Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Supporting Information

Efficient [5+1]-Strategy for the Assembly of 1,8-Naphthyridines by Domino Amination/Conjugate Addition Reactions of 1-(2-Chloropyridin-3-yl)prop-2-yn-1-ones with Amines

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(A) Experimental Section

The dry solvents DMF and THF were purchased directly from ACROS as AcroSeal bottles. Other solvents were purified by destination. All reactions were carried out under an inert atmosphere. For ^{1}H and ^{13}C NMR spectra the deuterated solvents indicated were used. Mass spectrometric data (MS) were obtained by electron ionization (EI, 70 eV), chemical ionization (CI, isobutane) or electrospray ionization (ESI). For preparative scale chromatography silica gel 60 (0.063-0.200 mm, 70–230 mesh) was used. The absorption spectra were measured on a Perkin Elmer UV/VIS Spectrometer Lambda 2 in dichloromethane ($c = 2.5 * 10^{-5}$ mol/l). The fluorescence spectra were recorded on a Hitachi F-4010 fluorescence spectrometer in dichloromethane ($c = 10^{-4}$ mol/l; excitation wavelength: 350 nm). The solvent was distilled before use. Compound **1** was obtained starting from commercially available 2-chloropyridine-3-carboxylic acid by the method described previously.[19] Acetylenes **2** and amines **4** are commercially available compounds.

Procedure A – General procedure 1-(2-chloropyridin-3-yl)prop-2-yn-1-ones (3): 1 g (6.35 mmol) of 2-chloronicotinic acid was refluxed in an excess of $SOCl_2$. After 3 h the $SOCl_2$ was removed in vacuo and the crude white residue used without further purification.
1.05 Equiv of the corresponding acetylene, 0.02 equiv (2 mol%) of $PdCl_2(PPh_3)_2$, 0.04 equiv (4 mol%) of CuI and 1.0 equiv of the chlorinated 2-chloropyridine-3-carboxylic acid chloride (**1**) are added to dry THF under argon atmosphere in a pressure tube. The mixture is cooled to 0 °C, 1.05 equiv NEt_3 are added and the mixture is stirred at room temperature. After 3 h the reaction mixture is washed with water and extracted with ethylacetate. The combined phases are dried over Na_2SO_4, the solvent is removed in vacuo and the residue purified by column chromatography (eluent : *n*-heptane/ethylacetate).

Procedure B – General procedure for alkylamines (5b-k, 5q-t, 5v, 5w): 2.0 equiv of the corresponding alkylamine, 2.0 equiv of K_2CO_3 and 1.0 equiv of the corresponding 1-(2-chloropyridin-3-yl)prop-2-yn-1-one are heated at 150 °C (100 °C if a TMS group is present in the molecule) in dry DMF under argon atmosphere in a pressure tube. After 16 h the solvent is removed in vacuo and the crude product is purified by column chromatography (eluent: *n*-heptane/ethylacetate).

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Procedure C – General procedure for anilines (5a, 5l-p, 5u): 2.0 equiv of the corresponding aniline, 2.0 equiv of K_2CO_3, 0.1 equiv (10 mol%) of $Pd(PPh_3)_4$ and 1.0 equiv of the corresponding 1-(2-chloropyridin-3-yl)prop-2-yn-1-one are heated at 150 °C in dry DMF under argon atmosphere in a pressure tube. After 16 h the solvent is removed in vacuo and the crude product is purified by column chromatography (eluent: *n*-heptane/ethylacetate).

Procedure D – General procedure for bromination (20): 1.0 equiv of the starting material, 1.5 equiv of bromine and 6.0 equiv of Na_2CO_3 in THF are stirred at room temperature for 6 h. The solvent is removed in vacuo and the crude product purified by column chromatography (eluent: *n*-heptane/ethylacetate).

Procedure E – General procedure for Suzuki-Coupling (21a-c): 1.0 equiv of the starting material, 1.1 equiv of the boronic acid, 0.05 equiv (5 mol%) $Pd(PPh_3)_4$ and 2.0 equiv K_2CO_3 are heated in DMF for 16 h at 120 °C. The solvent is removed in vacuo and the crude product is purified by column chromatography (eluent: *n*-heptane/ethylacetate).

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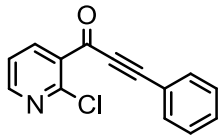
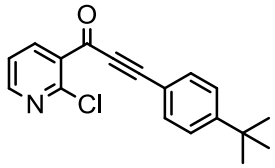
(B) Spectral data

1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (3a).[1]



Starting with 2-chloropyridine-3-carboxylic acid chloride (**1**) (0.200 g, 1.14 mmol), $PdCl_2(PPh_3)_2$ (0.016 g, 0.023 mmol), CuI (0.009 g, 0.046 mmol), NEt_3 (0.17 mL, 1.2 mmol) and phenylacetylene (0.13 mL, 1.2 mmol) in THF (10 mL), product **3a** was isolated as a white solid (0.220 g, 80 %); mp 68-70 °C (lit.[1] 69-71 °C); Procedure E. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 7.33-7.47 (m, 4H, H_{Ar}), 7.57-7.61 (m, 2H, H_{Ar}), 8.27 (dd, ^4J = 2.0 Hz, ^3J = 7.7 Hz, 1H, H_{Ar}), 8.50 (dd, ^4J = 2.0 Hz, ^3J = 4.8 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 87.9, 95.7, 119.6, 122.4, 128.8, 131.4, 132.6, 133.2, 140.7, 149.5, 152.3, 175.5.

3-(4-*tert*-butylphenyl)-1-(2-chloropyridin-3-yl)prop-2-yn-1-one (3b).[2]



Starting with 2-chloropyridine-3-carboxylic acid chloride (**1**) (0.200 g, 1.14 mmol), $PdCl_2(PPh_3)_2$ (0.016 g, 0.023 mmol), CuI (0.009 g, 0.046 mmol), NEt_3 (0.17 mL, 1.2 mmol) and 4-*tert*-butylphenylacetylene (0.22 mL, 1.2 mmol) in THF (10 mL), product **3b** was isolated as a white-brown solid (0.204 g, 60 %); mp 54-56 °C; Procedure E. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 1.26 (s, 9H, $C(CH_3)_3$), 7.32-7.39 (m, 3H, H_{Ar}), 7.51-

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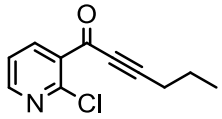
7.55 (m, 2H, H_{Ar}), 8.26 (dd, ^4J = 2.0 Hz, ^3J = 7.2 Hz, 1H, H_{Ar}), 8.70 (dd, ^4J = 2.0 Hz, ^3J = 4.8 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 31.0, 35.2, 87.9, 96.5, 116.5, 122.4, 125.9, 132.8, 133.2, 140.6, 149.5, 152.5, 155.3, 175.5. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3038 (w), 2963 (w), 2904 (w), 2866 (w), 2351 (w), 2292 (w), 2190 (s), 1938 (w), 1644 (s), 1600 (m), 1573 (m), 1556 (m), 1504 (w), 1463 (w), 1439 (w), 1400 (s), 1364 (w), 1291 (m), 1268 (w), 1258 (w), 1204 (m), 1185 (w), 1127 (w), 1113 (w), 1095 (m), 1062 (w), 1015 (w). *m/z* (%) = 297 ($M\text{-}H^+$, 25), 282 (100), 254 (6), 226 (7), 185 (4), 155 (7), 140 (7), 112 (4), 95 (5), 76 (3), 41 (3). Anal. calcd for $C_{18}H_{16}ClNO$ (297.78): C, 72.60 ; H, 5.42; N, 4.70. Found: C, 72.36 ; H, 5.53; N, 4.86.

1-(2-chloropyridin-3-yl)hex-2-yn-1-one (3c).



