

# Construction of All-Substituted Pyrrolidine Derivative with Multiple Stereogenic Centers and Betti-Base-derived $\gamma$ -Amino Alcohols by [1,2]-Wittig Rearrangement

Cai-Yun Wang<sup>a</sup>, Cheng Dong<sup>a</sup>, Zhan-Jiang Zheng<sup>\*a</sup>, Zheng Xu<sup>a</sup>, Ke-Fang Yang<sup>a</sup>, Li-Wen Xu<sup>\*a,b</sup>

<sup>a</sup> Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education (MOE), Hangzhou Normal University, Hangzhou 311121; Tel: +86-571-28867756; E-mail: liwenxu@hznu.edu.cn

<sup>b</sup> State Key Laboratory for Oxo Synthesis and Selective Oxidation Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou, P. R. China; E-mail: licpxulw@yahoo.com

## Supporting Information

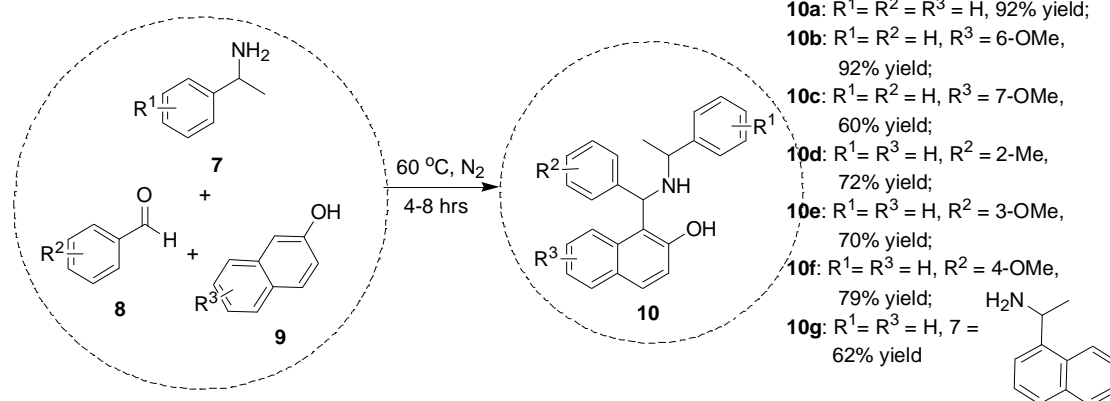
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## 1. General Information

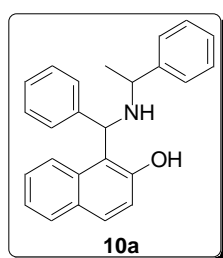
DCM was dried by  $\text{CaH}_2$ , distilled under Atmospheric pressure and stored under nitrogen. THF and  $\text{Et}_2\text{O}$  were dried by sodium benzophenone ketyl, distilled under Atmospheric pressure and stored under nitrogen. Reagents were purchased from commercial sources and were used as received unless mentioned otherwise. Reactions were monitored by thin layer chromatography using silica gel. All the reactions dealing with air or moisture sensitive compounds were carried out in a dry reaction vessel under positive pressure of argon. Air- and moisture-sensitive liquids and solutions were transferred via a syringe or a stainless steel cannula. NMR spectra were recorded on a Bruke Avance operating for  $^1\text{H}$  NMR at 400 MHz,  $^{13}\text{C}$  NMR at 100 MHz, and  $^{19}\text{F}$  NMR at 470 MHz, using TMS as internal standard. The peaks were internally referenced to TMS (0.00 ppm) or residual undeuterated solvent signal (77.16 ppm for  $^{13}\text{C}$  NMR). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet, b = broad. Mass spectroscopy data of the products were collected on an HRMS-TOF instrument or a low-resolution MS instrument using EI ionization.

## 2. Synthesis of various Betti base 10 under the classic reaction conditions.



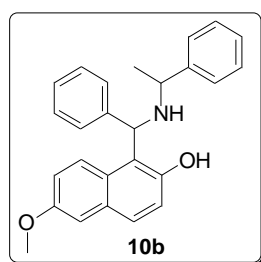
**General procedure for the synthesis of aminoalkynaphthol 10 (Betti base).** In the following typical procedure, a mixture of 2-naphthol (0.72 g, 5.0 mmol),

benzaldehyde (0.64g, 6.00 mmol), and 1-phenylethylamine (0.64 g, 5.25mmol) was stirred at 60 °C for 8 h under nitrogen atmosphere. Following the progress of the reaction by TLC and <sup>1</sup>H NMR, The reaction mixture was dispersed at room temperature with EtOH (5 mL). The white crystals separated were collected and washed with EtOH. The crystalline white residue, purified by crystallization from EtOAc/hexane, gives the pure **10**.



**1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-ol (10a):**

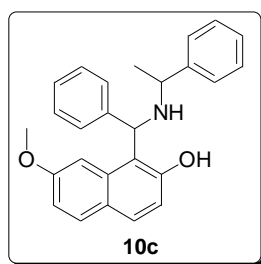
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.76-7.72 (m, 2H), 7.38 (t, *J* = 7.1 Hz, 4H), 7.30 – 7.12 (m, 10H), 5.49 (s, 1H), 3.91 (q, *J* = 6.4 Hz, 1H), 2.31 (s, 1H), 1.50 (d, *J* = 6.8 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.4, 143.2, 141.6, 129.8, 129.2, 129.1, 128.9, 128.1, 128.0, 127.8, 126.8, 122.5, 121.2, 120.2, 113.2, 60.4, 56.7, 23.1. IR (KBr) (ν<sub>max</sub>/ cm<sup>-1</sup>): 3273, 3060, 2963, 1622, 1452, 1239, 818, 744, 671. HRMS (EI) calcd. for C<sub>25</sub>H<sub>24</sub>NO [M+H]<sup>+</sup>, 354.1858, found 354.1840. Isolated yield: 92 %.



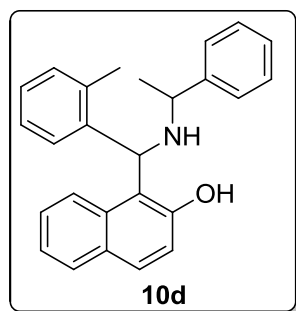
**6-methoxy-1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-ol (10b):**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 13.43 (s, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.34 – 7.16 (m, 10H), 7.09 (s, 1H), 6.93 (d, *J* = 9.2 Hz, 1H), 5.42 (s, 1H), 3.89 (d, *J* = 7.0 Hz, 1H), 3.86 (s, 3H), 2.28 (d, *J* = 9.8 Hz, 1H), 1.51 (d, *J* = 6.7 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 155.2, 148.3, 141.7, 129.7, 129.2, 129.1, 128.6, 128.1, 128.0, 127.8, 126.8, 122.8, 120.6, 118.7, 113.7, 107.4, 60.5, 56.7, 55.4, 23.1. IR (KBr) (ν<sub>max</sub>/ cm<sup>-1</sup>): 3423, 3312, 3021, 2959, 1606, 1519, 1493, 1385,

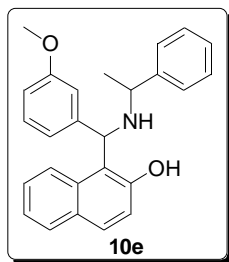
1242, 1100, 864, 700. **HRMS** (EI) calcd. for  $C_{26}H_{26}NO$   $[M+H]^+$ , 384.1964, found 384.1944. Isolated yield: 56 %.



**7-methoxy-1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-ol (10c):**  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  13.68 (s, 1H), 7.69-7.63 (m, 2H), 7.44-7.37 (m, 3H), 7.26-7.20 (m, 7H), 7.10 (d,  $J = 8.8$  Hz, 1H), 6.91 (d,  $J = 8.8$  Hz, 1H), 6.68 (s, 1H), 5.36 (s, 1H), 3.92 (q,  $J = 6.7$  Hz, 1H), 3.65 (s, 3H), 2.30 (s, 1H), 1.53 (d,  $J = 6.7$  Hz, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  158.2, 158.0, 143.3, 141.5, 130.3, 129.5, 129.2, 129.0, 128.1, 128.0, 127.7, 127.0, 124.1, 117.6, 114.2, 112.5, 101.0, 60.5, 56.7, 55.0, 22.9. **IR** (KBr) ( $\nu_{max}/cm^{-1}$ ): 3424, 3298, 3057, 3008, 1620, 1475, 1225, 835, 699. **HRMS** (EI) calcd. for  $C_{26}H_{26}NO$   $[M+H]^+$ , 384.1964, found 384.1962. Isolated yield: 60 %.

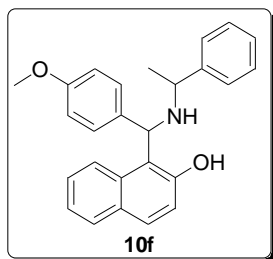


**1-(((1-phenylethyl)amino)(o-tolyl)methyl)naphthalen-2-ol (10d):**  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  13.77 (s, 1H), 7.74 (t,  $J = 8.8$  Hz, 2H), 7.41 – 6.93 (m, 14H), 5.67 (s, 1H), 3.88 (s, 1H), 1.92 (s, 3H), 1.52 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  157.9, 142.5, 138.8, 135.0, 132.7, 131.0, 129.8, 129.1, 129.0, 128.93, 128.88, 128.2, 128.1, 127.3, 127.0, 126.7, 122.6, 120.9, 120.2, 113.9, 56.9, 56.8, 21.7, 18.3. **IR** (KBr) ( $\nu_{max}/cm^{-1}$ ): 3412, 3279, 3062, 2964, 1956, 1623, 1470, 1239, 745, 720. **HRMS** (EI) calcd. for  $C_{26}H_{26}NO$   $[M+H]^+$ , 368.2014, found 368.2000. Isolated yield: 72 %.



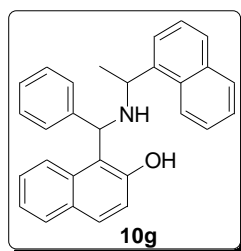
**1-((3-methoxyphenyl)((1-phenylethyl)amino)methyl)naphthalen**

**-2-ol (10e):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  13.56 (s, 1H), 7.76 (d,  $J = 8.7$  Hz, 2H), 7.42-7.36 (m, 4H), 7.27-7.22 (m, 5H), 7.17 (t,  $J = 7.8$  Hz, 1H), 6.82-6.74 (m, 3H), 5.46 (s, 1H), 3.92 (q,  $J = 6.6$  Hz, 1H), 3.71 (s, 3H), 1.53 (d,  $J = 6.6$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.1, 132.7, 130.2, 130.0, 129.1, 128.9, 128.8, 128.2, 127.0, 126.6, 122.6, 121.2, 120.1, 113.8, 113.3, 60.4, 57.0, 55.3, 22.9. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3427, 3290, 3059, 2965, 1601, 1456, 1264, 1096, 819. **HRMS** (EI) calcd. for  $\text{C}_{26}\text{H}_{26}\text{NO}$   $[\text{M}+\text{H}]^+$ , 384.1964, found 384.1953, **HRMS** (EI) calcd. for  $\text{C}_{26}\text{H}_{25}\text{NONa}$   $[\text{M}+\text{Na}]^+$ , 406.1783, found 406.1767. Isolated yield: 70 %.



**1-((4-methoxyphenyl)((1-phenylethyl)amino)methyl)naphtha**

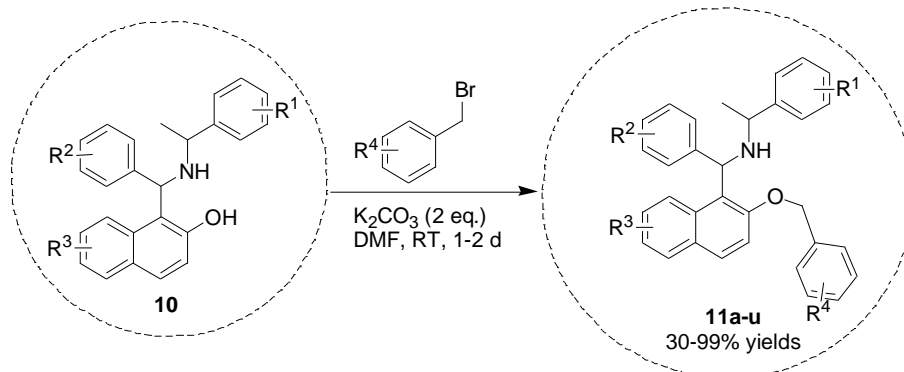
**len-2-ol (10f):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  13.43 (s, 1H), 7.73 (d,  $J = 8.5$  Hz, 2H), 7.42 – 7.08 (m, 10H), 6.82 – 6.64 (m, 3H), 5.43 (s, 1H), 3.89 (q,  $J = 6.7$  Hz, 1H), 3.67 (s, 3H), 1.50 (d,  $J = 6.7$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.1, 157.2, 142.58, 130.2, 130.0, 129.1, 128.9, 128.2, 127.0, 126.6, 122.6, 121.2, 120.1, 113.8, 113.3, 112.8, 60.4, 56.9, 55.2, 22.9. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3422, 3309, 3023, 2996, 2360, 1600, 1457, 1417, 1264, 1164, 1038, 915, 816, 699. **HRMS** (EI) calcd. for  $\text{C}_{26}\text{H}_{26}\text{NO}$   $[\text{M}+\text{H}]^+$ , 384.1964, found 384.1942. Isolated yield: 79 %.



**1-(((1-(naphthalen-1-yl)ethyl)amino)(phenyl)methyl)naphthalen-2-ol (10g)**

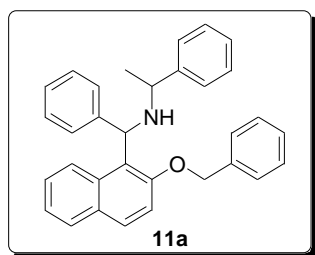
**n-2-ol (10g):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  13.94 (s, 1H), 7.82 (t,  $J = 6.8$  Hz, 2H), 7.71 (d,  $J = 8.9$  Hz, 1H), 7.68 – 7.42 (m, 4H), 7.35 (t,  $J = 7.3$  Hz, 1H), 7.29 – 7.04 (m, 9H), 6.98 (t,  $J = 7.6$  Hz, 1H), 5.47 (s, 1H), 4.84 (s, 1H), 2.55 (s, 1H), 1.56 (d,  $J = 6.3$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.3, 141.7, 129.9, 129.2, 128.7, 127.8, 126.4, 126.3, 125.9, 125.7, 122.4, 121.3, 120.2, 113.6, 61.3, 23.2. **IR** (KBr) ( $\nu_{\text{max}}$ / $\text{cm}^{-1}$ ): 3422, 3320, 3049, 2961, 2361, 1621, 1454, 1379, 1239, 1100, 780, 744. **HRMS** (EI) calcd. for  $\text{C}_{29}\text{H}_{26}\text{NO}$   $[\text{M}+\text{H}]^+$ , 404.2014, found 404.2011. Isolated yield: 62 %.

### 3. The synthesis of Betti base-derived benzyl ethers **11**.



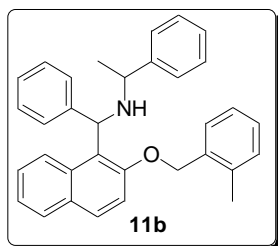
#### General procedure for the synthesis of 2-(benzyloxy)Aminoalkylnaphthalene **11**.

In the following typical procedure, a mixture of aminoalkylnaphthol **10** (Betti base), benzyl bromide (1.2 eq),  $\text{K}_2\text{CO}_3$  (2.0 eq) in *N,N*-dimethylformamide (DMF) at room temperature for 1-2 days, The reaction was quenched with water and resulted mixture was extracted with ethyl acetate, and washed with water and saturated NaCl solution. The organic layer was dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was purified by column chromatography (hexanes/ethylacetate = 5/1) to give **11** in varied yields (see Table 1).



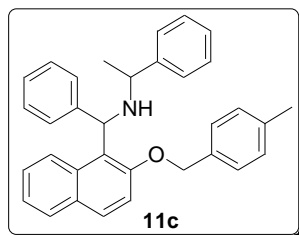
**N-((2-(benzyloxy)naphthalen-1-yl)(phenyl)methyl)-1-phen**

**ylethylamine (11a):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (s, 2H), 7.68 (s, 1H), 7.51 – 7.09 (m, 16H), 7.01 (s, 2H), 5.69 (s, 1H), 5.06 (d,  $J = 6.7$  Hz, 1H), 4.87 (d,  $J = 6.7$  Hz, 1H), 3.64 (s, 1H), 2.92 (s, 1H), 1.21 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.7, 146.4, 145.2, 137.0, 128.7, 128.6, 128.4, 127.9, 127.4, 127.3, 126.9, 123.7, 115.1, 55.8, 55.3, 26.0. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3427, 3348, 3054, 3026, 2967, 1621, 1574, 1492, 1237, 1066, 803, 696. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{30}\text{NO}$   $[\text{M}+\text{H}]^+$ , 444.2249, found 444.2348, **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{NONa}$   $[\text{M}+\text{Na}]^+$ , 466.2147, found 466.2165. Isolated yield: 85 %.

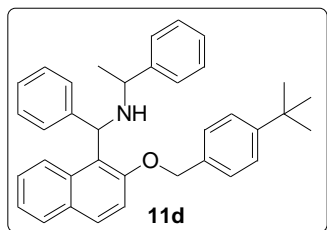


**N-((2-((2-methylbenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)**

**-1-phenylethylamine (11b):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 8.2$  Hz, 2H), 7.64 (s, 1H), 7.34-7.07 (m, 18H), 6.99 (d,  $J = 7.4$  Hz, 1H), 5.64 (s, 1H), 5.02 (d,  $J = 11.7$  Hz, 1H), 4.82 (d,  $J = 11.4$  Hz, 1H), 3.62 (d,  $J = 5.3$  Hz, 1H), 2.90 (s, 1H), 2.13 (s, 3H), 1.19 (d,  $J = 4.9$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.8, 136.1, 134.9, 128.7, 128.4, 128.2, 127.9, 127.3, 126.9, 126.1, 115.0, 69.5, 55.8, 55.3, 25.9, 18.7. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421.87, 3329.81, 2966.17, 1623.30, 1599.92, 1455.77, 1257.61, 1241.11, 1080.65, 741.43. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 458.2484, found 458.2473. Isolated yield: 65 %.

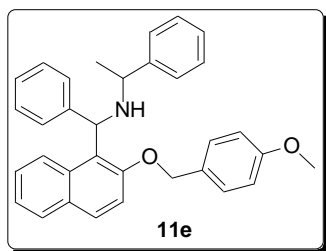


**N-((2-((4-methylbenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11c):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 – 7.70 (m, 2H), 7.64 (s, 1H), 7.40 (d,  $J = 7.0$  Hz, 2H), 7.34 – 7.09 (m, 12H), 7.04 (d,  $J = 7.5$  Hz, 2H), 6.86 (d,  $J = 7.4$  Hz, 2H), 5.64 (s, 1H), 5.00 (d,  $J = 11.5$  Hz, 1H), 4.79 (d,  $J = 11.4$  Hz, 1H), 3.62 (q,  $J = 6.3$  Hz, 1H), 2.97 (s, 1H), 2.30 (s, 3H), 1.19 (d,  $J = 6.2$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.7, 146.4, 145.2, 129.21, 129.16, 128.7, 128.4, 127.8, 127.5, 127.3, 127.0, 126.9, 126.5, 125.9, 123.6, 115.1, 71.0, 55.8, 55.3, 25.9, 21.3. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3422, 3334, 3056, 3016, 2921, 1595, 1511, 1492, 1234, 809, 700. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 458.2484, found 458.2484. Isolated yield: 85 %.



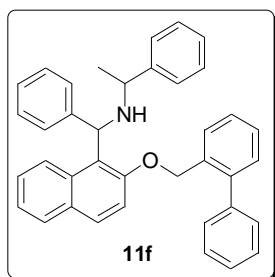
**N-((2-((4-(tert-butyl)benzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11d):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 (d,  $J = 8.6$  Hz, 2H), 7.65 (s, 1H), 7.46 – 7.10 (m, 15H), 6.96 (d,  $J = 7.7$  Hz, 2H), 5.65 (s, 1H), 5.04 (d,  $J = 11.6$  Hz, 1H), 4.83 (d,  $J = 11.6$  Hz, 1H), 3.62 (q,  $J = 6.2$  Hz, 1H), 2.90 (s, 1H), 1.31 (s, 9H), 1.19 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.8, 150.9, 146.4, 145.2, 134.0, 128.4, 127.9, 127.3, 127.2, 127.0, 125.5, 123.6, 115.2, 71.1, 55.9, 34.7, 31.57, 26.0. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 3362, 3024, 1622, 1513, 1252, 1070, 1015, 698. **HRMS** (EI) calcd. for  $\text{C}_{36}\text{H}_{37}\text{NONa}$   $[\text{M}+\text{Na}]^+$ , 522.2773, found 522.2784. Isolated yield: 99 %.





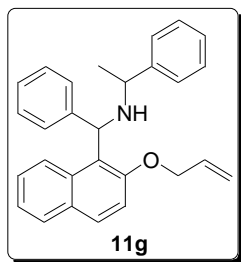
**N-((2-((4-methoxybenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11e):**

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 8.3$  Hz, 2H), 7.63 (s, 1H), 7.51 – 7.07 (m, 15H), 6.90 (d,  $J = 7.7$  Hz, 2H), 6.77 (d,  $J = 8.0$  Hz, 2H), 5.62 (s, 1H), 5.00 (d,  $J = 11.1$  Hz, 1H), 4.77 (d,  $J = 10.8$  Hz, 1H), 3.78 (s, 3H), 3.61 (q,  $J = 5.8$  Hz, 1H), 2.90 (s, 1H), 1.19 (d,  $J = 5.2$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.4, 154.7, 129.2, 129.0, 128.4, 127.9, 127.8, 127.4, 127.0, 126.6, 125.9, 123.6, 115.1, 113.9, 70.9, 55.8, 55.4, 25.9. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3423, 3337, 3057, 2999, 1618, 1513, 1246, 811, 702. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 474.2433, found 474.2449. Isolated yield: 80 %.

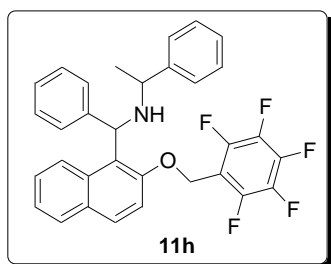


**N-((2-([1,1'-biphenyl]-2-ylmethoxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11f):**

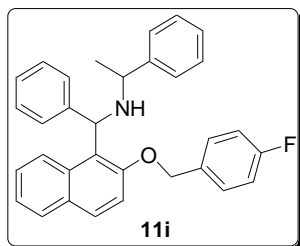
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (d,  $J = 7.8$  Hz, 1H), 7.72 (d,  $J = 9.0$  Hz, 1H), 7.62 (s, 1H), 7.44 – 7.10 (m, 21H), 7.08 (d,  $J = 8.9$  Hz, 1H), 6.95 (s, 1H), 5.65 (s, 1H), 5.00 (d,  $J = 10.8$  Hz, 1H), 4.73 (d,  $J = 9.0$  Hz, 1H), 3.62 (s, 1H), 2.98 (s, 1H), 1.22 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.5, 146.4, 145.2, 141.6, 140.5, 129.9, 129.3, 129.2, 128.7, 128.4, 127.9, 127.8, 127.4, 126.9, 123.6, 114.8, 69.0, 55.8, 55.2, 26.0. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3416, 3349, 3025, 2886, 1621, 1593, 1254, 1068, 1016, 770, 702. **HRMS** (EI) calcd. for  $\text{C}_{38}\text{H}_{34}\text{NO}$   $[\text{M}+\text{H}]^+$ , 520.2640, found 520.2636. Isolated yield: 90 %.



**N-((2-(allyloxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11g):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 (d,  $J = 8.1$  Hz, 2H), 7.62 (s, 1H), 7.41 (d,  $J = 5.1$  Hz, 2H), 7.37 – 7.04 (m, 11), 5.65 (d,  $J = 11.2$  Hz, 2H), 5.13 (t,  $J = 13.9$  Hz, 2H), 4.49 (s, 1H), 4.30 (s, 1H), 3.61 (s, 1H), 2.93 (s, 1H), 1.24 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.7, 133.3, 129.5, 129.2, 128.7, 128.4, 127.9, 127.4, 126.9, 126.6, 127.0, 123.7, 117.5, 115.3, 70.2, 55.9, 55.2, 25.9. **IR** (KBr) ( $\nu_{\text{max}}$ /  $\text{cm}^{-1}$ ): 3431, 3339, 3056, 2864, 2361, 1594, 1491, 1248, 805, 704. **HRMS** (EI) calcd. for  $\text{C}_{28}\text{H}_{28}\text{NO}$   $[\text{M}+\text{H}]^+$ , 394.2171, found 394.2169. Isolated yield: 99 %.

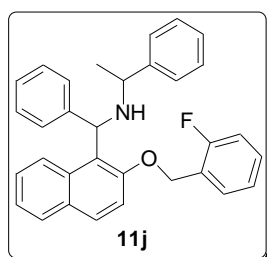


**N-((2-((perfluorophenyl)methoxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11h):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87-7.82 (m, 2H), 7.62 (d,  $J = 6.0$  Hz, 1H), 7.42 – 7.02 (m, 13H), 5.53 (s, 1H), 5.04 (d,  $J = 10.6$  Hz, 1H), 4.85 (d,  $J = 10.1$  Hz, 1H), 3.57 (q,  $J = 6.2$  Hz, 1H), 2.64 (s, 1H), 1.21 (d,  $J = 6.0$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.1, 146.7, 146.2, 145.1, 144.2, 138.7, 136.2, 133.7, 130.0, 129.6, 128.8, 128.3, 127.8, 127.2, 126.8, 126.4, 125.9, 124.2, 123.9, 115.1, 110.1, 100.1, 55.8, 55.8, 54.9, 25.9.  $^{19}\text{F NMR}$  (470 MHz,  $\text{CDCl}_3$ )  $\delta$  -142.07 (dd,  $J = 26.1, 5.9$  Hz, 2F), -153.00 (t,  $J = 23.0$  Hz, 1F), -160.33 – -162.08 (m, 2F). **IR** (KBr) ( $\nu_{\text{max}}$ /  $\text{cm}^{-1}$ ): 3423, 3368, 3064, 2957, 1595, 1512, 1256, 1131, 1023, 938, 618. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{24}\text{NOF}_5$   $[\text{M}+\text{Na}]^+$ , 556.1676, found: 556.1654. Isolated yield: 62 %.



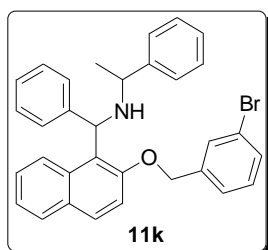
**N-((2-((4-fluorobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)**

**-1-phenylethanamine (11i):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 8.4$  Hz, 2H), 7.64 (s, 1H), 7.47 – 7.06 (m, 13H), 6.94 – 6.82 (m, 4H), 5.64 (s, 1H), 5.00 (d,  $J = 11.3$  Hz, 1H), 4.77 (d,  $J = 11.1$  Hz, 1H), 3.59 (q,  $J = 5.8$  Hz, 1H), 2.84 (s, 1H), 1.18 (d,  $J = 5.5$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.5 (d,  $J_{\text{C-F}} = 244.0$  Hz) 154.5, 146.3, 145.2, 132.6, 131.7, 129.3 (d,  $J_{\text{C-F}} = 8.0$  Hz), 128.8, 128.4, 128.0, 127.3, 126.9, 126.7, 126.0, 123.8, 115.4 (d,  $J_{\text{C-F}} = 22$  Hz), 115.0, 70.5, 55.8, 55.2, 26.0.  $^{19}\text{F NMR}$  (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -114.21 (s, 1F). **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3422, 3344, 3056, 2960, 2362, 1597, 1512, 1228, 1078, 1020, 703. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{NOF}$   $[\text{M}+\text{H}]^+$ , 462.2233, found 462.2235. Isolated yield: 82 %.



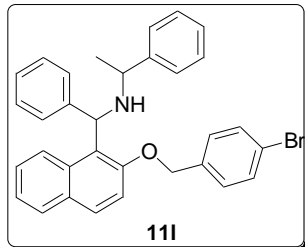
**N-((2-((2-fluorobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-**

**1-phenylethanamine (11j):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.6$  Hz, 2H), 7.67 (s, 1H), 7.42 (d,  $J = 6.5$  Hz, 2H), 7.36 – 6.88 (m, 14H), 6.80 (d,  $J = 6.8$  Hz, 1H), 5.69 (s, 1H), 5.16 (d,  $J = 12.1$  Hz, 1H), 4.84 (d,  $J = 11.9$  Hz, 1H), 3.63 (q,  $J = 5.9$  Hz, 1H), 2.90 (s, 1H), 1.21 (d,  $J = 6.0$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.5 (d,  $J_{\text{C-F}} = 240.0$  Hz), 154.4, 145.7 (d,  $J_{\text{C-F}} = 120.0$  Hz), 129.7 (d,  $J_{\text{C-F}} = 3$  Hz), 129.6 (d,  $J_{\text{C-F}} = 20$  Hz), 128.8, 128.4, 127.9, 127.2, 126.9, 126.6, 125.9, 124.3 (d,  $J_{\text{C-F}} = 4$  Hz), 124.1, 124.0, 123.7, 115.2 (d,  $J_{\text{C-F}} = 21$  Hz), 114.8, 64.6, 55.8, 55.2, 25.9.  $^{19}\text{F NMR}$  (470 MHz,  $\text{CDCl}_3$ )  $\delta$  -118.59 (s, 1F). **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 3363, 3057, 2923, 1621, 1593, 1494, 1238, 804, 704. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{NOF}$   $[\text{M}+\text{H}]^+$ , 462.2233, found 462.2225. Isolated yield: 80 %.



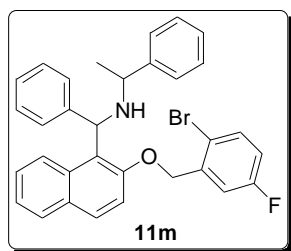
**N-((2-((3-bromobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-**

**1-phenylethanamine (11k):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (d,  $J = 8.4$  Hz, 2H), 7.69 (s, 1H), 7.49 – 7.06 (m, 16H), 6.89 (d,  $J = 7.4$  Hz, 1H), 5.67 (s, 1H), 5.03 (d,  $J = 11.9$  Hz, 1H), 4.78 (d,  $J = 11.8$  Hz, 1H), 3.63 (q,  $J = 5.7$  Hz, 1H), 2.85 (s, 1H), 1.23 (d,  $J = 5.7$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.4, 139.2, 131.1, 130.3, 130.2, 128.4, 128.0, 127.3, 126.8, 125.9, 123.9, 115.0, 70.4, 55.8, 55.1, 26.0. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3338, 3061, 3023, 2958, 2360, 1596, 1513, 1235, 1070, 877, 801, 743, 696. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{NOBr}$   $[\text{M}+\text{H}]^+$ , 524.1433, found 524.1428. Isolated yield: 60 %.



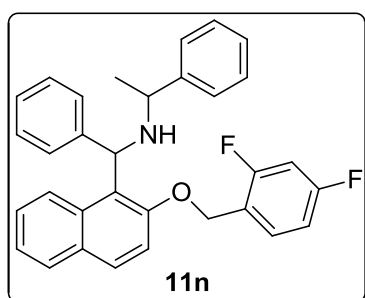
**N-((2-((4-bromobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-**

**1-phenylethanamine (11l):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 (d,  $J = 8.5$  Hz, 2H), 7.64 (s, 1H), 7.47 – 7.09 (m, 15), 6.76 (d,  $J = 7.0$  Hz, 2H), 5.64 (s, 1H), 4.98 (d,  $J = 11.5$  Hz, 1H), 4.75 (d,  $J = 11.2$  Hz, 1H), 3.59 (q,  $J = 5.1$  Hz, 1H), 2.81 (s, 1H), 1.18 (d,  $J = 4.4$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.4, 135.8, 131.7, 129.4, 129.1, 128.8, 128.4, 128.0, 127.3, 126.9, 126.7, 126.1, 123.9, 121.9, 114.8, 70.4, 55.8, 55.2, 26.0 (s). **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 3370, 3063, 3023, 1594, 1490, 1215, 1069, 800, 701. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{NOBr}$   $[\text{M}+\text{H}]^+$ , 524.1433, found 524.1428. Isolated yield: 68 %.



