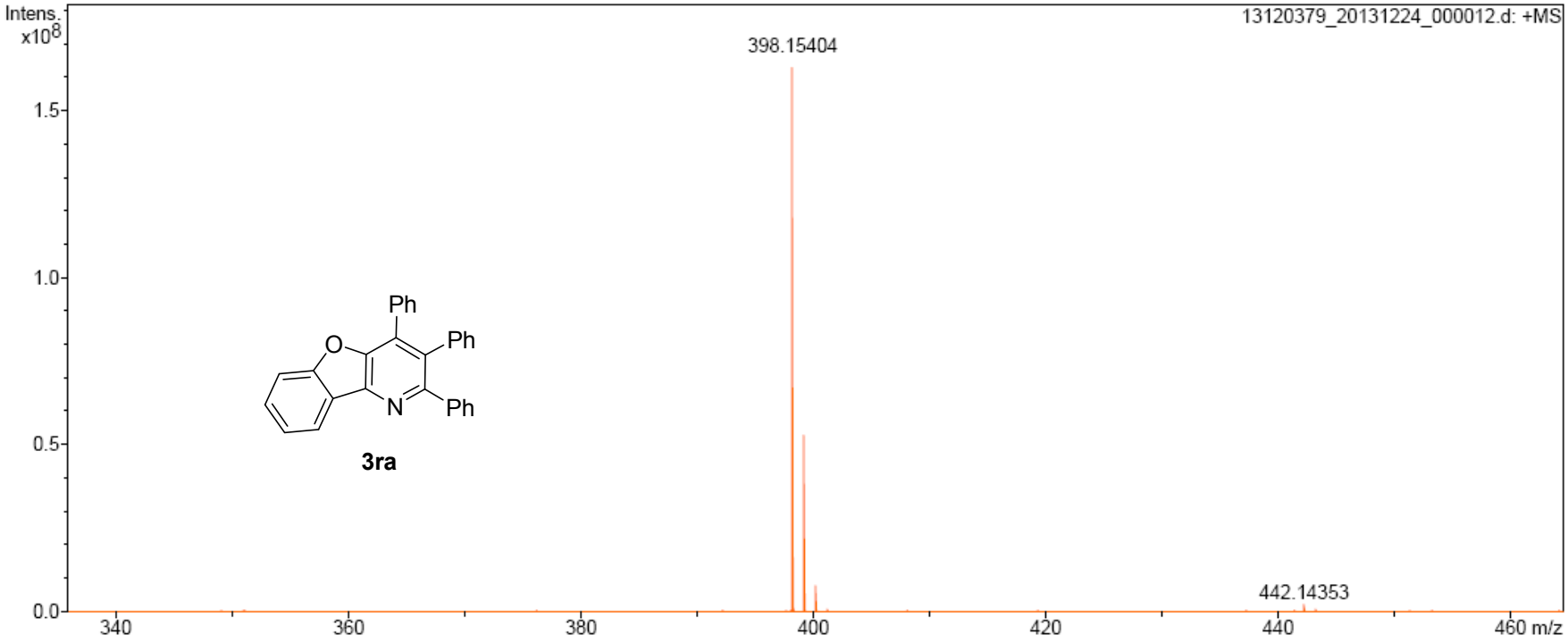

8.279
8.260
7.499
7.499
7.479
7.462
7.442
7.373
7.354
7.337
7.285
7.276
7.266
7.211
7.204
7.194
7.165
7.135
7.125
6.997
6.983
6.965
6.863
6.863
6.845
1.574
Ph
Ph
Ph
O
N
3ra
5.00
3.12
3.23
2.06
2.36
2.09
0.96
1.11
10
8
6
4
2
0
PPM


158.115
155.194
147.198
142.982
141.256
137.729
133.285
133.143
133.044
131.847
131.004
130.460
130.242
129.038
127.997
127.665
127.630
127.221
126.654
123.812
123.521
121.607
112.300
77.340
77.032
76.707
Ph
Ph
Ph
O
N
3ra
200
150
100
50
0
PPM

Peking University Mass Spectrometry Sample Analysis Report

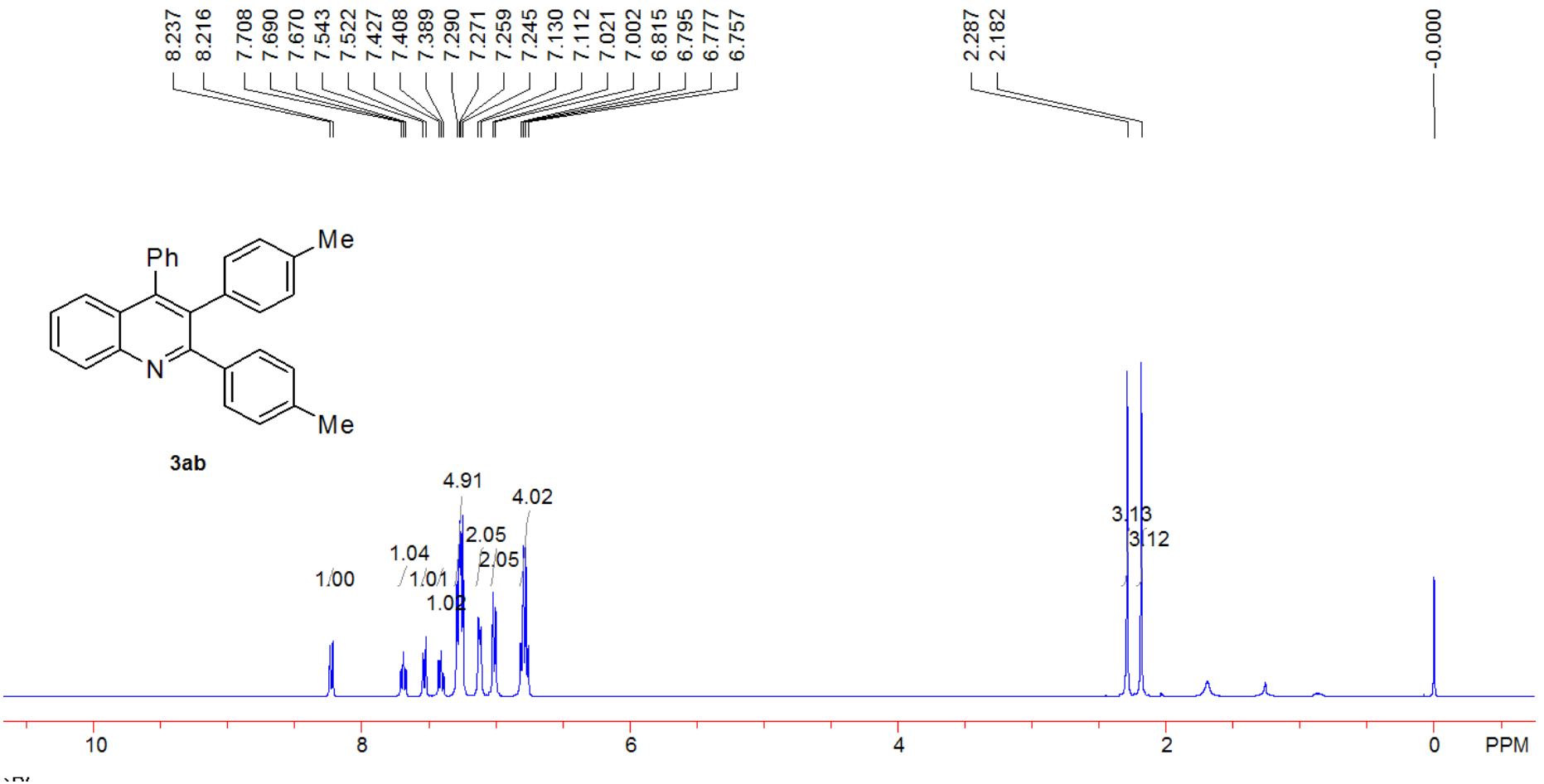
Analysis Info

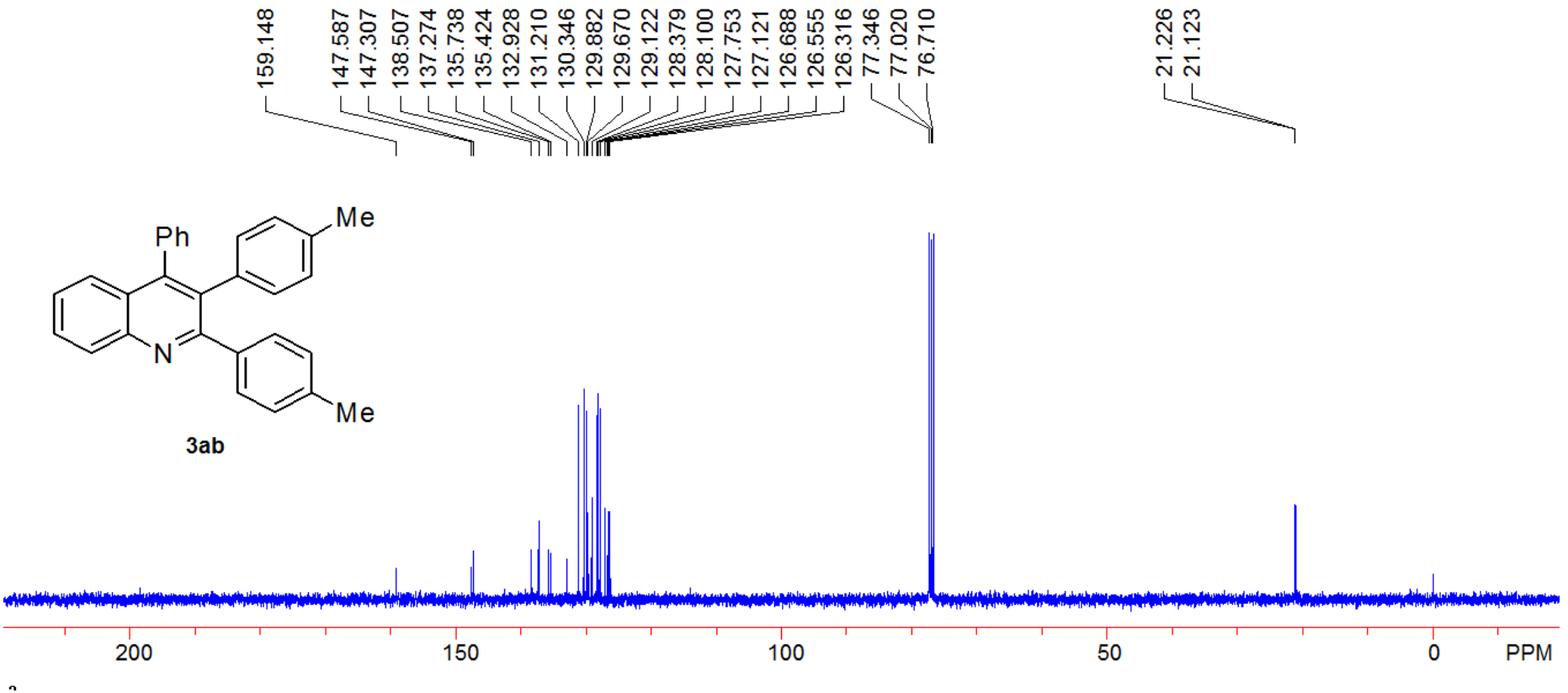
Analysis Name	13120379_20131224_000012.d	Acquisition Date	12/24/2013 11:38:36 AM
Sample	I	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ra