Starting with 2-chloropyridine-3-carboxylic acid chloride (**1**) (0.200 g, 1.14 mmol), $PdCl_2(PPh_3)_2$ (0.016 g, 0.023 mmol), CuI (0.009 g, 0.046 mmol), NEt_3 (0.17 mL, 1.2 mmol) and 1-pentyne (0.12 mL, 1.2 mmol) in THF (10 mL), product **3c** was isolated as a brown oil (0.140 g, 59 %); Procedure E. ^1H NMR ($CDCl_3$, 250 MHz): δ = 0.99 (t, ^3J = 7.4 Hz, 3H, CH_3), 1.58-1.68 (m, 2H, CH_2), 2.40 (t, ^3J = 7.1 Hz, 2H, CH_2), 7.31 (dd, ^3J = 4.8 Hz, ^3J = 7.7 Hz, 1H), 8.20 (dd, ^3J = 7.7 Hz, ^4J = 2.0 Hz, 1H, H_{Ar}), 8.46 (dd, ^3J = 4.8 Hz , ^4J = 2.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 13.6, 21.1, 21.3, 80.8, 99.5, 122.2, 132.6, 140.7, 149.3, 152.1, 175.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3046 (w), 2965 (w), 2934 (w), 2905 (w), 2874 (w), 2278 (w), 2217 (m), 2201 (m), 1656 (s), 1572 (m), 1558 (m), 1462 (w), 1443 (w), 1421 (w), 1397 (s), 1338 (w), 1325 (w), 1287 (m), 1266 (m), 1234 (m), 1138 (m), 1128 (m), 1069 (m), 1024 (m). *m/z* (%) = 207 (M^+, 18), 192 (3), 179 (34), 164 (5), 140 (16), 112 (14), 95 (100), 76 (12), 66 (12), 53 (13), 39 (9). HRMS (ESI): calcd for $C_{11}H_{11}{}^{35}ClNO$ ($[M+H]^+$) 208.0524, found 208.0521, $C_{11}H_{11}{}^{37}ClNO$ ($[M+H]^+$) 209.0421, found 209.0423.

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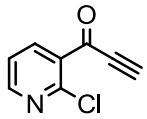
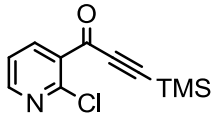
1-(2-chloropyridin-3-yl)prop-2-yn-1-one (3d).[2]



1-(2-chloropyridin-3-yl)-3-(trimethylsilyl)prop-2-yn-1-one (**3e**) (0.800 g, 3.36 mmol), KF (1.900 g, 33.6 mmol) and dibenzo-18-crown-6 (0.030 mg, 0.083 mmol) are stirred at room temperature in THF (30 mL). After 2 h the solvent is removed in vacuo and the crude product is purified by column chromatography (eluent: *n*-heptane/ethylacetate). The reaction afforded product **3d** as a white solid (0.100 g, 18 %, product is unstable); mp 98-100 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.52 (s, 1H, C≡CH), 7.35 (dd, ^{3}J = 4.8 Hz, ^{3}J = 2.0 Hz, 1H, H_{Ar}), 8.30 (dd, ^{4}J = 2.0 Hz, ^{3}J = 7.8 Hz, 1H, H_{Ar}), 8.49 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.8 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 80.7, 82.9, 122.3, 131.3, 141.4, 149.7, 152.7, 174.7. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3059 (w), 3066 (w), 2922 (w), 2852 (w), 2077 (m), 1683 (w), 1656 (s), 1570 (m), 1556 (s), 1443 (w), 1403 (s), 1265 (m), 1221 (m), 1133 (w), 1108 (s), 1064 (m). *m/z* (%) = 165 (M^+, 100), 137 (97), 130 (10), 113 (13), 102 (61), 85 (11), 76 (31), 62 (6), 53 (64), 50 (27). HRMS (ESI): calcd for $C_8H_5{}^{35}ClNO$ ($[M+H]^+$) 166.00542, found 166.00502, $C_8H_5{}^{37}ClNO$ ($[M+H]^+$) 168.00262, found 168.00247.

1-(2-chloropyridin-3-yl)-3-(trimethylsilyl)prop-2-yn-1-one (3e).



Starting with 2-chloropyridine-3-carboxylic acid chloride (**1**) (0.200 g, 1.14 mmol), $PdCl_2(PPh_3)_2$ (0.016 g, 0.023 mmol), CuI (0.009 g, 0.046 mmol), NEt_3 (0.17 mL, 1.2 mmol) and ethynyltrimethylsilane (0.17 mL, 1.2 mmol) in THF (10 mL), product **3e** was isolated as a brown solid (0.163 g, 60 %); mp 32-34 °C; Procedure E. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 0.20 (s, 9H, $Si(CH_3)_3$), 7.10 (dd, 1H, ^{3}J = 4.8 Hz, ^{3}J = 7.6 Hz, 1H,

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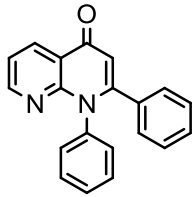
H_{Ar}), 7.70 (dd, 1H, ^{4}J = 2.0 Hz, ^{3}J = 7.6 Hz, 1H, H_{Ar}), 8.22 (dd, 1H, ^{4}J = 2.0 Hz, ^{3}J = 4.8 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 0.0, 102.1, 104.5, 123.3, 132.9, 142.0, 150.5, 153.3, 176.0. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3046 (w), 2964 (w), 2901 (w), 2152 (w), 1658 (m), 1572 (w), 1555 (w), 1401 (m), 1279 (w), 1268 (w), 1248 (m), 1232 (w), 1221 (w), 1128 (w), 1109 (m), 1098 (w), 1061 (w), 1005 (m). *m/z* (%) = 236 ($M\text{-}H^+$, 13), 222 (100), 194 (21), 194 (21), 179 (7), 158 (20), 143 (39), 130 (27), 117 (10), 93 (12), 76 (11), 63 (10), 53 (6), 43 (7). Anal. calcd for $C_{11}H_{12}NOClSi$ (237.76): C, 55.57; H, 5.09; N, 5.89. Found: C, 55.35; H, 4.86; N, 6.29.

1,2-diphenyl-1,8-naphthyridin-4(1*H*)-one (5a).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), $Pd(PPh_3)_4$ (0.072 g, 0.062 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and aniline (0.11 mL, 1.24 mmol) in DMF (10 mL) product **5a** was isolated as a brown solid (0.083 g, 45 %); mp 290-292 °C; Procedure B; ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 6.43 (s, 1H, C=CH), 7.06-7.31 (m, 11H, H_{Ar}), 8.56 (dd, ^{4}J = 2.1 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}), 8.72 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.1 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 113.5, 120.0, 120.8, 127.9, 128.3, 128.8, 128.8, 129.0, 130.1, 135.5, 135.6, 138.8, 151.9, 152.5, 155.1, 178.2. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3055 (w), 2953 (w), 2922 (w), 2852 (w), 1631 (m), 1595 (w), 1491 (w), 1481 (w), 1437 (w), 1412 (m), 1336 (w), 1309 (w), 1275 (w), 1191 (w), 1118 (w), 1070 (w), 1036 (w). *m/z* (%) = 297 ($M\text{-}H^+$, 100), 269 (9), 195 (5), 167 (4), 140 (3), 77 (5), 51 (3). HRMS (ESI): calcd for $C_{20}H_{14}N_2O$ ($[M+H]^+$) 299.1179, found 299.1180.

1-benzyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5b).