**N-((2-((2-bromo-5-fluorobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11m):**

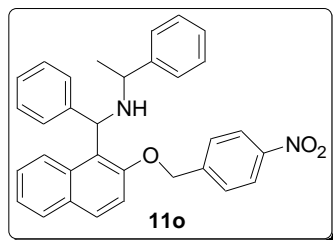
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.81 (d, *J* = 8.6 Hz, 2H), 7.72 (s, 1H), 7.58 – 7.05 (m, 15H), 6.82 (t, *J* = 8.2 Hz, 1H), 6.55 (d, *J* = 7.9 Hz, 1H), 5.72 (s, 1H), 5.08 (d, *J* = 13.7 Hz, 1H), 4.80 (d, *J* = 13.7 Hz, 1H), 3.61 (q, *J* = 6.1 Hz, 1H), 2.77 (s, 1H), 1.23 (d, *J* = 6.1 Hz, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 162.2 (d, *J*<sub>C-F</sub> = 246.0 Hz), 154.0, 146.2, 145.0, 138.6 (d, *J*<sub>C-F</sub> = 8 Hz), 133.6 (d, *J*<sub>C-F</sub> = 8 Hz), 129.8, 129.5, 128.8, 128.4, 128.1, 127.2, 127.0, 126.8, 126.2, 124.0, 116.4, 116.1 (d, *J*<sub>C-F</sub> = 8 Hz), 115.8, 115.4, 114.8, 70.2, 55.8, 55.0, 26.1. **<sup>19</sup>F NMR** (471 MHz, CDCl<sub>3</sub>) δ -113.36 (s, 1F). **IR** (KBr) (ν<sub>max</sub>/ cm<sup>-1</sup>): 3420, 3335, 3026, 2937, 1594, 1491, 1284, 1027, 806, 721, 701. Isolated yield: 77%.



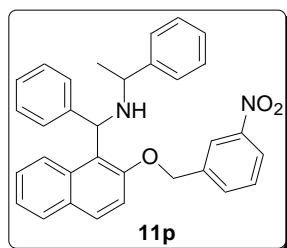
**N-((2-((2,4-difluorobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11n):**

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.84 – 7.76 (m, 2H), 7.64 (s, 1H), 7.45 – 7.08 (m, 13H), 6.75 (t, *J* = 9.5 Hz, 1H), 6.65 (d, *J* = 6.9 Hz, 2H), 5.64 (s, 1H), 5.11 (d, *J* = 11.3 Hz, 1H), 4.77 (d, *J* = 10.7 Hz, 1H), 3.59 (q, *J* = 4.2 Hz, 1H), 2.77 (s, 1H), 1.19 (s, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 164.0 (d, *J*<sub>C-F</sub> = 12.0 Hz), 161.5 (t, *J*<sub>C-F</sub> = 20.0 Hz), 159.1 (d, *J*<sub>C-F</sub> = 12.0 Hz), 154.3, 146.3, 145.2, 133.7, 130.9, 129.7, 129.4, 128.8, 128.4, 128.0, 127.3, 126.9, 126.7, 126.0, 123.9, 120.1 (d, *J*<sub>C-F</sub> = 10.0 Hz), 114.8, 111.5 (dd, *J*<sub>C-F</sub> = 23.0 Hz, 3 Hz), 103.7 (t, *J*<sub>C-F</sub> = 25.0 Hz), 64.2, 55.8, 55.1, 26.0. **<sup>19</sup>F NMR** (470 MHz, CDCl<sub>3</sub>) δ -110.26 (s, 1F), -114.70 (s, 1F). **IR** (KBr) (ν<sub>max</sub>/ cm<sup>-1</sup>): 3425, 3025, 2923, 2368, 1622, 1508, 1253, 1098, 962, 849, 804, 701. **HRMS** (EI) calcd. for C<sub>32</sub>H<sub>28</sub>NOF<sub>2</sub> [M+H]<sup>+</sup>, 480.2139,

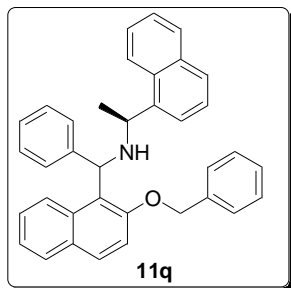
found 480.2142. Isolated yield: 73 %.



**N-((2-((4-nitrobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11o):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J = 7.9$  Hz, 2H), 7.80 (d,  $J = 8.6$  Hz, 2H), 7.66 (s, 1H), 7.47 – 7.09 (m, 13H), 6.99 (d,  $J = 7.5$  Hz, 2H), 5.67 (s, 1H), 5.11 (d,  $J = 12.4$  Hz, 1H), 4.87 (d,  $J = 12.5$  Hz, 1H), 3.57 (q,  $J = 4.9$  Hz, 1H), 2.69 (s, 1H), 1.18 (d,  $J = 3.9$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.0, 147.6, 144.2, 129.5, 128.8, 128.5, 128.1, 127.7, 127.2, 126.9, 126.2, 124.1, 123.8, 114.7, 70.0, 55.8, 55.0, 26.2. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3427, 2366, 2332, 1625, 1522, 1345, 1112, 1085, 1028, 805, 701. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ , 489.2178, found 489.2180. Isolated yield: 36 %.

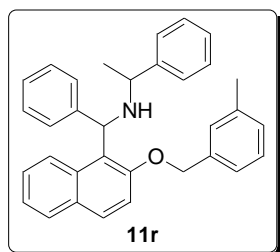


**N-((2-((3-nitrobenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11p):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10 (d,  $J = 8.1$  Hz, 1H), 7.99 (s, 1H), 7.83 (d,  $J = 8.7$  Hz, 2H), 7.71 (s, 1H), 7.43 (d,  $J = 7.1$  Hz, 2H), 7.40 – 7.06 (m, 13H), 5.70 (s, 1H), 5.12 (d,  $J = 12.0$  Hz, 1H), 4.81 (d,  $J = 11.9$  Hz, 1H), 3.63 (q,  $J = 6.2$  Hz, 1H), 2.75 (s, 1H), 1.23 (d,  $J = 5.6$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.1, 148.3, 138.9, 133.4, 129.6, 128.4, 128.0, 127.2, 126.76 (s), 124.1, 122.9, 122.1, 115.0, 70.1, 55.8, 55.0, 26.0. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3446, 2918, 2850, 2363, 1734, 1653, 1559, 1508, 1348, 1240, 1093, 803. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ , 489.2178, found 489.2177. Isolated yield: 30 %.



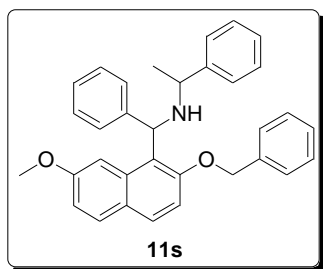
**(1S)-N-((2-(benzyloxy)naphthalen-1-yl)(phenyl)methyl)-1-(naphthalen-1-yl)ethanamine (11q):**

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.93 – 7.04 (m, 31H), 5.54 (d, *J* = 12.0 Hz, 1H), 5.30 (d, *J* = 12.0 Hz, 1H), 5.24 (d, *J* = 12.1 Hz, 1H), 5.03 (d, *J* = 11.6 Hz, 1H, diastereomeric isomer mixtures), 3.63 (q, *J* = 6.3 Hz, 1H), 2.83 (s, 1H), 1.21 (d, *J* = 6.5 Hz, 1H, diastereomeric isomer mixtures), 1.14 (d, *J* = 6.4 Hz, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 154.9, 146.4, 145.1, 128.80, 128.3, 127.8, 127.3, 126.8, 126.6, 125.9, 125.8, 125.5, 123.7, 123.4, 115.2, 69.7, 63.1, 55.9, 25.9. **IR** (KBr) (ν<sub>max</sub>/ cm<sup>-1</sup>): 3446, 3032, 2920, 2362, 1717, 1653, 1623, 1541, 1508, 1457, 1238, 1068, 801, 779, 700. **HRMS** (EI) calcd. for C<sub>36</sub>H<sub>32</sub>NO [M+H]<sup>+</sup>, 494.2484, found 494.2485. Dr = 67:37; Isolated yield: 83%.

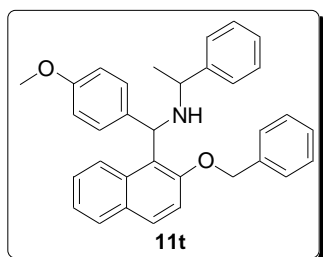


**N-((2-((3-methylbenzyl)oxy)naphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11r):**

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.84 (d, *J* = 8.1 Hz, 2H), 7.68 (s, 1H), 7.44 (d, *J* = 6.6 Hz, 2H), 7.41 – 7.16 (m, 13H), 7.11 (d, *J* = 7.3 Hz, 1H), 6.87 (s, 2H), 5.68 (s, 1H), 5.08 (d, *J* = 11.6 Hz, 1H), 4.88 (d, *J* = 11.5 Hz, 1H), 3.66 (q, *J* = 5.5 Hz, 1H), 3.00 (s, 1H), 2.32 (s, 3H), 1.24 (d, *J* = 5.3 Hz, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 154.7, 146.4, 145.2, 138.2, 136.9, 128.7, 128.5, 128.4, 128.1, 127.9, 127.4, 127.0, 124.5, 115.1, 71.2, 55.8, 55.3, 26.0, 21.5. **IR** (KBr) (ν<sub>max</sub>/ cm<sup>-1</sup>): 3422, 2961, 2866, 2362, 1623, 1559, 1490, 1457, 1253, 1068, 804, 700. Isolated yield: 86 %.

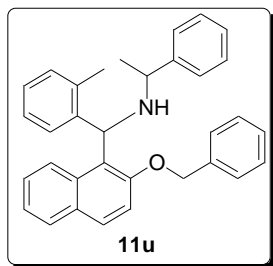


**N-((2-(benzyloxy)-7-methoxynaphthalen-1-yl)(phenyl)methyl)-1-phenylethanamine (11s):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (dd,  $J = 14.2, 8.9$  Hz, 2H), 7.47 (d,  $J = 6.4$  Hz, 2H), 7.35 (d,  $J = 7.4$  Hz, 3H), 7.32 – 7.15 (m, 10H), 7.00 (d,  $J = 8.0$  Hz, 3H), 5.63 (s, 1H), 5.08 (d,  $J = 11.7$  Hz, 1H), 4.87 (d,  $J = 11.4$  Hz, 1H), 3.66 (q,  $J = 5.8$  Hz, 1H), 3.50 (s, 3H), 2.91 (s, 1H), 1.24 (d,  $J = 5.8$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.3, 155.3, 146.6, 145.4, 137.0, 130.2, 128.5, 128.4, 128.0, 127.4, 127.3, 126.9, 116.9, 112.3, 70.9, 55.7, 55.3, 54.9, 26.2. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3446, 3058, 3026, 2953, 2361, 1626, 1515, 1420, 1229, 1029, 970, 826, 700. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 474.2355, found 474.2429. Isolated yield: 60 %.



**N-((2-(benzyloxy)naphthalen-1-yl)(4-methoxyphenyl)methyl)-1-phenylethanamine (11t):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 (s, 1H), 7.37 (d,  $J = 9.2$  Hz, 2H), 7.33-7.26 (m, 14H), 7.12 – 7.00 (m, 3H), 5.63 (d,  $J = 9.5$  Hz, 1H), 5.15 (d,  $J = 11.6$  Hz, 1H), 5.08 (d,  $J = 11.6$  Hz, 1H), 3.69 (q,  $J = 6.4$  Hz, 1H), 2.76 (s, 1H), 1.97 (s, 3H), 1.21 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.9, 145.7, 141.9, 130.6, 129.3, 128.7, 128.3, 128.2, 128.1, 127.6, 127.0, 126.5, 125.6, 123.5, 114.5, 71.1, 55.9, 54.8, 24.8, 19.9. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 2361, 1653, 1559, 1508, 1457, 1262, 1221, 1023, 806, 700. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 474.2433, found 474.2433. Isolated yield: 68 %.

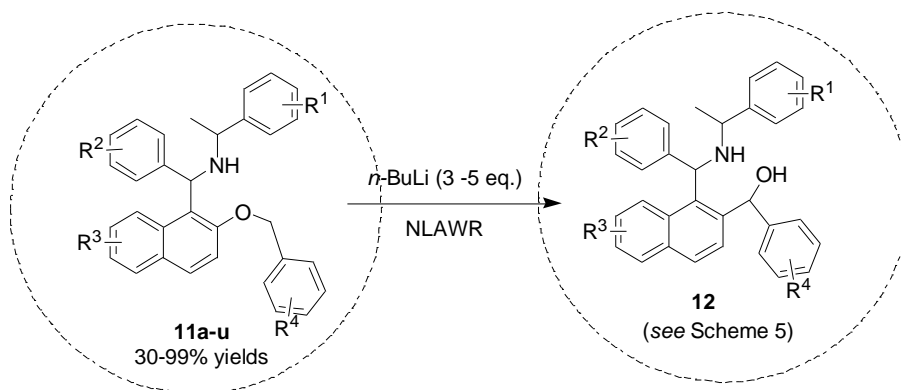




**N-((2-(benzyloxy)naphthalen-1-yl)(o-tolyl)methyl)-1-phenylet**

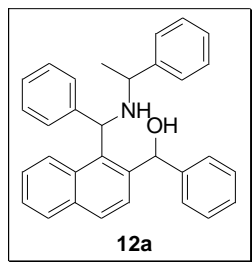
**hanamine: (11u)**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 7.8$  Hz, 2H), 7.66 (s, 1H), 7.36-7.06 (m, 15H), 6.86 (d,  $J = 6.8$  Hz, 1H), 6.69 (d,  $J = 7.6$  Hz, 1H), 5.63 (s, 1H), 5.07 (d,  $J = 11.6$  Hz, 1H), 4.86 (d,  $J = 11.4$  Hz, 1H), 3.70 (s, 3H), 3.62 (d,  $J = 5.9$  Hz, 1H), 1.19 (d,  $J = 6.0$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.6, 154.7, 147.2, 146.4, 137.0, 129.2, 128.8, 128.7, 128.5, 128.4, 127.9, 127.4, 127.3, 126.9, 126.6, 123.7, 119.5, 115.1, 113.0, 111.1, 71.2, 55.8, 55.2, 26.0. **IR** (KBr) ( $\nu_{\text{max}}$ /  $\text{cm}^{-1}$ ): 3430, 3333, 3030, 2964, 2835, 1609, 1454, 1434, 1283, 1235, 1144, 1046, 808, 768, 703. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 458.2484, found 458.2485. Isolated yield: 40 %.

#### 4. The synthesis of Betti base-derived amino alcohols **12**.



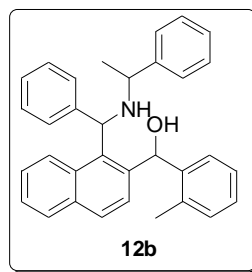
Under argon atmosphere, to a solution of **11** (2 mmol) in the dry THF (10 ml) at  $-78$   $^{\circ}\text{C}$ , the *n*-BuLi (4 mL, 10 mmol, 2.5 M in hexane) was added slowly in 15 min. After the addition, the solution was allowed to stir at  $-78$   $^{\circ}\text{C}$  for 1-2 h. And then the reaction solution was warmed to room temperature slowly. After quenched with saturated  $\text{NH}_4\text{Cl}$  solution, the resulted mixture was extracted with ethyl acetate, and washed with water and saturated NaCl solution. The organic layer was dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was purified by column chromatography (hexanes/ethyl

acetate = 20/1) to give **12** as a colorless powder.



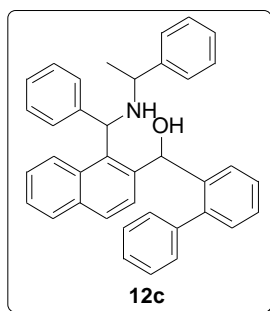
**phenyl(1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-**

**yl)methanol (12a):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (d,  $J = 8.1$  Hz, 1H), 7.71 (t,  $J = 6.8$  Hz, 2H), 7.51 (d,  $J = 6.8$  Hz, 1H), 7.42-7.15 (m, 17H), 6.32 (s, 1H), 6.09 (s, 1H), 3.62 (q,  $J = 5.6$  Hz, 1H), 2.11 (s, 1H), 1.43 (d,  $J = 5.6$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.4, 143.3, 142.9, 142.1, 137.0, 133.1, 128.8, 128.7, 128.6, 128.0, 127.6, 127.5, 126.9, 126.7, 126.4, 126.3, 126.0, 125.7, 123.9, 70.8, 56.5, 56.2, 24.5. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3407, 3058, 3025, 2963, 2359, 1725, 1710, 1600, 1449, 1030, 818, 700. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{30}\text{NO}$   $[\text{M}+\text{H}]^+$ , 444.22, found 444.2313, **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{29}\text{NO}$   $[\text{M}+\text{Na}]^+$ , 466.2147, found 466.2118. Isolated yield: 76 %.



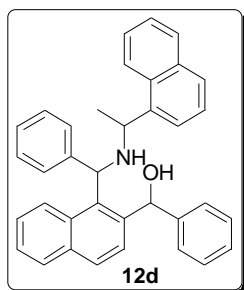
**(1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-yl)(o-to**

**lyl)methanol (12b):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 7.6$  Hz, 1H), 7.81 (d,  $J = 8.1$  Hz, 1H), 7.64 (d,  $J = 8.5$  Hz, 2H), 7.45 (d,  $J = 6.9$  Hz, 3H), 7.38 – 7.13 (m, 10H), 7.00 (d,  $J = 5.6$  Hz, 2H), 6.94 – 6.81 (m, 2H), 6.20 (s, 1H), 6.16 (s, 1H), 3.59 (q,  $J = 6.5$  Hz, 1H), 1.50 (d,  $J = 5.7$  Hz, 3H), 0.89 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.5, 141.0, 135.1, 133.5, 133.3, 130.0, 129.3, 129.0, 128.9, 128.7, 128.5, 127.8, 127.0, 126.9, 126.6, 126.5, 126.4, 125.9, 125.9, 124.0, 68.4, 55.9, 55.5, 24.6, 18.4. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3428, 3054, 2368, 2344, 1636, 1449, 1385, 1031, 737, 700. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 458.2484, found 458.2475. Isolated yield: 56 %.

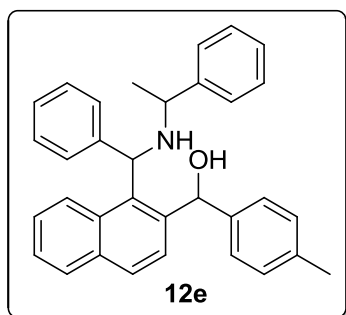


**[1,1'-biphenyl]-2-yl(1-(phenyl((1-phenylethyl)amino)methyl)**

**naphthalen-2-yl)methanol (12c):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (d,  $J = 6.7$  Hz, 1H), 7.88 (d,  $J = 8.1$  Hz, 1H), 7.78 (d,  $J = 8.6$  Hz, 2H), 7.60 – 6.59 (m, 19H), 6.06 (s, 1H), 3.51 (q,  $J = 6.4$  Hz, 1H), 2.09 (s, 1H), 1.35 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.4, 140.8, 140.7, 133.6, 133.1, 130.7, 128.9, 128.8, 128.6, 128.5, 128.4, 127.9, 127.7, 127.6, 127.4, 126.8, 126.7, 126.2, 126.0, 125.5, 124.9, 69.7, 56.0, 31.7, 22.8. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3426, 3058, 3025, 2958, 2923, 2856, 2368, 2344, 2332, 1624, 1508, 1449, 1099, 1028, 819, 748, 701. **HRMS** (EI) calcd. for  $\text{C}_{38}\text{H}_{34}\text{NO}$   $[\text{M}+\text{H}]^+$ , 520.2640, found 520.2642. Isolated yield: 79 %.

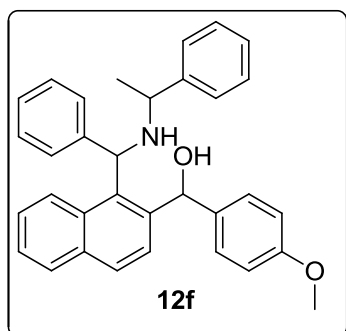


**1-(((1-(naphthalen-1-yl)ethyl)amino)(phenyl)methyl)naphthalen-2-yl(phenyl)methanol (12d):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 8.1$  Hz, 2H), 7.69 (d,  $J = 8.4$  Hz, 2H), 7.58 (d,  $J = 7.5$  Hz, 1H), 7.54 – 6.99 (m, 21H), 6.76 (s, 1H, mixture of diastereomers), 6.23 (s, 2H), 4.59 (s, 1H), 0.98 (d,  $J = 6.6$  Hz, 1H, mixture of diastereomers), 0.92 – 0.85 (m, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.4, 142.9, 141.8, 140.3, 137.2, 134.1, 133.1, 131.5, 128.8, 128.7, 128.6, 128.5, 128.1, 127.8, 127.6, 127.4, 127.0, 126.4, 126.9, 126.4, 126.1, 126.0, 125.9, 125.7, 125.6, 122.4, 122.2, 71.0, 56.5, 24.5, 14.3. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3433, 3057, 2918, 2850, 2364, 1699, 1653, 1636, 1541, 1508, 1457, 1110, 1030, 778, 728. **HRMS** (EI) calcd. for  $\text{C}_{36}\text{H}_{31}\text{NO}$   $[\text{M}+\text{H}]^+$ , 494.2484, found 494.2483. Isolated yield: 62 %.



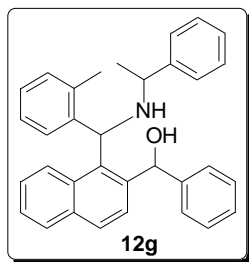
**(1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-**

**-yl)(p-tolyl)methanol (12e):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (d,  $J = 8.1$  Hz, 1H), 7.74 (d,  $J = 8.5$  Hz, 1H), 7.67 (s, 1H), 7.48 (d,  $J = 6.7$  Hz, 1H), 7.42 (d,  $J = 7.2$  Hz, 2H), 7.38 – 7.14 (m, 10H), 7.09 (d,  $J = 5.1$  Hz, 2H), 7.02 (d,  $J = 4.1$  Hz, 2H), 6.25 (s, 1H), 6.09 (s, 1H), 3.6 (b, 1H), 2.34 (d,  $J = 2.3$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.1, 139.9, 136.4, 133.2, 129.1, 128.93, 128.85, 128.7, 128.3, 128.0, 127.8, 127.1, 127.0, 126.5, 126.3, 126.2, 125.8, 123.8, 70.7, 56.7, 24.4, 21.2. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 3025, 2965, 2362, 1653, 1508, 1457, 1262, 1030, 909, 761, 700. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}$   $[\text{M}+\text{H}]^+$ , 458.2484, found 458.2485. Isolated yield: 42 %.

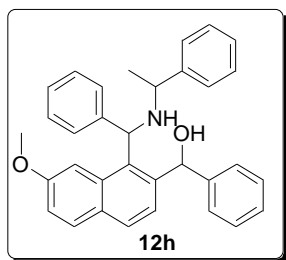


**(4-methoxyphenyl)(1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-yl)methanol (12f):**

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (d,  $J = 8.1$  Hz, 1H), 7.74 (d,  $J = 8.7$  Hz, 1H), 7.63 (d,  $J = 8.2$  Hz, 1H), 7.57 (d,  $J = 7.6$  Hz, 1H), 7.50 – 7.10 (m, 11H), 7.02 (d,  $J = 8.1$  Hz, 2H), 6.93 (d,  $J = 7.6$  Hz, 1H), 6.81 (d,  $J = 7.8$  Hz, 2H), 6.20 (s, 1H), 6.07 (s, 1H), 3.79 (s, 3H), 3.68 – 3.58 (m, 1H), 1.46 (d,  $J = 5.4$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.6, 142.1, 134.9, 133.2, 130.5, 129.9, 129.2, 129.0, 128.9, 128.8, 128.3, 128.0, 127.8, 127.5, 127.2, 127.1, 126.6, 126.3, 125.9, 123.8, 114.0, 113.6, 70.5, 56.8, 55.4, 24.3. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 3309, 2930, 2654, 2164, 1624, 1508, 1457, 1262, 1230, 1032, 840, 700. **HRMS** (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 474.2355, found HRMS+H: 474.2433. Isolated yield: 20 %.

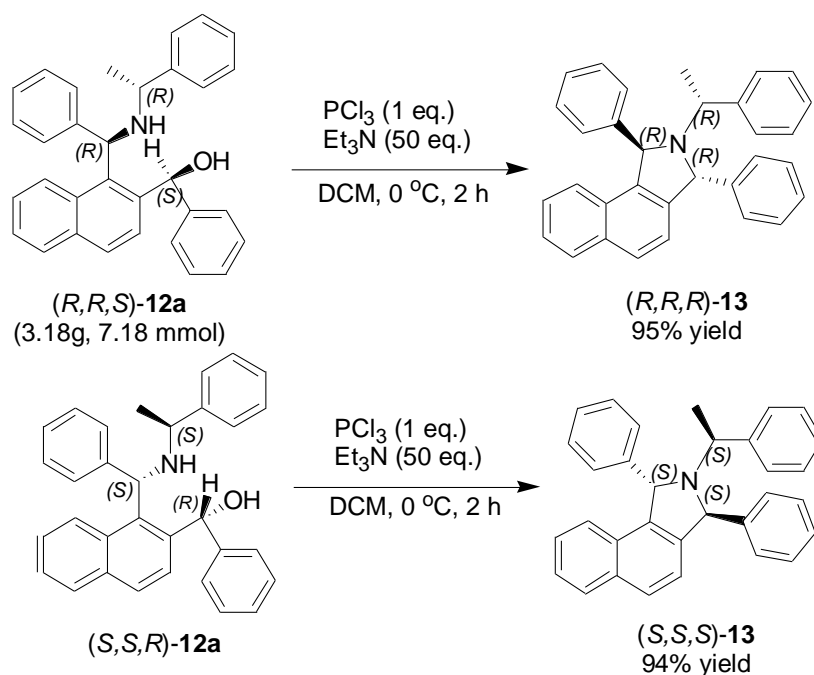


**phenyl(1-(((1-phenylethyl)amino)(o-tolyl)methyl)naphthalen-2-yl)methanol (12g):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.1$  Hz, 1H), 7.67-7.61 (m, 2H), 7.40 (t,  $J = 7.4$  Hz, 1H), 7.36 – 7.07 (m, 12H), 7.04 (d,  $J = 8.5$  Hz, 1H), 6.91 (s, 1H), 6.84 (d,  $J = 7.7$  Hz, 1H), 6.71 (d,  $J = 8.2$  Hz, 1H), 6.23 (s, 1H), 5.94 (s, 1H), 3.66 (s, 3H), 3.52 (d,  $J = 6.6$  Hz, 1H), 1.99 (s, 1H), 1.34 (d,  $J = 6.2$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.0, 143.0, 129.7, 128.9, 128.9, 128.1, 127.7, 126.9, 126.5, 126.5, 125.8, 118.7, 112.8, 111.8, 70.9, 56.6, 56.5, 55.4, 24.5. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3447, 2967, 2920, 2166, 1636, 1508, 1457, 1261, 1101, 1048, 767, 698. Isolated yield: 28 %.



**(7-methoxy-1-(phenyl((1-phenylethyl)amino)methyl)naphthalen-2-yl)methanol (12h):**  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.9$  Hz, 1H), 7.65 (d,  $J = 8.5$  Hz, 1H), 7.43 (d,  $J = 7.6$  Hz, 2H), 7.38 – 7.19 (m, 10H), 7.15 (d,  $J = 7.4$  Hz, 2H), 7.10 (d,  $J = 7.3$  Hz, 2H), 6.96 – 6.86 (m, 2H), 6.22 (s, 1H), 5.98 (s, 1H), 3.60 (q,  $J = 6.5$  Hz, 1H), 3.51 (s, 3H), 2.06 (s, 1H), 1.43 (d,  $J = 6.5$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 143.0, 130.3, 128.9, 128.8, 128.6, 128.1, 127.6, 126.9, 126.4, 126.0, 118.8, 102.1, 70.7, 56.5, 56.0, 54.9, 24.9. **IR** (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3421, 2164, 1624, 1559, 1507, 1457, 1262, 1230, 1032, 840. HRMS (EI) calcd. for  $\text{C}_{33}\text{H}_{32}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 474.2355, found IR . HRMS+H 474.2433. Isolated yield: 20 %.

**5. The synthesis of optically pure and all-substituted pyrrolidine derivative 13 through intramolecular cyclization.**



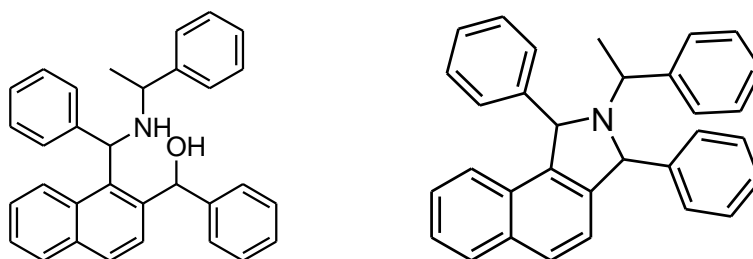
A 100 mL three-necked flask was charged with freshly distilled  $\text{PCl}_3$  (986.5 mg, 7.18 mmol) in anhydrous  $\text{CH}_2\text{Cl}_2$  (12 mL). The solution was cooled to 0 °C, and  $\text{NEt}_3$  (5 mL, 359 mmol) was added dropwise to the solution. And then a solution of **12a** (3.18g, 7.18 mol) in  $\text{CH}_2\text{Cl}_2$  (30 mL) was slowly added over 30 min to the reaction mixture, and the reaction solution was kept at 0 °C. After completing the addition, the ice bath was removed, and the resulting suspension was stirred for 90 min at room temperature. The reaction was quenched with  $\text{H}_2\text{O}$  (30 mL). The aqueous phase was extracted once with  $\text{CH}_2\text{Cl}_2$  (40 mL). The combined organic phases were dried over  $\text{Na}_2\text{SO}_4$ , the salt was removed by filtration, and the solution was evaporated to afford the crude product, which was purified by flash chromatography under pressure of argon:  $R_f = 0.4$  (3:1 (v/v) pentane/ $\text{CH}_2\text{Cl}_2$ ). The solvent was evaporated, and the product was dried under vacuum (0.04 mm) to afford **5** as a white powder.

**1,3-diphenyl-2-(1-phenylethyl)-2,3-dihydro-1H-benzo[e]isoindole:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 8.1$  Hz, 1H), 7.67 (d,  $J = 7.4$  Hz, 2H), 7.63 (d,  $J = 8.4$  Hz, 1H), 7.45 – 7.08 (m, 16H), 7.01 (d,  $J = 8.4$  Hz, 1H), 5.68 (s, 1H), 5.48 (s, 1H), 4.22 (q,  $J = 6.7$  Hz, 1H), 1.23 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.3, 140.6, 136.6, 133.6, 129.4, 128.8, 128.7, 128.6, 128.5, 128.3, 128.3, 128.0, 127.3, 127.0,

126.9, 126.1, 125.0, 124.2, 121.1, 70.6, 60.0, 20.4. **IR** (KBr) ( $\nu_{\text{max}}$ /  $\text{cm}^{-1}$ ): 3420, 3059, 3028, 2970, 2369, 1680, 1600, 1492, 1453, 1145, 1026, 809, 700. **HRMS** (EI) calcd. for  $\text{C}_{32}\text{H}_{28}\text{N}$   $[\text{M}+\text{H}]^+$ , 426.2222, found 426.2213. Isolated yield: 95 %.

## 6. CD Spectroscopic Data of Chiral Products 12a and 13

Computational details: The Gaussian 03 software package was used to carry out gas phase density functional theory (DFT) geometry optimizations<sup>[1]</sup>. The hybrid B3LYP functional was selected and 6-31G(d) basis sets were used. The same functional and basis set was used to obtain excitation energies and oscillator strengths from time dependent density functional theory (TD-DFT) calculations. The (R)- and (S)-silane are both taken as models for calculation. The calculated CD spectra were shown by the SpecDis software package (Version 1.51) software to yield higher-quality images, with comparison to the measured ones.<sup>[2]</sup>

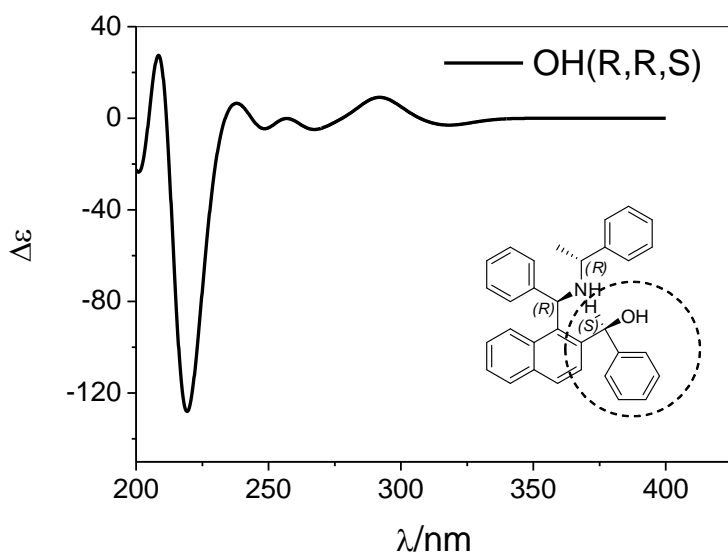


### References:

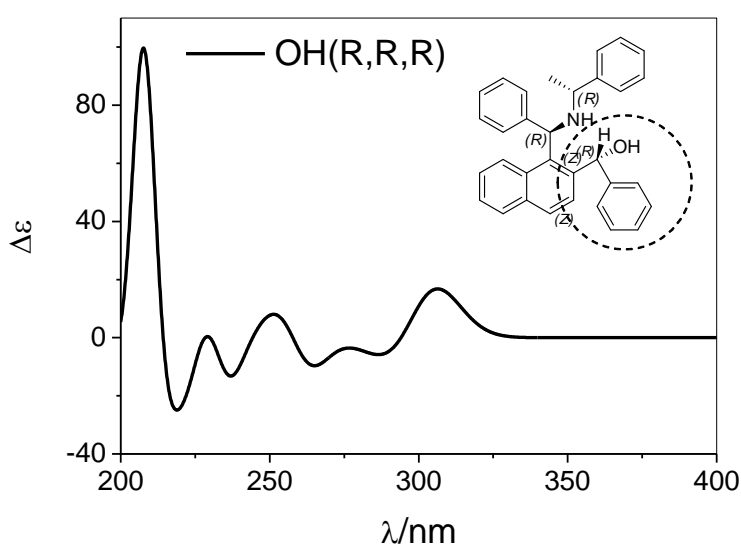
- [1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M. E.; Replogle, S.; Pople, J. A. Gaussian 03, Inc., Pittsburgh PA, 2003.
- [2] a) Stephens, P.J.; Harada, N. *Chirality* 2010, 22, 229-233. b) Bringmann, G.; Bruhm, T.; Maksimenka, K.; Hemberger, Y. *Eur. J. Org. Chem.* 2009, 2717-2727. c) Bringmann, G.; Gulder, T. A. M.; Reichert, M.; Gulder, T. *Chirality* 2008, 20, 628-642.