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
398.15404	166246432	C 29 H 20 N O	398.15394	-0.1	-0.2	6.9	20.5	even	ok

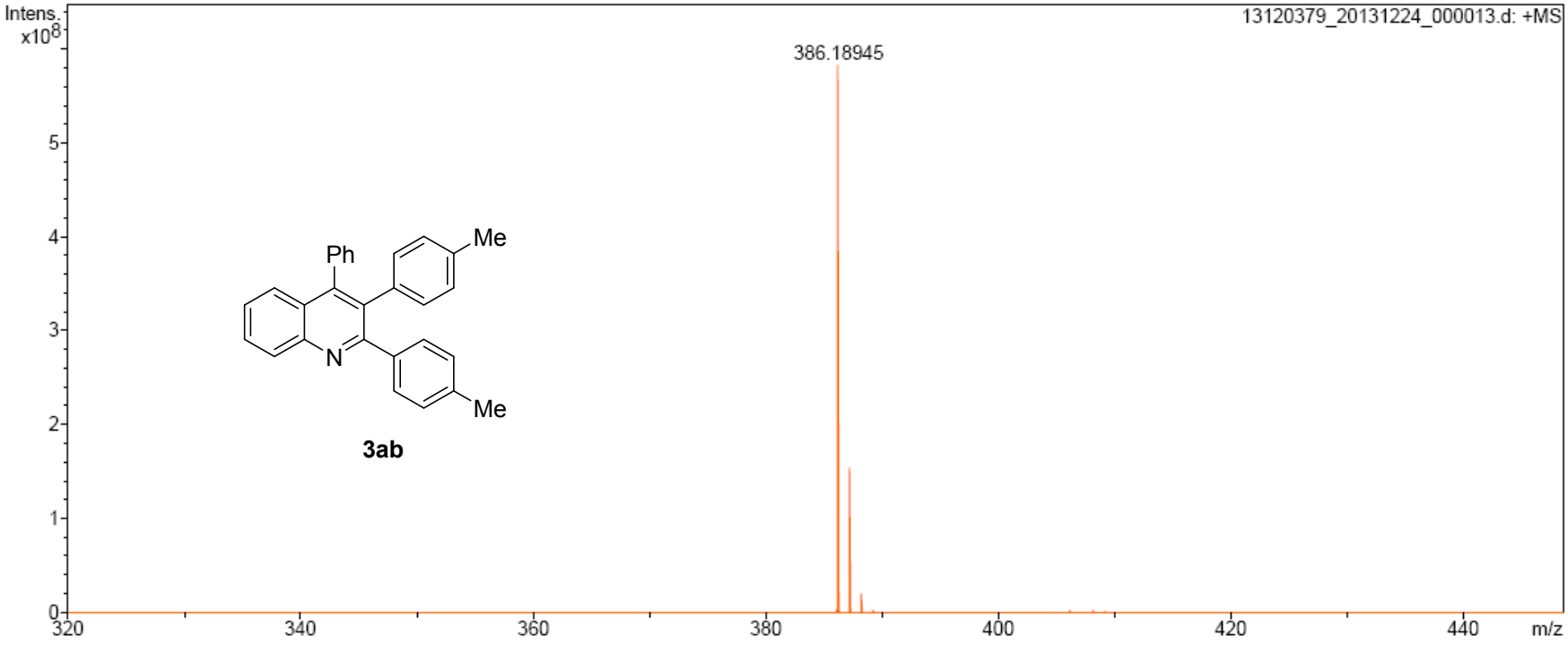

8.237
8.216
7.708
7.690
7.670
7.543
7.522
7.427
7.408
7.389
7.290
7.271
7.259
7.245
7.130
7.112
7.021
7.002
6.815
6.795
6.777
6.757
2.287
2.182
-0.000
Ph
Me
N
Me
3ab
4.91
4.02
2.05
2.05
1.04
1.00
1.01
1.02
3.13
3.12
10
8
6
4
2
0
PPM


159.148
147.587
147.307
138.507
137.274
135.738
135.424
132.928
131.210
130.346
129.882
129.670
129.122
128.379
128.100
127.753
127.121
126.688
126.555
126.316
77.346
77.020
76.710
21.226
21.123
Ph
Me
N
Me
3ab
200
150
100
50
0
PPM

Peking University Mass Spectrometry Sample Analysis Report

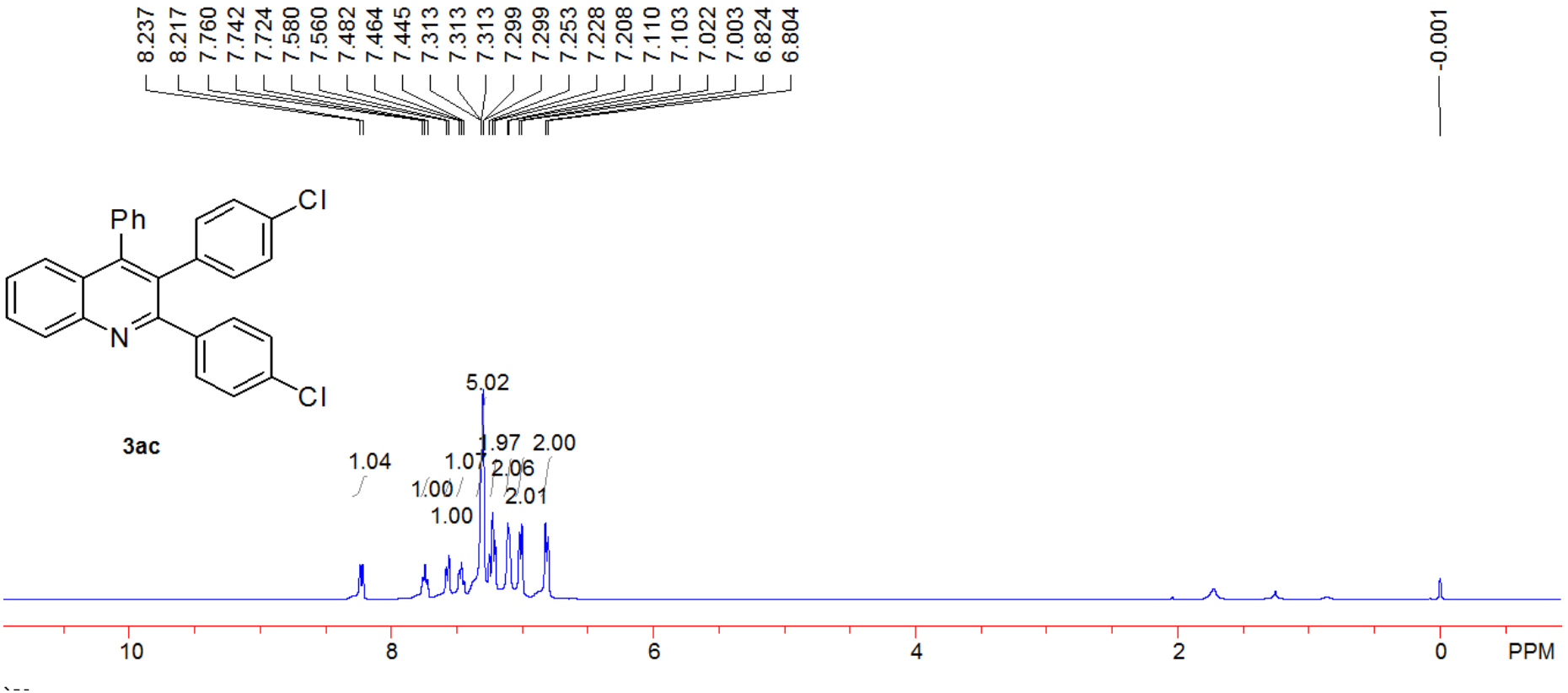
Analysis Info

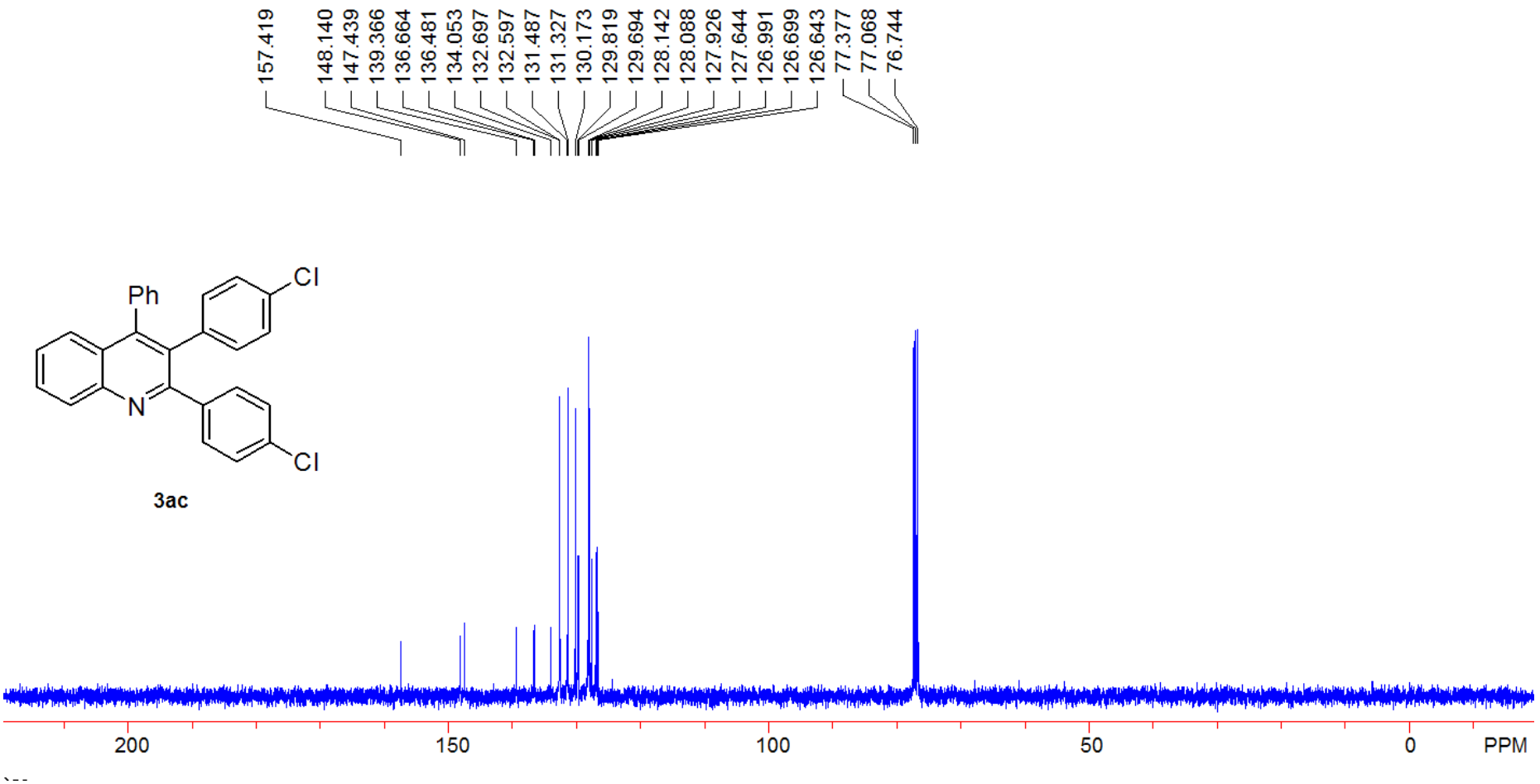
Analysis Name	13120379_20131224_000013.d	Acquisition Date	12/24/2013 11:39:40 AM
Sample	J	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ab