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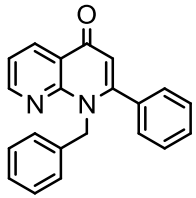
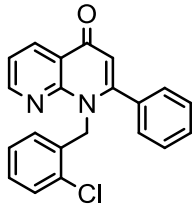


Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and benzylamine (0.14 mL, 1.24 mmol) in DMF (10 mL), product **5b** was isolated as a white solid (0.190 g, 98 %); mp 134-136 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 5.57 (s, 2H, CH_2), 6.27 (s, 1H, C=CH), 6.70-6.73 (m, 2H, H_{Ar}), 7.08-7.19 (m, 5H, H_{Ar}), 7.26-7.36 (m, 4H, H_{Ar}), 8.64 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.4 Hz, 1H, H_{Ar}), 8.71 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 49.5, 114.0, 120.0, 121.4, 126.3, 127.2, 128.4, 128.4, 128.5, 129.6, 135.2, 135.9, 137.6, 150.9, 152.4, 155.8, 177.8. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3049 (w), 3025 (w), 2958 (w), 1633 (m), 1615 (w), 1591 (m), 1575 (m), 1484 (m), 1453 (w), 1440 (w), 1426 (m), 1411 (m), 1361 (w), 1335 (w), 1327 (w), 1315 (w), 1291 (w), 1254 (w), 1235 (w), 1225 (w), 1185 (w), 1139 (w), 1077 (w), 1057 (w), 1043 (w), 1034 (w), 1027 (w). *m/z* (%) = 311 (M-H$^+$, 100), 283 (4), 233 (10), 181 (3), 91 (54), 65 (7). Anal. calcd for $C_{21}H_{17}N_2O$ (312.37): C, 80.75 ; H, 5.16; N, 8.97. Found: C, 80.38; H, 5.05; N, 8.98.

1-(2-chlorobenzyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5c).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 2-chlorobenzylamine (0.15 mL, 1.24 mmol) in DMF (10 mL), product **5c** was isolated as a white solid (0.181 g, 84 %); mp 175-178 °C;

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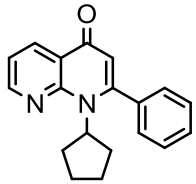
Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 5.57 (s, 2H, CH_2), 6.32 (s, 1H, C=CH), 6.52-6.56 (m, 1H, H_{Ar}), 6.99-7.13 (m, 4H, H_{Ar}), 7.22-7.39 (m, 5H, H_{Ar}), 8.61 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}), 8.73 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 47.8, 114.0, 120.2, 126.8, 126.9, 127.9, 128.2, 128.6, 129.4, 129.7, 131.9, 134.7, 135.2, 135.9, 150.8, 152.7, 155.8, 177.7. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3050 (w), 3036 (w), 3025 (w), 2953 (w), 2920 (w), 2850 (w), 1632 (s), 1615 (w), 1591 (m), 1575 (w), 1548 (w), 1483 (m), 1472 (w), 1441 (w), 1441 (w), 1423 (m), 1409 (s), 1339 (w), 1314 (w), 1294 (w), 1255 (w), 1235 (w), 1224 (w), 1138 (w), 1127 (w), 1038 (m). *m/z* (%) = 345 ($M\text{-}H^+$, 23), 311 (100), 233 (9), 155 (6), 125 (34), 89 (7), 77 (3). Anal. calcd for $C_{21}H_{15}ClN_2O$ (346.81): C, 72.73; H, 4.36; N, 8.08. Found: C, 72.61 ; H, 4.40 ; N, 8.02.

1-cyclopentyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5d).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and cyclopentylamine (0.12 mL, 1.24 mmol) in DMF (10 mL), product **5d** was isolated as a white solid (0.173 g, 96 %); mp 223-224 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 1.40-1.48 (m, 2H, CH_2), 1.65-1.75 (m, 2H, CH_2), 2.00-2.09 (m, 2H, CH_2), 2.41-2.53 (m, 2H, CH_2), 4.49-4.58 (m, 1H, CH), 6.17 (s, 1H, C=CH), 7.24-7.28 (m, 1H, H_{Ar}), 7.36-7.45 (m, 5H, H_{Ar}), 8.64-8.68 (m, 2H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 25.9, 30.6, 63.1, 113.6, 119.4, 122.5, 127.7, 128.8, 129.4, 135.8, 136.8, 150.7, 150.7, 156.6, 177.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3055 (w), 3035 (w), 3001 (w), 2951 (w), 2867 (w), 1633 (s), 1614 (m), 1605 (m), 1591 (s), 1553 (w) 1532 (w), 1484 (s), 1454 (m), 1442 (m), 1429 (m), 1393 (m), 1325 (m), 1301 (m), 1247 (m), 1233 (m), 1191 (m), 1168 (w), 1157 (w), 1138 (m), 1040 (m), 1035 (m). *m/z* (%) = 290 (M^+, 11), 261 (2),

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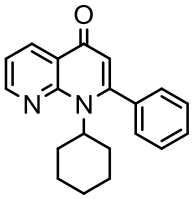
247 (2), 222 (100), 194 (44), 166 (4), 145 (2), 117 (2), 91 (3), 78 (2), 67 (2), 41 (3). Anal. calcd for $C_{19}H_{18}N_2O$ (290.36): C, 78.59; H, 6.25; N, 9.65. Found: C, 78.49 ; H, 6.26 ; N, 9.69.

1-cyclohexyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5e).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and cyclohexylamine (0.14 mL, 1.24 mmol) in DMF (10 mL), product **5e** was isolated as a white solid (0.185 g, 98 %); mp 262-263 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 0.81-0.98 (m, 2H, $H_{Cyclohexyl}$), 1.11-1.27 (m, 1H, $H_{Cyclohexyl}$), 1.46-1.51 (m, 1H, $H_{Cyclohexyl}$), 1.63-1.72 (m, 4H, $H_{Cyclohexyl}$), 2.83-2.98 (m, 2H, $H_{Cyclohexyl}$), 3.94-4.04 (m, 1H, $H_{Cyclohexyl}$), 6.18 (s, 1H, C=CH), 7.24-7.46 (m, 6H, H_{Ar}), 8.64-8.68 (m, 2H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 25.1, 26.5, 30.7, 63.9, 113.7, 119.5, 122.2, 127.6, 128.7, 129.4, 135.5, 136.8, 150.8, 151.5, 156.4, 177.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3053 (w), 3035 (w), 2981 (w), 2947 (w), 2916 (w), 2847 (w), 1635 (m), 1604 (w), 1591 (m), 1574 (w), 1483 (m), 1455 (w), 1444 (w), 1427 (w), 1421 (w), 1393 (m), 1340 (w), 1393 (m), 1340 (w), 1320 (w), 1303 (w), 1252 (m), 1238 (w), 1227 (w), 1189 (w), 1121 (w), 1060 (w), 1044 (w), 1060 (w), 1044 (w). *m/z* (%) = 304 ($M\text{-}H^+$, 7), 222 (100), 194 (28), 166 (3), 145 (3), 117 (3), 91 (3), 67 (3), 55 (3), 41 (4). Anal. calcd for $C_{20}H_{20}N_2O$ (304.39): C, 78.92; H, 6.62; N, 9.20. Found: C, 78.85; H, 6.63; N, 9.08.

1-phenethyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5f).

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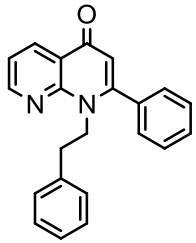
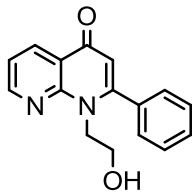


Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 2-phenylethylamine (0.16 mL, 1.24 mmol) in DMF (10 mL), product **5f** was isolated as a white solid (0.186 g, 92 %); mp 163-165 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 2.84 (t, 2H, ^{3}J = 7.7 Hz, CH_2), 4.47 (t, 2H, ^{3}J = 7.7 Hz, CH_2), 6.21 (s, 1H, C=CH), 6.73-6.76 (m, 2H, H_{Ar}), 7.09-7.2 (m, 5H, H_{Ar}), 7.31-7.44 (m, 4H, H_{Ar}), 8.69-8.77 (m, 2H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 35.5, 48.1, 113.4, 119.8, 121.6, 126.6, 128.2, 128.5, 128.6, 128.8, 129.5, 135.4, 135.9, 137.9, 150.5, 152.3, 155.4, 177.6. IR(ATR, cm^{-1}): $\tilde{\nu}$ = 3062 (w), 3045 (w), 3023 (w), 2994 (w), 2958 (w), 1621 (m), 1589 (m), 1553 (m), 1486 (m), 1453 (m), 1442 (m), 1433 (m), 1414 (m), 1368 (m), 1333 (m), 1314 (m), 1230 (m), 1256 (m), 1244 (m), 1230 (m), 1198 (m), 1174 (w), 1154 (w), 1144 (m), 1135 (m), 1041 (m), 1027 (m), 1000 (m). *m/z* (%) = 326 (M^+, 7), 235 (91), 222 (100), 194 (14), 166 (2), 133 (6), 106 (11), 91 (4), 78 (12), 65 (2), 51 (4). Anal. calcd for $C_{22}H_{18}N_2O$ (326.39): C, 80.53; H, 5.85; N, 8.42. Found: C, 80.96; H, 5.56 ; N, 8.58.