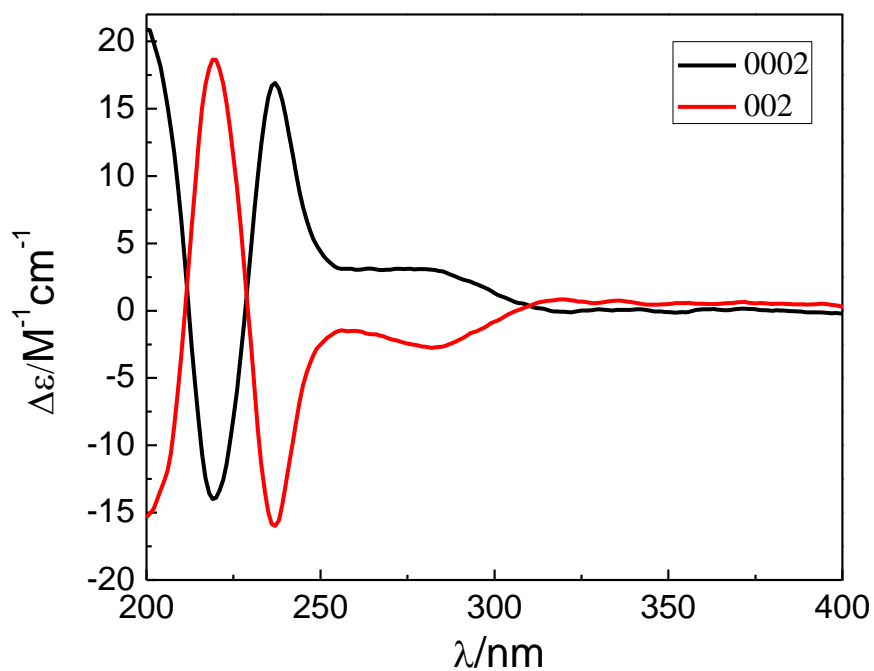
**Figure S1.** The experimental and calculated CD spectrum of chiral product **12a**: The absolute configuration of **12a** could be confirmed as corresponding configuration in comparison to that of the following calculated CD spectrum.



(a) Calculated CD spectra

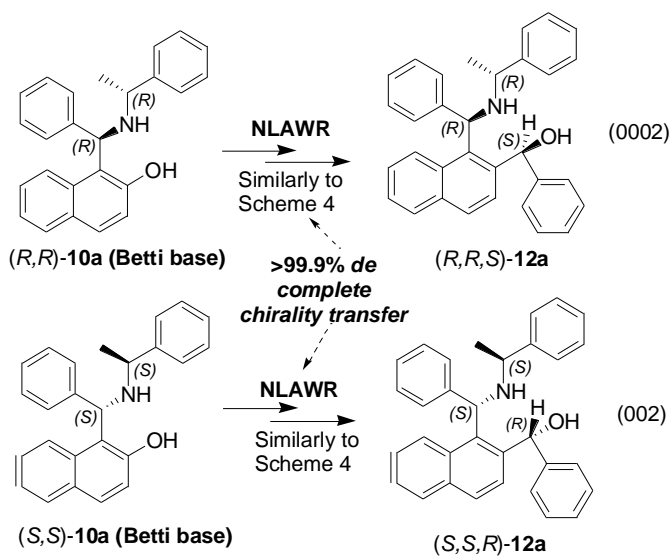


(b) Calculated CD spectra

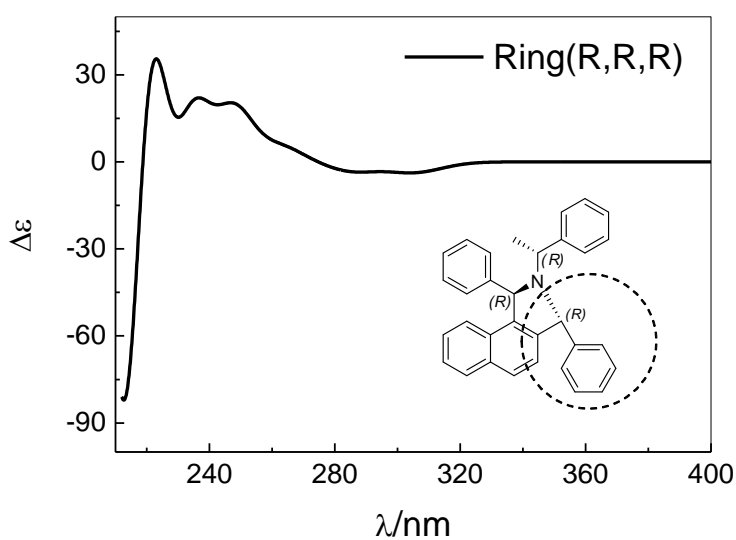


(c) Experimental CD spectra: Band width 2 nm; Response 1 sec; Sensitivity Standard;  
Data pitch 0.1 nm; Scanning speed 500 nm/min.  $c = 0.125\text{mmol/L}$ .

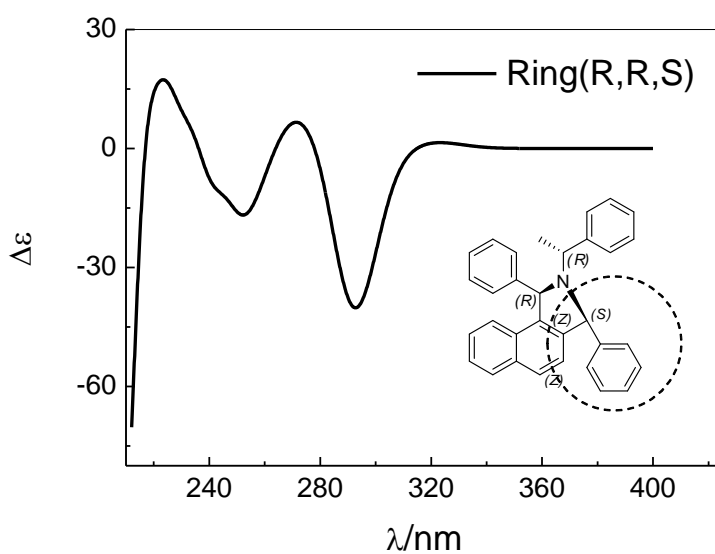
Results:



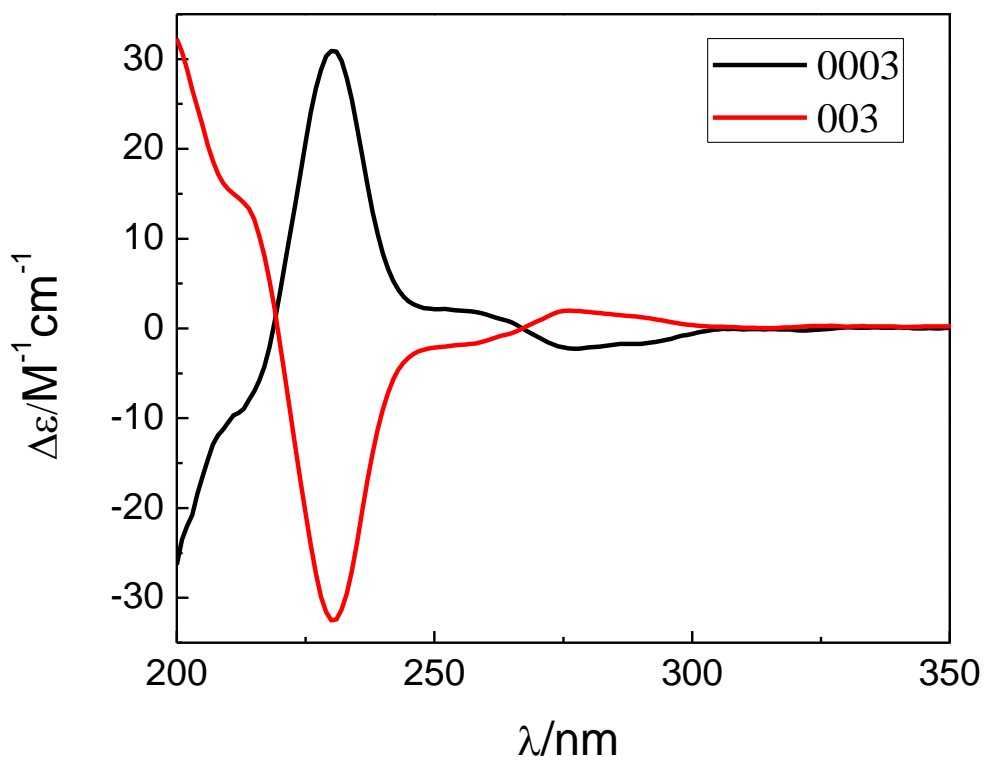
**Figure S2.** The experimental and calculated CD spectrum of chiral product **13**: The absolute configuration of **13** could be confirmed as corresponding configuration in comparison to that of the following calculated CD spectrum.



(a) Calculated spectra

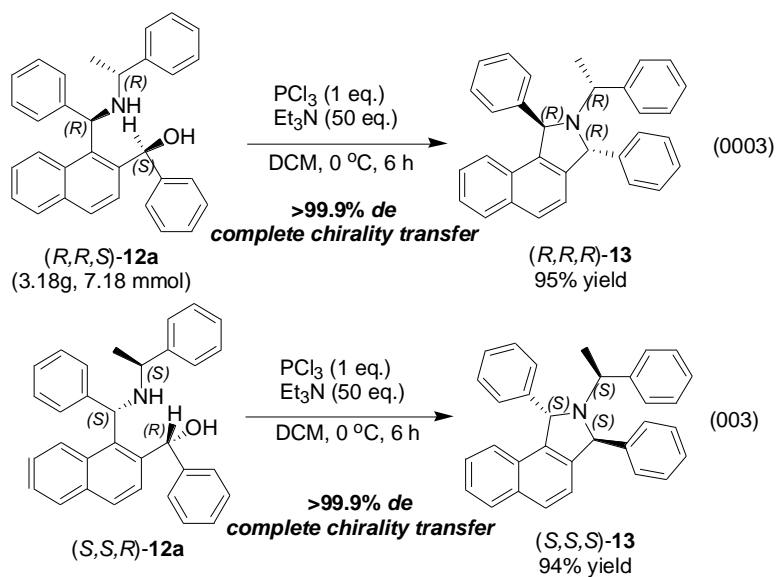


(b) Calculated spectra



(c) Experimental CD spectra: Band width 2 nm; Response 1 sec; Sensitivity Standard; Data pitch 0.1 nm; Scanning speed 500 nm/min.  $c = 0.125\text{mmol/L}$ .

Result:



## 7. NMR and HRMS Charts of Betti bases and it derivatives

### Mass Spectrum SmartFormula Report

#### Analysis Info

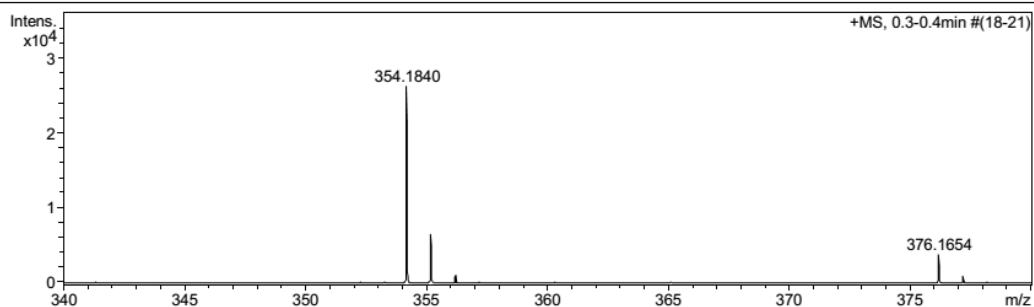
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 Comment

Acquisition Date 3/5/2014 3:03:56 PM

Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

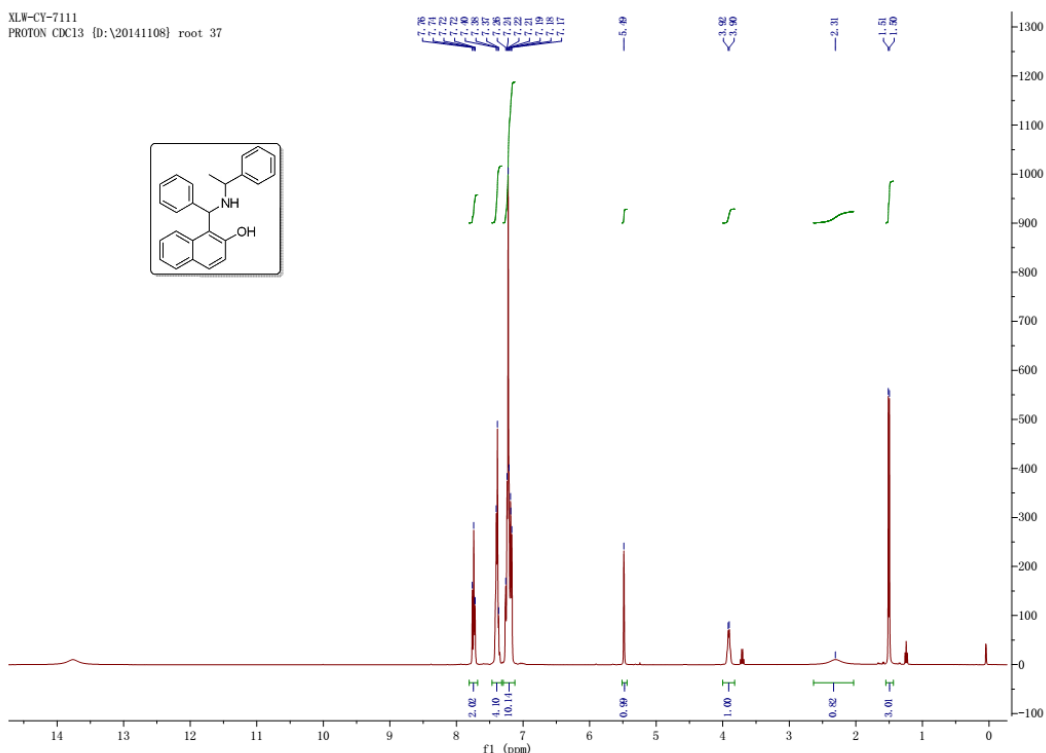
#### Acquisition Parameter

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Scan End	600 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

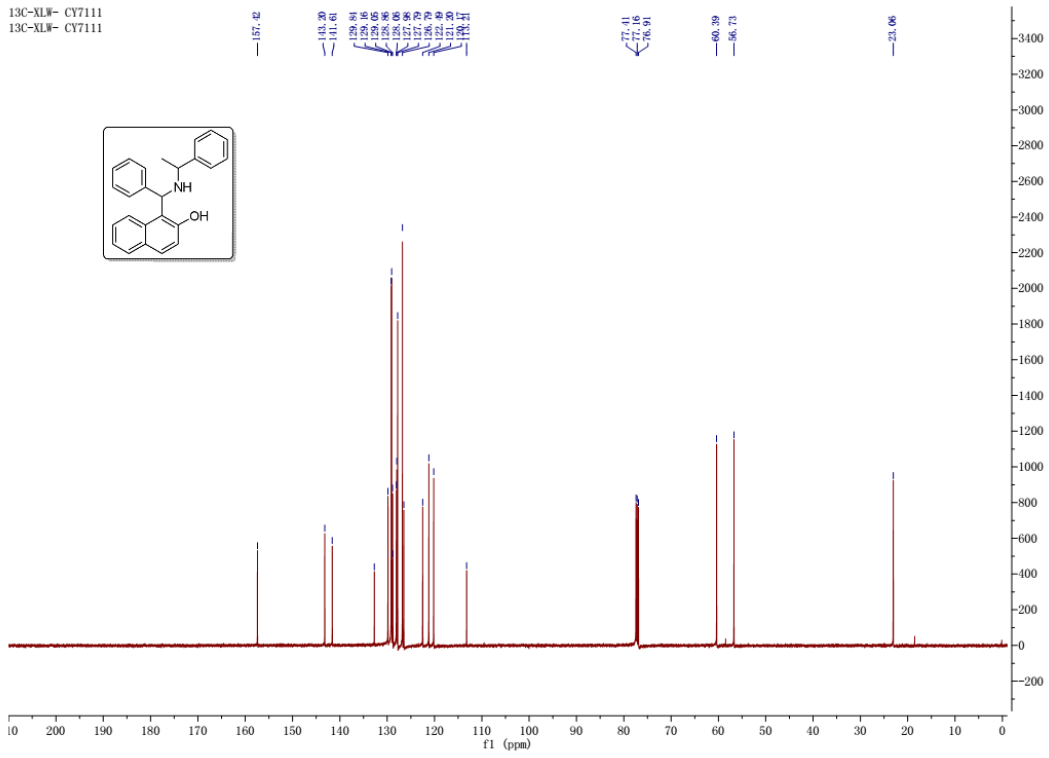


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376.1654	1	C 25 H 23 N Na O	100.00	376.1672	1.8	4.8	4.3	14.5	even	ok

XLW-CY-7111  
 PROTON CDCl3 {D:\20141108} root 37



13C-XLW- CY7111  
13C-XLW- CY7111



## Mass Spectrum SmartFormula Report

**Analysis Info**

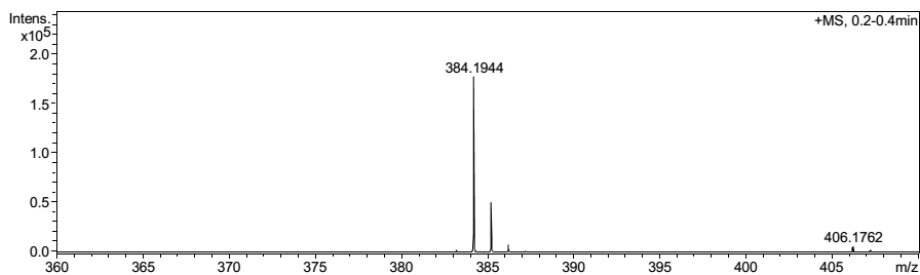
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 Comment

Acquisition Date 1/15/2015 2:44:16 PM

Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

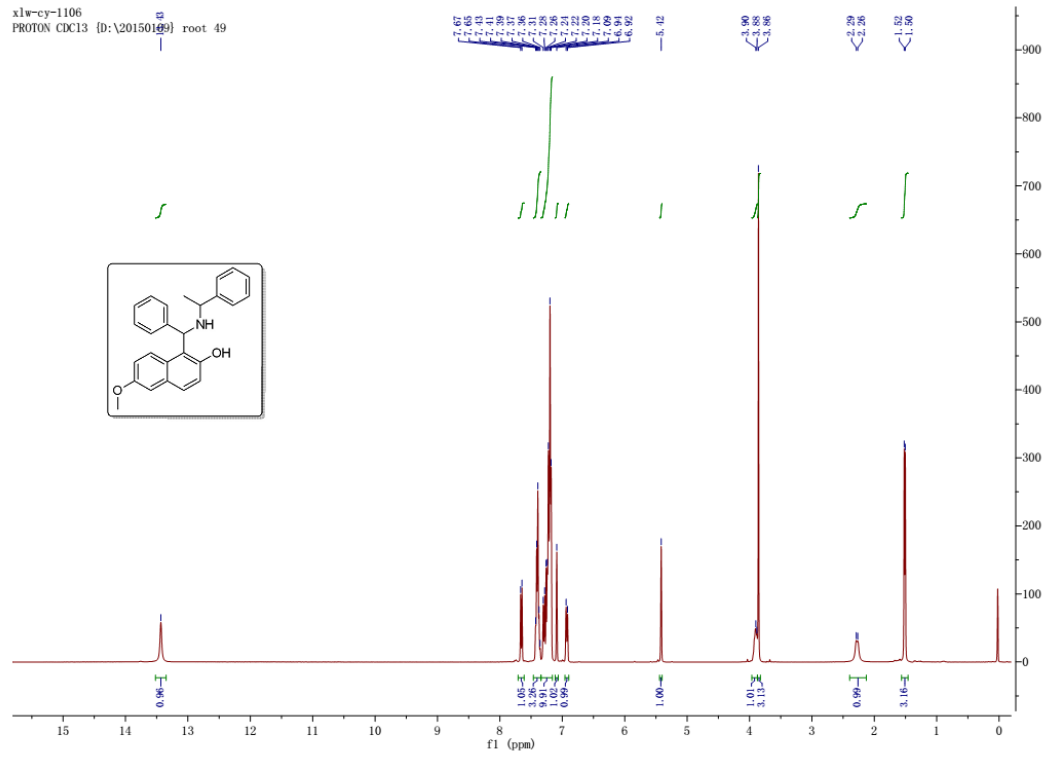
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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

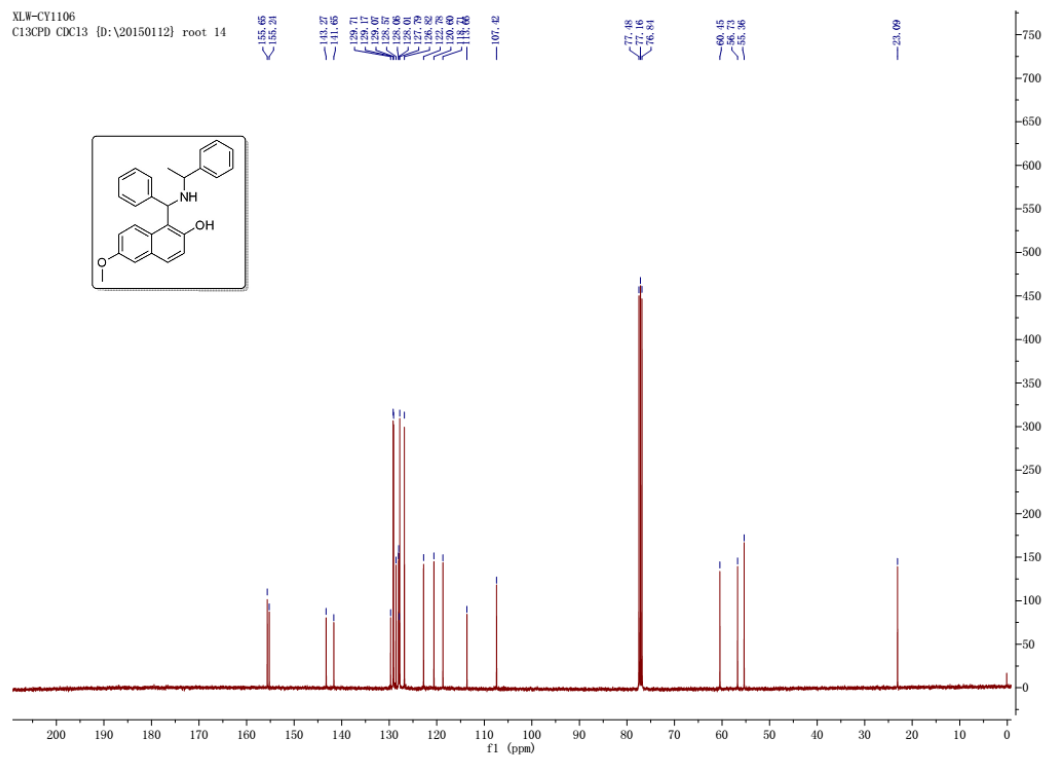


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
384.1944	1	C <sub>26</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>	100.00	384.1958	1.4	3.5	2.7	14.5	even	ok
406.1762	1	C <sub>26</sub> H <sub>25</sub> N <sub>2</sub> NaO <sub>2</sub>	100.00	406.1778	1.6	3.9	5.2	14.5	even	ok

xlw-cy-1106  
PROTON CDC13 {D:\20150109} root 49



XLW-CY1106  
C13CPD CDC13 {D:\20150112} root 14





## Mass Spectrum SmartFormula Report

**Analysis Info**

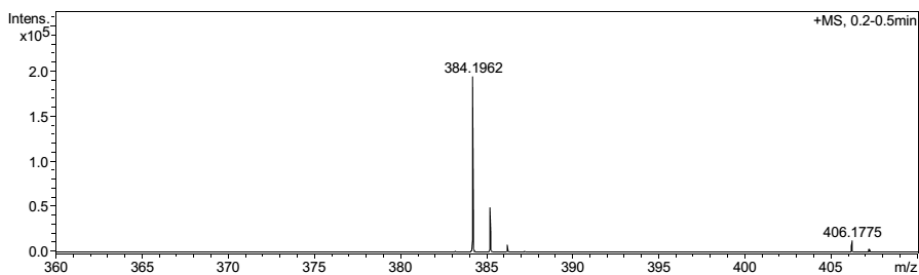
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 Comment

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Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
384.1962	1	C <sub>26</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>	100.00	384.1958	-0.4	-1.1	17.0	14.5	even	ok
406.1775	1	C <sub>26</sub> H <sub>25</sub> N <sub>2</sub> NaO <sub>2</sub>	100.00	406.1778	0.3	0.6	10.5	14.5	even	ok



## Mass Spectrum SmartFormula Report

**Analysis Info**

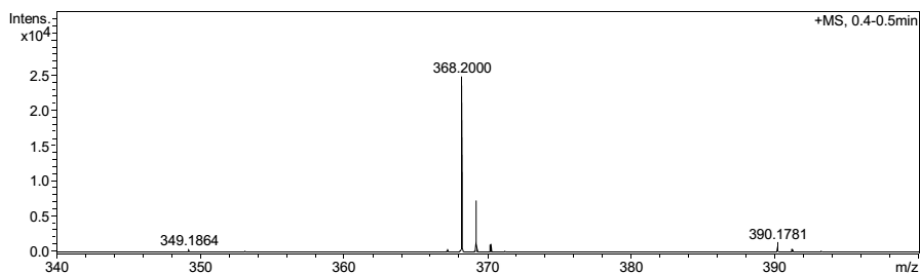
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 Comment

Acquisition Date 1/15/2015 2:26:09 PM

Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
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## Mass Spectrum SmartFormula Report

**Analysis Info**

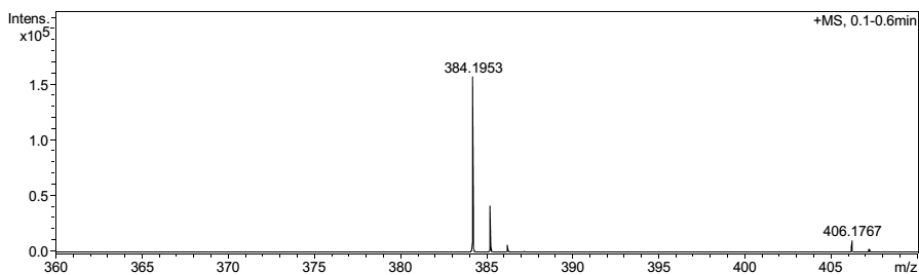
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Acquisition Date 1/15/2015 2:23:43 PM

Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
384.1953	1	C <sub>26</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>	100.00	384.1958	0.5	1.4	11.8	14.5	even	ok
406.1767	1	C <sub>26</sub> H <sub>25</sub> N <sub>2</sub> NaO <sub>2</sub>	100.00	406.1778	1.1	2.6	10.0	14.5	even	ok

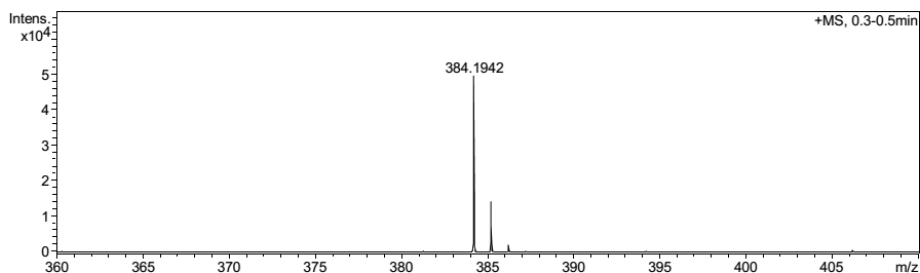


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Comment

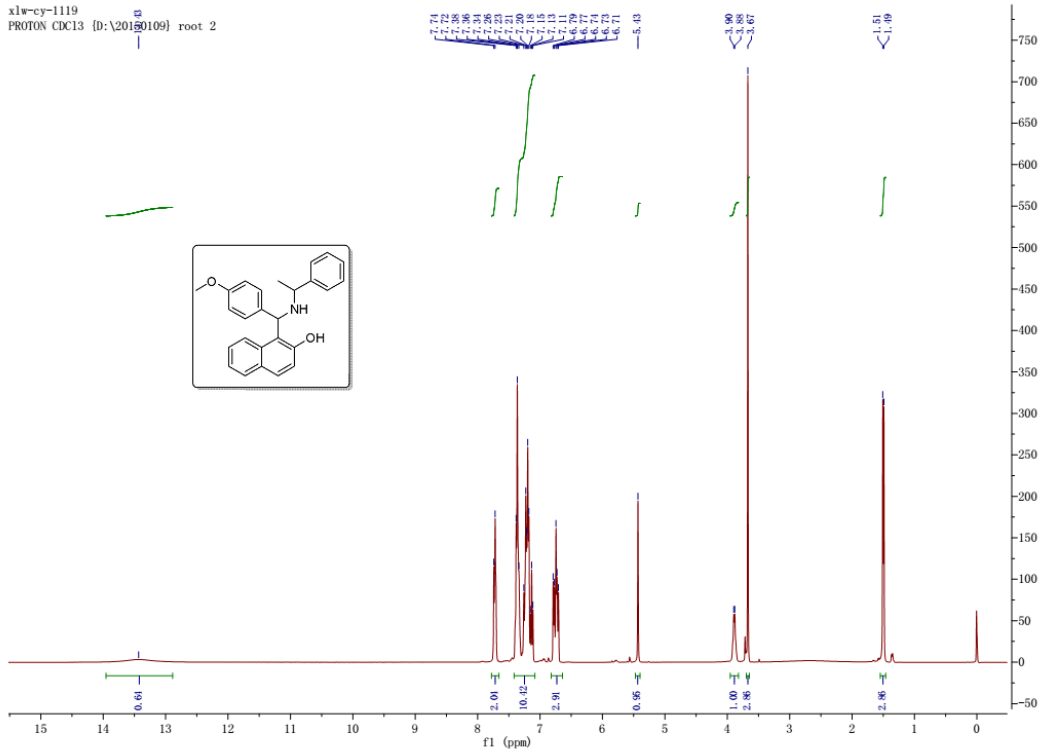
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Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

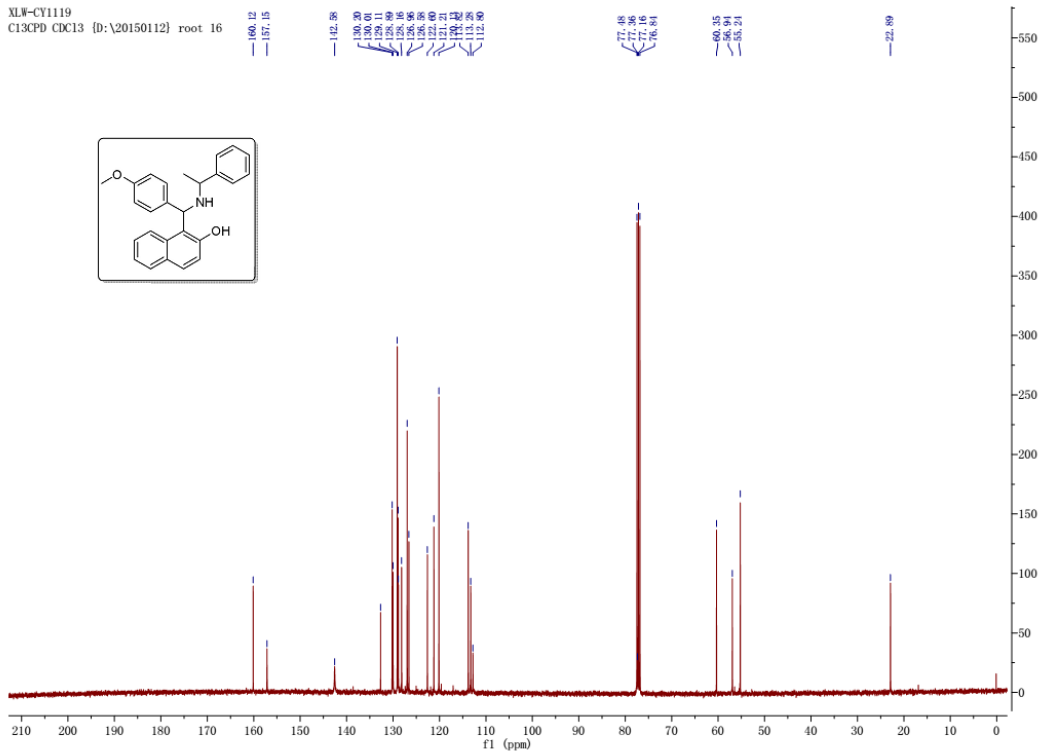


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
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XLW-CY1119  
C13CPD CDC13 {D:\20150112} root 16