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
386.18945	583493504	C 29 H 24 N	386.19033	0.9	2.3	27.4	18.5	even	ok

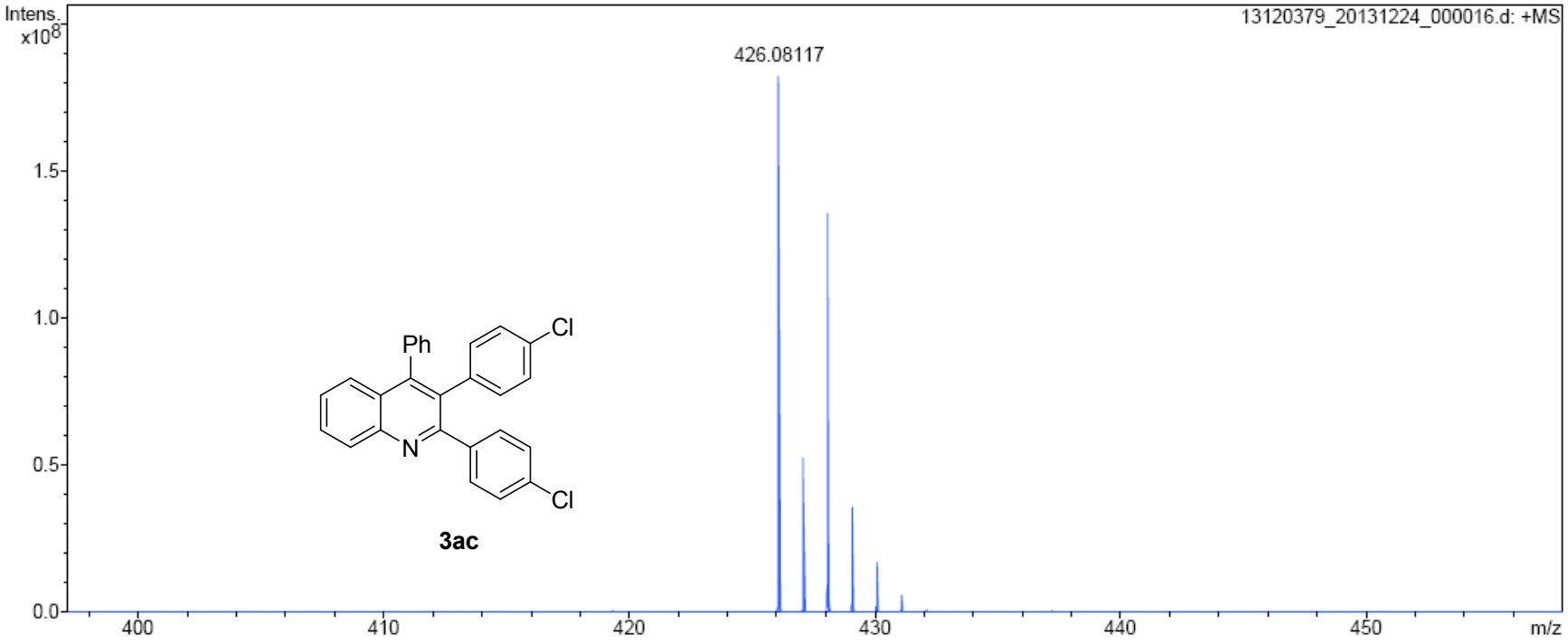

8.237
8.217
7.760
7.742
7.724
7.580
7.560
7.482
7.464
7.445
7.313
7.313
7.313
7.299
7.299
7.253
7.228
7.208
7.110
7.103
7.022
7.003
6.824
6.804
-0.001
Ph
Cl
N
Cl
3ac
5.02
1.97
2.00
1.04
1.07
2.06
1.00
2.01
1.00
10
8
6
4
2
0
PPM


157.419
148.140
147.439
139.366
136.664
136.481
134.053
132.697
132.597
131.487
131.327
130.173
129.819
129.694
128.142
128.088
127.926
127.644
126.991
126.699
126.643
77.377
77.068
76.744
Ph
Cl
N
Cl
3ac
200
150
100
50
0
PPM

Peking University Mass Spectrometry Sample Analysis Report

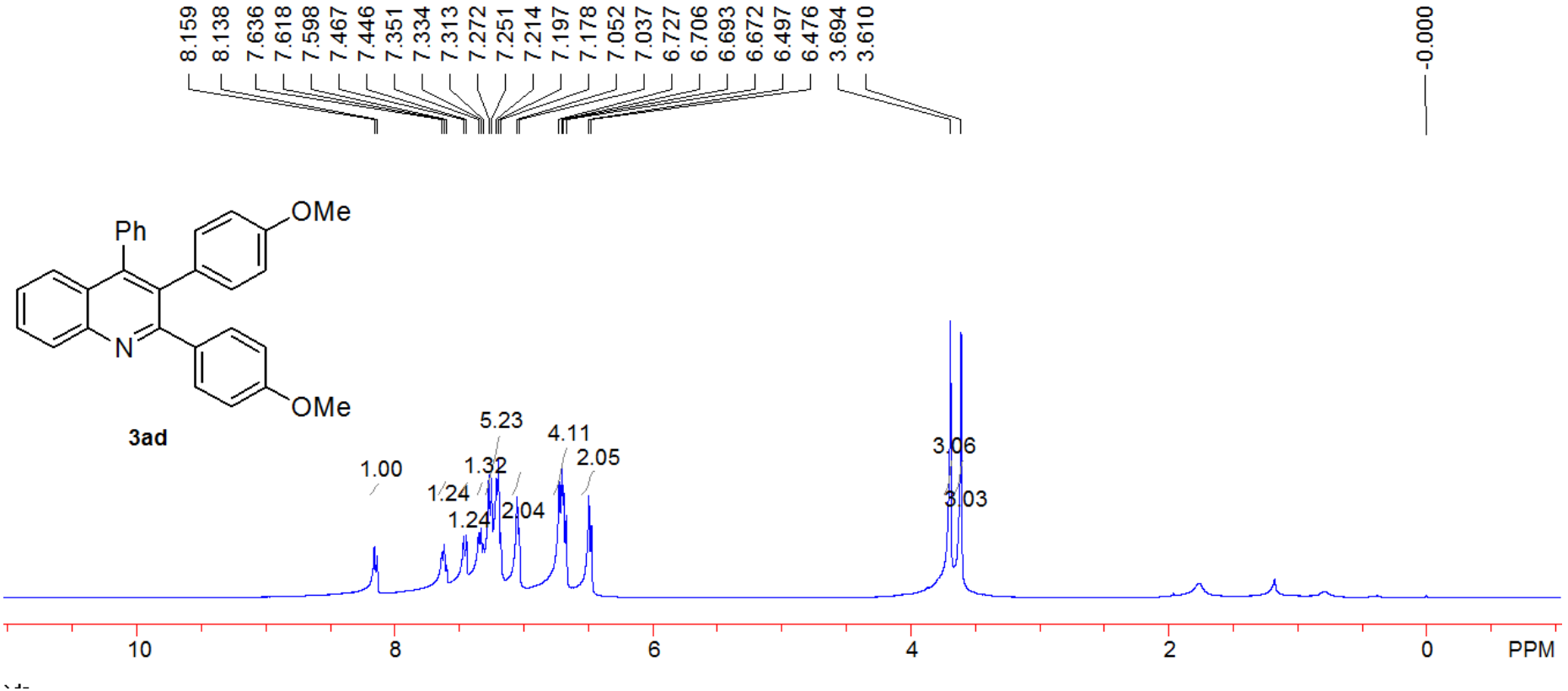
Analysis Info

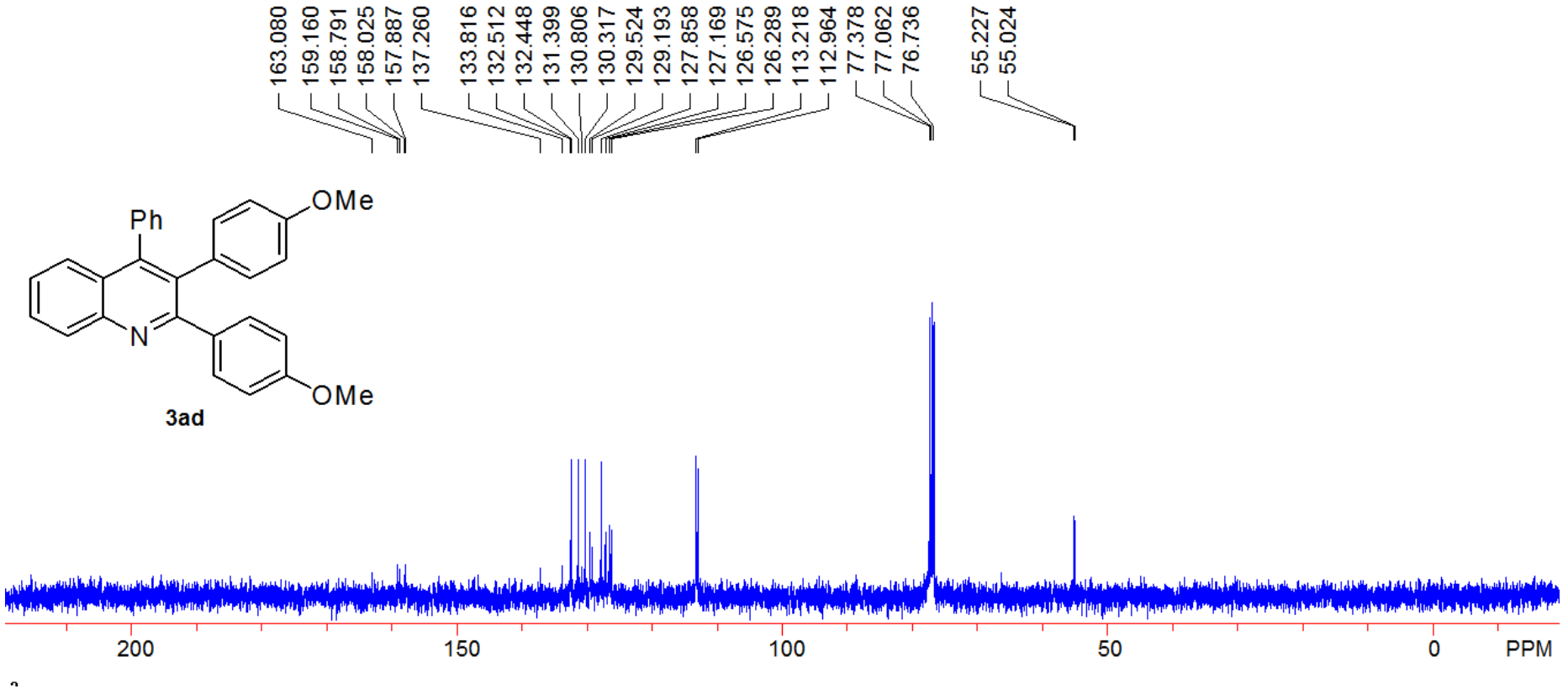
Analysis Name	13120379_20131224_000016.d	Acquisition Date	12/24/2013 11:43:03 AM
Sample	M	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