1-(2-hydroxyethyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5g).



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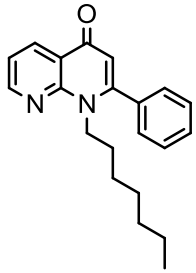
Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and ethanolamine (0.075 mL, 1.24 mmol) in DMF (10 mL), product **5g** was isolated as a white solid (0.101 g, 61 %); mp 174-175 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.82 (t, ^{3}J = 5.1 Hz, 2H, CH_2), 4.39 (t, ^{3}J = 5.1 Hz, 2H, CH_2), 6.15 (s, 1H, C=CH), 7.25-7.29 (m, 1H, H_{Ar}), 7.35-7.44 (m, 5H, H_{Ar}), 8.51 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}), 8.65 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 49.7, 61.5, 113.6, 119.8, 121.4, 128.6, 128.7, 129.5, 135.5, 136.0, 150.9, 151.9, 156.3, 177.2. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3210 (w), 3071 (w), 2957 (w), 2921 (w), 2864 (w), 1610 (m), 1593 (s), 1562 (w), 1557 (w), 1538 (w), 1494 (w), 1486 (m), 1445 (w), 1428 (w), 1411 (m), 1323 (w), 1316 (w), 1301 (w), 1258 (w), 1248 (w), 1234 (w), 1205 (w), 1143 (w), 1043 (s), 1013 (w). *m/z* (%) = 266 (M^+, 20), 247 (20), 235 (100), 222 (80), 205 (9), 194 (22), 166 (3), 133 (8), 106 (12), 78 (13), 51 (5). Anal. calcd for $C_{16}H_{14}N_2O_2$ (266.29): C, 72.16; H, 5.30; N, 10.52. Found: C, 72.31; H, 5.28; N, 10.28.

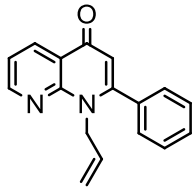
1-heptyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5h).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and *n*-heptylamine (0.18 mL, 1.24 mmol) in DMF (10 mL), product **5h** was isolated as a white solid (0.191 g, 96 %); mp 144-146 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 0.73-0.78 (t, ^{3}J = 7.0 Hz, 3H, CH_3), 1.02-1.14 (m, 8H, CH_2), 1.51-1.56 (m, 2H, CH_2), 4.23 (t, ^{3}J = 8.0 Hz, 2H, CH_2), 6.22 (s, 1H, C=CH), 7.28-7.45 (m, 6H, H_{Ar}), 8.67-8.71 (m, 2H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 14.0, 22.4, 26.4, 28.3, 29.7, 31.5,

46.7, 113.5, 119.7, 121.6, 128.2, 129.0, 129.4, 135.6, 135.7, 150.5, 152.1, 155.4, 177.5. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3101 (w), 3057 (w), 2956 (w), 2920 (w), 2852 (w), 2352 (w), 2163 (w), 2126 (w), 2071 (w), 1962 (w), 1930 (w), 1796 (w), 1756 (w), 1609 (s), 1589 (s), 1532 (m), 1494 (m), 1474 (w), 1456 (m), 1443 (w), 1432 (w), 1415 (w), 1380 (m), 1340 (m), 1303 (w), 1233 (m), 1155 (w), 1130 (w), 1091 (w), 1048 (w), 1024 (w). *m/z* (%) = 320 (27, M^+), 277 (5), 263 (8), 249 (10), 235 (57), 222 (100), 207 (6), 194 (25), 166 (4), 133 (4), 106 (7), 78 (6), 41 (4). Anal. calcd for $C_{21}H_{24}N_2O$ (320.43): C, 78.71; H, 7.55; N, 8.74. Found: C, 78.87; H, 7.57; N, 8.53.

1-allyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5j).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and allylamine (0.054 mL, 1.24 mmol) in DMF (10 mL), product **5j** was isolated as a white-brown solid (0.120 g, 74 %); mp 79-81 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 4.69 (dd, ^{3}J = 17.0 Hz, ^{2}J = 0.9 Hz, 1H, CH_2-CH=C*H*H), 4.86-4.88 (m, 2H, C*H*$_2$-CH=CHH), 5.00-5.04 (dd, ^{3}J = 10.3 Hz, ^{2}J = 0.9 Hz, 1H, CH_2-CH=CH*H*), 5.75-5.87 (m, 1H, CH_2-C*H*=CHH), 6.25 (s, 1H, O=C-C*H*=C), 7.29-7.44 (m, 6H, H_{Ar}), 8.68-8.70 (m, 2H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 48.6, 113.6, 116.9, 119.8, 128.3, 128.3, 128.4, 129.6, 133.2, 135.1, 135.8, 150.4, 152.2, 155.5, 177.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3145 (w), 3053 (w), 2979 (w), 2950 (w), 1631 (s), 1614 (m), 1602 (m), 1590 (s), 1575 (m), 1548 (w), 1483 (s), 1442 (w), 1424 (m), 1409 (s), 1360 (w), 1333 (w), 1312 (w), 1289 (w), 1254 (m), 1236 (m), 1224 (m), 1186 (w), 1159 (w), 1145 (w), 1074 (w), 1041 (w), 1033 (w), 1001 (w). *m/z* (%) = 261 (M-H^+, 91), 247 (100), 233 (10), 194 (76), 166 (9), 139 (6), 97 (13), 76 (4). Anal. calcd for $C_{17}H_{14}N_2O$ (262.31): C, 77.84; H, 5.38; N, 10.68. Found: C, 77.75; H, 5.44; N, 10.98.

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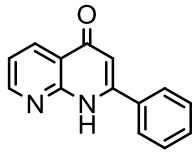
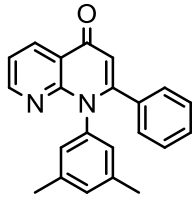
2-phenyl-1,8-naphthyridin-4(1*H*)-one (5k).



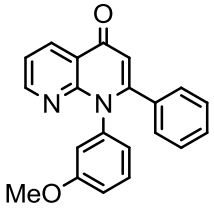
Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and ammonia (7 N solution in methanol, 0.18 mL, 1.26 mmol) in DMF (10 mL), product **5k** was isolated as a white-brown solid (0.098 g, 71 %); mp 224-226 °C °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 6.39 (s, 1H, C=CH), 7.42 (dd, ^4J = 4.4 Hz, ^3J = 8.0 Hz, 1H, H_{Ar}), 7.52-7.58 (m, 3H, H_{Ar}), 7.82-7.86 (m, 2H, H_{Ar}), 8.47 (dd, ^4J = 1.9 Hz, ^3J = 7.9 Hz, 1H, H_{Ar}), 8.78 (dd, ^4J = 1.9 Hz, ^3J = 3.2 Hz, 1H, H_{Ar}), 12.34 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 108.5 (CH), 119.3 (C), 119.9 (CH), 127.7 (CH), 128.8 (CH), 130.6 (CH), 133.6 (C), 134.5 (CH), 151.3 (C), 151.5 (C), 153.1 (CH), 177.2 (C=O). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3218 (w), 3130 (w), 3076 (w), 3052 (w), 2919 (w), 2867 (w), 2810 (w), 2748 (w), 1643 (w), 1627 (w), 1592 (m), 1580 (m), 1549 (m), 1504 (m), 1495 (m), 1442 (w), 1424 (m), 1403 (w), 1393 (w), 1335 (w), 1314 (m), 1258 (w), 1234 (w), 1223 (w), 1190 (w), 1144 (w), 1119 (w), 1090 (w), 1039 (w), 1028 (w), 1000 (w). *m/z* (%) = 222 (M^+, 100), 194 (83), 166 (12), 139 (7), 97 (8), 91 (6), 84 (4), 76 (4), 63 (4), 51 (4). Anal. calcd for $C_{14}H_{10}N_2O$ (222.24): C, 75.66; H, 4.54; N, 12.60. Found: C, 75.80; H, 4.86; N, 12.47.