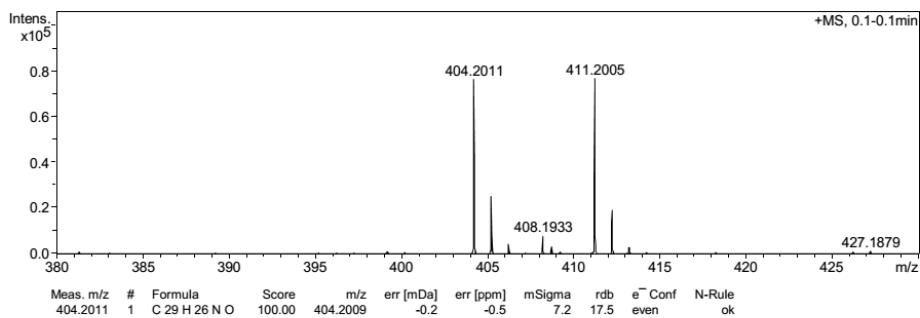


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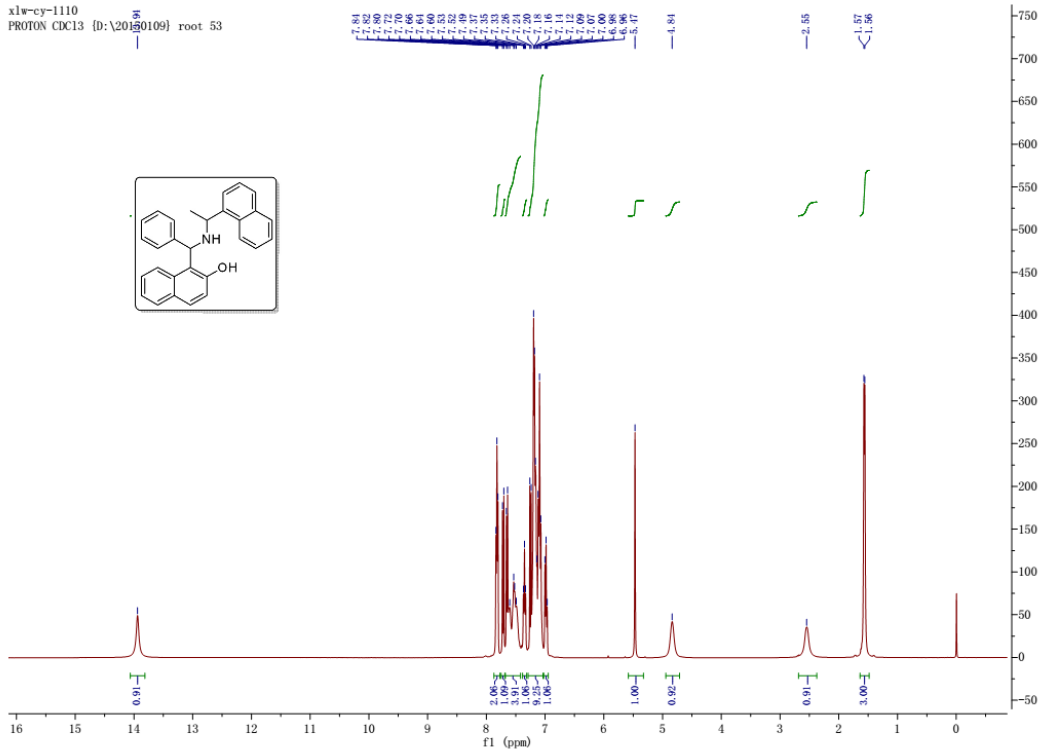
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Instrument / Ser#: micrOTOF-Q II 10324

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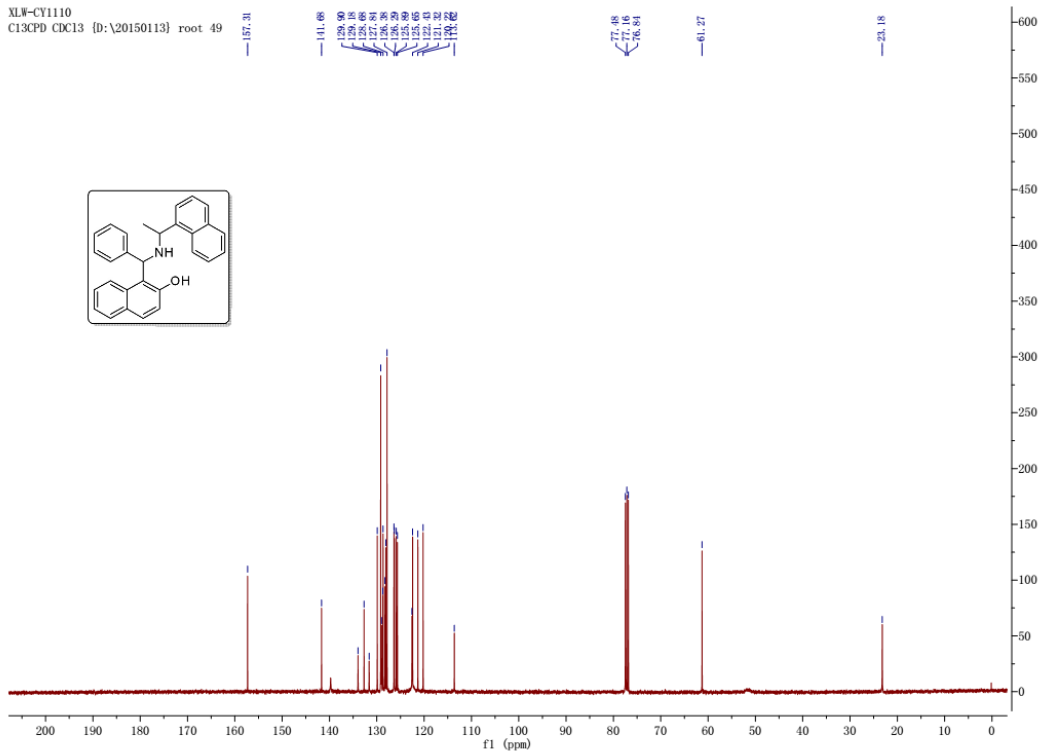
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Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



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XLW-CY1110  
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## Mass Spectrum SmartFormula Report

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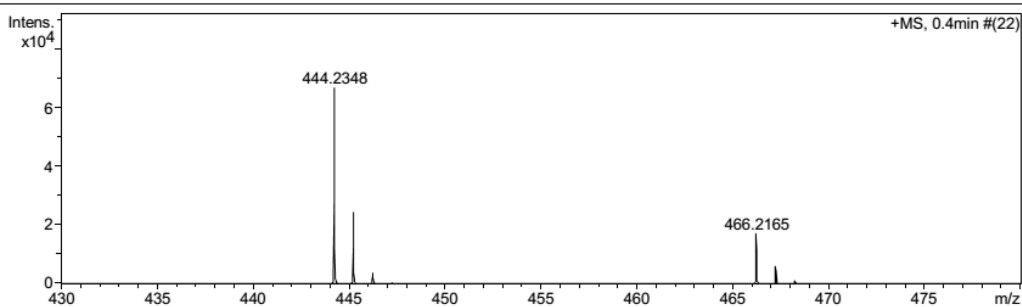
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Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

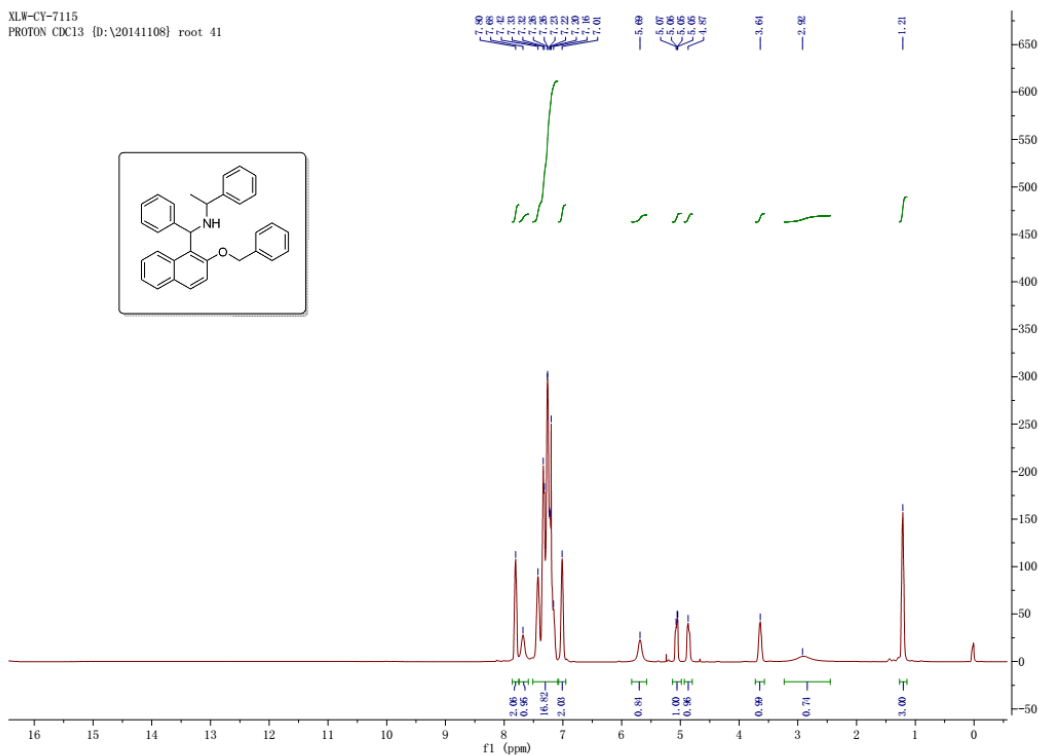
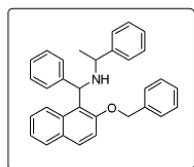
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Scan End	600 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

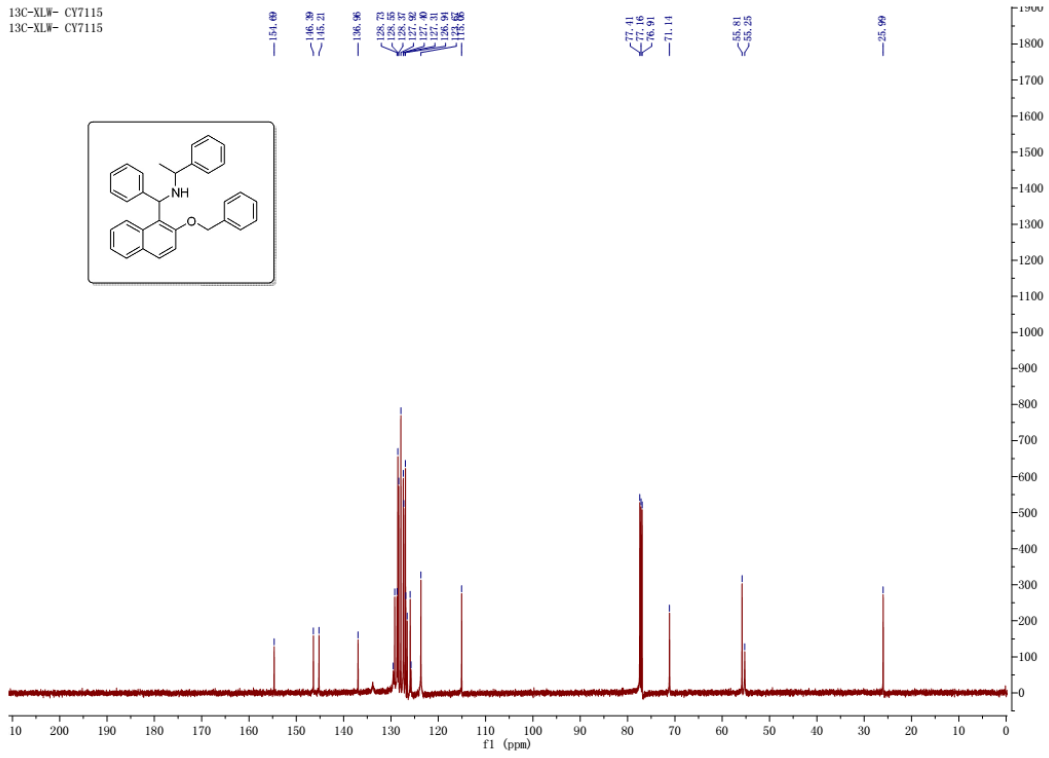


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466.2165	1	C 32 H 29 N Na O	28.64	466.2141	-2.4	-5.1	1.8	18.5	even	ok

XLW-CY-7115  
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13C-XLM- CY7115  
13C-XLM- CY7115

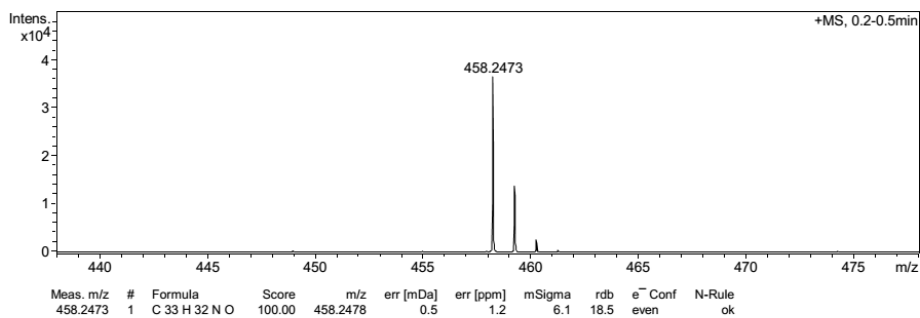


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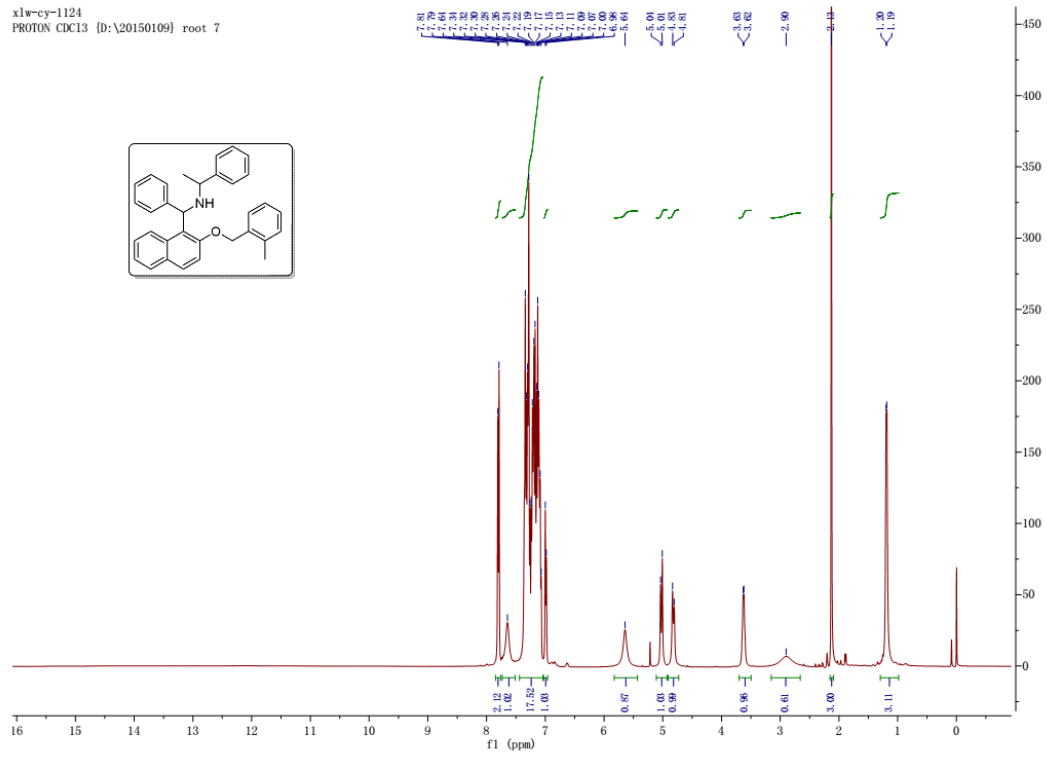
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Comment  
Acquisition Date 1/15/2015 2:07:04 PM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

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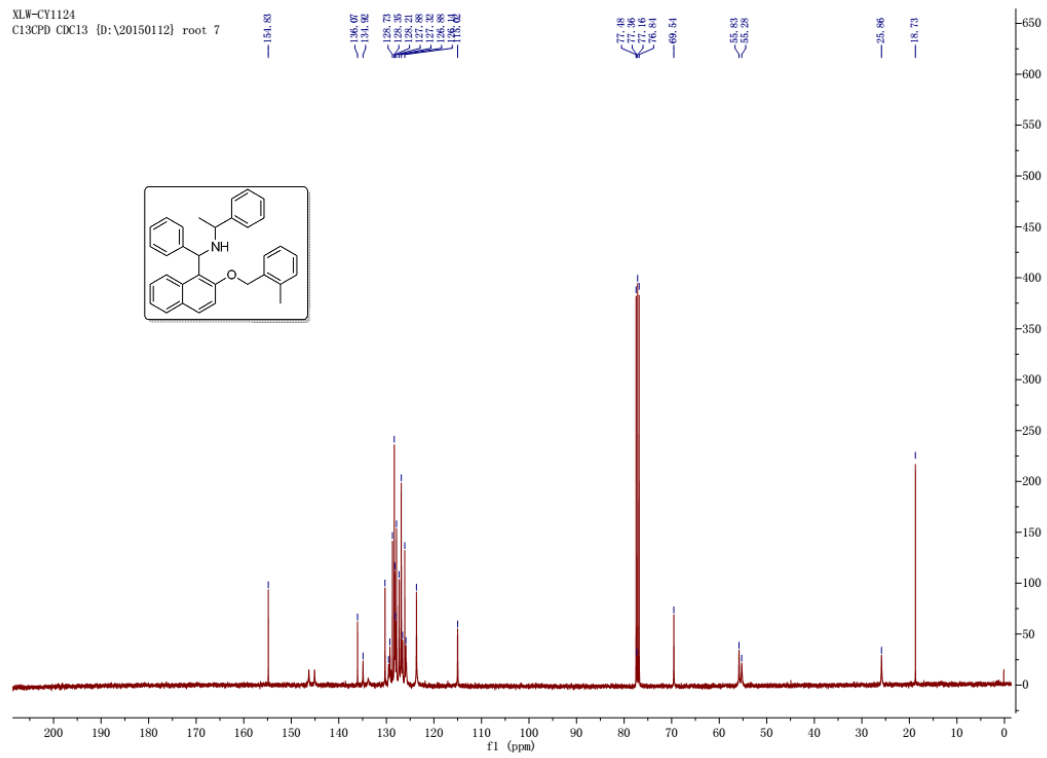
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xlw-cy-1124  
PROTON CDC13 {D:\20150109} root 7



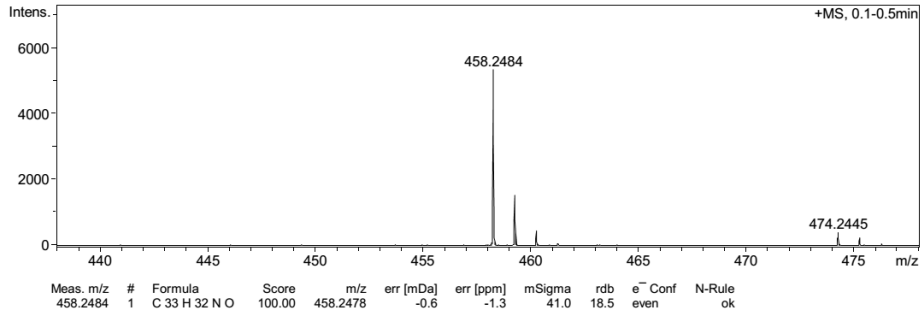
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Comment:  
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Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

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Ion Polarity: Positive  
Set Capillary: 4500 V  
Set End Plate Offset: -500 V  
Set Collision Cell RF: 120.0 Vpp  
Set Nebulizer: 0.4 Bar  
Set Dry Heater: 200 °C  
Set Dry Gas: 2.2 l/min  
Set Divert Valve: Source







## Mass Spectrum SmartFormula Report

**Analysis Info**

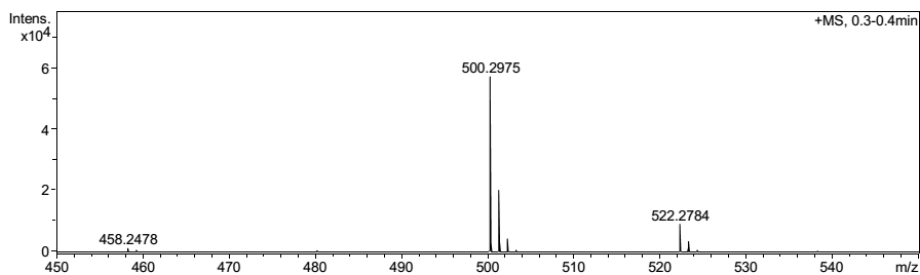
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 Comment

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Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

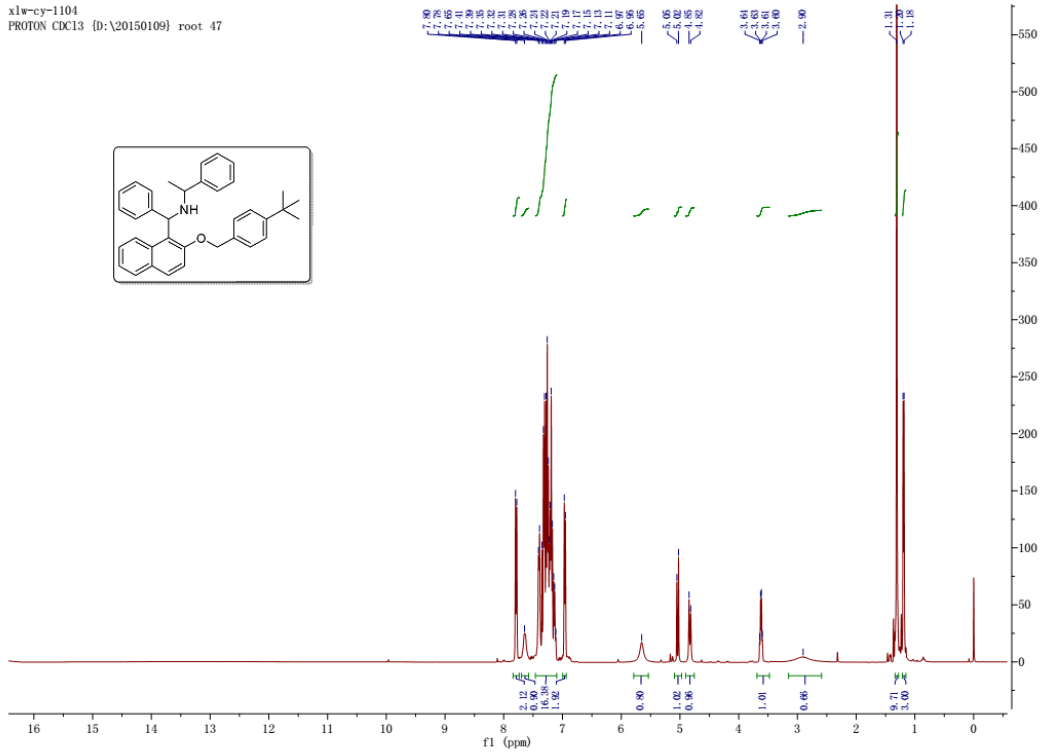
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Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

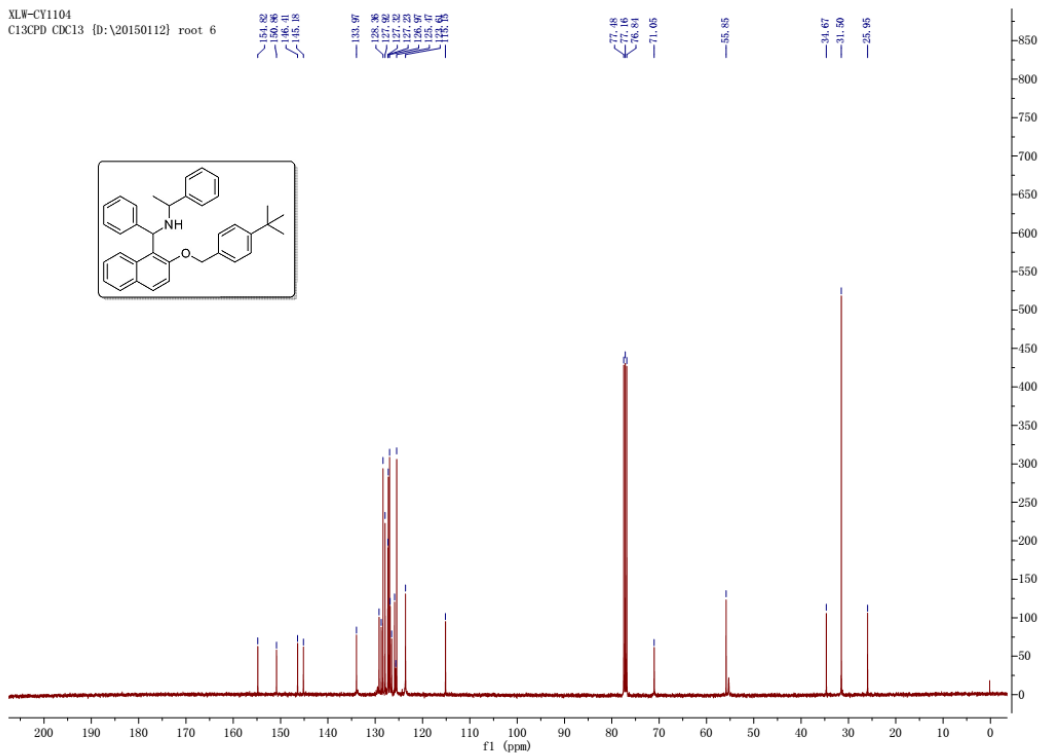


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522.2784	1	C 36 H 37 N Na O	100.00	522.2767	-1.6	-3.1	9.9	18.5	even	ok

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XLW-CY1104  
C13CPD CDC13 {D:\20150112} root 6

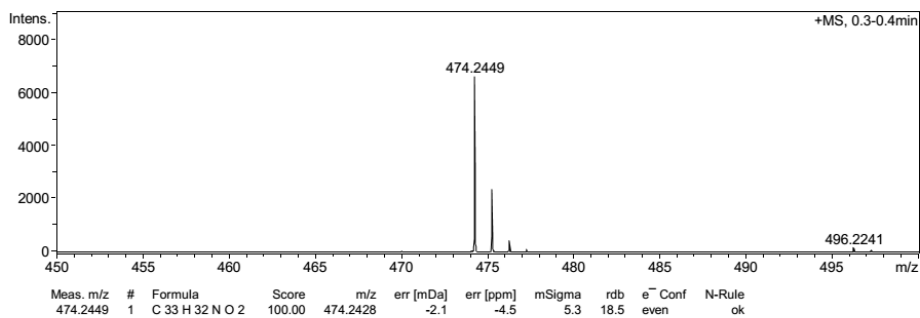


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Sample Name trz-7 Instrument / Ser# micrOTOF-Q II 10324  
Comment

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



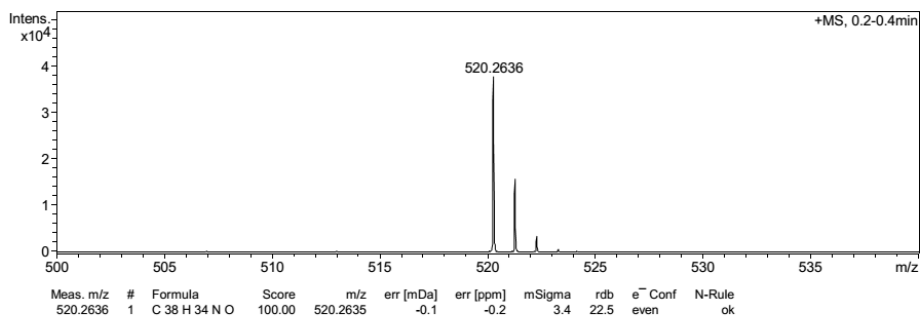


## Mass Spectrum SmartFormula Report

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Sample Name trz-7 Instrument / Ser# micrOTOF-Q II 10324  
Comment

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

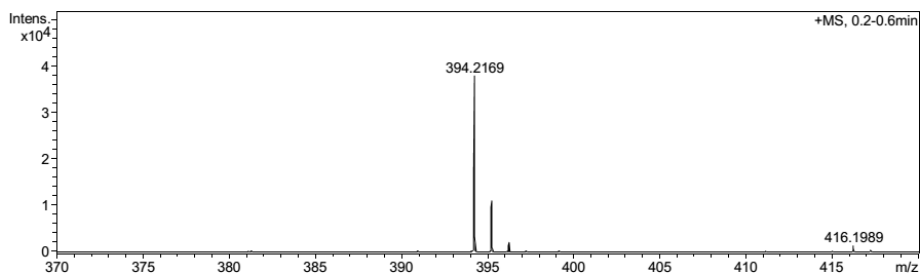




## Mass Spectrum SmartFormula Report

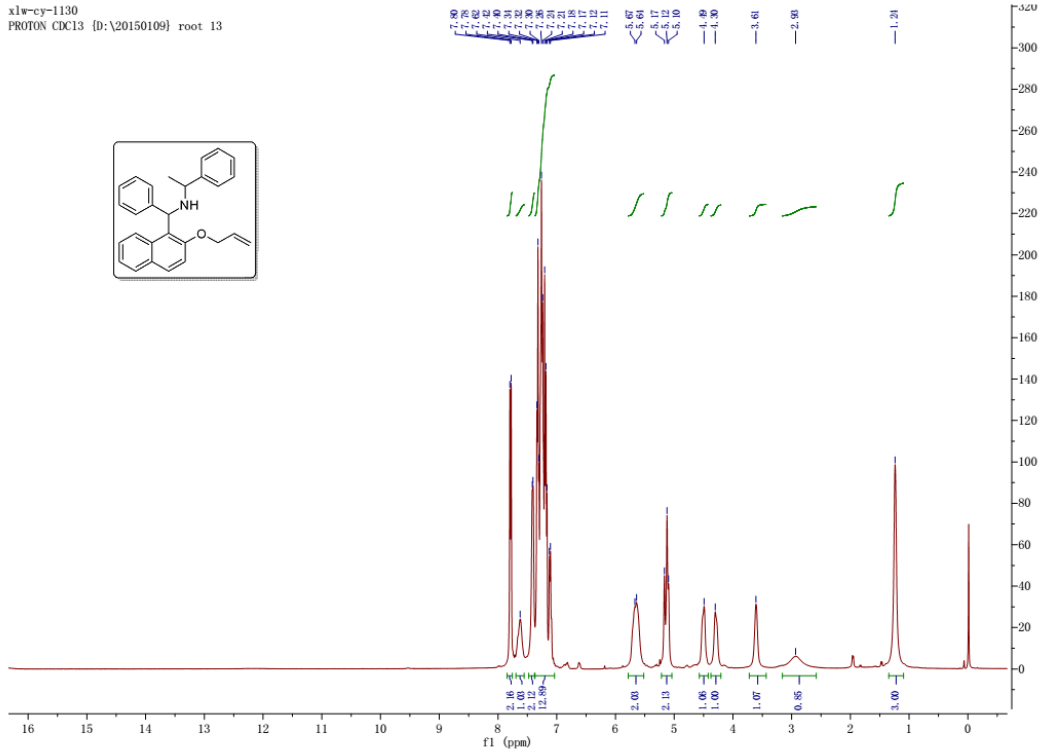
**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150115-wcy-1130\_01.d  
Method tune\_100-550\_pos150115.m  
Sample Name trz-7  
Comment  
Acquisition Date 1/15/2015 2:01:37 PM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**  
Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Active Set Capillary 4500 V Set Dry Heater 200 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 2.2 l/min  
Scan End 550 m/z Set Collision Cell RF 120.0 Vpp Set Divert Valve Source