3ac

Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
426.08117	186053712	C 27 H 18 Cl 2 N	426.08108	-0.1	-0.2	23.4	18.5	even	ok

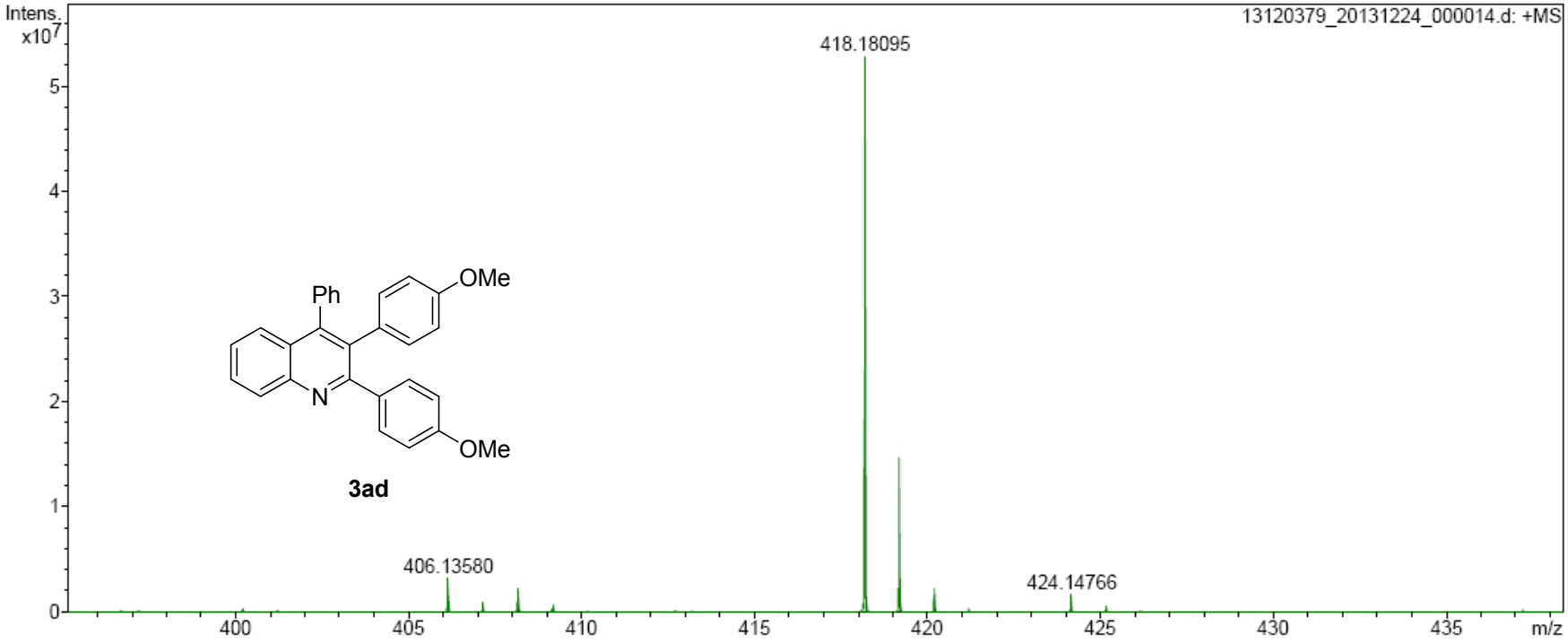

8.159
8.138
7.636
7.618
7.598
7.467
7.446
7.351
7.334
7.313
7.272
7.251
7.214
7.197
7.178
7.052
7.037
6.727
6.706
6.693
6.672
6.497
6.476
3.694
3.610
-0.000
Ph
OMe
N
OMe
3ad
1.00
1.24
1.32
1.24
5.23
2.04
4.11
2.05
3.06
3.03
10
8
6
4
2
0
PPM


163.080
159.160
158.791
158.025
157.887
137.260
133.816
132.512
132.448
131.399
130.806
130.317
129.524
129.193
127.858
127.169
126.575
126.289
113.218
112.964
77.378
77.062
76.736
55.227
55.024
Ph
OMe
N
OMe
3ad
200
150
100
50
0
PPM

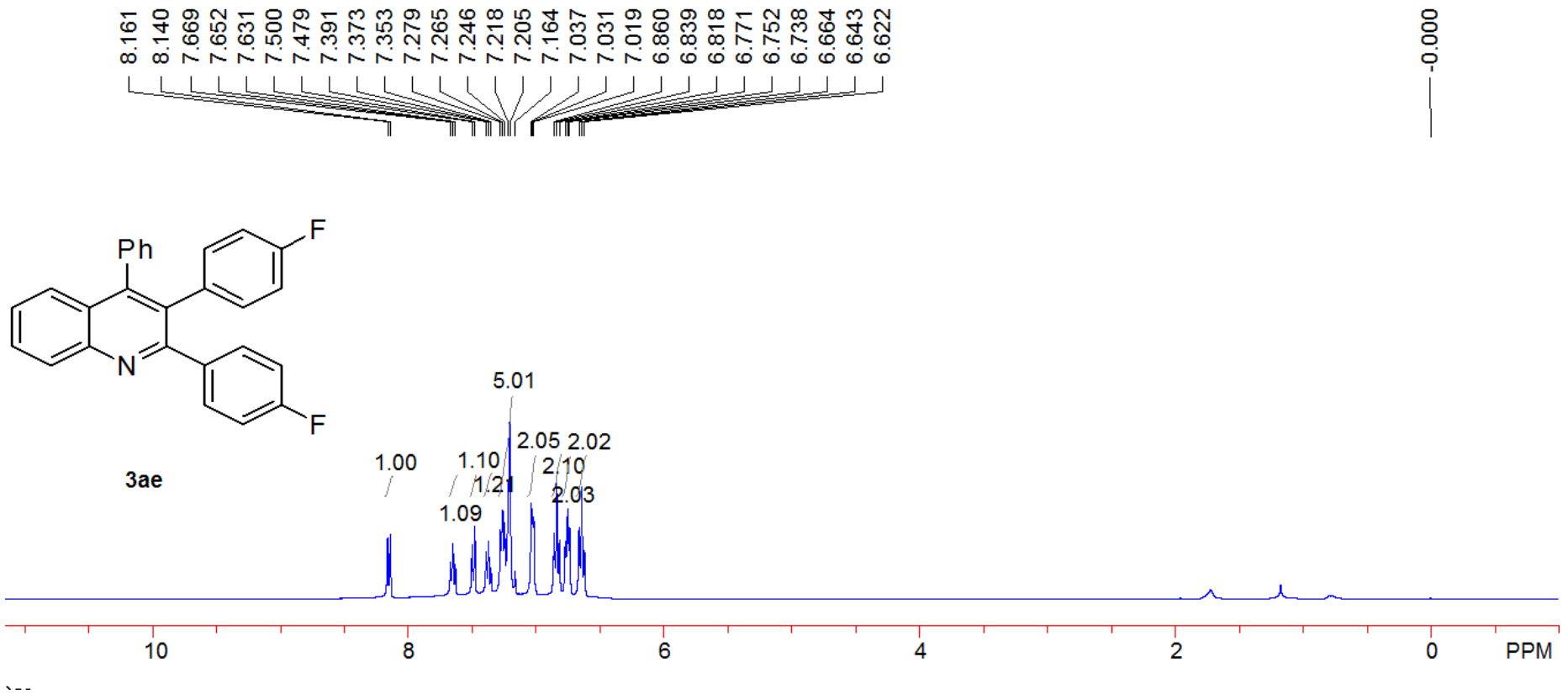
Peking University Mass Spectrometry Sample Analysis Report

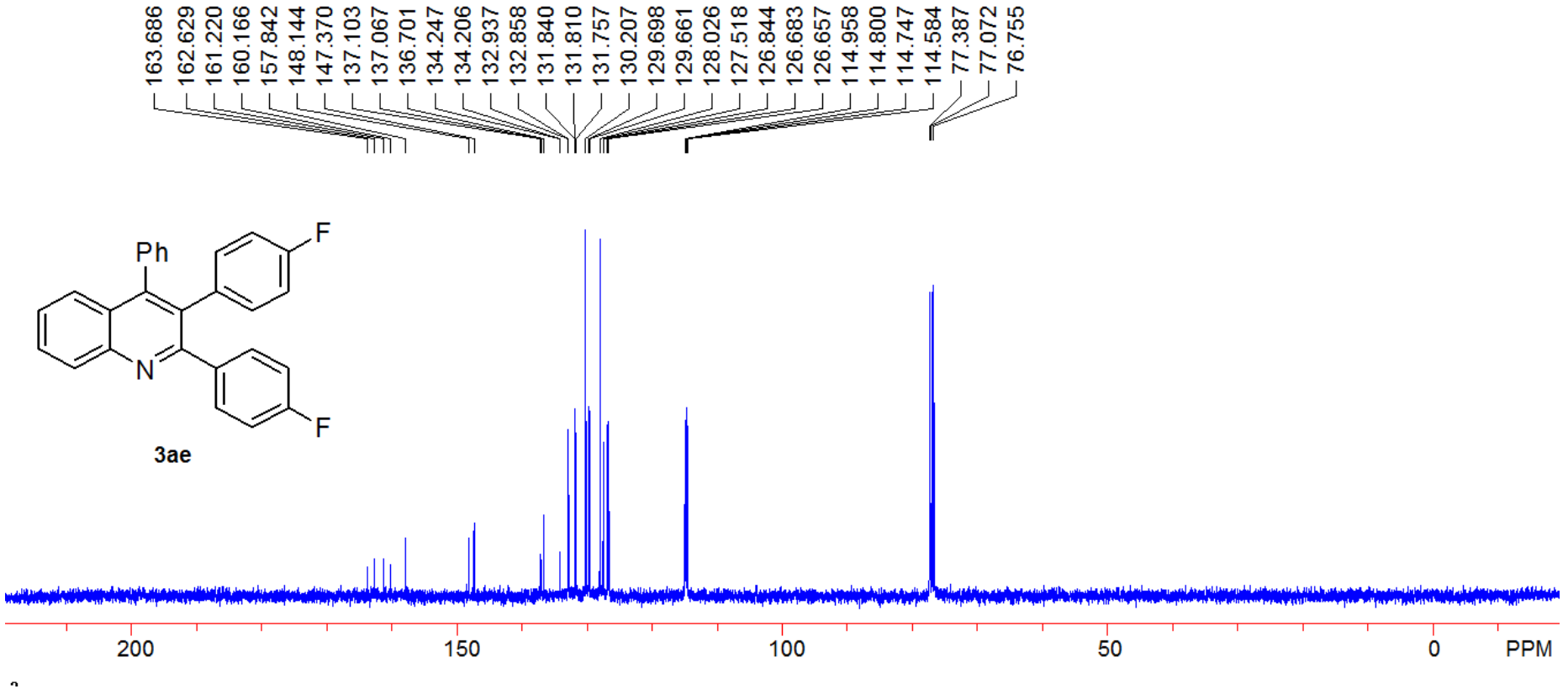
Analysis Info

Analysis Name	13120379_20131224_000014.d	Acquisition Date	12/24/2013 11:40:41 AM
Sample	K	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
418.18095	52998176	C 29 H 24 N O 2	418.18016	-0.8	-1.9	19.7	18.5	even	ok