1-(3,5-dimethylphenyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5l).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), $Pd(PPh_3)_4$ (0.072 g, 0.062 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 3,5-dimethylaniline (0.15 mL, 1.24 mmol) in DMF (10 mL), product **5l** was isolated as a brown solid (0.083 g, 41 %); mp 188-190 °C; Procedure B. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.15 (s, 6H, CH_3), 6.41 (s, 1H, H_{Ar}), 6.67 (s, 2H, H_{Ar}), 6.81 (s, 1H, H_{Ar}), 7.09-7.16 (m, 5H, H_{Ar}), 7.25-7.29 (dd, ^{3}J = 4.5 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}), 8.58 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}), 8.71 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 21.1, 113.4, 119.9, 120.8, 127.7, 127.8, 128.7, 128.9, 130.1, 135.6, 138.4, 138.5, 152.0, 152.6, 155.4, 178.1. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3054 (w), 3040 (w), 3010 (w), 2918 (w), 2852 (w), 1633 (s), 1615 (m), 1592 (s), 1558 (w), 1492 (w), 1479 (m), 1445 (w), 1405 (s), 1377 (w), 1338 (w), 1295 (m), 1248 (w), 1226 (w), 1175 (w), 1135 (w), 1108 (w), 1077 (w), 1037 (w), 1027 (w). *m/z* (%) = 325 (M-H$^+$, 100), 297 (5), 282 (5), 223 (3), 195 (4), 163 (2), 140 (2), 103 (2), 77 (3). Anal. calcd for $C_{22}H_{18}N_2O$ (326.39): C, 80.96; H, 5.56; N, 8.58. Found: C, 80.56; H, 4.45; N, 8.55.

1-(3-methoxyphenyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5m).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), $Pd(PPh_3)_4$ (0.072 g, 0.062 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 3-methoxylaniline (0.14 mL, 1.24 mmol) in DMF (10 mL), product **5m** was isolated as a white solid (0.126 g, 62 %); mp 254-255 °C; Procedure B. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 3.62 (s, 1H, OCH_3), 6.41 (s, 1H, C=C*H*), 6.59-6.61 (m, 1H, H_{Ar}), 6.68-6.76 (m, 2H, H_{Ar}), 7.12-7.17 (m, 6H, H_{Ar}), 7.26-7.30 (m, 1H, H_{Ar}), 8.57 (dd, ^{4}J = 2.0 Hz, ^{3}J = 7.9 Hz, 1H, H_{Ar}), 8.70 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 55.4, 113.5, 114.1, 116.1, 120.0, 120.8, 122.5, 128.0, 128.9, 128.9, 129.3, 135.5, 135.7, 139.8, 151.9, 152.5, 155.1,

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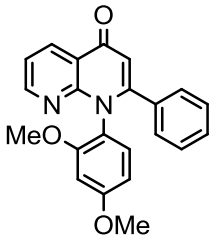
159.8, 178.2. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3049 (w), 3037 (w), 3007 (w), 2963 (w), 2936 (w), 2837 (w), 1632 (s), 1602 (m), 1593 (m), 1574 (w), 1545 (w), 1480 (m), 1439 (w), 1427 (w), 1405 (s), 1336 (w), 1310 (w), 1280 (m), 1244 (m), 1222 (s), 1189 (w), 1171 (m), 1147 (w), 1138 (w), 1084 (w), 1049 (m), 1038 (m). *m/z* (%) = 327 ($M\text{-}H^+$, 100), 312 (6), 184 (3), 255 (4), 211 (2), 155 (3), 128 (3), 113 (3), 98 (2), 77 (2). Anal. calcd for $C_{21}H_{16}N_2O_2$ (328.36): C, 76.81; H, 4.91; N, 8.53. Found: C, 76.78 ; H, 5.02 ; N, 8.34.

1-(2,4-dimethoxyphenyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5n).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), $Pd(PPh_3)_4$ (0.072 g, 0.062 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 2,4-dimethoxylaniline (0.18 mL, 1.24 mmol) in DMF (10 mL), product **5n** was isolated as a white-brown solid (0.138 g, 62 %); mp 150-152 °C; Procedure B. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.53 (s, 3H, OCH_3), 3.69 (s, 3H, OCH_3), 6.27-6.35 (m, 2H, H_{Ar}), 6.39 (s, 1H, C=CH), 6.93 (d, ^{3}J = 8.6 Hz, 1H, H_{Ar}), 7.12-7.16 (m, 5H, H_{Ar}), 7.23-7.27 (dd, ^{4}J = 4.5 Hz, ^{3}J = 7.8 Hz, 1H, H_{Ar}), 8.56 (dd, ^{3}J = 4.5 Hz, ^{4}J = 2.0 Hz, 1H, H_{Ar}), 8.69 (dd, ^{3}J = 7.9 Hz, ^{4}J = 2.0 Hz, 1H, H_{Ar}). ^{13}C-NMR ($CDCl_3$, 63 MHz) : δ = 55.4, 55.4, 99.1, 104.2, 113.0, 115.8, 119.8, 120.9, 127.6, 128.4, 128.8, 131.3, 135.5, 135.6, 152.0, 152.6, 156.0, 156.3, 160.9, 178.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3064 (w), 3006 (w), 2962 (w), 2928 (w), 2835 (w), 1627 (s), 1589 (m), 1510 (m), 1477 (m), 1455 (w), 1436 (w), 1423 (w), 1405 (s), 1314 (w), 1276 (m), 1255 (w), 1244 (m), 1211 (s), 1161 (s), 1135 (m), 1098 (w), 1044 (w), 1028 (m). *m/z* (%) = 358 (M^+, 4), 327 (100), 312 (5), 283 (2), 197 (3), 163 (3), 128 (3). Anal. calcd for $C_{22}H_{18}N_2O_3$ (358.39): C, 73.73; H, 5.06; N, 7.82. Found: C, 73.55; H, 4.93; N, 7.71.

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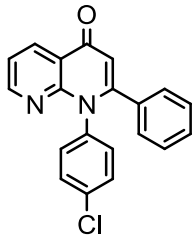
1-(4-chlorophenyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5o).



Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), $Pd(PPh_3)_4$ (0.072 g, 0.062 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 4-chloroaniline (0.158 g, 1.24 mmol) in DMF (10 mL), product **5o** was isolated as a white solid (0.083 g, 40 %); mp 243-244 °C; Procedure B. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 6.42 (s, 1H, C=CH), 7.00-7.31 (m, 10H, H_{Ar}), 8.55 (dd, ^4J = 2.1 Hz, ^3J = 4.5 Hz, 1H, H_{Ar}), 8.70 (dd, ^4J = 2.0 Hz, ^3J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 113.7, 120.2, 120.8, 128.2, 129.0, 129.0, 129.0, 131.4, 134.2, 135.1, 135.8, 137.3, 151.8, 152.4, 154.8, 178.1. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3061 (w), 3049 (w), 3031 (w), 2963 (w), 2918 (w), 2849 (w), 1630 (s), 1611 (m), 1591 (m), 1573 (m), 1546 (m), 1491 (m), 1476 (s), 1445 (w), 1410 (m), 1399 (s), 1338 (w), 1308 (w), 1272 (m), 1240 (w), 1180 (w), 1136 (w), 1095 (w), 1085 (w), 1040 (w), 1031 (w), 1022 (m). *m/z* (%) = 333 (41, M-H$^+$, ^{37}Cl), 331 (100, M-H$^+$, ^{35}Cl), 295 (9), 268 (15), 229 (6), 201 (5), 166 (4), 134 (5), 111 (3), 75 (5). HRMS (ESI): calcd for $C_{20}H_{14}{}^{35}ClN_2O$ ($[M+H]^+$) 333.0796, found 333.0789, $C_{20}H_{14}{}^{37}ClN_2O$ ($[M+H]^+$) 335.0767, found 335.0771.