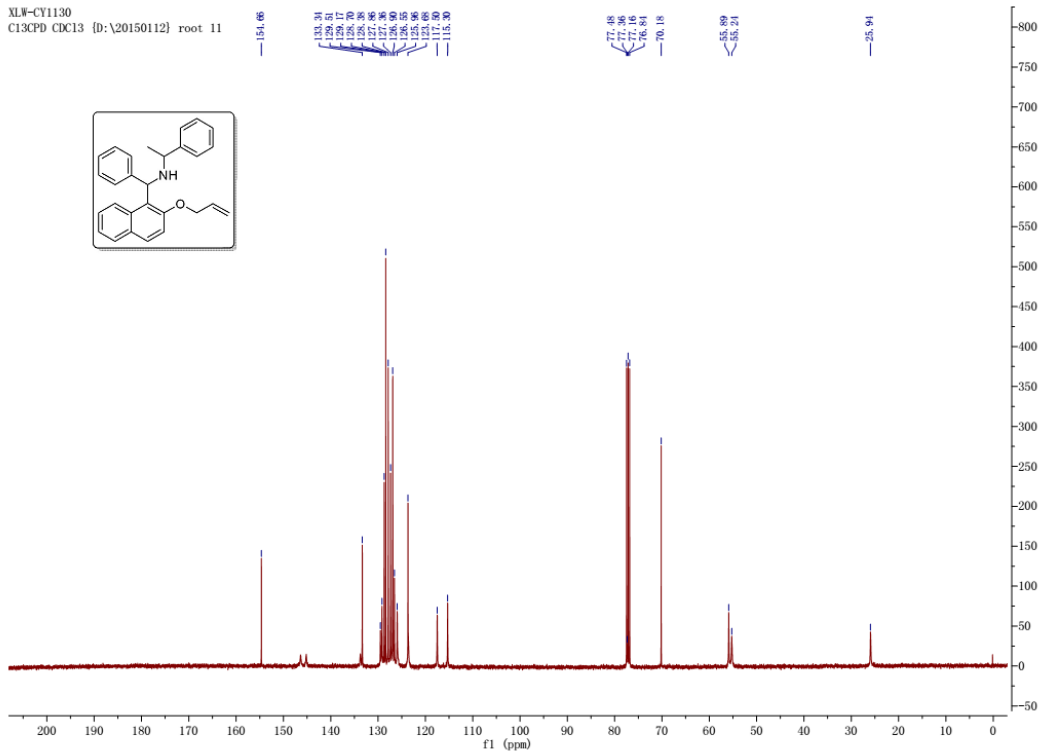


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
394.2169	1	C <sub>28</sub> H <sub>28</sub> N <sub>2</sub> O	100.00	394.2165	-0.3	-0.8	8.9	15.5	even	ok

xlw-cy-1130  
PROTON CDC13 {D:\20150109} root 13



XLW-CY1130  
C13CPD CDC13 {D:\20150112} root 11





## Mass Spectrum SmartFormula Report

**Analysis Info**

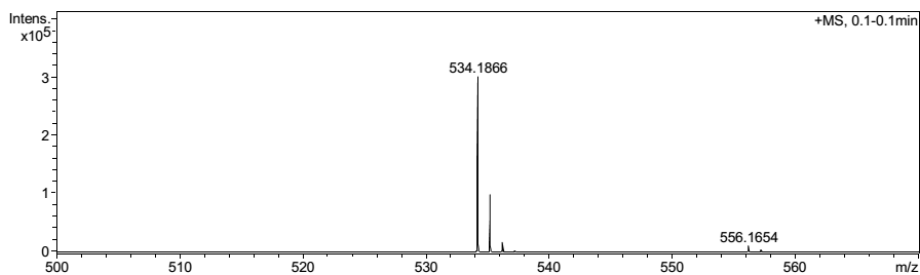
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150115-wcy-1143\_03.d  
 Method tune\_100-550\_pos150115.m  
 Sample Name trz-7  
 Comment

Acquisition Date 1/15/2015 2:47:25 PM

Operator Jiang  
 Instrument / Ser# micrOTOF-Q II 10324

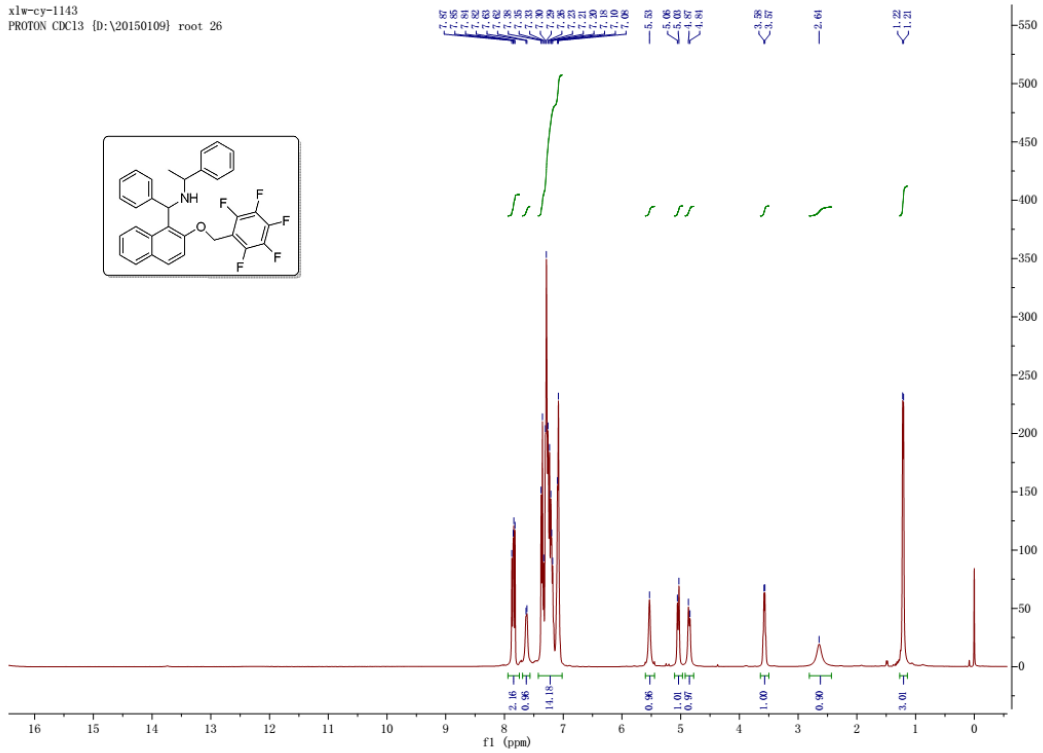
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	600 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

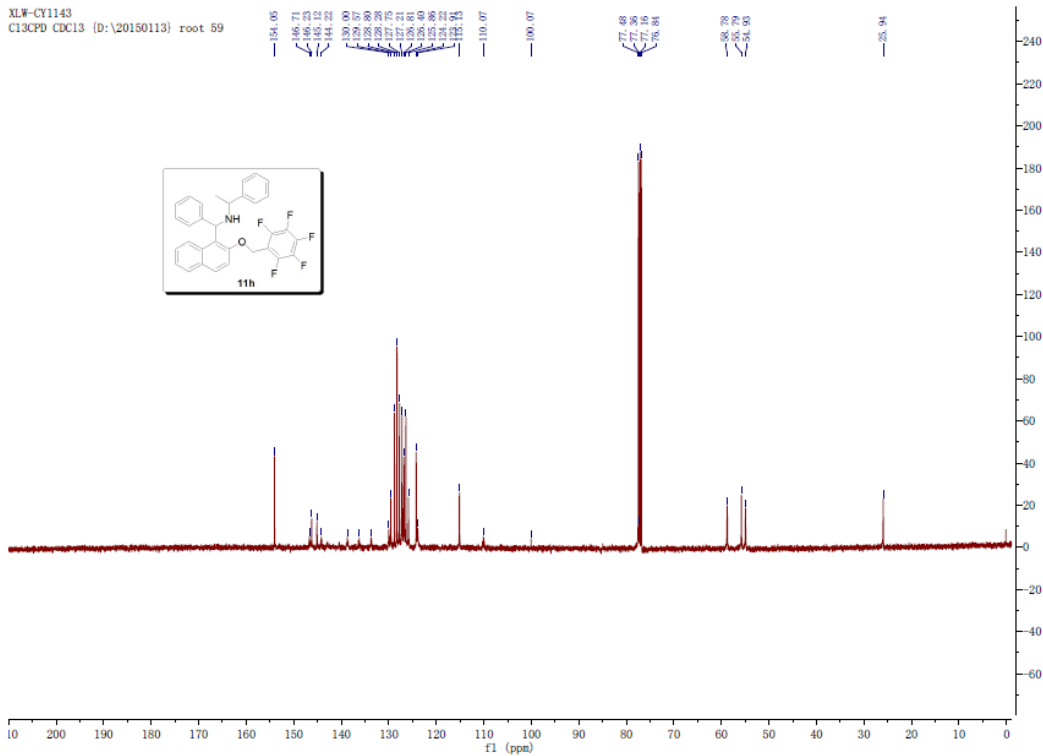


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
534.1866	1	C <sub>32</sub> H <sub>25</sub> F <sub>5</sub> N <sub>1</sub> O	100.00	534.1851	-1.5	-2.8	11.1	18.5	even	ok
556.1654	1	C <sub>32</sub> H <sub>24</sub> F <sub>5</sub> N <sub>1</sub> NaO	100.00	556.1670	1.6	2.8	14.2	18.5	even	ok

xlw-cy-1143  
PROTON CDC13 {D:\20150109} root 26



XLW-CY1143  
C13CPD CDC13 {D:\20150113} root 59



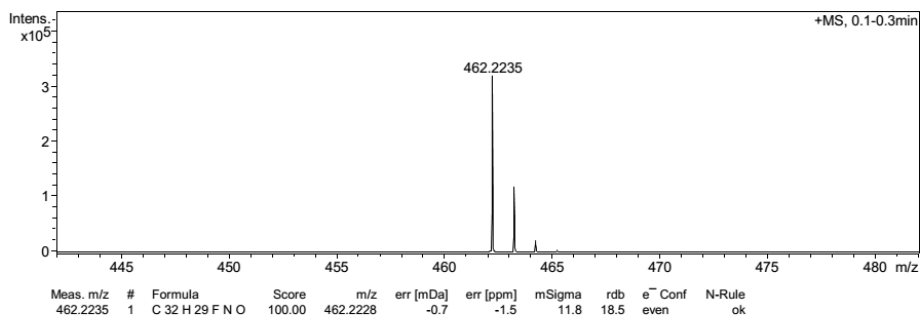


## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150115-wcy-1145\_01.d Acquisition Date 1/15/2015 2:49:58 PM  
Method tune\_100-550\_pos150115.m Operator Jiang  
Sample Name trz-7 Instrument / Ser# micrOTOF-Q II 10324  
Comment

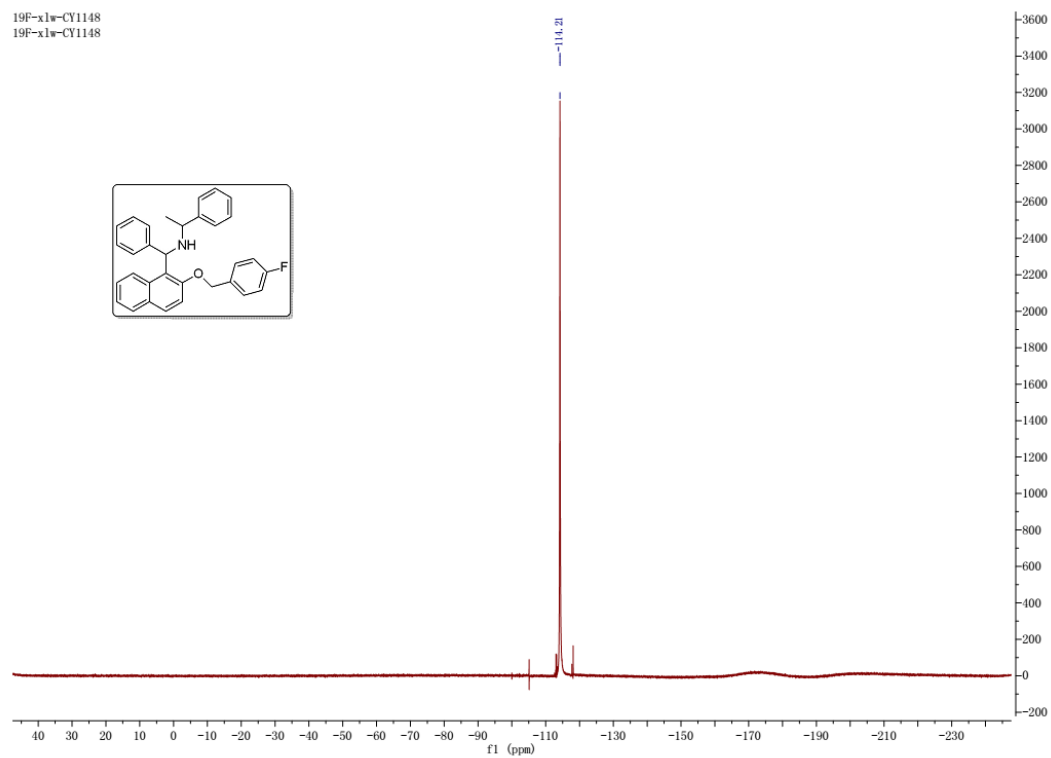
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	600 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source





19F-xlw-CY1148  
19F-xlw-CY1148



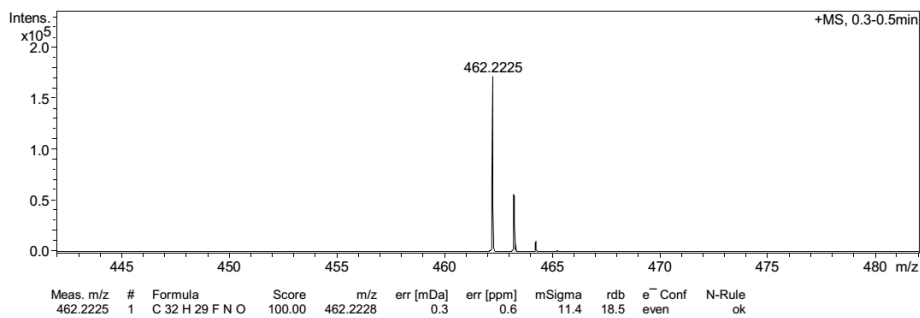
## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-9\_01.d  
Method tune\_100-550\_pos150120.m  
Sample Name  
Comment

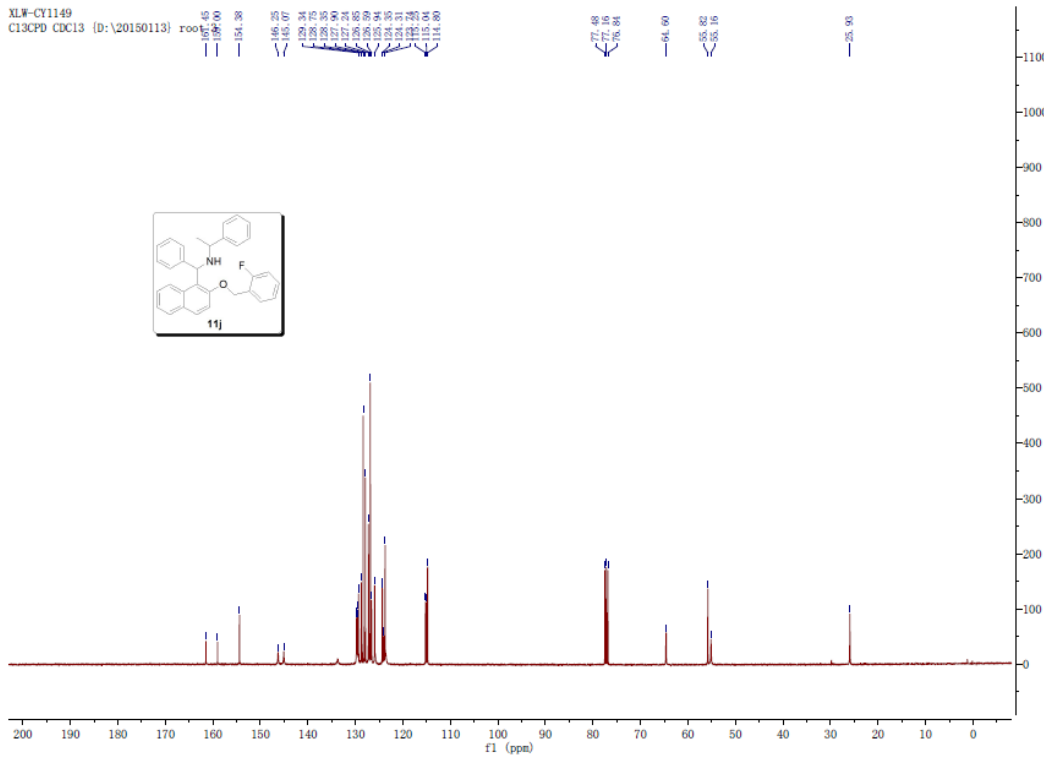
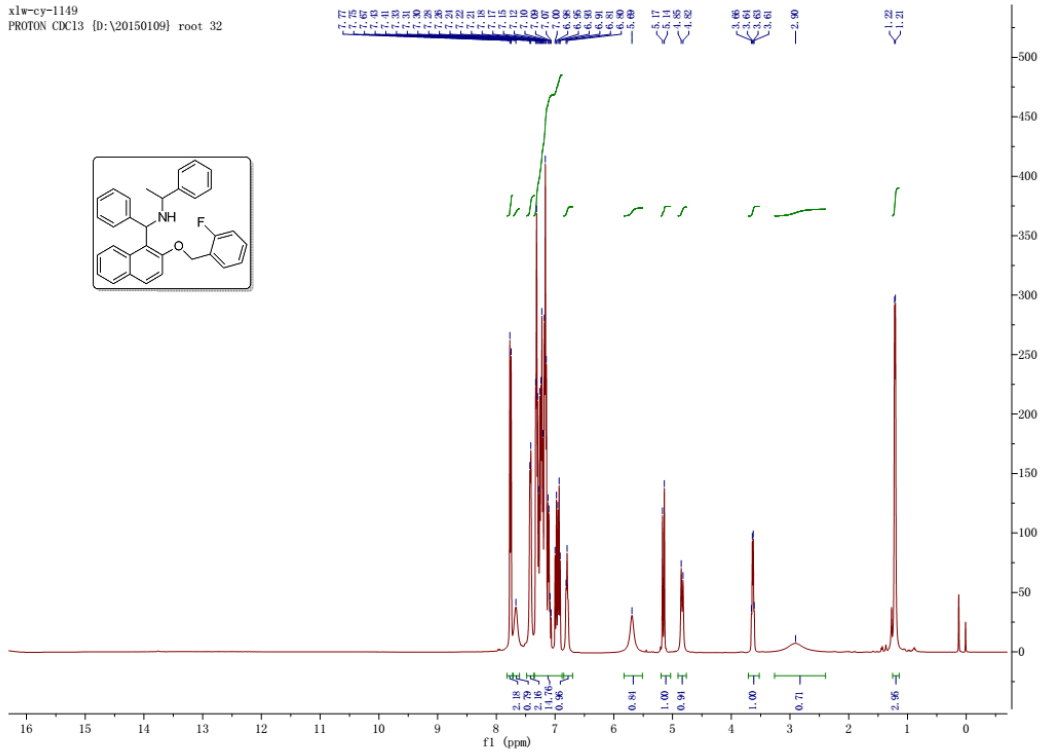
Acquisition Date 1/20/2015 3:03:21 PM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

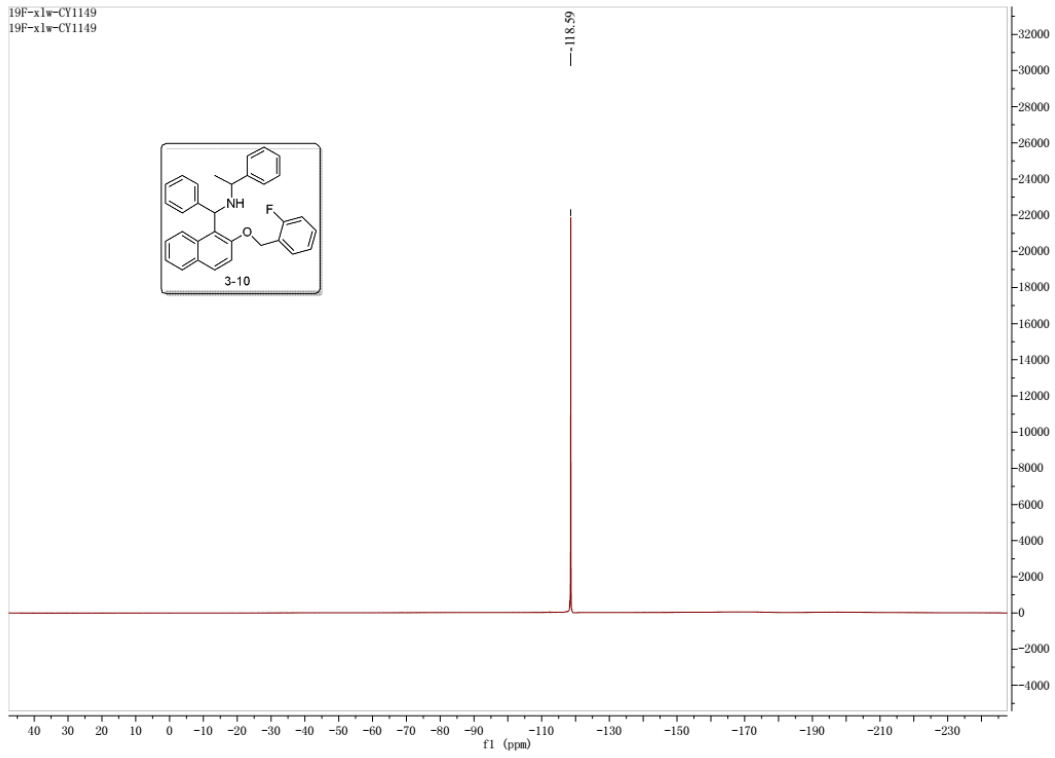
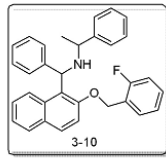


xlw-cy-1149  
PROTON CDC13 [D:\20150109] root 32





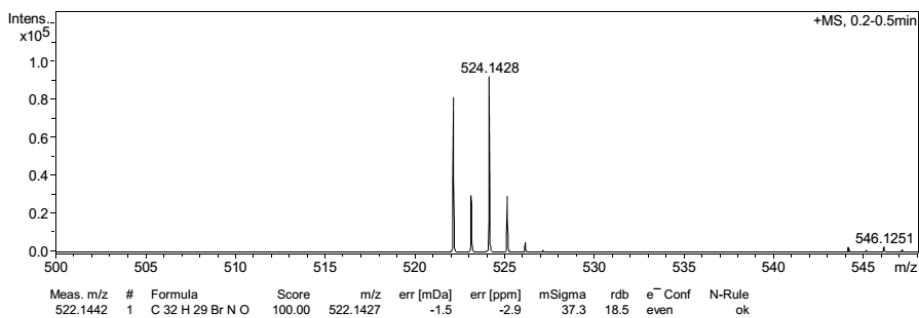
19F-xlw-CY1149  
19F-xlw-CY1149



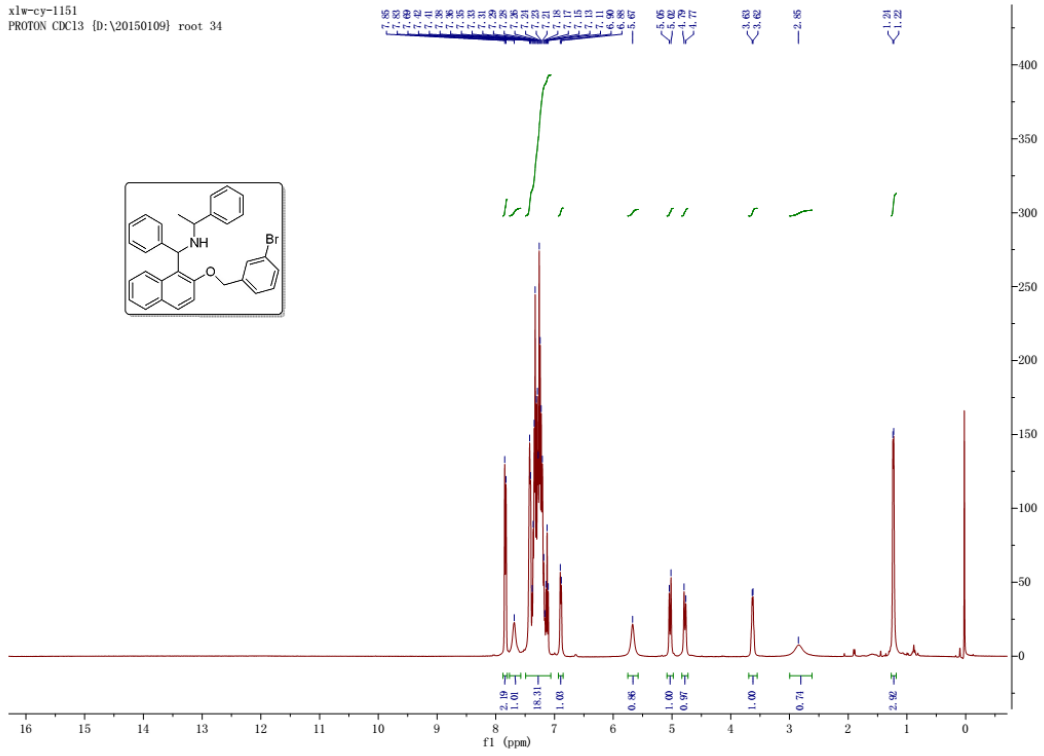
# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150115-wcy-1151\_01.d  
Method: tune\_100-550\_pos150115.m  
Sample Name: trz-7  
Comment:  
Acquisition Date: 1/15/2015 1:52:55 PM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

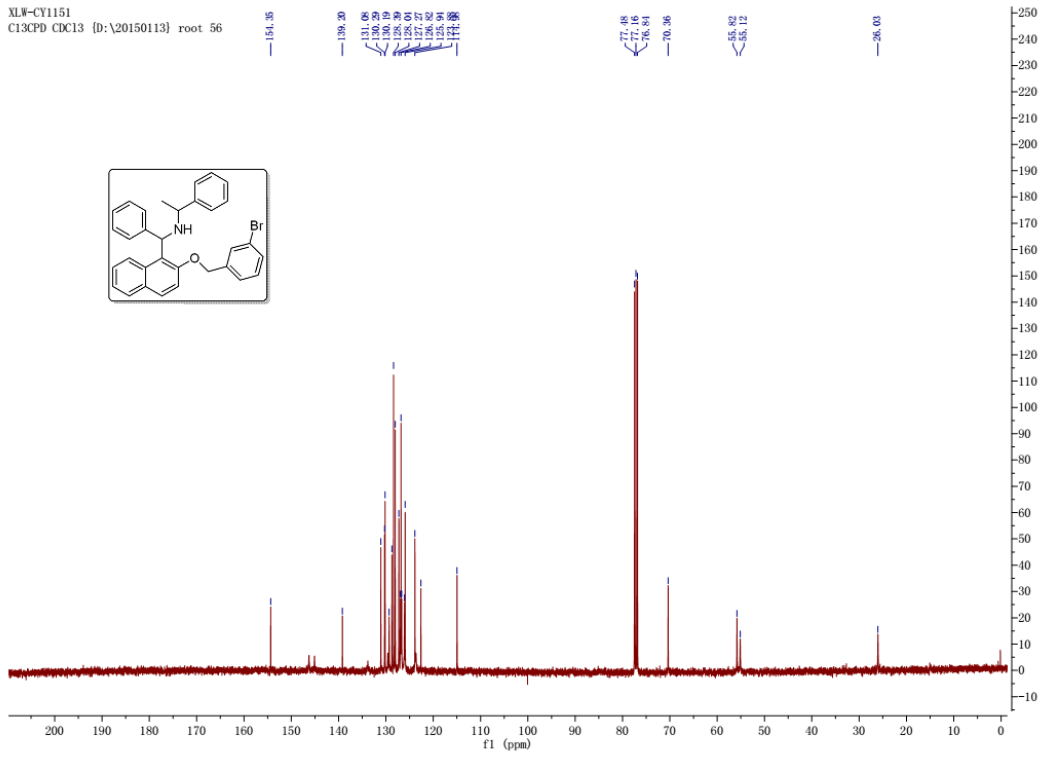
**Acquisition Parameter**  
Source Type: ESI  
Focus: Active  
Scan Begin: 50 m/z  
Scan End: 550 m/z  
Ion Polarity: Positive  
Set Capillary: 4500 V  
Set End Plate Offset: -500 V  
Set Collision Cell RF: 120.0 Vpp  
Set Nebulizer: 0.4 Bar  
Set Dry Heater: 200 °C  
Set Dry Gas: 2.2 l/min  
Set Divert Valve: Source



xlw-cy-1151  
PROTON CDC13 {D:\20150109} root 34



XLW-CY1151  
C13CPD CDC13 {D:\20150113} root 56

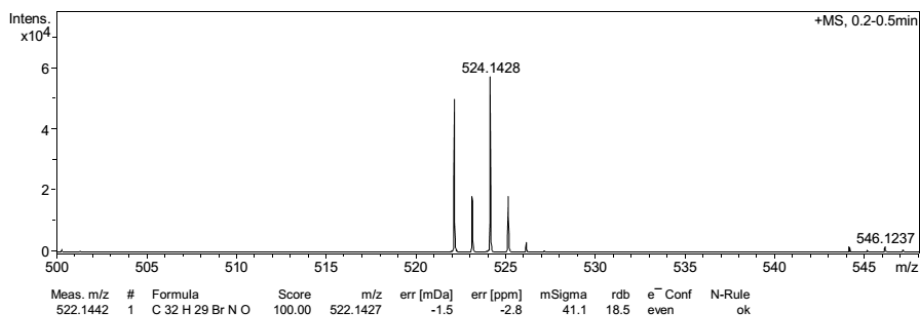


## Mass Spectrum SmartFormula Report

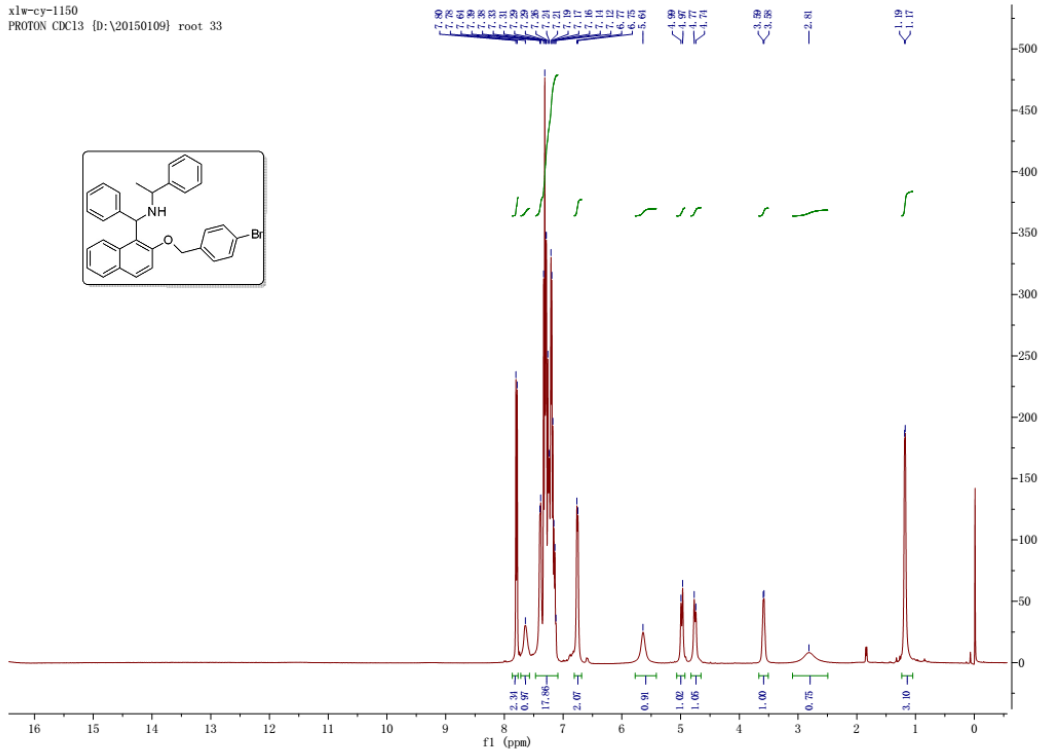
**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150115-wcy-1150\_01.d Acquisition Date 1/15/2015 1:58:44 PM  
Method tune\_100-550\_pos150115.m Operator Jiang  
Sample Name trz-7 Instrument / Ser# micrOTOF-Q II 10324  
Comment