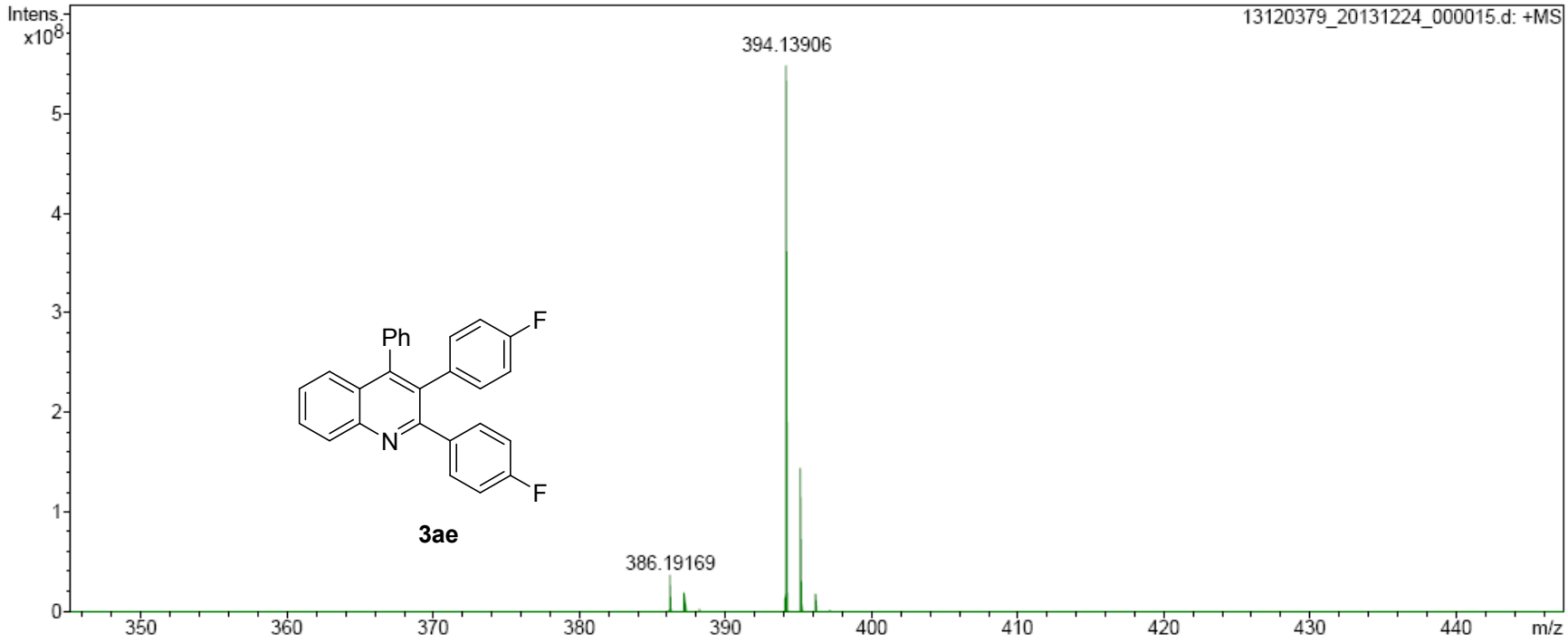

8.161
8.140
7.669
7.652
7.631
7.500
7.479
7.391
7.373
7.353
7.279
7.265
7.246
7.218
7.205
7.164
7.037
7.031
7.019
6.860
6.839
6.818
6.771
6.752
6.738
6.664
6.643
6.622
-0.000
Ph
F
N
F
3ae
1.00
1.10
1.09
1.21
5.01
2.05
2.02
2.10
2.03
10
8
6
4
2
0
PPM


163.686
162.629
161.220
160.166
157.842
148.144
147.370
137.103
137.067
136.701
134.247
134.206
132.937
132.858
131.840
131.810
131.757
130.207
129.698
129.661
128.026
127.518
126.844
126.683
126.657
114.958
114.800
114.747
114.584
77.387
77.072
76.755
Ph
F
N
F
3ae
200
150
100
50
0
PPM

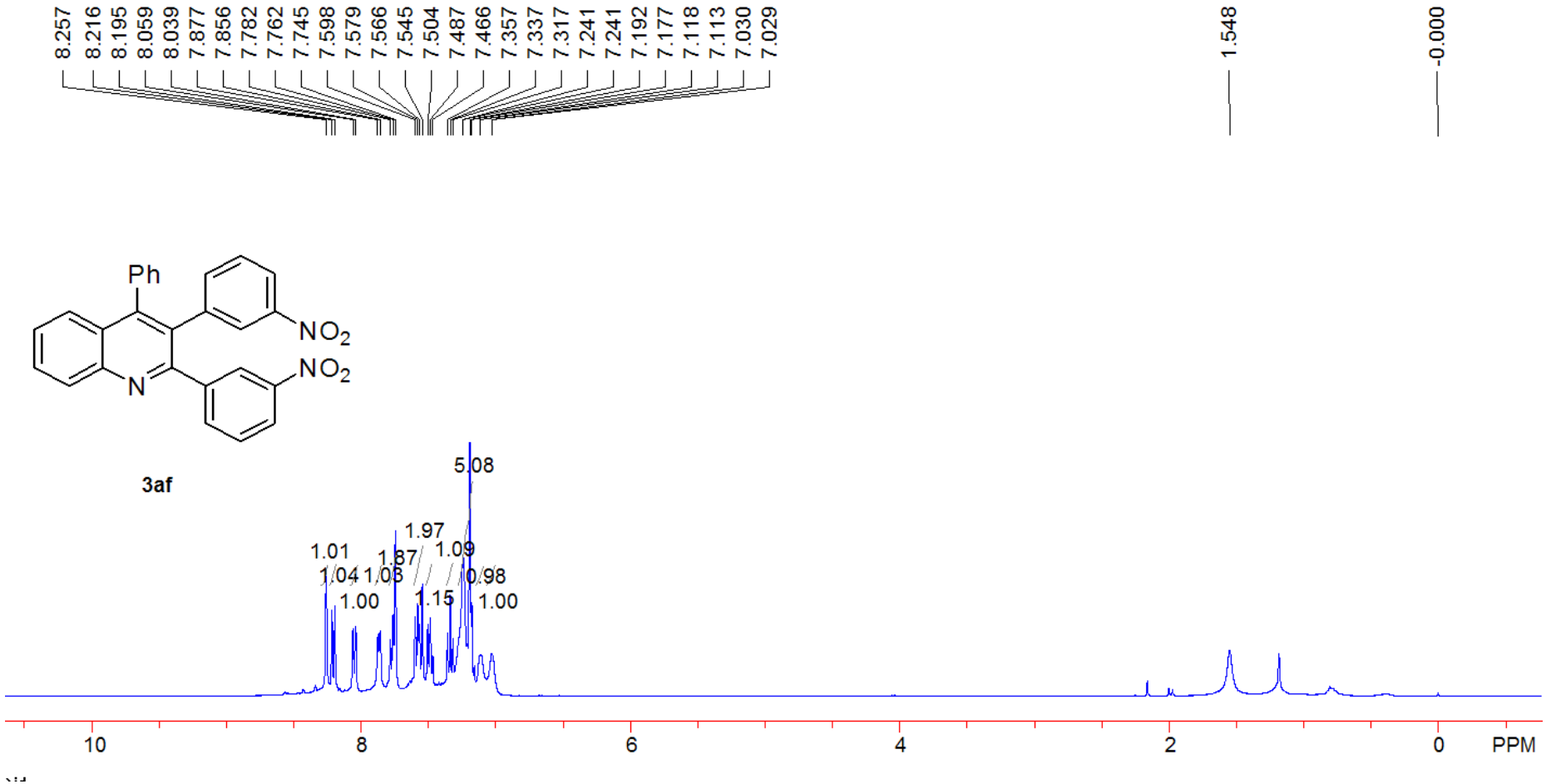
Peking University Mass Spectrometry Sample Analysis Report