1-(4-bromophenyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (5p).

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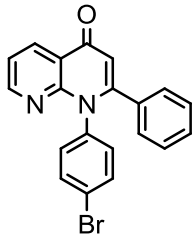
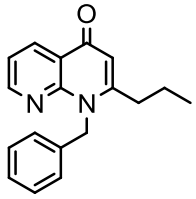


Starting with 1-(2-chloropyridin-3-yl)-3-phenylprop-2-yn-1-one (**3a**) (0.150 g, 0.62 mmol), $Pd(PPh_3)_4$ (0.072 g, 0.062 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 4-bromoaniline (0.213 g, 1.24 mmol) in DMF (10 mL), product **5p** was isolated as a white solid (0.082 g, 35 %); mp 223-225 °C; Procedure B. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 6.42 (s, 1H, C=CH), 6.94-6.97 (m, 2H, H_{Ar}), 7.08-7.17 (m, 4H, H_{Ar}), 7.27-7.38 (m, 4H, H_{Ar}), 8.54 (dd, ^4J = 2.0 Hz, ^3J = 4.4 Hz, 1H, H_{Ar}), 8.70 (dd, ^4J = 2.0 Hz, ^3J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 112.5, 120.3, 120.5, 121.3, 128.1, 129.0, 129.2, 131.6, 132.8, 135.0, 135.3, 138.5, 151.7, 152.7, 154.8, 176.8. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3058 (w), 3028 (w), 1730 (w), 1630 (s), 1610 (w), 1592 (m), 1545 (w), 1489 (m), 1477 (m), 1444 (w), 1410 (m), 1402 (m), 1336 (w), 1308 (m), 1271 (m), 1183 (w), 1155 (w), 1136 (w), 1070 (w), 1040 (w), 1031 (w), 1019 (w). *m/z* (%) = 379 (95, M^+, ^{81}Br), 377 (100, M^+, ^{79}Br), 295 (21), 268 (29), 247 (4), 207 (5), 167 (9), 148 (19), 102 (5), 76 (8), 63 (3), 44 (5). Anal. calcd for $C_{20}H_{13}BrN_2O$ (377.23): C, 63.68; H, 3.47; N, 7.43. Found: C, 63.72; H, 3.65; N, 7.44.

1-benzyl-2-propyl-1,8-naphthyridin-4(1*H*)-one (5q).



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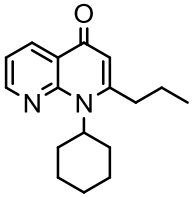
Starting with 1-(2-chloropyridin-3-yl)hex-2-yn-1-one (**3c**) (0.129 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and benzylamine (0.14 mL, 1.24 mmol) in DMF (10 mL), product **5q** was isolated as a white solid (0.161 g, 93 %); mp 82-84 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 0.92 (t, ^{3}J = 7.4 Hz, 3H, CH_3), 1.57-1.69 (m, 2H, CH_2), 2.58 (t, ^{3}J = 7.4 Hz, 2H, CH_2), 5.80 (s, 2H, CH_2), 6.34 (s, 1H, C=CH), 6.92-6.94 (m, 2H, H_{Ar}), 7.22-7.29 (m, 4H, H_{Ar}), 8.58 (dd, ^{4}J = 1.9 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}), 8.66 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 18.7, 26.6, 39.7, 51.9, 115.9, 125.2, 125.4, 130.8, 132.3, 133.9, 140.3, 142.9, 155.8, 157.6, 161.7, 181.3. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3058 (w), 3030 (w), 2960 (w), 2929 (w), 2870 (w), 1681 (w), 1618 (m), 1592 (m), 1546 (w), 1492 (m), 1452 (w), 1426 (w), 1412 (m), 1363 (w), 1307 (w), 1278 (w), 1244 (w), 1227 (w), 1188 (w), 1138 (w), 1119 (m), 1049 (w), 1028 (w), 1000 (w). *m/z* (%) = 278 (M^+, 87), 263 (20), 250 (28), 235 (6), 187 (37), 91 (100), 65 (13). Anal. calcd for $C_{18}H_{18}N_2O$ (278.35): C, 77.67; H, 6.52; N, 10.06. Found: C, 77.83 ; H, 6.49 ; N, 10.07.

1-cyclohexyl-2-propyl-1,8-naphthyridin-4(1*H*)-one (5r).



Starting with 1-(2-chloropyridin-3-yl)hex-2-yn-1-one (**3c**) (0.129 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and cyclohexylamine (0.14 mL, 1.24 mmol) in DMF (10 mL), product **5r** was isolated as a white solid (0.163 g, 97 %); mp 114-116 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 1.02 (t, ^{3}J = 7.4 Hz, 3H, CH_3), 1.28-1.34 (m, 3H, CH_2), 1.61-1.73 (m, 5H, CH_2), 1.87-1.90 (m, 2H, CH_2), 2.68 (t, ^{3}J = 7.4 Hz, 2H, CH_2), 3.00-3.13 (m, 2H, CH_2), 4.12-4.20 (m, 1H, $CH_{Cyclohexyl}$), 6.28 (s, 1H, C=CH), 7.22-7.24 (m, 1H, H_{Ar}), 8.58-8.65 (m, 2H, H_{Ar}). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 13.4, 21.7, 24.9, 26.0, 30.0, 36.3, 60.4, 111.5, 119.4, 120.8, 134.5, 150.7, 151.1, 156.3, 175.7. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3076 (w), 3020 (w), 2961 (w), 2916 (w), 2862 (w), 2849 (w), 1623 (s), 1589 (s), 1571 (m), 1547 (w), 1483 (m), 1459 (w), 1435 (w), 1415 (m), 1389

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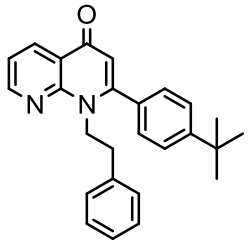
(m), 1380 (m), 1337 (w), 1299 (w), 1287 (w), 1258 (w), 1244 (w), 1225 (w), 1199 (w), 1149 (w), 1117 (s), 1048 (w). *m/z* (%) = 270 (M^+, 17), 188 (44), 173 (13), 160 (100), 131 (8), 78 (4), 55 (4). HRMS (ESI): calcd for $C_{17}H_{23}N_2O$ ($[M+H]^+$) 271.18049, found 271.18042.

2-(4-*tert*-butylphenyl)-1-phenethyl-1,8-naphthyridin-4(1*H*)-one (5s).



Starting with 3-(4-*tert*-butylphenyl)-1-(2-chloropyridin-3-yl)prop-2-yn-1-one (**3b**) (0.185 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 2-phenylethylamine (0.16 mL, 1.24 mmol) in DMF (10 mL), product **5s** was isolated as a white solid (0.232 g, 98 %); mp 202-204 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.33 (s, 9H, $C(CH_3)_3$), 2.82 (t, ^3J = 7.9 Hz, 2H, CH_2), 4.48 (t, ^3J = 7.9 Hz, 2H, CH_2), 6.25 (s, 1H, C=CH), 6.70- 6.73 (m, 2H, H_{Ar}), 7.07-7.11 (m, 3H, H_{Ar}), 7.16-7.19 (m, 2H, H_{Ar}), 7.30-7.35 (m, 1H, H_{Ar}), 7.41-7.45 (m, 2H, H_{Ar}), 8.70 (dd, ^4J = 2.0 Hz, ^3J = 8.0 Hz, 1H, H_{Ar}), 8.75 (dd, ^4J = 2.0 Hz, ^3J = 4.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 31.3, 34.9, 35.6, 48.0, 113.5, 119.7, 121.6, 125.5, 126.5, 128.1, 128.4, 128.7, 132.4, 135.8, 138.0, 150.5, 152.2, 152.8, 155.5, 177.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3051 (w), 3028 (w), 3000 (w), 2960 (w), 2902 (w), 2867 (w), 1622 (s), 1601 (w), 1589 (s), 1556 (w), 1504 (w), 1468 (m), 1451 (w), 1431 (w), 1414 (s), 1366 (w), 1332 (w), 1313 (w), 1299 (w), 1257 (w), 1246 (w), 1232 (m), 1197 (w), 1188 (w), 1134 (m), 1110 (w), 1049 (w), 1038 (w), 1027 (w). *m/z* (%) = 382 (M^+, 7), 291 (3), 278 (100), 263 (25), 235 (91), 205 (3), 133 (5), 106 (8), 91 (3), 78 (7), 57 (16). Anal. calcd for $C_{26}H_{26}N_2O$ (383.50): C, 81.64; H, 6.85; N, 7.32. Found: C, 81.42; H, 6.63; N, 7.50.