**Acquisition Parameter**

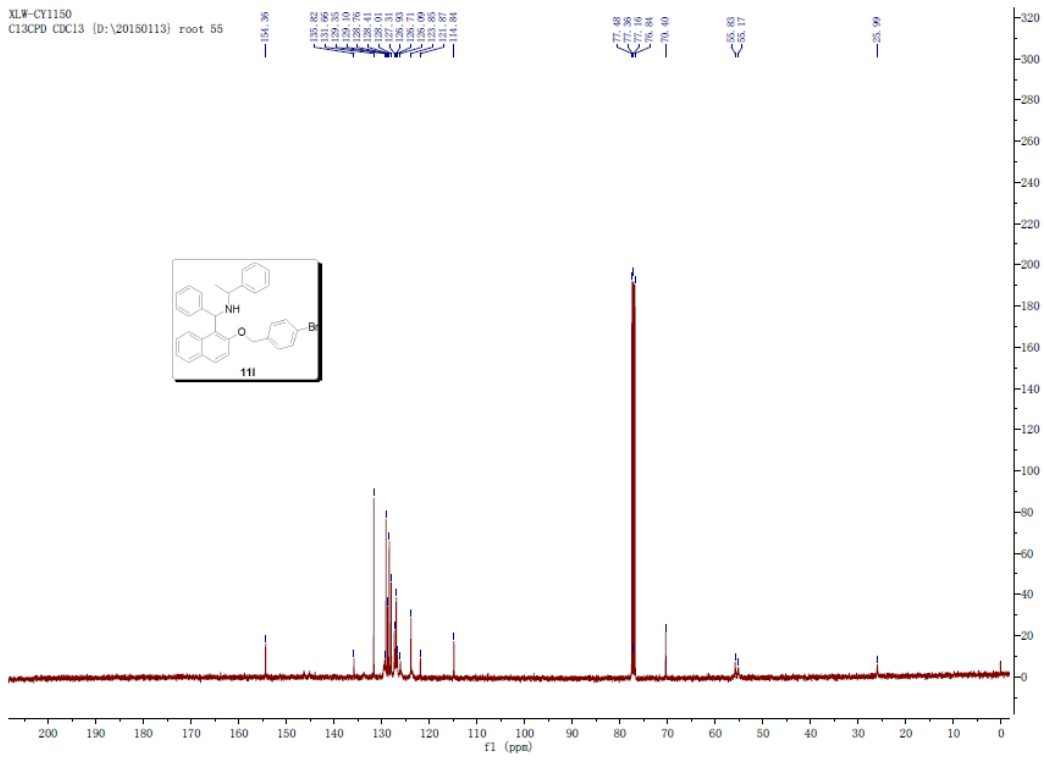
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



xlw-cy-1150  
PROTON CDC13 {D:\20150109} root 33



XLW-CY1150  
C13CPD CDC13 {D:\20150113} root 55

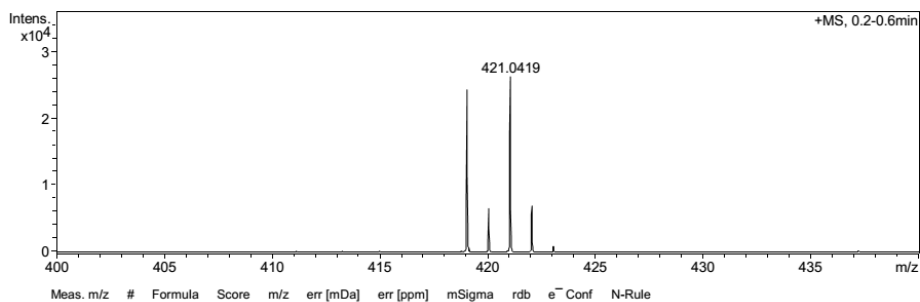


## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150115-wcy-1152\_01.d  
Method tune\_100-550\_pos150115.m  
Sample Name trz-7  
Comment  
Acquisition Date 1/15/2015 2:52:41 PM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

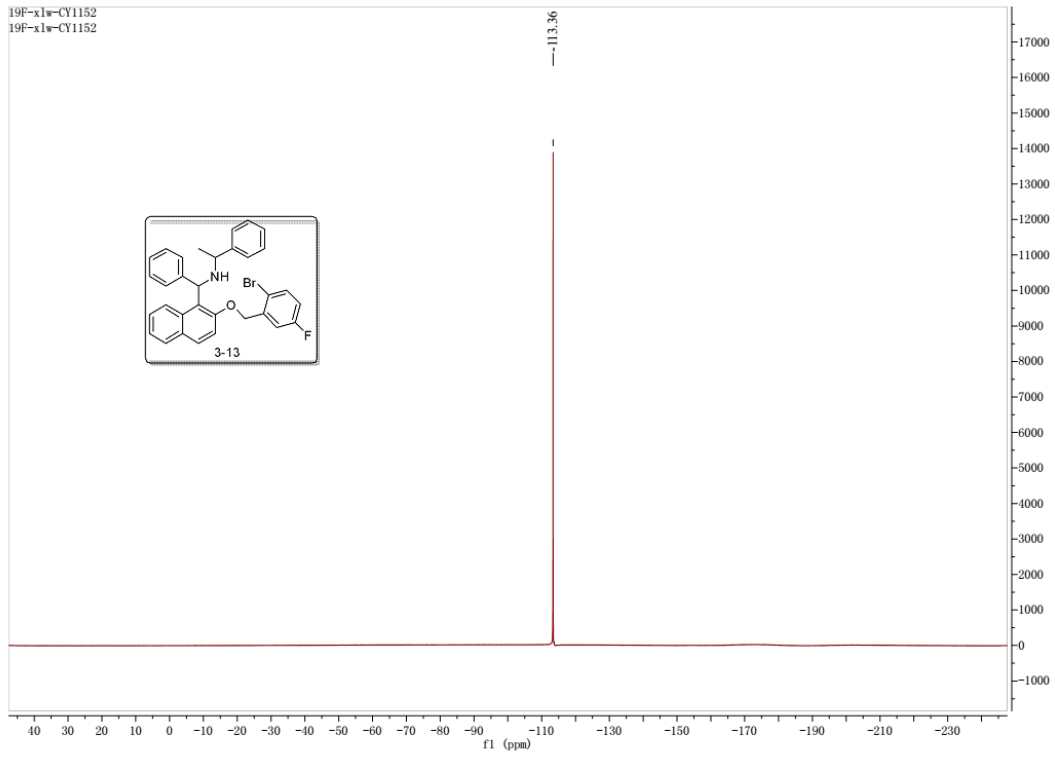
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	600 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source





19F-xlw-CY1152  
19F-xlw-CY1152





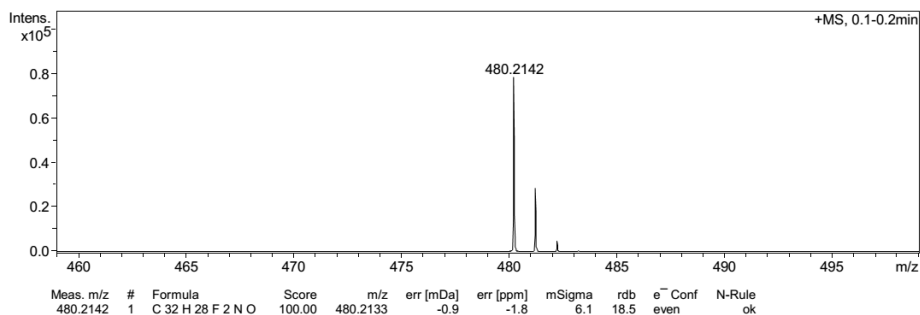
## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-7\_01.d  
Method tune\_100-550\_pos150120.m  
Sample Name  
Comment

Acquisition Date 1/20/2015 2:51:37 PM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

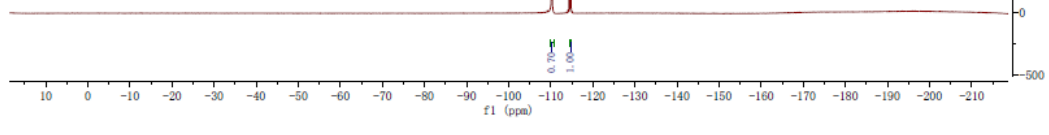
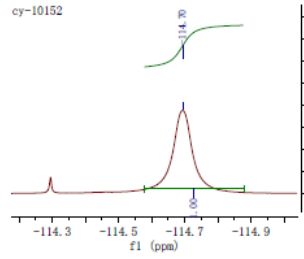
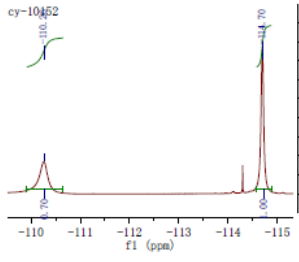
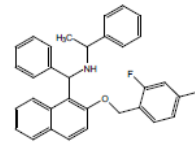
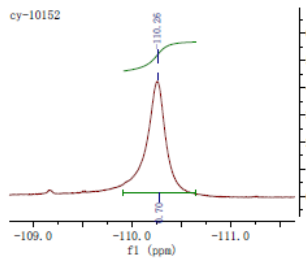
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source





cy-10152



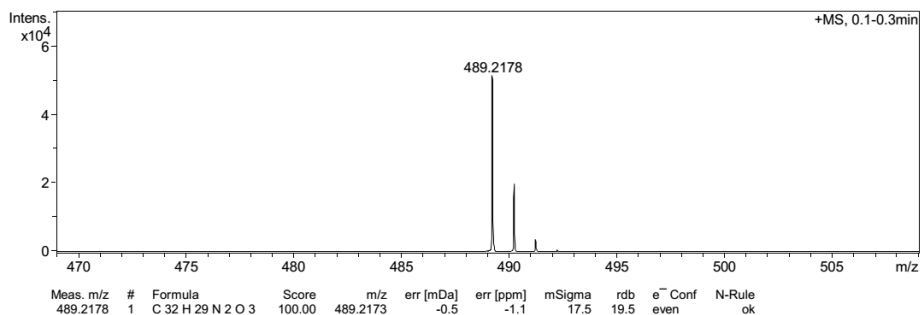
## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-4\_01.d  
Method tune\_100-550\_pos150120.m  
Sample Name  
Comment

Acquisition Date 1/20/2015 2:55:33 PM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



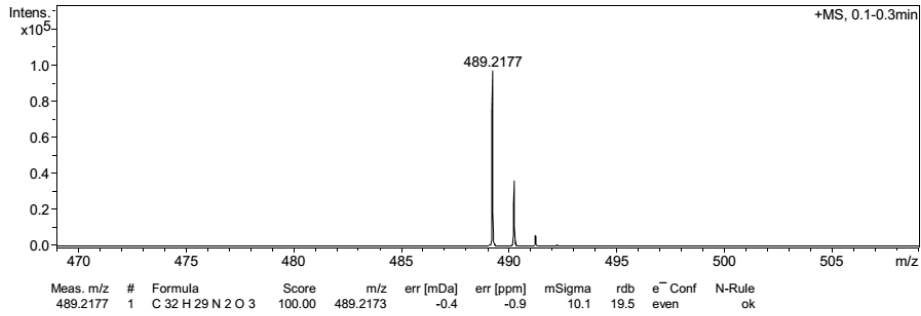


# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-8\_01.d  
Method: tune\_100-550\_pos150120.m  
Sample Name:  
Comment:  
Acquisition Date: 1/20/2015 3:01:31 PM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



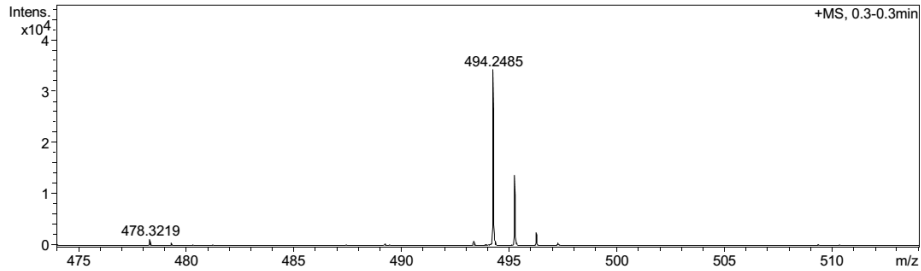


# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-3\_01.d  
Method: tune\_100-550\_pos150120.m  
Sample Name:  
Comment:  
Acquisition Date: 1/20/2015 2:49:07 PM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

**Acquisition Parameter**

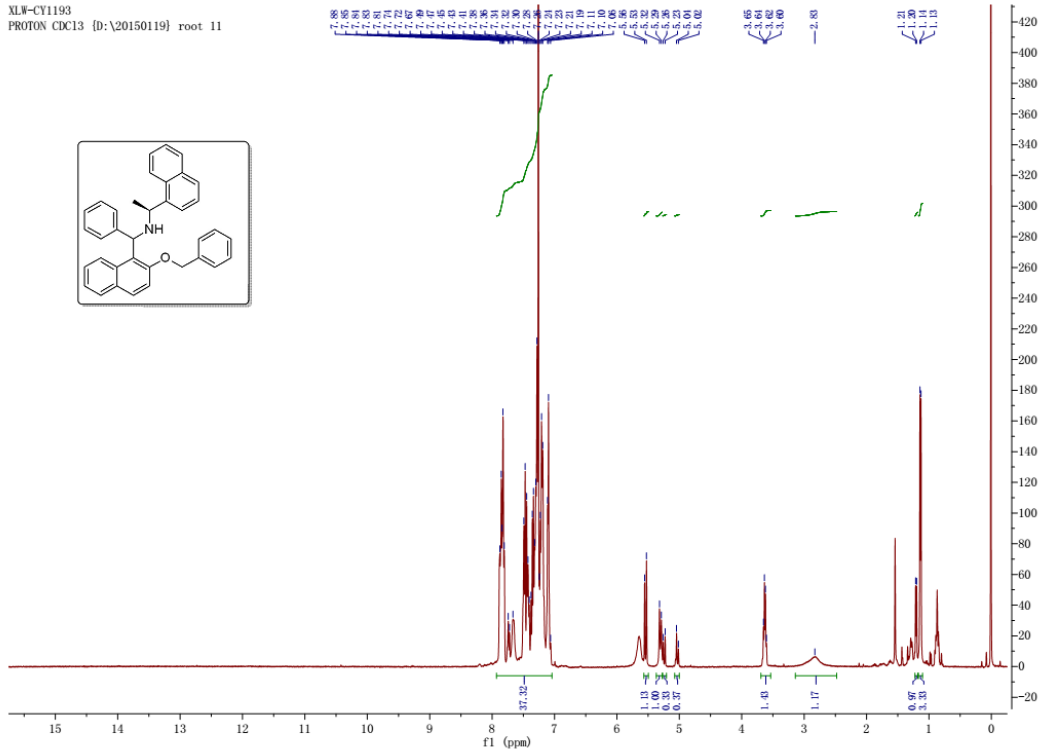
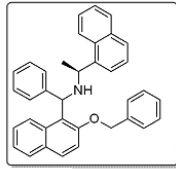
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



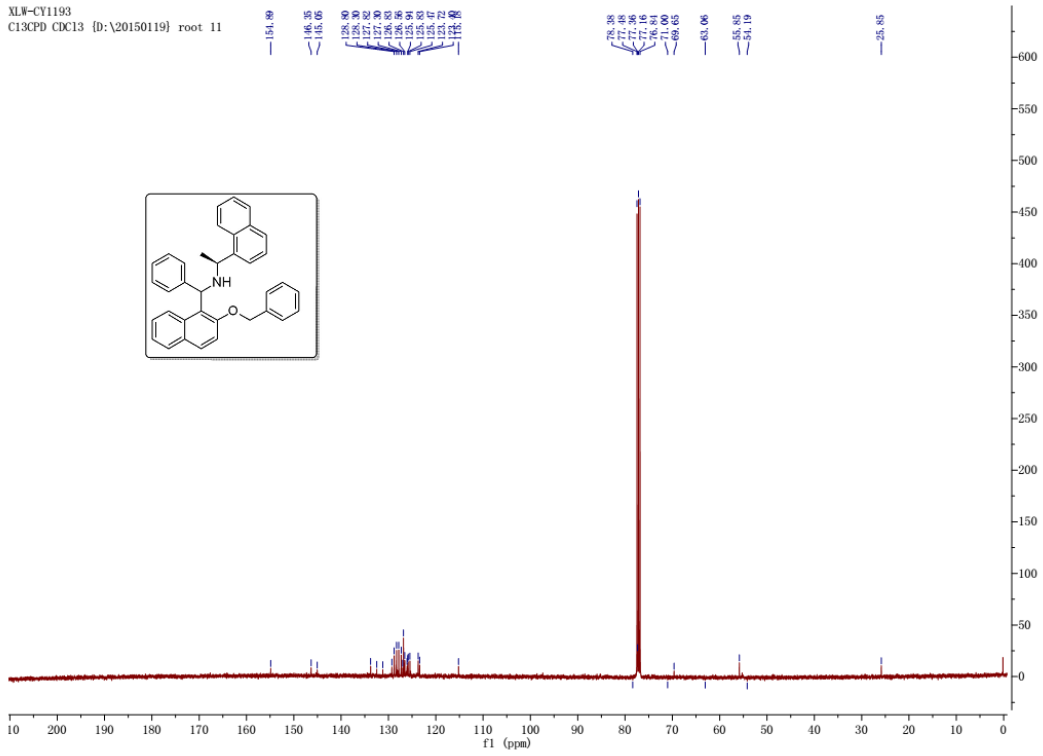
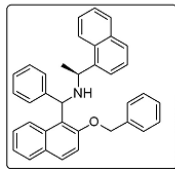
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
494.2485	1	C <sub>36</sub> H <sub>32</sub> N <sub>2</sub> O	100.00	494.2478	-0.7	-1.3	3.8	21.5	even	ok



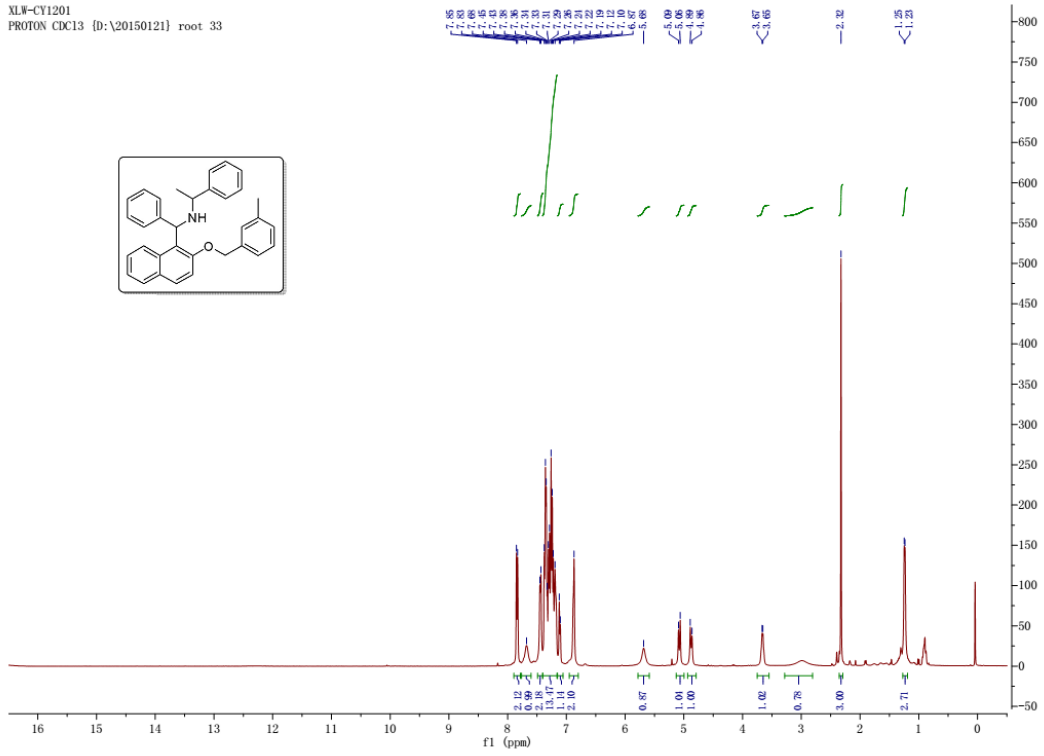
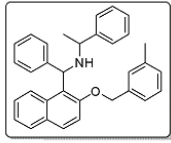
XLW-CY1193  
PROTON CDC13 {D:\20150119} root 11



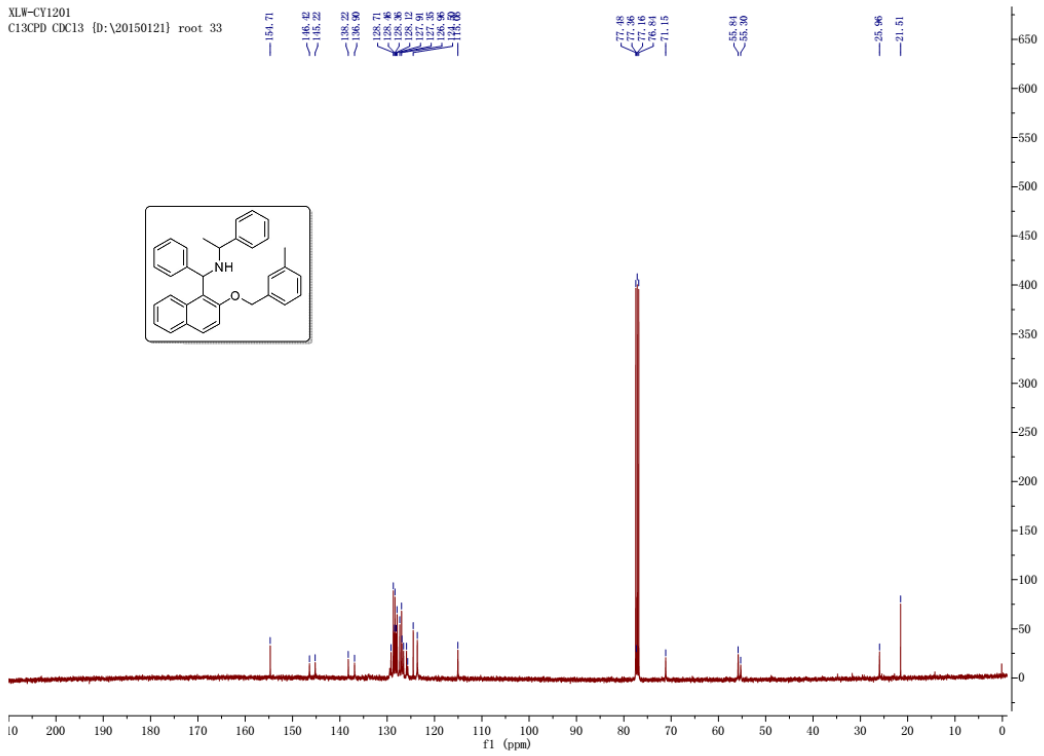
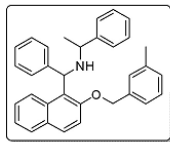
XLW-CY1193  
C13CPD CDC13 {D:\20150119} root 11



XLW-CY1201  
PROTON CDC13 {D:\20150121} root 33



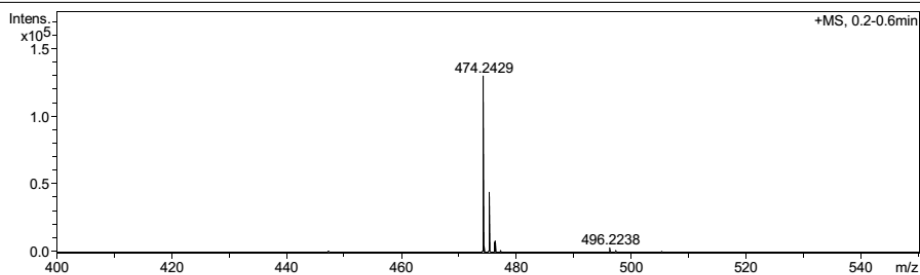
XLW-CY1201  
C13CPD CDC13 {D:\20150121} root 33



# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150205-cy1252\_01.d  
Method: tune\_100-550\_pos150205.m  
Sample Name: wxy1501-3  
Acquisition Date: 2/5/2015 9:44:08 AM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324  
Comment:

**Acquisition Parameter**  
Source Type: ESI  
Focus: Active  
Scan Begin: 50 m/z  
Scan End: 550 m/z  
Ion Polarity: Positive  
Set Capillary: 4500 V  
Set End Plate Offset: -500 V  
Set Collision Cell RF: 120.0 Vpp  
Set Nebulizer: 0.4 Bar  
Set Dry Heater: 200 °C  
Set Dry Gas: 2.2 l/min  
Set Divert Valve: Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
474.2429	1	C <sub>33</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>	100.00	474.2428	-0.2	-0.4	11.0	18.5	even	ok

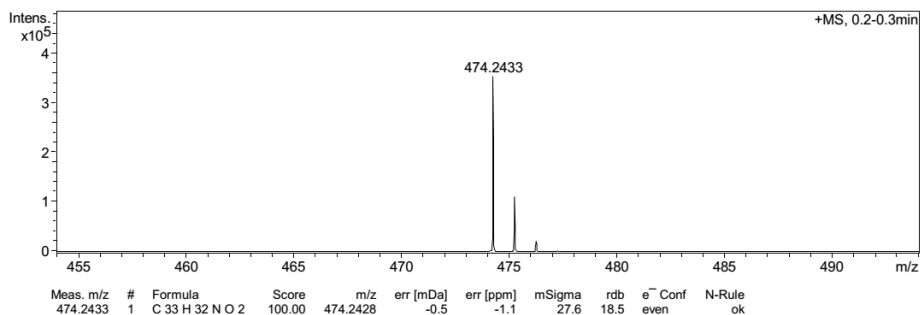


# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150123-wcy-1216\_01.d  
Method: tune\_100-550\_pos150120.m  
Sample Name:  
Comment:  
Acquisition Date: 1/23/2015 10:49:23 AM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

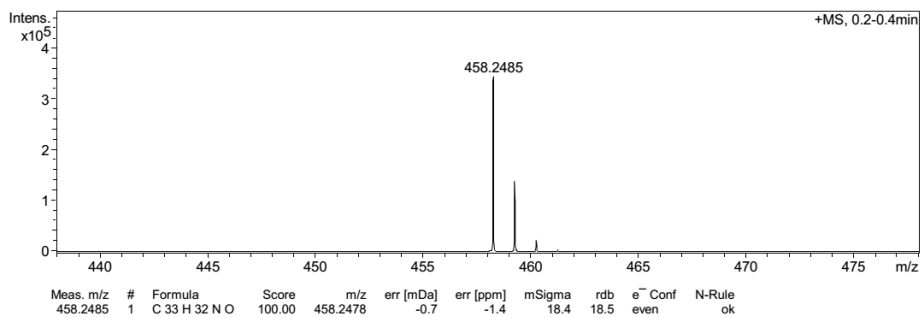




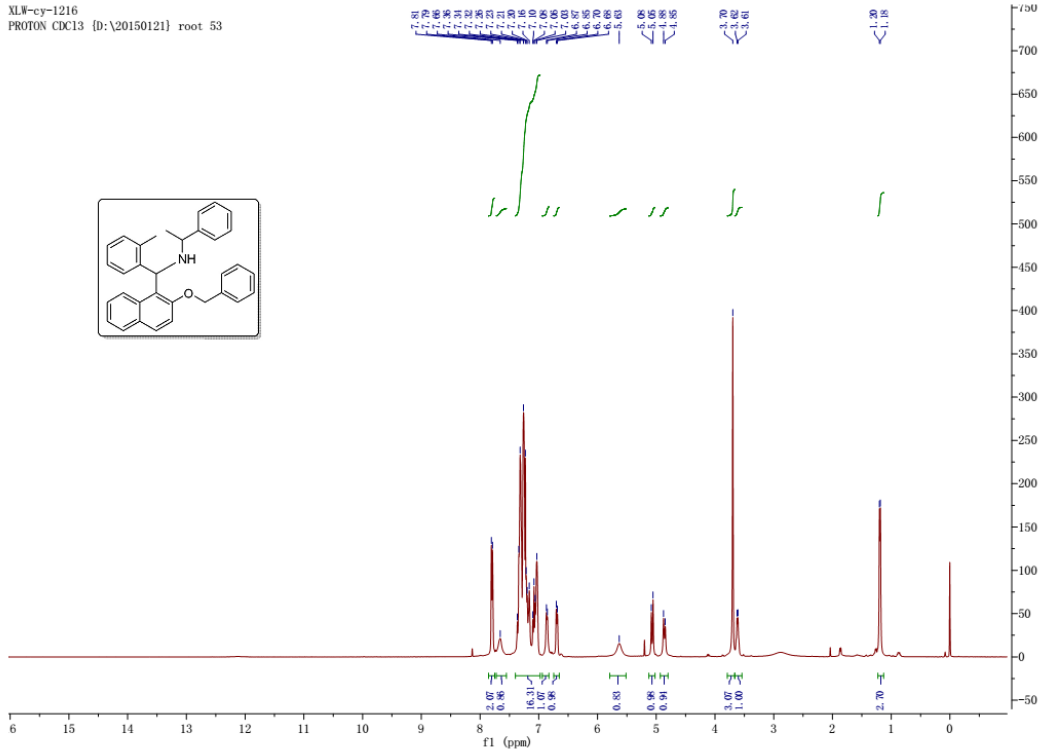
# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150123-wcy-1215\_01.d  
Method: tune\_100-550\_pos150120.m  
Sample Name:  
Comment:  
Acquisition Date: 1/23/2015 10:47:31 AM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

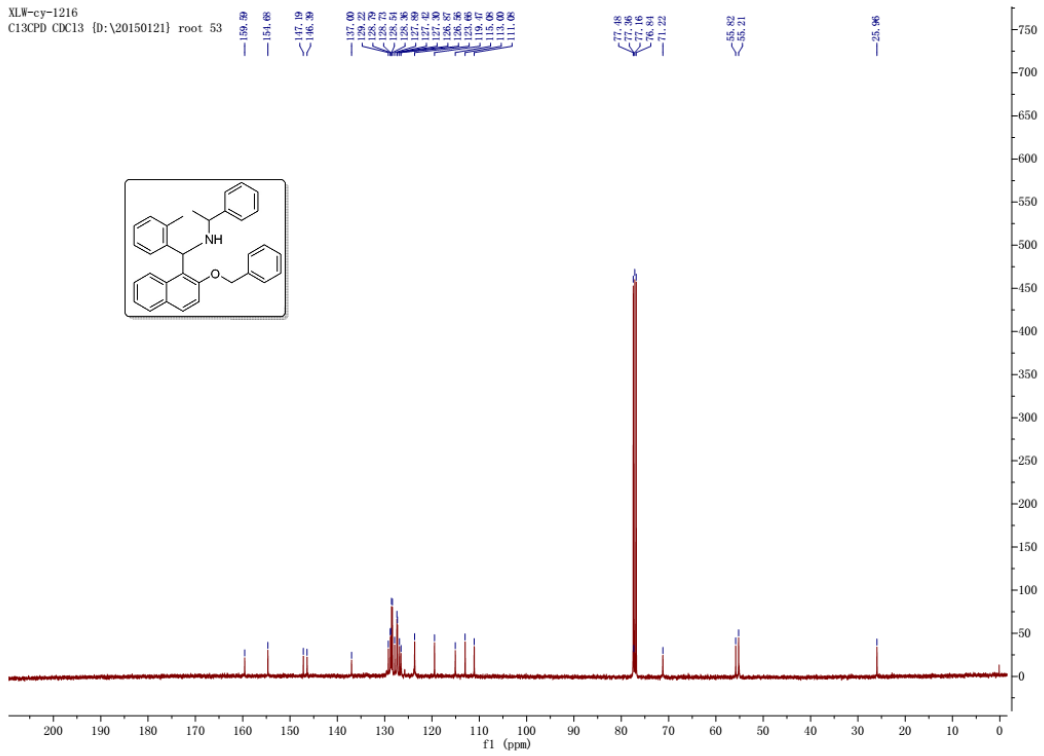
**Acquisition Parameter**  
Source Type: ESI  
Focus: Active  
Scan Begin: 50 m/z  
Scan End: 550 m/z  
Ion Polarity: Positive  
Set Capillary: 4500 V  
Set End Plate Offset: -500 V  
Set Collision Cell RF: 120.0 Vpp  
Set Nebulizer: 0.4 Bar  
Set Dry Heater: 200 °C  
Set Dry Gas: 2.2 l/min  
Set Divert Valve: Source



XLW-cy-1216  
PROTON CDC13 {D:\20150121} root 53



XLW-cy-1216  
C13CPD CDC13 {D:\20150121} root 53





# Mass Spectrum SmartFormula Report

**Analysis Info**

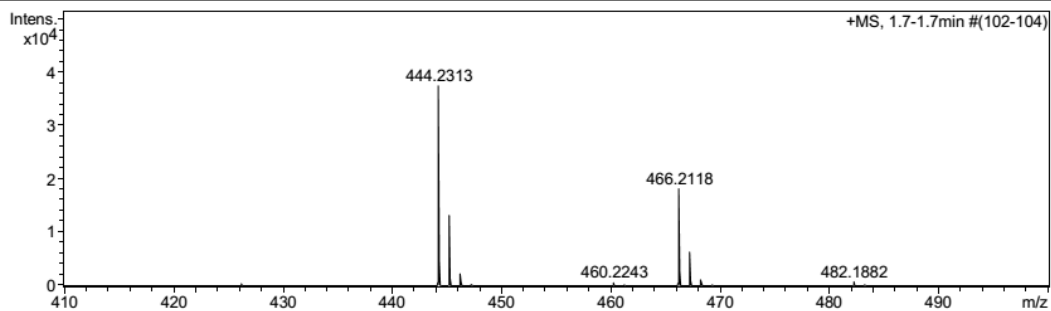
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw140106-wcy-CTWSBnCP\_01.d  
 Method: tune-pos\_100-500\_140106.m  
 Sample Name: CTWSBnCP  
 Comment:

Acquisition Date: 1/6/2014 12:57:11 PM

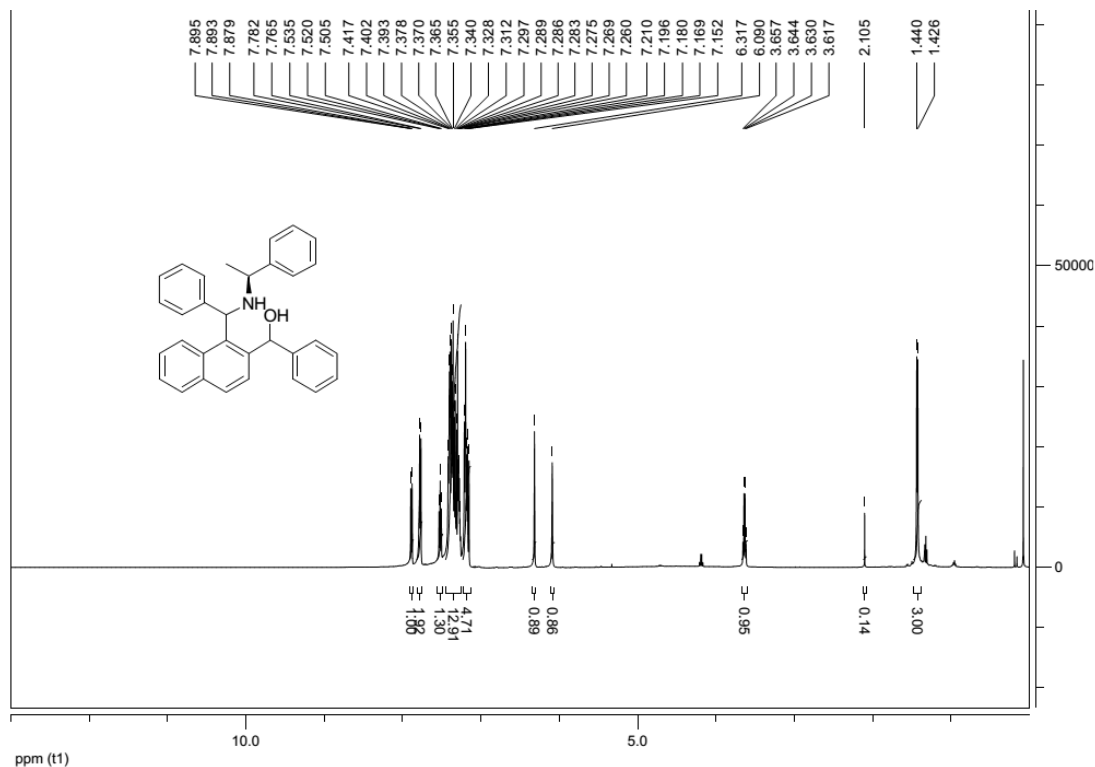
Operator: Jiang  
 Instrument / Ser#: micrOTOF-Q II 10324

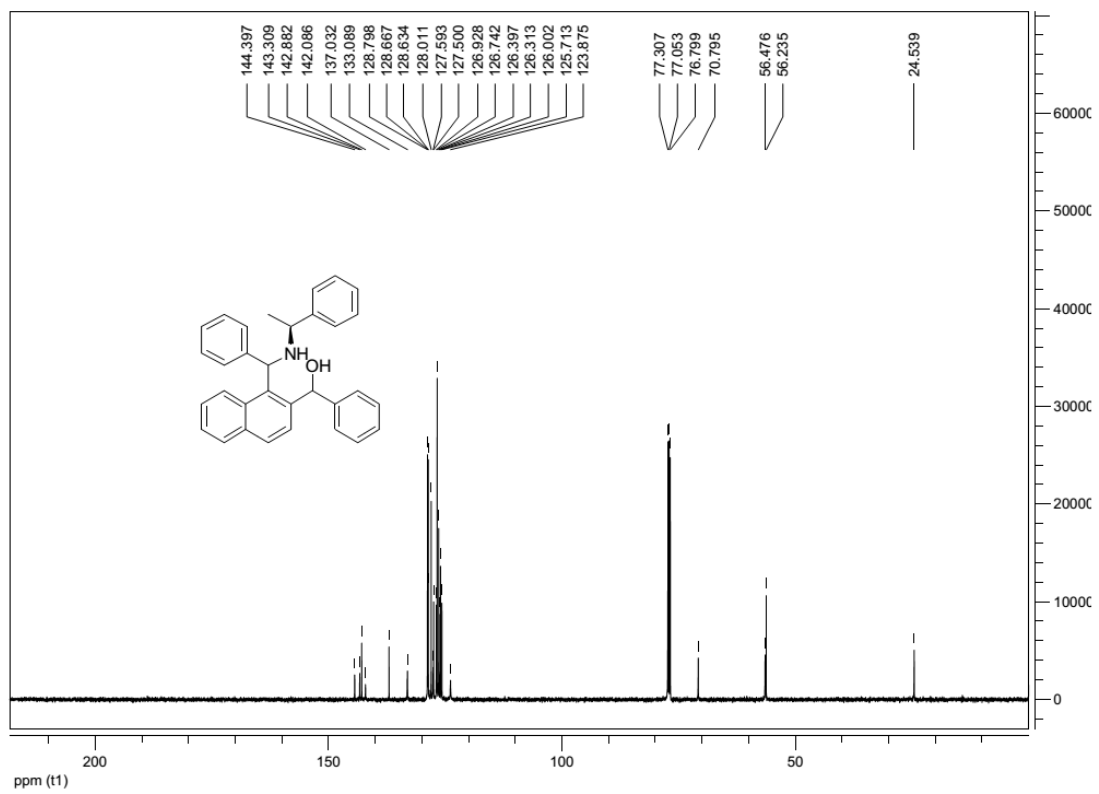
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
444.2313	1	C 32 H 30 N O	100.00	444.2322	0.9	2.1	1.9	18.5	even	ok
466.2118	1	C 32 H 29 N Na O	100.00	466.2141	2.3	5.0	2.3	18.5	even	ok





# Mass Spectrum SmartFormula Report

## Analysis Info

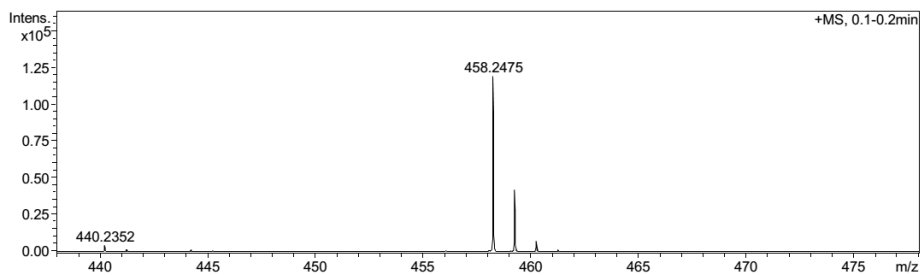
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-6\_01.d  
Method tune\_100-550\_pos150120.m  
Sample Name  
Comment

Acquisition Date 1/20/2015 2:53:33 PM

Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

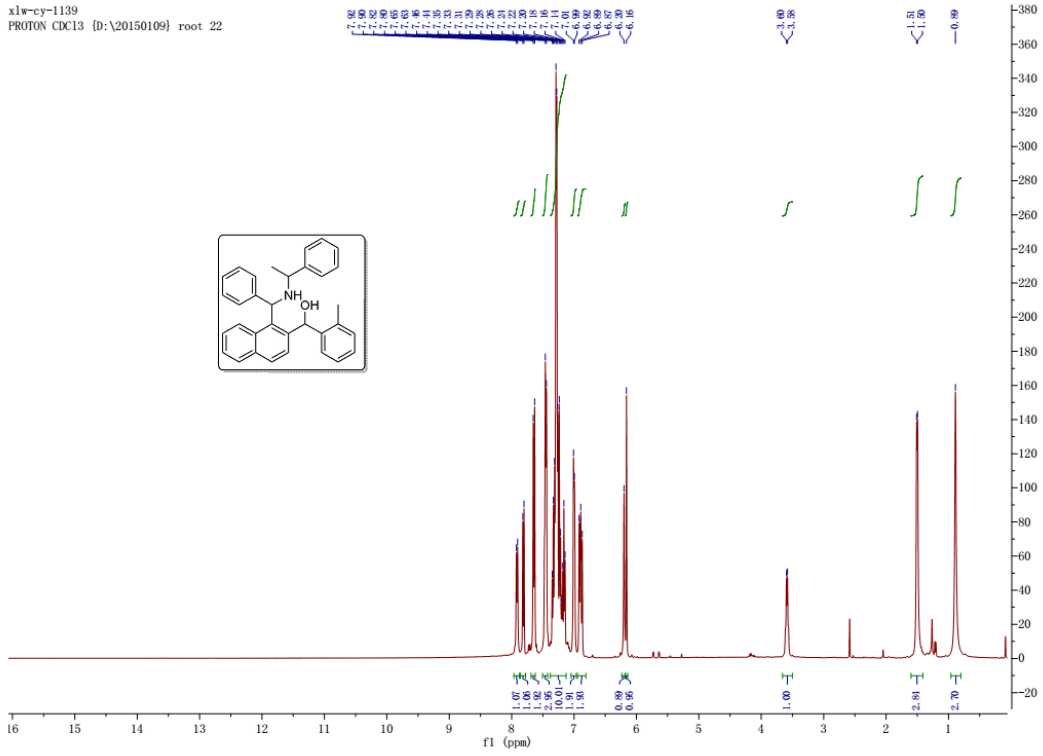
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

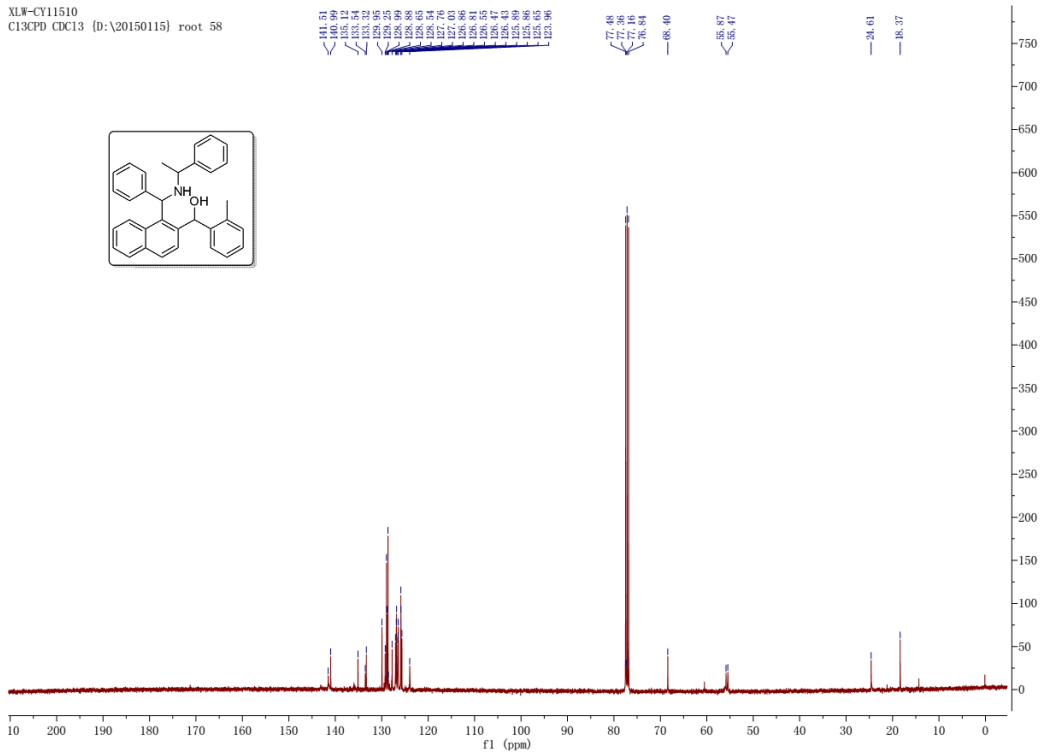


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
458.2475	1	C <sub>33</sub> H <sub>32</sub> N <sub>2</sub> O	100.00	458.2475	0.3	0.7	5.9	18.5	even	ok

xlw-cy-1139  
PROTON CDC13 {D:\20150109} root 22



XLW-CY11510  
C13CPD CDC13 {D:\20150115} root 58

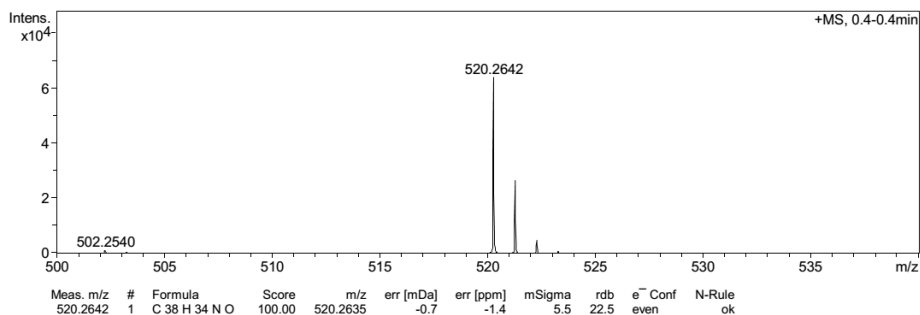


## Mass Spectrum SmartFormula Report

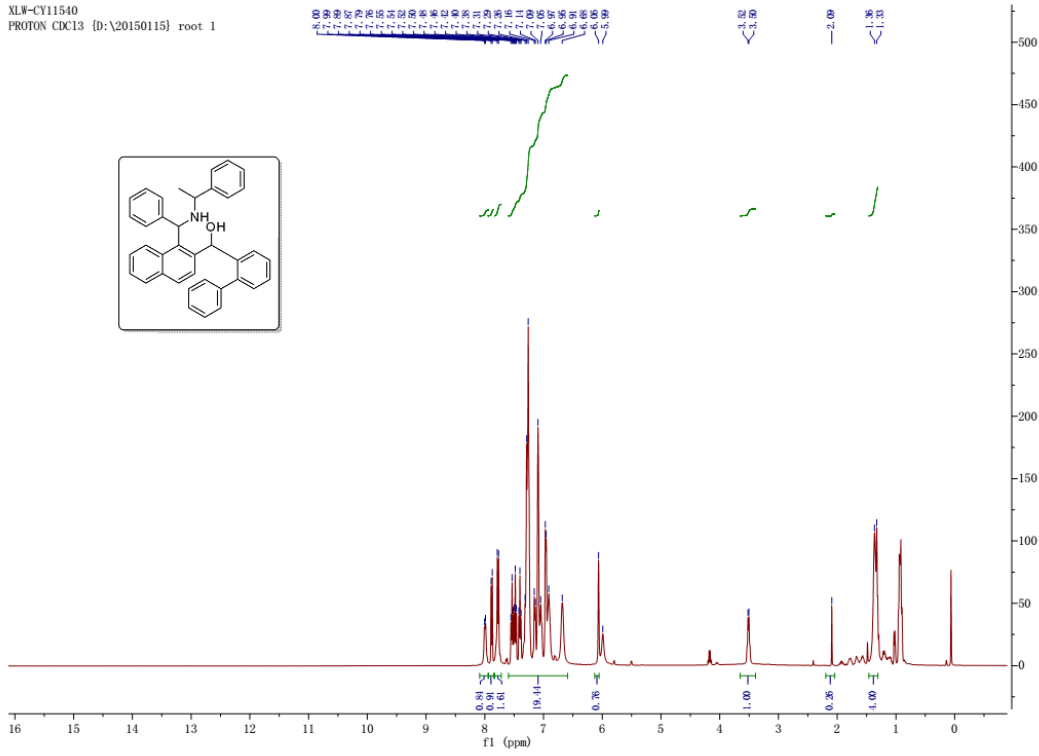
**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150120-cy119-5\_01.d  
Method: tune\_100-550\_pos150120.m  
Sample Name:  
Comment:  
Acquisition Date: 1/20/2015 2:57:36 PM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

**Acquisition Parameter**

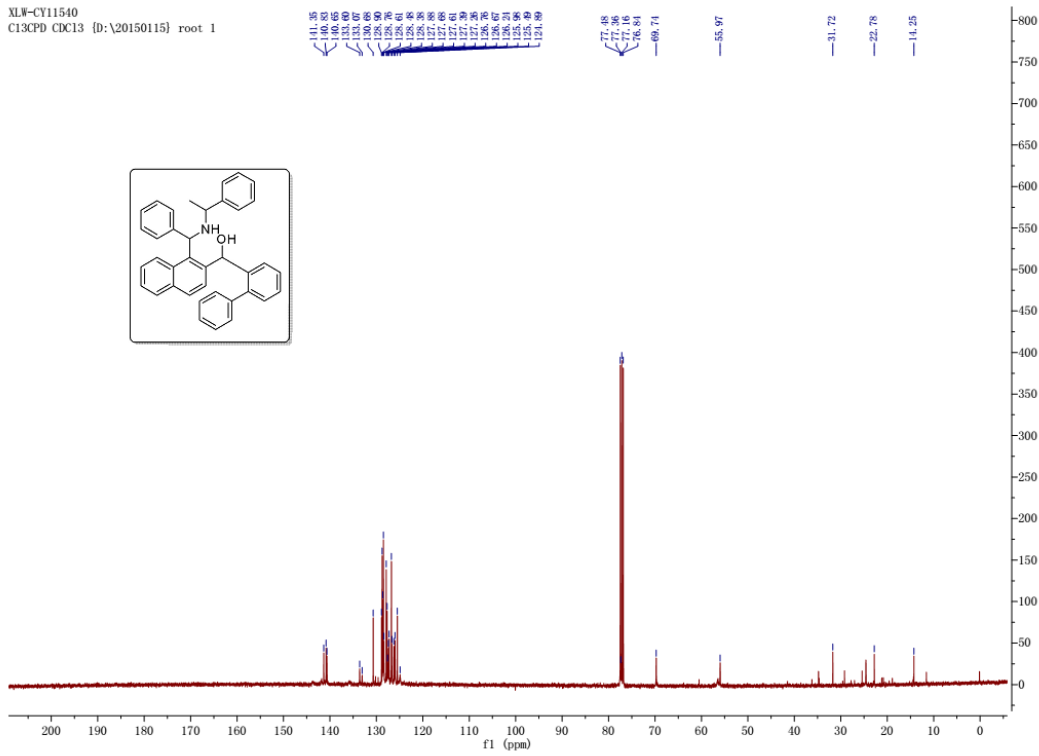
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



XLW-CY11540  
PROTON CDC13 {D:\20150115} root 1



XLW-CY11540  
C13CPD CDC13 {D:\20150115} root 1



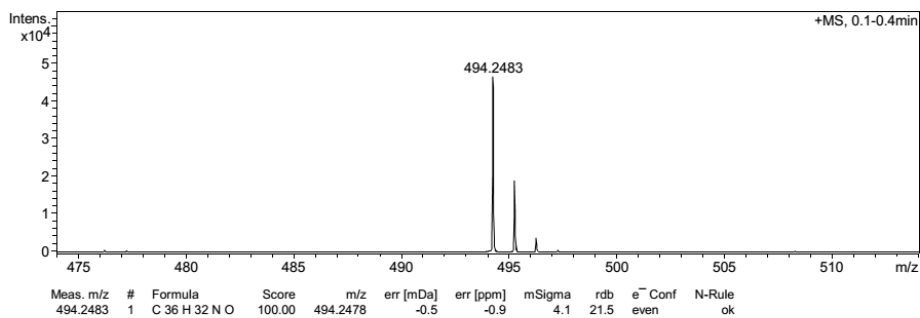
## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150123-wcy-1211\_01.d  
Method tune\_100-550\_pos150120.m  
Sample Name  
Comment

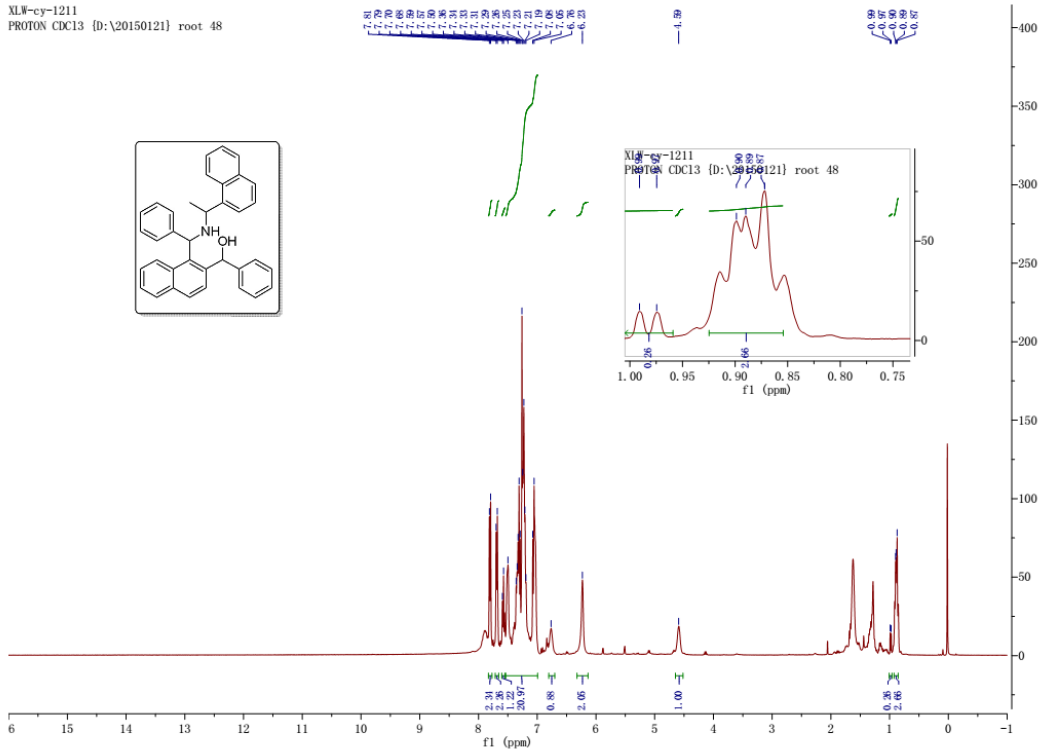
Acquisition Date 1/23/2015 10:45:44 AM  
Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

**Acquisition Parameter**

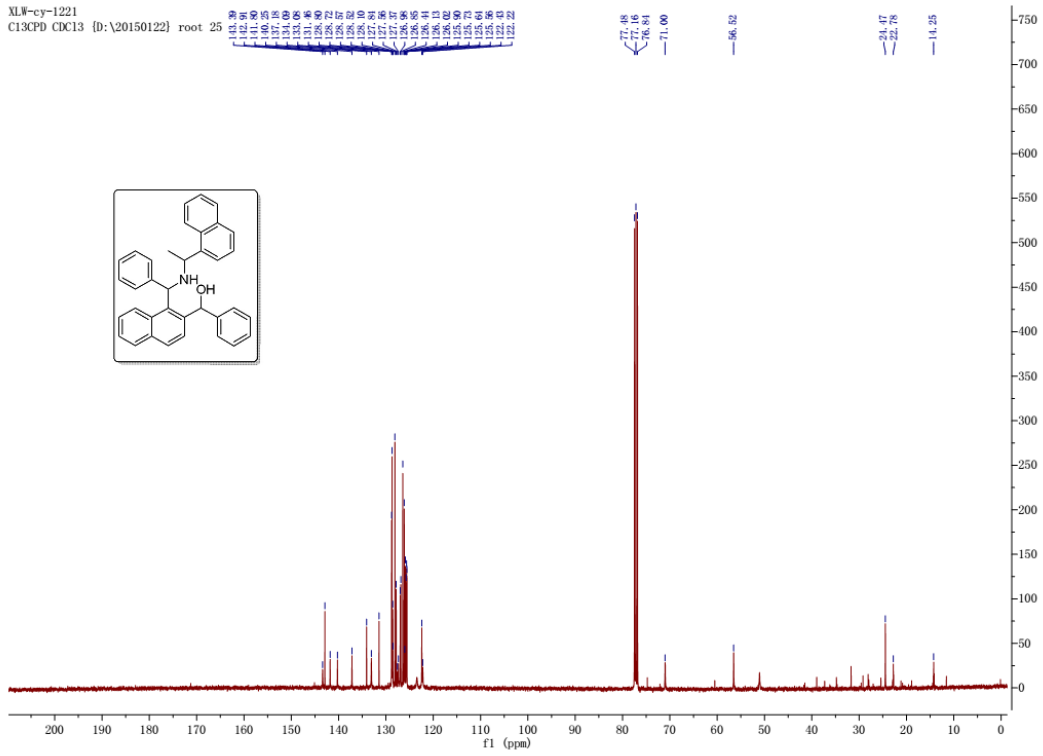
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



XLW-cy-1211  
PROTON CDC13 {D:\20150121} root 48



XLW-cy-1221  
C13CPD CDC13 {D:\20150122} root 25

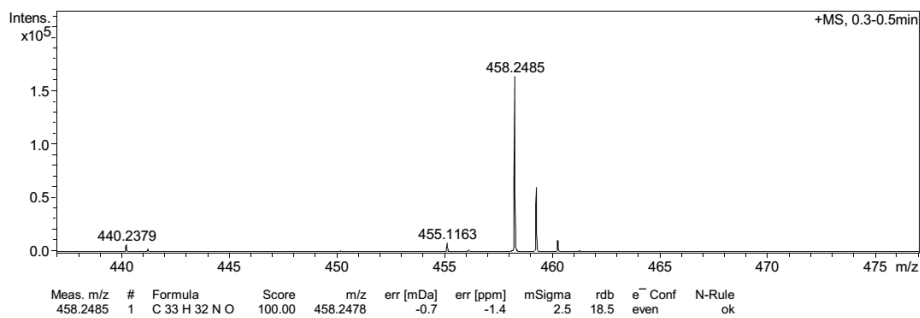




## Mass Spectrum SmartFormula Report

<b>Analysis Info</b>	Acquisition Date 1/23/2015 10:43:38 AM
Analysis Name D:\Data\Xuliwen\Q-TOF-lizf150122-2015d_01.d	
Method tune_100-550_pos150120.m	Operator Jiang
Sample Name	Instrument / Ser# micrOTOF-Q II 10324
Comment	

<b>Acquisition Parameter</b>					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.2 l/min
Scan End	550 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

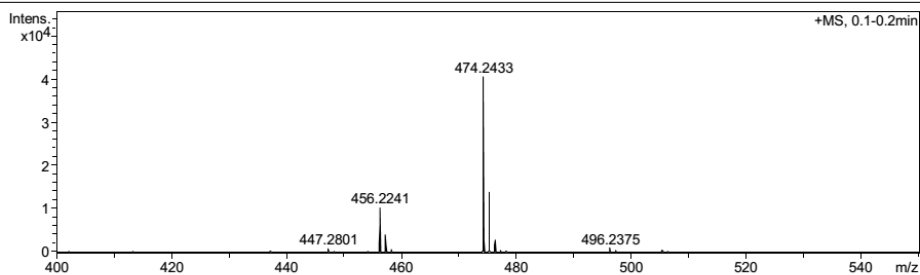




## Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw150205-cy1253\_01.d Acquisition Date 2/5/2015 9:47:09 AM  
Method tune\_100-550\_pos150205.m Operator Jiang  
Sample Name wxy1501-3 Instrument / Ser# micrOTOF-Q II 10324  
Comment

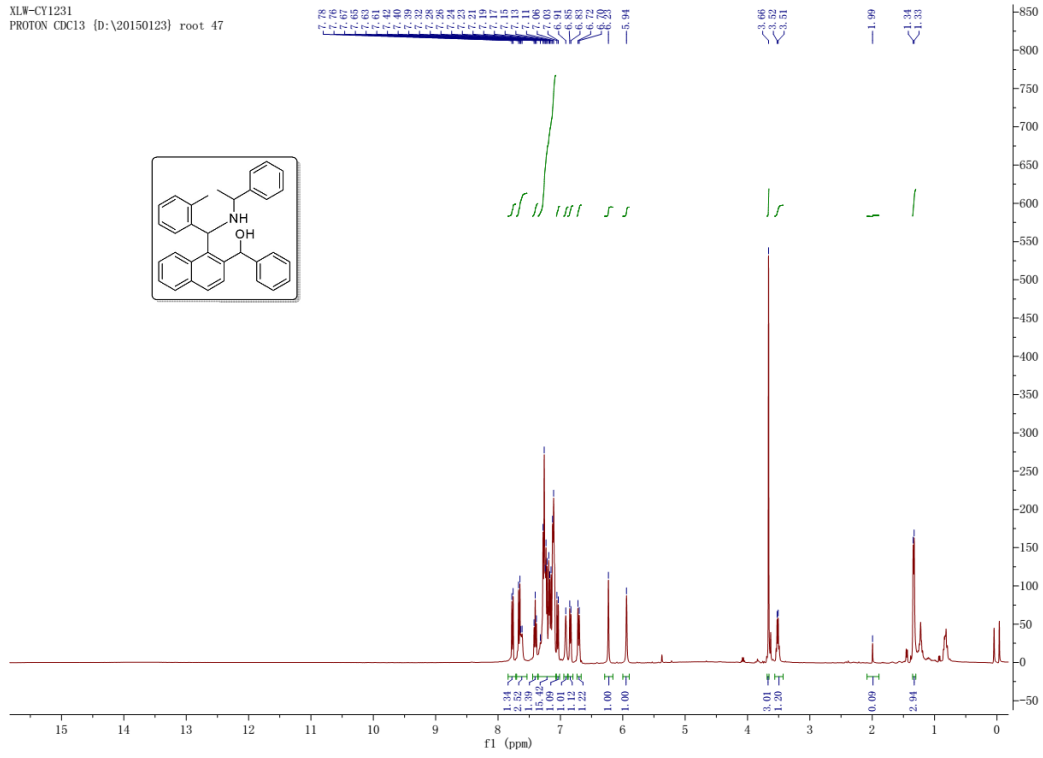
**Acquisition Parameter**  
Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Active Set Capillary 4500 V Set Dry Heater 200 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 2.2 l/min  
Scan End 550 m/z Set Collision Cell RF 120.0 Vpp Set Divert Valve Source



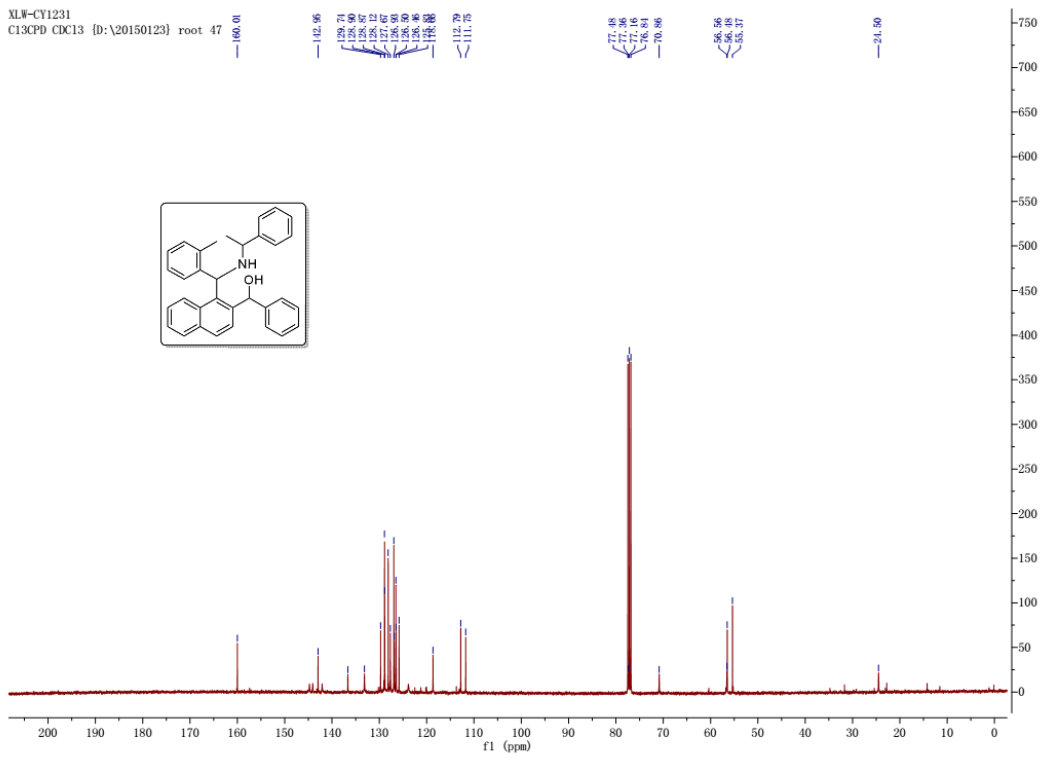
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
474.2433	1	C <sub>33</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>	100.00	474.2428	-0.5	-1.1	11.0	18.5	even	ok