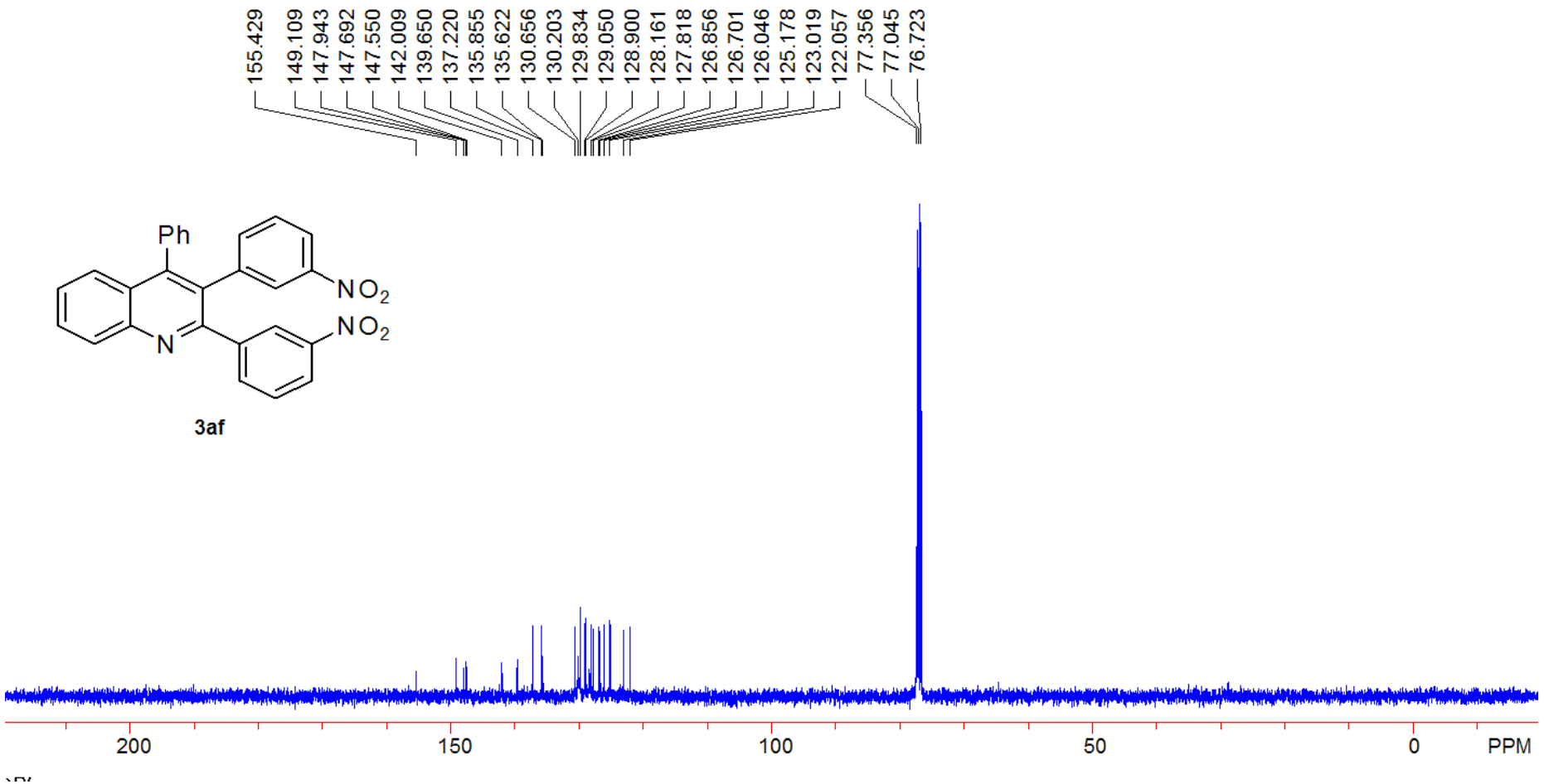
Analysis Info

Analysis Name	13120379_20131224_000015.d	Acquisition Date	12/24/2013 11:42:00 AM
Sample	L	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
394.13906	557029376	C 27 H 18 F 2 N	394.14018	1.1	2.8	18.1	18.5	even	ok


8.257
8.216
8.195
8.059
8.039
7.877
7.856
7.782
7.762
7.745
7.598
7.579
7.566
7.545
7.504
7.487
7.466
7.357
7.337
7.317
7.241
7.241
7.192
7.177
7.118
7.113
7.030
7.029
1.548
-0.000
Ph
NO2
NO2
N
3af
5.08
1.97
1.09
1.01
1.04
1.03
1.87
0.98
1.00
1.15
1.00
10
8
6
4
2
0
PPM

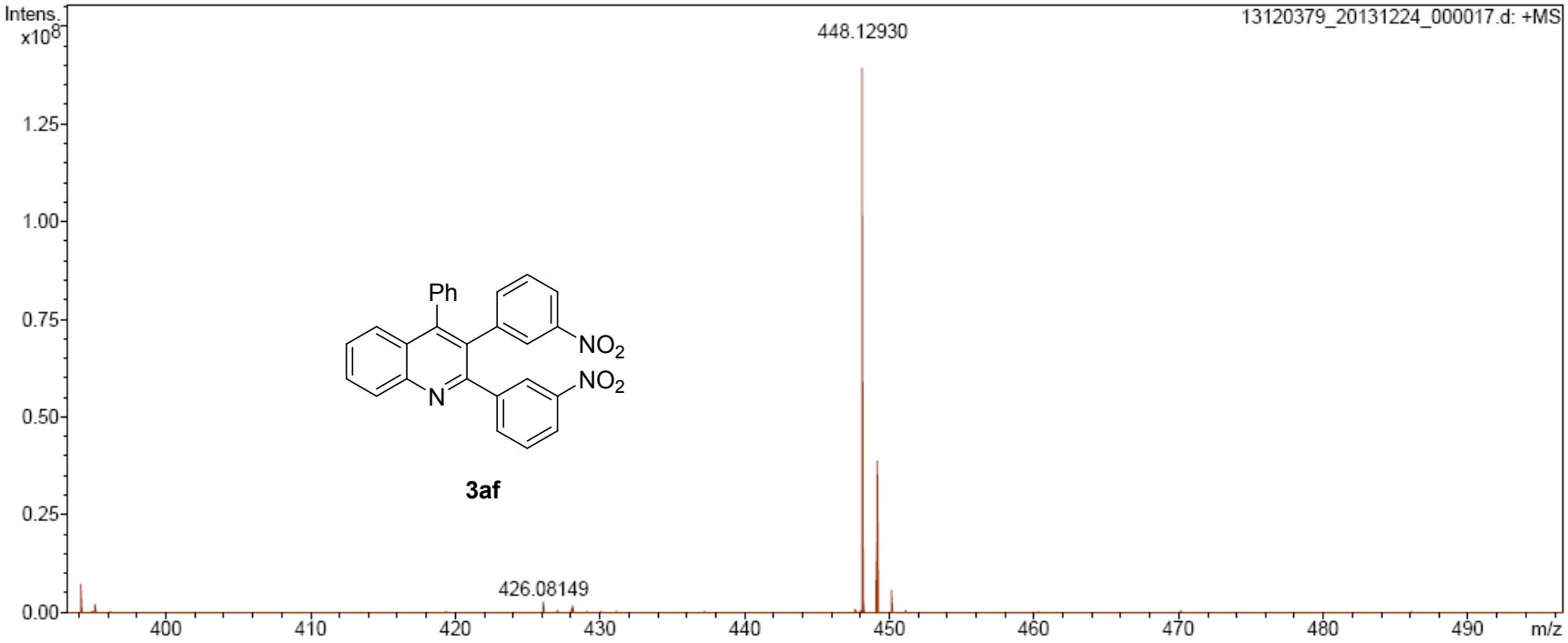

155.429
149.109
147.943
147.692
147.550
142.009
139.650
137.220
135.855
135.622
130.656
130.203
129.834
129.050
128.900
128.161
127.818
126.856
126.701
126.046
125.178
123.019
122.057
77.356
77.045
76.723
Ph
NO2
NO2
N
200
150
100
50
0
PPM