2-(4-*tert*-butylphenyl)-1-cyclohexyl-1,8-naphthyridin-4(1*H*)-one (5t).

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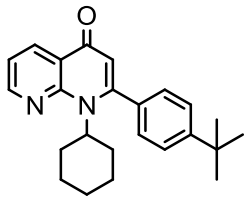
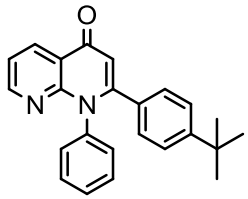


Starting with 3-(4-*tert*-butylphenyl)-1-(2-chloropyridin-3-yl)prop-2-yn-1-one (**3b**) (0.185 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 2- cyclohexylamine (0.14 mL, 1.24 mmol) in DMF (10 mL), product **5t** was isolated as a white solid (0.210 g, 94 %); mp 185-187 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 0.83-0.97 (m, 4H, CH_2), 1.32 (s, 9H, $C(CH_3)_3$), 1.52-1.73 (m, 4H, CH_2), 2.84-3.00 (m, 2H, CH_2), 3.99-4.08 (m, 1H, $CH_{Cyclohexyl}$), 6.18 (s, 1H, C=CH), 7.19-7.27 (m, 3H, H_{Ar}), 7.42-7.45 (m, 2H, H_{Ar}), 8.64-8.67 (m, 2H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 25.2, 26.6, 30.7, 31.3, 34.8, 63.9, 113.8, 119.4, 122.2, 125.6, 127.4, 133.8, 135.5, 150.8, 151.6, 152.7, 156.7, 177.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3041 (w), 2957 (w), 2925 (w), 2852 (w), 1639 (s), 1589 (m), 1556 (w), 1506 (w), 1486 (m), 1456 (w), 1431 (w), 1397 (m), 1363 (w), 1337 (w), 1303 (w), 1255 (w), 1230 (w), 1201 (w), 1140 (w), 1127 (w), 1109 (w), 1063 (w), 1044 (w), 1024 (w). *m/z* (%) = 360 (M^+, 10), 278 (100), 263 (66), 235 (9), 207 (4), 117 (4), 103 (3), 78 (2), 55 (3), 41 (3). Anal. calcd for $C_{24}H_{28}N_2O$ (360.49): C, 79.96; H, 7.83; N, 7.77. Found: C, 80.19; H, 7.75; N, 7.45.

2-(4-*tert*-butylphenyl)-1-phenyl-1,8-naphthyridin-4(1*H*)-one (5u).



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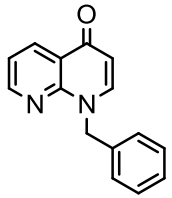
Starting with 3-(4-*tert*-butylphenyl)-1-(2-chloropyridin-3-yl)prop-2-yn-1-one (**3b**) (0.185 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and aniline (0.11 mL, 1.24 mmol) in DMF (10 mL), product **5u** was isolated as a white solid (0.092 g, 42 %); mp 247-249 °C; Procedure B. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.16 (s, 9H, $C(CH_3)_3$), 6.44 (s, 1H, C=CH), 7.00-7.14 (m, 6H, H_{Ar}), 7.19-7.29 (m, 4H, H_{Ar}), 8.54 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.6 Hz, 1H, H_{Ar}), 8.71 (dd, ^{4}J = 2.0 Hz, ^{3}J = 7.9 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 31.1, 34.6, 113.5, 119.9, 120.8, 124.8, 128.2, 128.6, 128.8, 130.1, 132.5, 135.6, 138.9, 152.0, 152.0, 152.4, 155.4, 178.2. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3062 (w), 3049 (w), 2961 (w), 2902 (w), 2866 (w), 1635 (s), 1613 (w), 1594 (m), 1577 (w), 1506 (w), 1495 (m), 1477 (m), 1410 (s), 1361 (w), 1338 (w), 1305 (w), 1270 (m), 1202 (w), 1178 (w), 1155 (w), 1134 (w), 1115 (w), 1037 (w), 1025 (w). *m/z* (%) = 353 ($M\text{-}H^+$, 100), 339 (19), 297 (4), 197 (6), 155 (8), 140 (2), 77 (3). Anal. calcd for $C_{24}H_{22}N_2O$ (354.44): C, 81.33; H, 6.26; N, 7.90. Found: C, 81.55 ; H, 6.31 ; N, 7.70.

1-benzyl-1,8-naphthyridin-4(1*H*)-one (5v).



Starting with 1-(2-chloropyridin-3-yl)-3-(trimethylsilyl)prop-2-yn-1-one (**3e**) (0.147 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and benzylamine (0.14 mL, 1.24 mmol) in DMF (10 mL) at 100 °C, product **5v** was isolated as a white solid (0.119 g, 81 %); mp 113-115 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 5.62 (s, 2H, CH_2), 6.19 (d, ^{3}J = 7.9 Hz, 1H, C=C*H*-C=O), 7.27-7.32 (m, 5H, H_{Ar}), 7.41-7.45 (m, ^{4}J = 4.5 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}), 8.20 (d, ^{3}J = 7.9 Hz, 1H, C=C*H*-N), 8.52 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}), 8.76 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 51.8, 110.1, 119.6, 121.1, 127.0, 127.2, 128.3, 135.0, 137.1, 144.2, 149.5, 152.1, 176.9. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3060 (w), 3047 (w), 3025 (w), 2991 (w), 2952 (w), 2923 (w), 2850 (w), 1643 (w), 1617 (s), 1580 (s), 1551 (w), 1489 (m), 1454 (w), 1434 (m), 1412 (m), 1401 (m), 1358 (w), 1327 (w), 1300 (w), 1289 (w), 1252 (w), 1235 (s), 1216 (w), 1184 (w), 1155 (w), 1135 (w),

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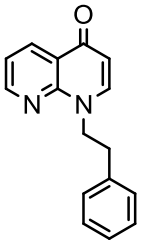
1120 (w), 1085 (w), 1047 (w), 1027 (w). *m/z* (%) = 236 (M^+, 79), 207 (4), 117 (2), 91 (100), 65 (12), 51 (4). Anal. calcd for $C_{15}H_{12}N_2O$ (236.27): C, 76.25; H, 5.12; N, 11.86. Found: C, 76.31 ; H, 5.42 ; N, 11.44.

1-phenethyl-1,8-naphthyridin-4(1*H*)-one (5w).