XLW-CY1231  
PROTON CDC13 [D:\20150123] root 47



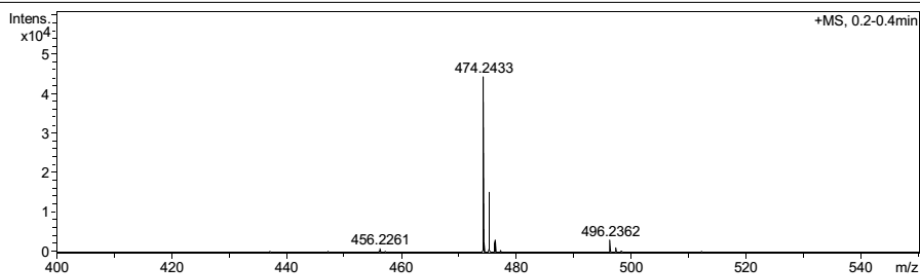
XLW-CY1231  
C13CPD CDC13 [D:\20150123] root 47



# Mass Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\Xuliwen\Q-TOF-xulw150205-cy1255\_01.d  
Method: tune\_100-550\_pos150205.m  
Sample Name: wxy1501-3  
Comment:  
Acquisition Date: 2/5/2015 9:54:58 AM  
Operator: Jiang  
Instrument / Ser#: micrOTOF-Q II 10324

**Acquisition Parameter**  
Source Type: ESI  
Focus: Active  
Scan Begin: 50 m/z  
Scan End: 550 m/z  
Ion Polarity: Positive  
Set Capillary: 4500 V  
Set End Plate Offset: -500 V  
Set Collision Cell RF: 120.0 Vpp  
Set Nebulizer: 0.4 Bar  
Set Dry Heater: 200 °C  
Set Dry Gas: 2.2 l/min  
Set Divert Valve: Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
474.2433	1	C <sub>33</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>	100.00	474.2428	-0.5	-1.1	11.2	18.5	even	ok



# Mass Spectrum SmartFormula Report

## Analysis Info

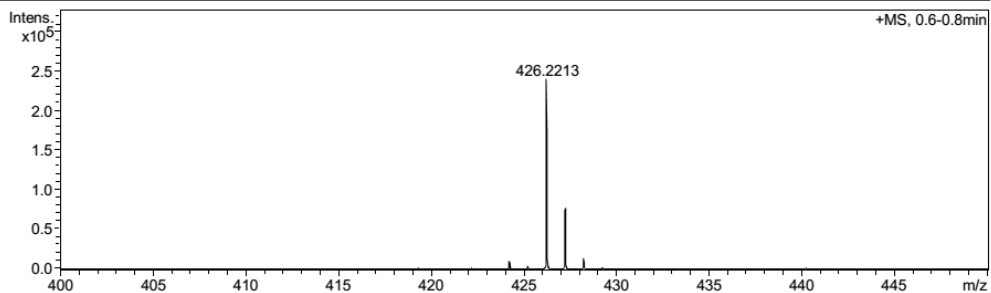
Analysis Name D:\Data\Xuliwen\Q-TOF-xulw-20141022-CY-2\_01.d  
Method tune-posAPCI-100-700\_140930.m  
Sample Name CY-2  
Comment

Acquisition Date 10/22/2014 6:00:05 PM

Operator Jiang  
Instrument / Ser# micrOTOF-Q II 10324

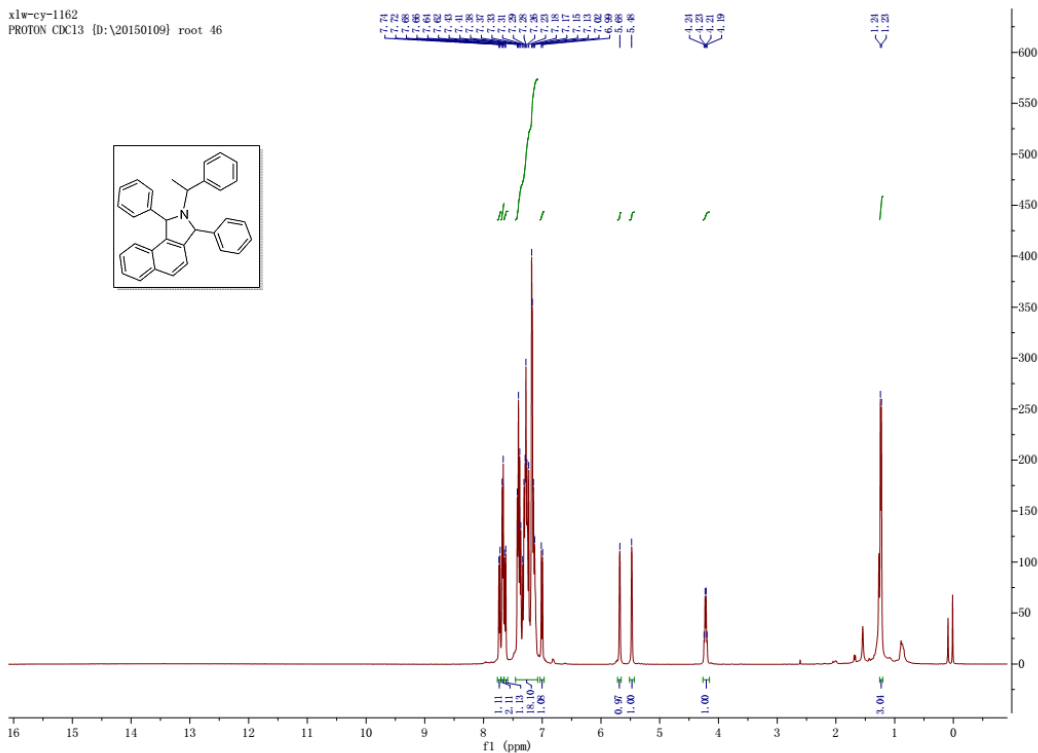
## Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste



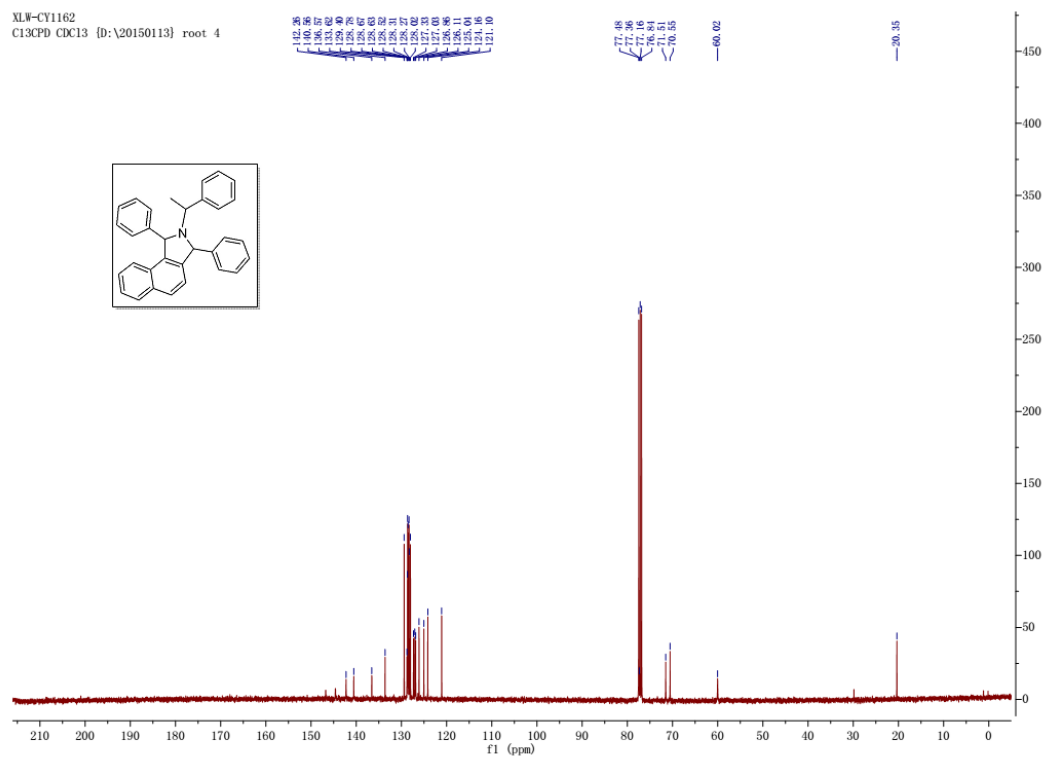
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
426.2213	1	C 32 H 28 N	100.00	426.2216	0.3	0.8	13.3	19.5	even	ok

xlw-cy-1162  
PROTON CDC13 {D:\20150109} root 46

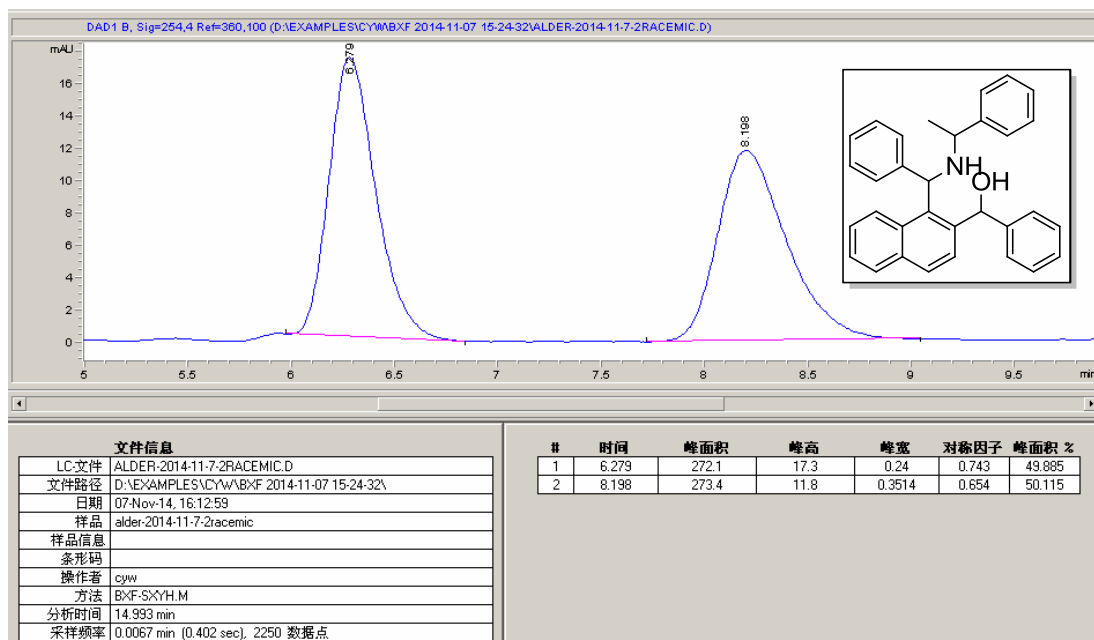
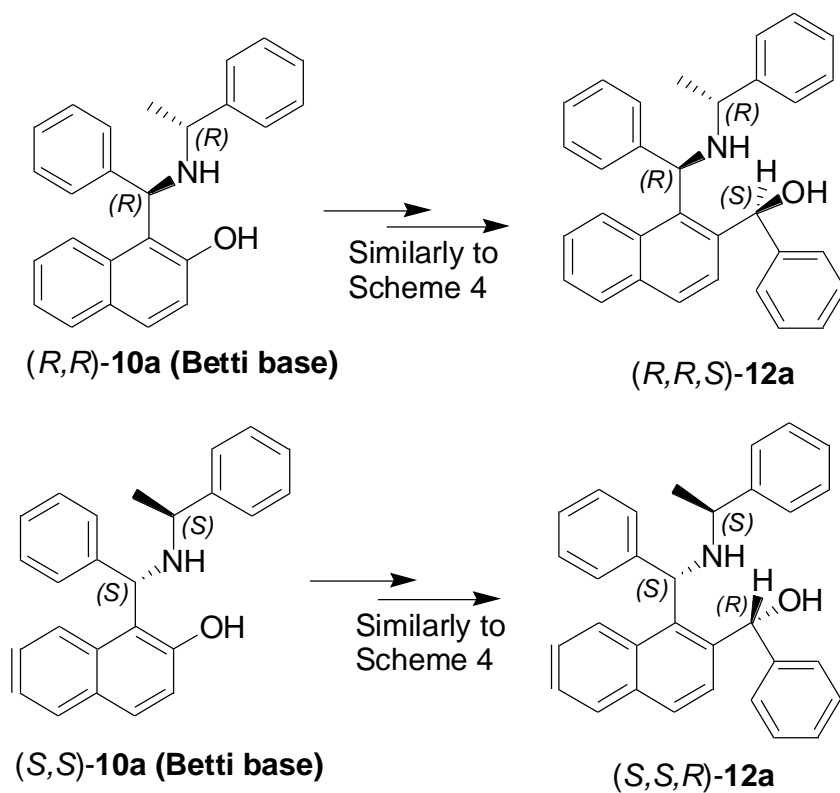


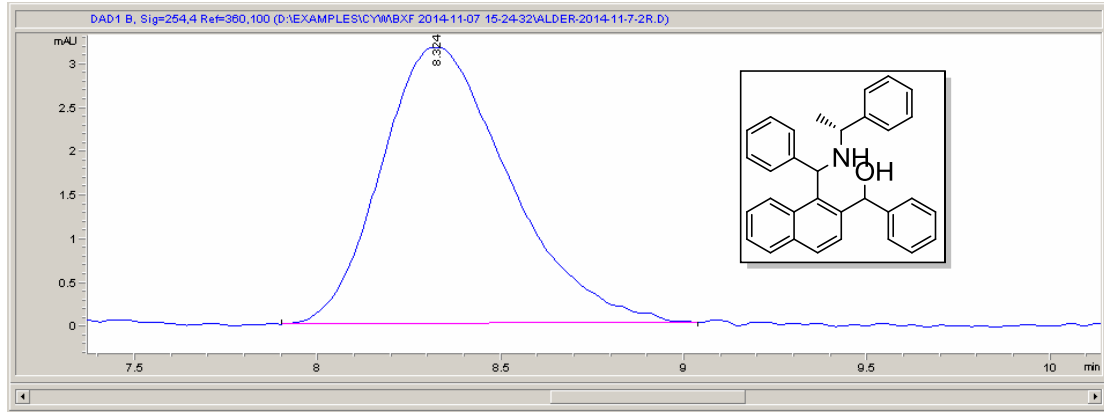


XLW-CY1162  
C13CPD CDC13 {D:\20150113} root 4

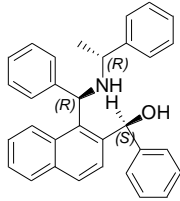


## 8. HPLC of chiral Betti base-derived amino alcohols 12a and all-substituted pyrrolidine derivative 13

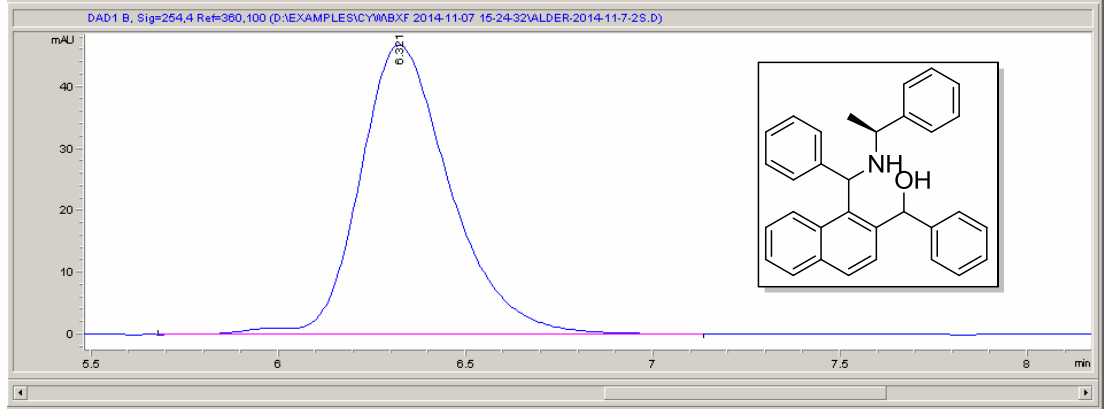




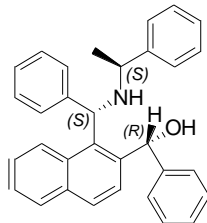
文件信息		#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
LC-文件	ALDER-2014-11-7-2R.D	1	8.324	77	3.2	0.3142	0.766	100.000
文件路径	D:\EXAMPLES\CYW\B\F 2014-11-07 15-24-32\							
日期	07-Nov-14, 16:28:52							
样品	alder-2014-11-7-2r							
样品信息								
条形码								
操作者	CYW							
方法	B\F-S\YH.M							
分析时间	14.993 min							
采样频率	0.0067 min (0.402 sec), 2250 数据点							



(R,R,S)-12a

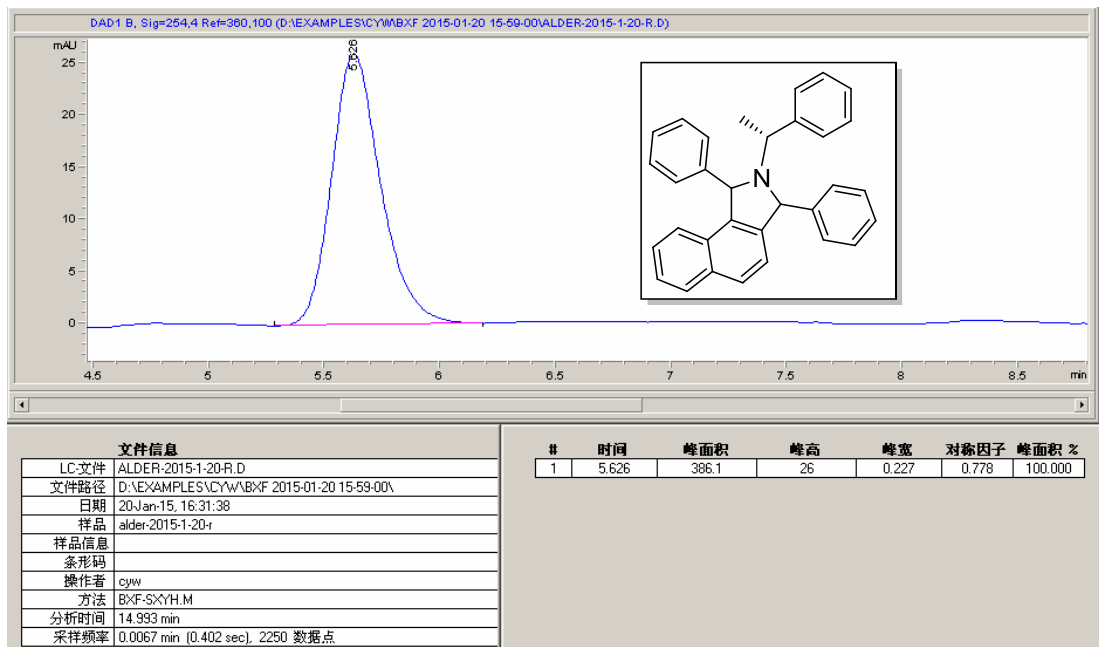
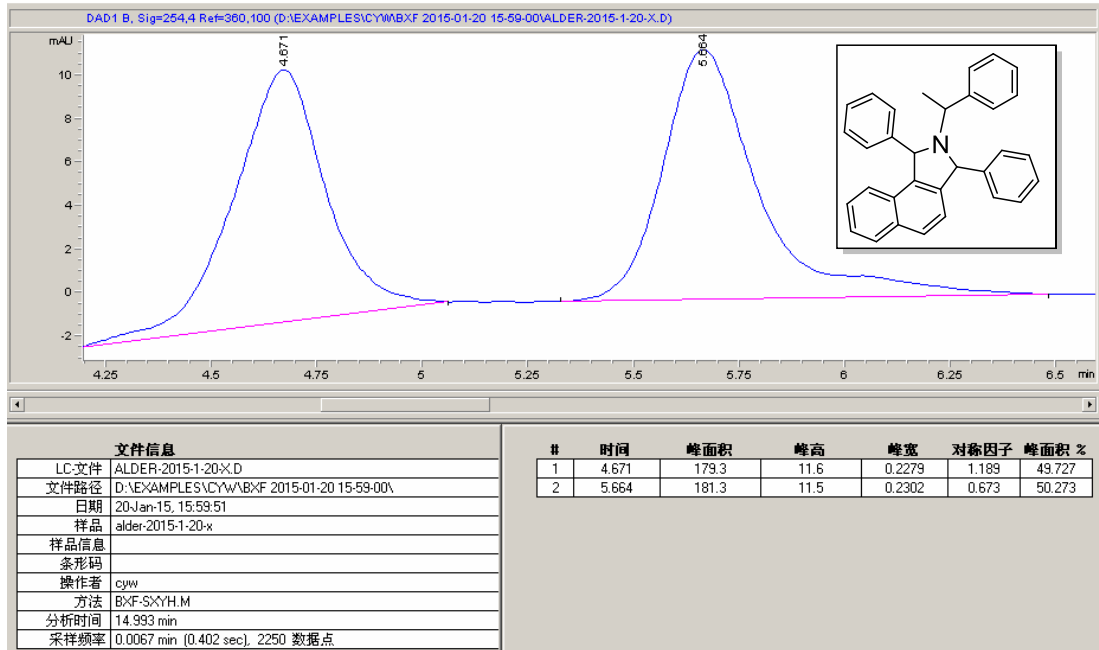
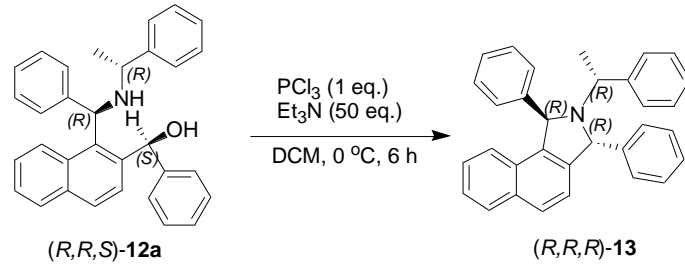


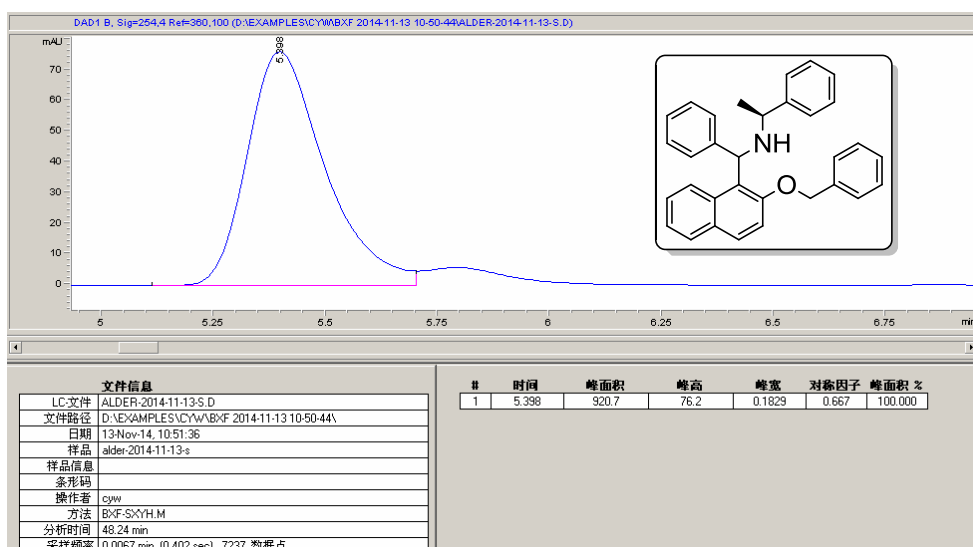
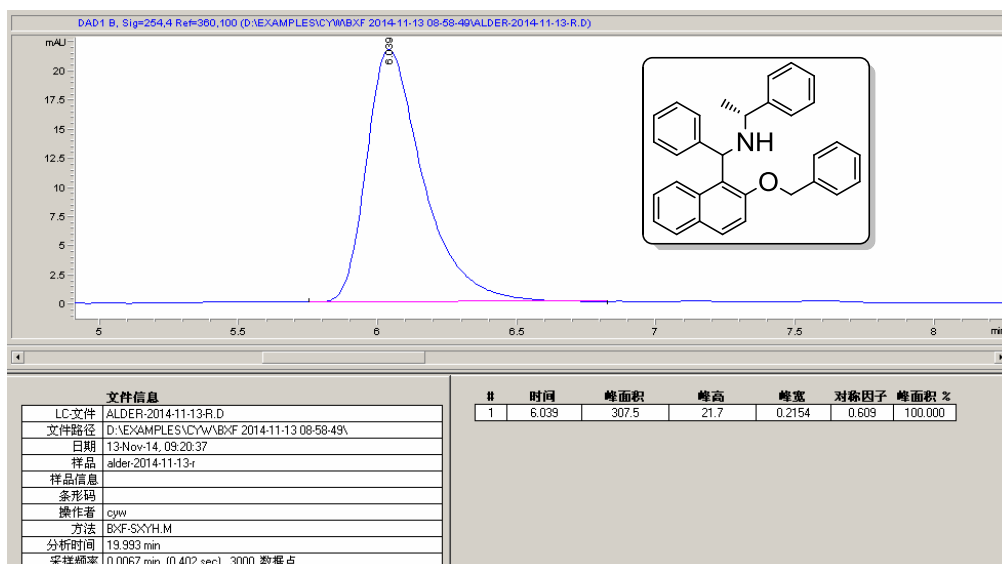
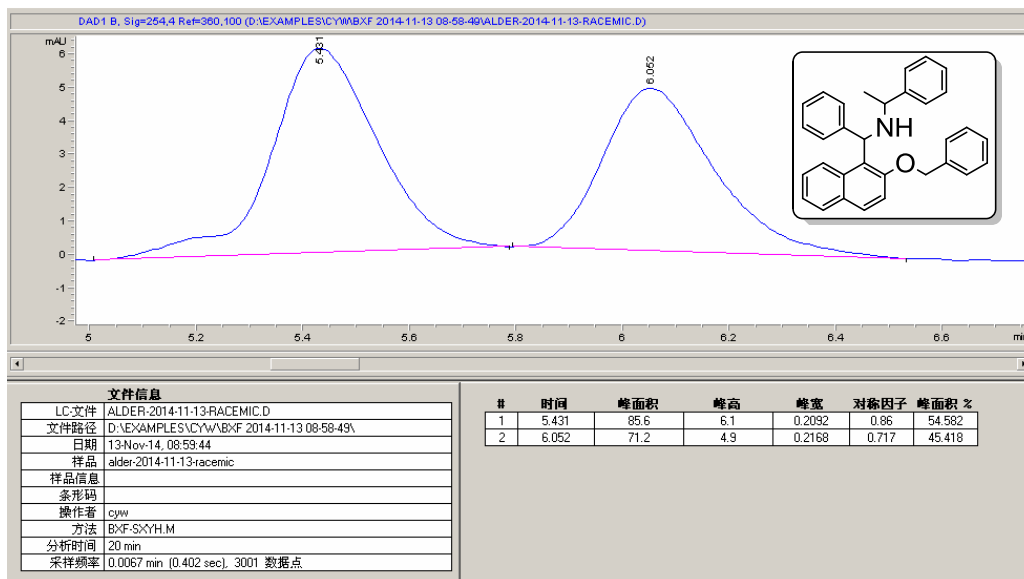
文件信息		#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
LC-文件	ALDER-2014-11-7-2S.D	1	6.321	785.6	46.8	0.254	0.738	100.000
文件路径	D:\EXAMPLES\CYW\B\F 2014-11-07 15-24-32\							
日期	07-Nov-14, 16:44:44							
样品	alder-2014-11-7-2s							
样品信息								
条形码								
操作者	CYW							
方法	B\F-S\YH.M							
分析时间	9.993 min							
采样频率	0.0067 min (0.402 sec), 1500 数据点							

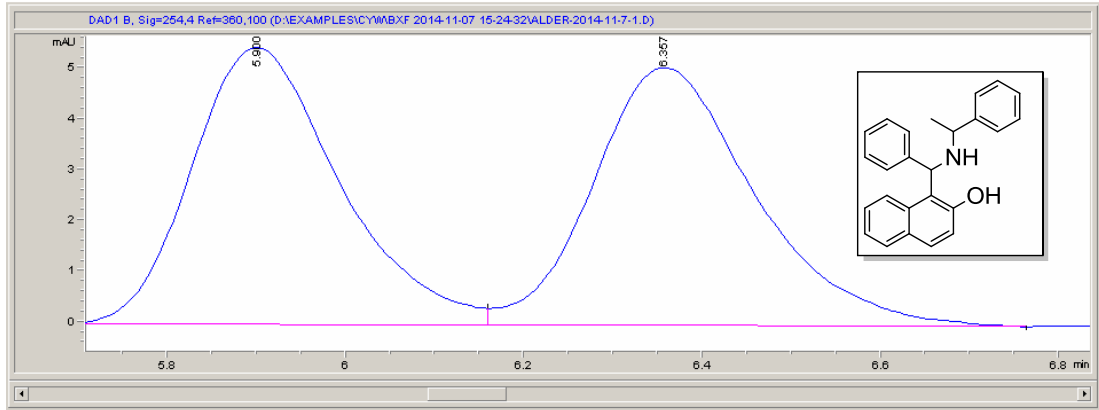


(S,S,R)-12a

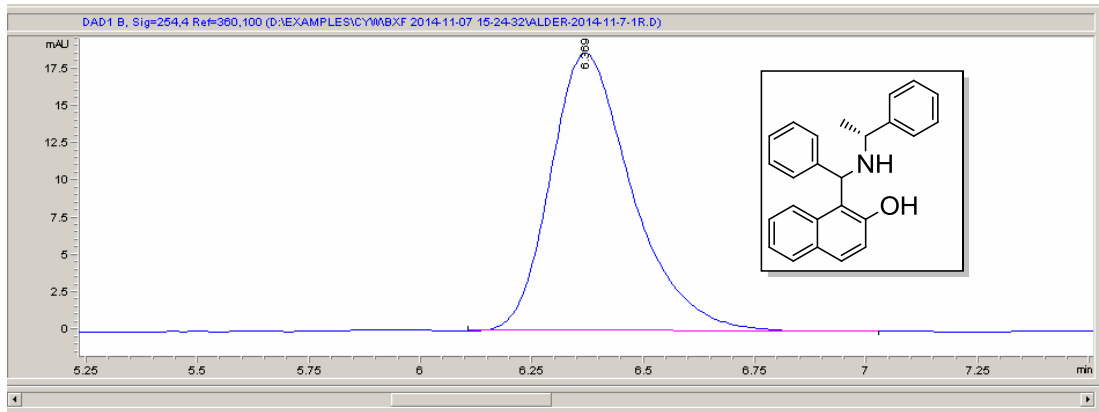
S107



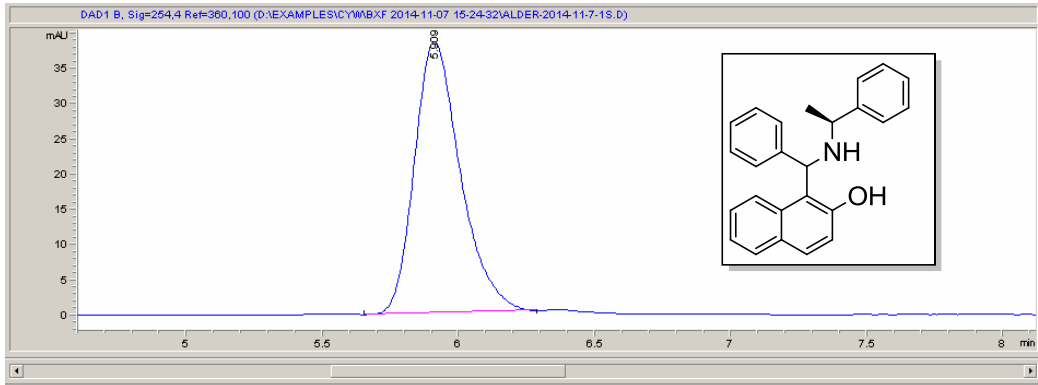




文件信息		峰数据						
LC文件	ALDER-2014-11-7-1.D	#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
文件路径	D:\EXAMPLES\CYW\BXF 2014-11-07 15-24-32\	1	5.9	62.9	5.5	0.1742	0.739	49.468
日期	07-Nov-14, 15:25:22	2	6.367	64.3	5.1	0.1913	0.746	50.532
样品	alder-2014-11-7-1							
样品信息								
条形码								
操作者	CYW							
方法	BXF-SXYH.M							
分析时间	15 min							
采样频率	0.0067 min (0.402 sec), 2251 数据点							



文件信息		峰数据						
LC文件	ALDER-2014-11-7-1R.D	#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
文件路径	D:\EXAMPLES\CYW\BXF 2014-11-07 15-24-32\	1	6.369	237.5	18.6	0.1927	0.697	100.000
日期	07-Nov-14, 15:41:12							
样品	alder-2014-11-7-1r							
样品信息								
条形码								
操作者	CJW							
方法	BXF-SXYH.M							
分析时间	15 min							
采样频率	0.0067 min (0.402 sec), 2251 数据点							



文件信息		#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
LC文件	ALDER-2014-11-7-1S.D	1	5.909	451	38.6	0.1784	0.718	100.000
文件路径	D:\EXAMPLES\CY\WAB\F 2014-11-07 15:24:32\							
日期	07-Nov-14, 15:57:04							
样品	alder-2014-11-7-1s							
样品信息								
条形码								
操作者	CJW							
方法	B\F-S\YH.M							
分析时间	14.993 min							
采样频率	0.0067 min (0.402 sec), 2250 数据点							