3af

Peking University Mass Spectrometry Sample Analysis Report

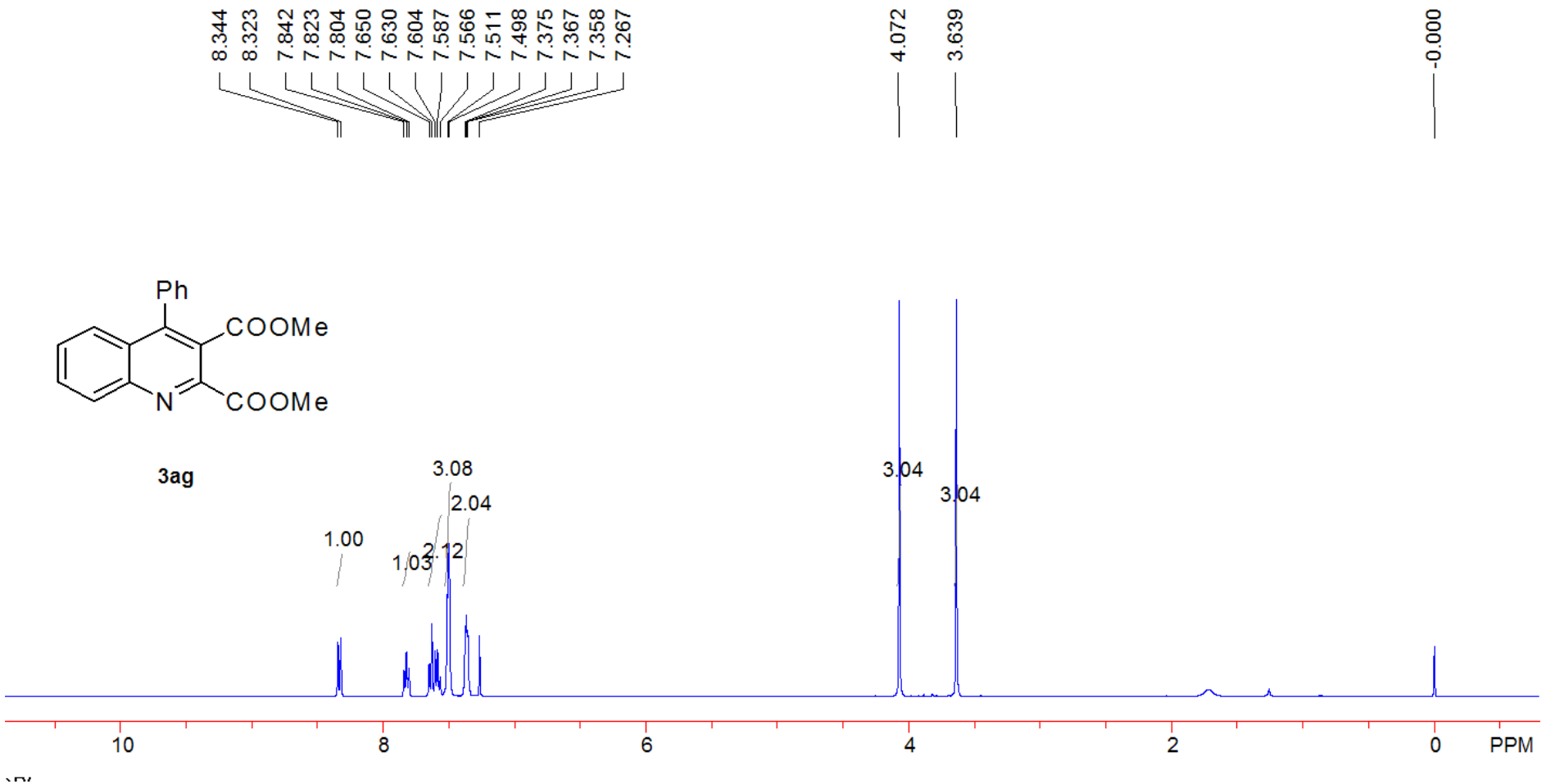
Analysis Info

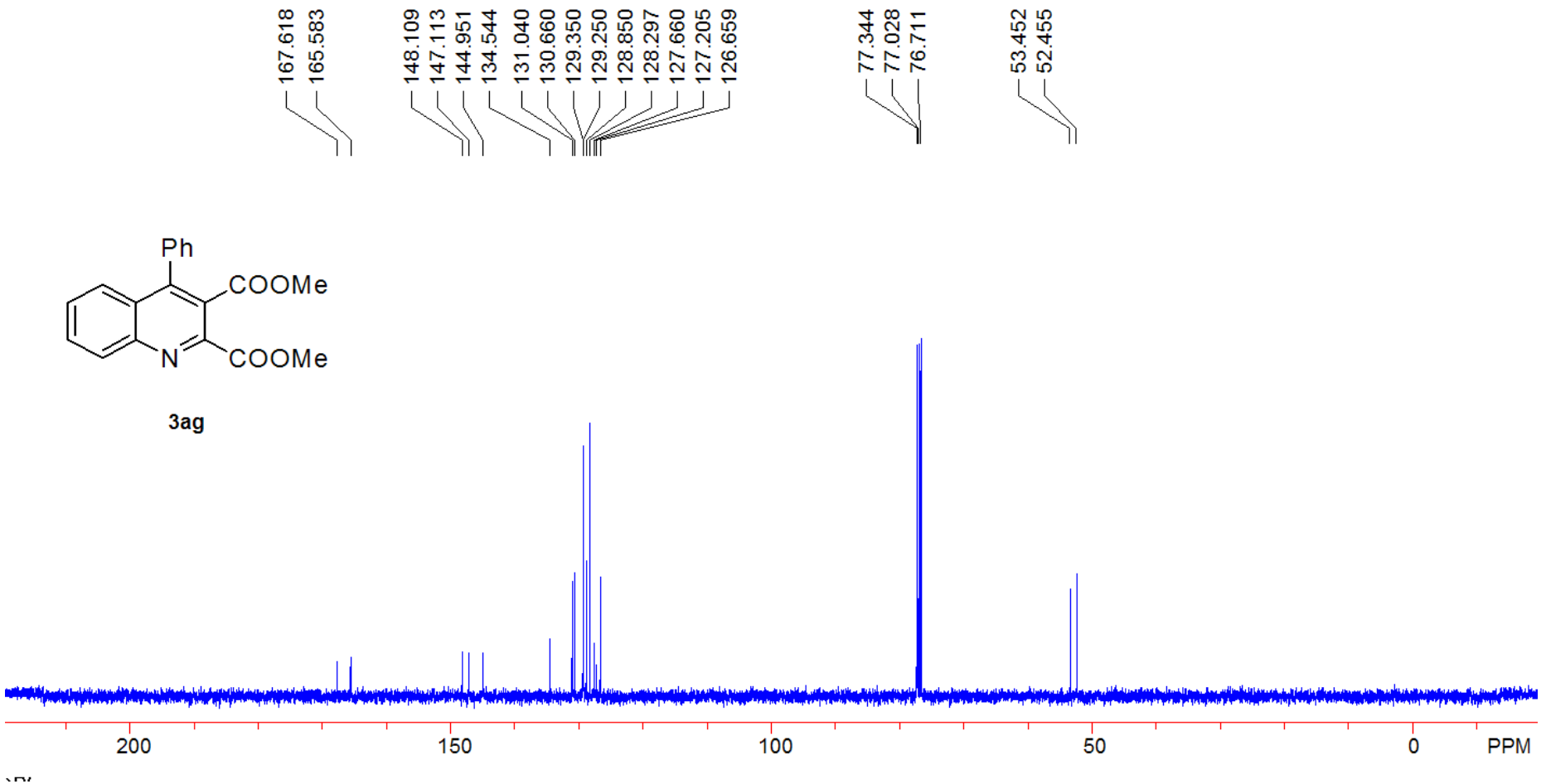
Analysis Name	13120379_20131224_000017.d	Acquisition Date	12/24/2013 11:44:12 AM
Sample	N	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University

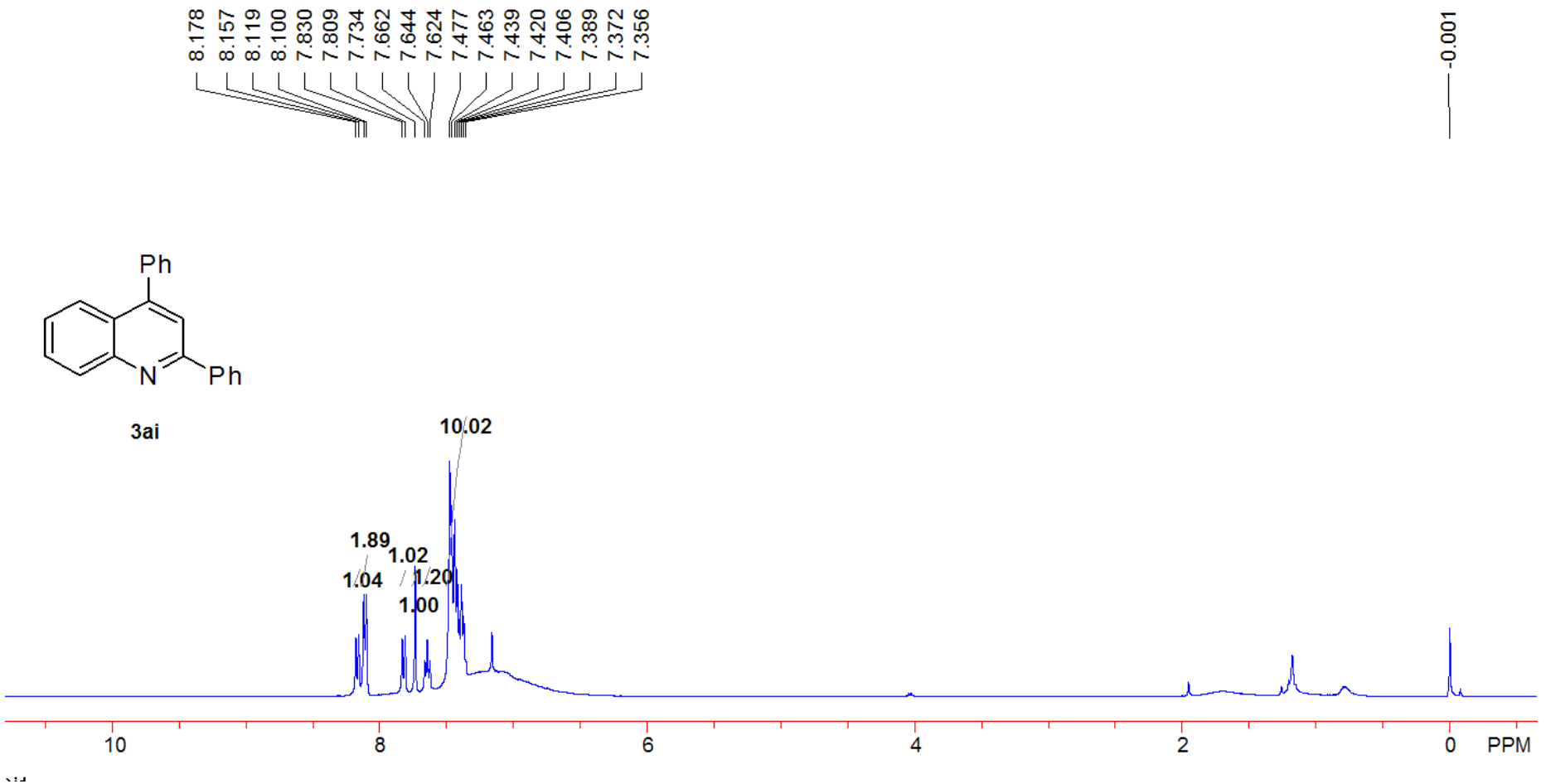


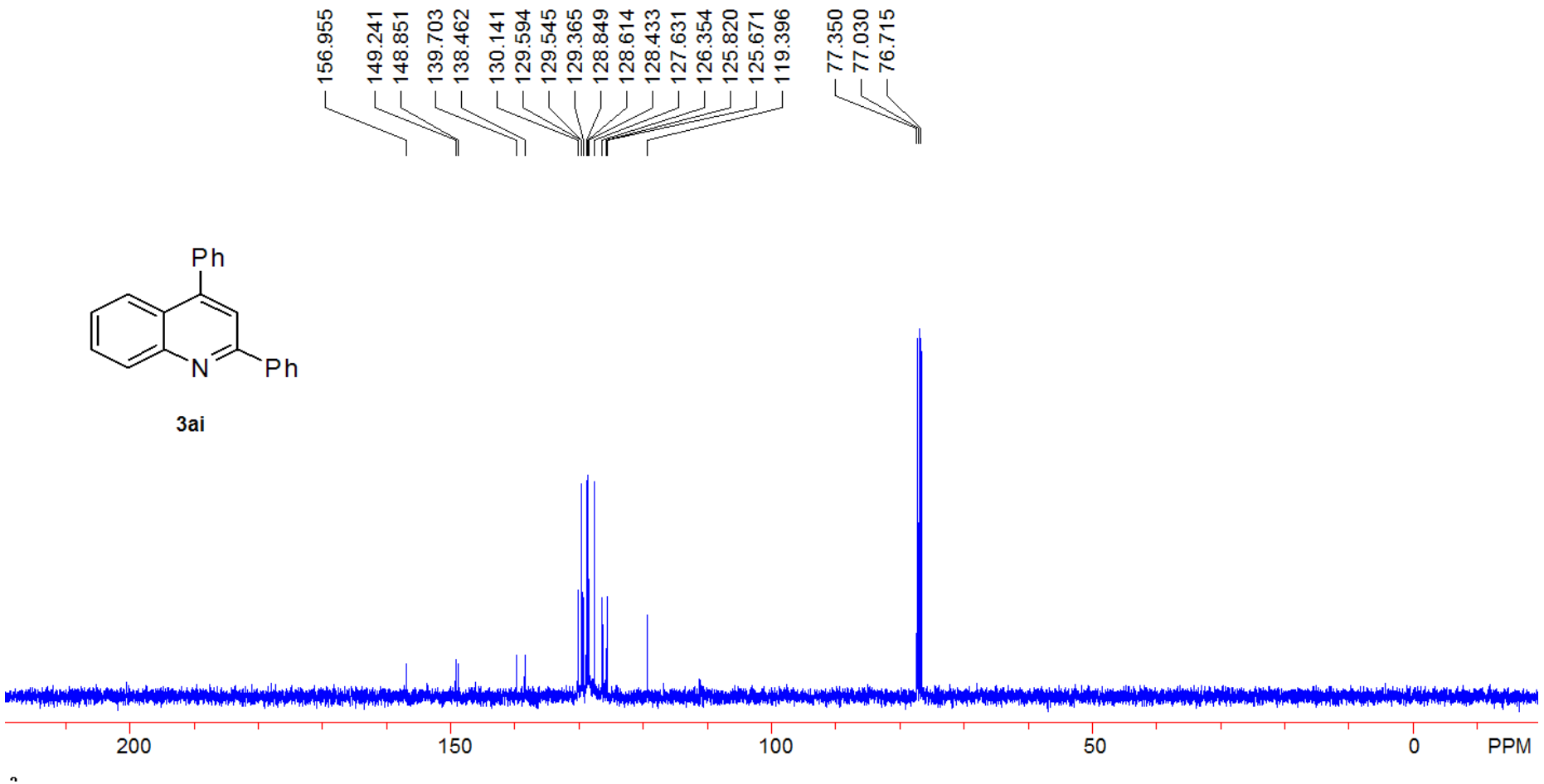
3af

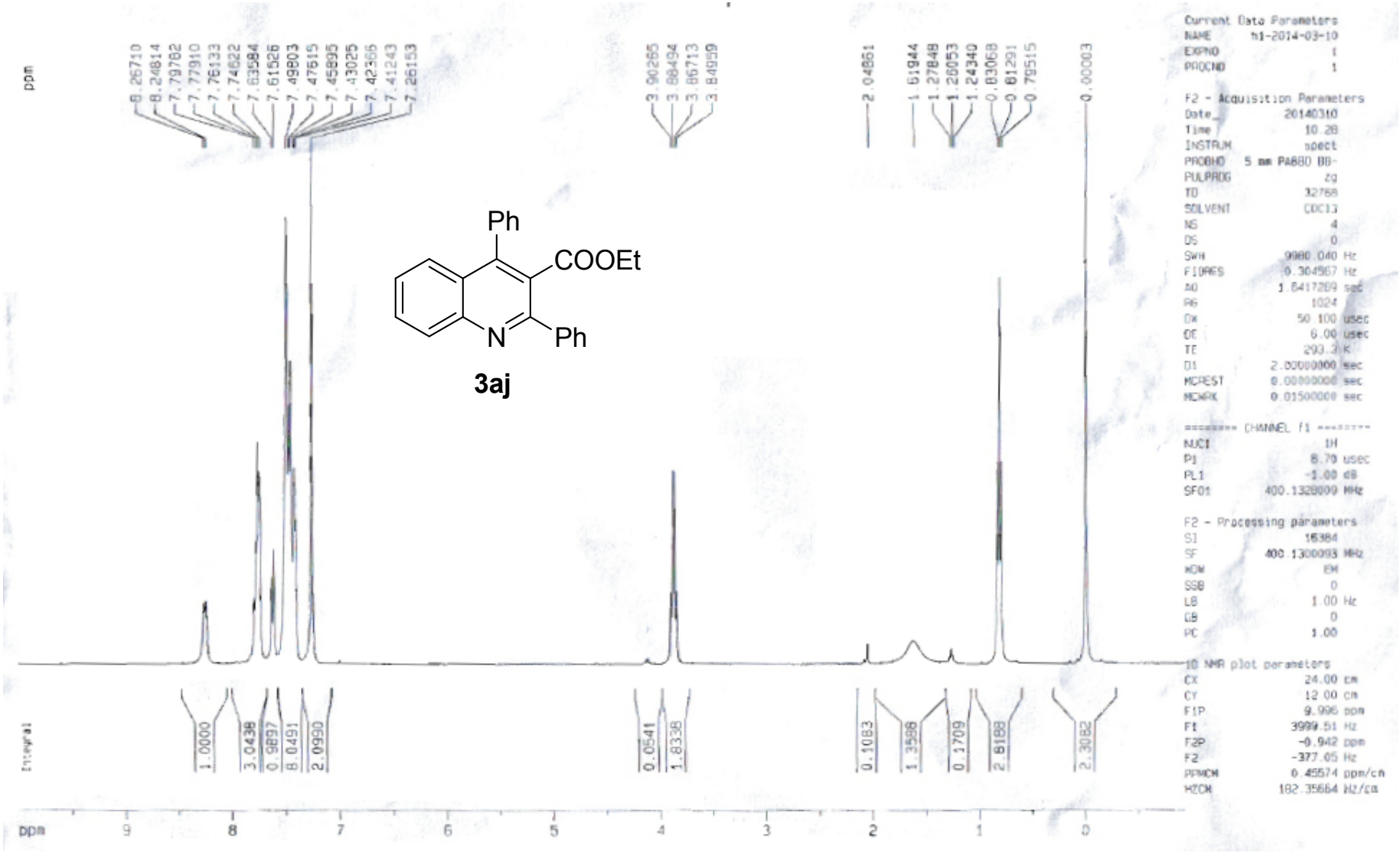
Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
448.12930	145751232	C 27 H 18 N 3 O 4	448.12918	-0.1	-0.3	15.4	20.5	even	ok

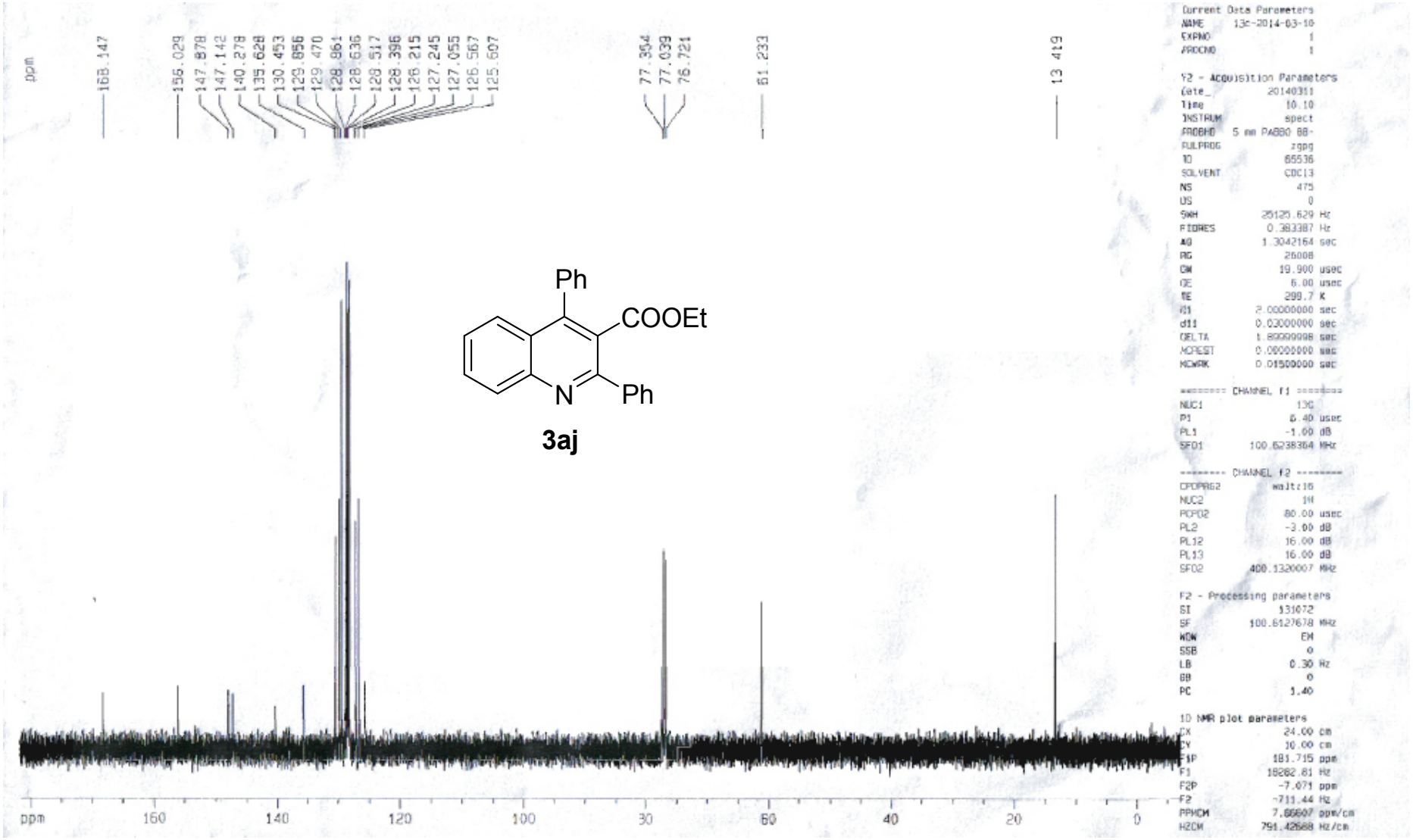

8.344
8.323
7.842
7.823
7.804
7.650
7.630
7.604
7.587
7.566
7.511
7.498
7.375
7.367
7.358
7.267
4.072
3.639
-0.000
Ph
COOMe
COOMe
N
3ag
3.08
2.04
1.00
1.03
2.12
3.04
3.04
10
8
6
4
2
0
PPM


167.618
165.583
148.109
147.113
144.951
134.544
131.040
130.660
129.350
129.250
128.850
128.297
127.660
127.205
126.659
77.344
77.028
76.711
53.452
52.455
Ph
COOMe
COOMe
N
3ag
200
150
100
50
0
PPM


8.178
8.157
8.119
8.100
7.830
7.809
7.734
7.662
7.644
7.624
7.477
7.463
7.439
7.420
7.406
7.389
7.372
7.356
-0.001
Ph
N
Ph
3ai
10.02
1.89
1.02
1.04
1.20
1.00
10
8
6
4
2
0
PPM


156.955
149.241
148.851
139.703
138.462
130.141
129.594
129.545
129.365
128.849
128.614
128.433
127.631
126.354
125.820
125.671
119.396
77.350
77.030
76.715
Ph
N
Ph
3ai
200
150
100
50
0
PPM


8.26710
8.24814
7.79782
7.77910
7.76133
7.74622
7.63584
7.61526
7.49803
7.47615
7.45895
7.43025
7.42366
7.41243
7.26153
3.90265
3.88494
3.86713
3.84959
2.04861
1.61944
1.27848
1.26053
1.24340
0.83068
0.81291
0.79515
0.00003
Ph
COOEt
N
Ph
3aj
1.0000
3.0438
0.9897
8.0491
2.0990
0.0541
1.8338
0.1083
1.3586
0.1709
2.8188
2.3082
ppm
Integral
Current Data Parameters
NAME h1-2014-03-10
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140310
Time 10.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 9000.040 Hz
FIDRES 0.304567 Hz
AQ 1.8417289 sec
RG 1024
DW 50.100 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -1.00 dB
SF01 400.1320009 MHz
F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 24.00 cm
CY 12.00 cm
F1P 9.996 ppm
F1 3999.51 Hz
F2P -0.942 ppm
F2 -377.05 Hz
PPMCM 0.45574 ppm/cm
HZCM 182.35664 Hz/cm


ppm
168.147
156.029
147.878
147.142
140.278
135.628
130.453
129.856
129.470
128.961
128.636
128.517
128.396
126.215
127.245
127.055
126.567
125.607
77.364
77.039
76.721
61.233
13.419
Ph
COOEt
N
Ph
3aj
ppm
160
140
120
100
30
60
40
20
0
Current Data Parameters
NAME 13c-2014-03-10
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140311
Time 10.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 475
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 26008
DW 19.900 usec
DE 6.00 usec
TE 299.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 6.40 usec
PL1 -1.00 dB
SFO1 100.6238364 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
PL13 16.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 131072
SF 100.6127678 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 10.00 cm
F1P 181.715 ppm
F1 18282.81 Hz
F2P -7.071 ppm
F2 -711.44 Hz
PPMCM 7.66607 ppm/cm
HZCM 791.42688 Hz/cm