Starting with 1-(2-chloropyridin-3-yl)-3-(trimethylsilyl)prop-2-yn-1-one (**3e**) (0.147 g, 0.62 mmol), K_2CO_3 (0.171 g, 1.24 mmol) and 2-phenylethylamine (0.16 mL, 1.24 mmol) in DMF (10 mL) at 100 °C, product **5w** was isolated as a white solid (0.101 g, 65 %); mp 98-100 °C; Procedure A. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.06 (t, ^{3}J = 7.0 Hz, 2H, CH_2), 4.50 (t, ^{3}J = 7.0 Hz, 2H, CH_2), 6.07 (d, ^{3}J = 7.9 Hz, 1H, C=CH), 7.00-7.03 (m, 2H, H_{Ar}), 7.12-7.17 (m, 2H, H_{Ar}), 7.12-7.30 (m, 3H, H_{Ar}), 8.64 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.0 Hz, 1H, H_{Ar}), 8.69 (dd, ^{4}J = 2.0 Hz, ^{3}J = 4.5 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 35.7, 52.7, 110.5, 119.7, 121.9, 126.9, 128.7, 128.9, 136.0, 137.7, 143.4, 149.6, 152.3, 178.7. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3040 (w), 3028 (w), 2958 (w), 2944 (w), 2864 (w), 1616 (s), 1600 (w), 1579 (s), 1485 (s), 1454 (w), 1429 (m), 1409 (s), 1393 (w), 1370 (w), 1312 (w), 1298 (w), 1286 (w), 1264 (m), 1239 (s), 1224 (m), 1199 (w), 1190 (m), 1151 (w), 1128 (w), 1084 (w), 1048 (w), 1031 (w), 1023 (w). *m/z* (%) = 250 (M^+, 12), 159 (54), 146 (100), 133 (8), 118 (10), 106 (9), 91 (6), 78 (11), 65 (4), 51 (5). Anal. calcd for $C_{16}H_{14}N_2O$ (250.29): C, 76.78; H, 5.64; N, 11.19. Found: C, 76.72 ; H, 5.64 ; N, 11.18.

1-(3-(trifluoromethyl)phenyl)-2-phenyl-1,8-naphthyridin-4(1H)-one (5x)

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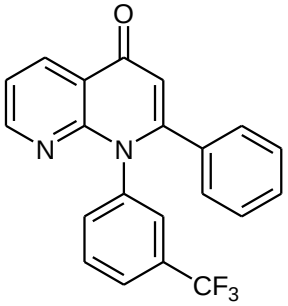
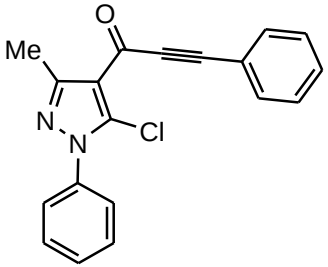


Yellow solid, mp 207-209 ^{0}C.^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.49 (s, 1H, CH_{Ar}), 7.12-7.21 (m, 2H, C*H*$_{Ar}$), 7.34-7.53 (m, 7H, C*H*$_{Ar}$), 7.62-7.69 (m, 1H, C*H*$_{Ar}$), 8.57-8.60 (m, 1H, CH_{Ar}), 8.77 (dd, 1H, ^{3}J = 7.9 Hz, ^{4}J = 2.0 Hz, CH_{Ar}).
^{19}F NMR (282 MHz, $CDCl_3$): δ = -62.9.
^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 113.8, 120.3 (CH), 123.3 (q, ^{1}J = 273 Hz, CF_3), 124.9 (q, ^{3}J = 3.7 Hz, *C*HCCF$_3$), 127.4 (q, ^{3}J = 3.7 Hz, *C*HCCF$_3$), 128.2, 128.4, 128.6, 128.9, 129.1 (CH), 131.3 (q, ^{2}J = 32 Hz, *C*CF$_3$), 131.9 (C), 132.0, 132.1 (CH), 134.9 (C), 139.4, 151.6 (C), 152.4 (CH), 154.7, 178.2 (C).
MS (GC, 70eV): *m/z* (%) = 366 (M^+, 100).
HRMS (EI): calcd for $C_{21}H_{13}F_3N_2O$ (M^+) 366.33593, found 366.33595.
IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3057 (w), 1636 (s), 1593 (m), 1496 (m), 1477 (m), 1446 (m), 1404 (s), 1328 (s), 1304 (m), 1265 (m), 1170 (s), 1137 (m), 1116 (s), 1074 (s), 1042 (m), 989 (m), 928 (w), 846 (m), 829 (m), 813 (m), 769 (s), 721 (s), 699 (s), 653 (s), 540 (s).

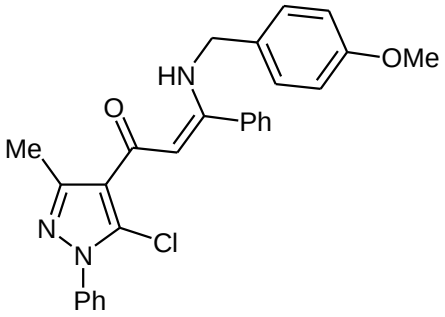
1-(5-chloro-3-methyl-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-yn-1-one (9)



Brown solid 80%. Mp 78 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 2.64 (s, 3H, Me), 7.37–7.57 (m, 8H), 7.62-7.65 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 15.4, 88.3, 92.4, 118.2, 120.3, 125.6, 128.6, 129.1, 130.7, 131.6, 132.8, 137.2, 152.4, 164.0, 170.3. MS (GC, 70 eV) *m/z* (%) 320

(M$^+$, 46), 319 (100), 189 (11), 129 (15), 77 (31); HRMS (EI): calcd for $C_{19}H_{13}ClN_2O$ (M$^+$) 320.07125, found 320.07127; IR (ATR, cm^{-1}) $\tilde{\nu}$ 3035 (w), 2199 (m), 1620 (s), 1520 (m), 1489 (m), 1462 (s), 1415 (m), 1382 (m), 1369 (s), 1299 (m), 1205 (w), 1101 (w), 1072 (w), 1027 (m), 1014 (m), 986 (s), 907 (w), 815 (w), 786 (m), 752 (s), 684 (s), 645 (m), 605 (s).

3-(4-methoxybenzylamino)-1-(5-chloro-3-methyl-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (10)



Wiht solid 60%. mp 155-157°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 2.40 (s, 3H, Me), 2.40 (s, 3H, OMe), 4.34 (d, 1H, ^3J = 6.3 Hz, CH_2), 5.60 (s, 1H, OCCH), 6.89-6.92 (m, 2H), 7.13-7.16 (m, 2H), 7.48-7.55 (m, 10H), 11.35 (t, 1H, ^3J = 6.3 Hz, NH); ^{13}C NMR (75 MHz, DMSO-d_6) δ 14.5, 47.1, 55.0, 96.2, 114.0, 119.0, 120.0, 127.6, 128.5, 128.7, 129.1, 129.7, 130.3, 134.8, 137.4, 149.6, 158.6, 165.5, 181.9. MS (GC, 70 eV) *m/z* (%) 457 (M$^+$, 4), 422 (100), 121 (65); HRMS (EI): calcd for $C_{27}H_{24}ClN_3O_2$ (M$^+$) 457.1632, found 457.1634; IR (ATR, cm^{-1}) $\tilde{\nu}$ 2928 (w), 1607 (w), 1557 (m), 1506 (m), 1484 (m), 1454 (m), 1411 (m), 1361 (m), 1303 (m), 1250 (m), 1182 (m), 1141 (w), 1104 (w), 1070 (w), 1033 (m), 889 (w), 818 (m), 774 (s), 736 (m), 697 (s), 613 (w).

(Z)-3-(3-(trifluoromethyl)phenylamino)-1-(2-chloropyridin-3-yl)-3-phenylprop-2-en-1-one (11)

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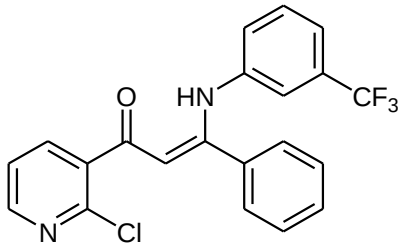
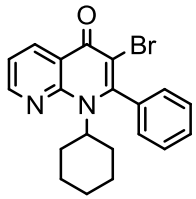


Yellow solid 61%. mp 183-185°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.84 (s, 1H, CC*H*C), 6.89-6.92 (m, 1H), 6.98 (br.s, 1H), 7.19-7.21 (m, 2H), 7.26-7.35 (m, 6H), 7.87 (dd, 1H, ^{3}J = 7.5 Hz, ^{4}J = 2.0 Hz), 8.38 (dd, 1H, ^{3}J = 4.7 Hz, ^{4}J = 1.9 Hz), 12.61 (s, 1H, NH); ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.1; ^{13}C NMR (75 MHz, $CDCl_3$) δ 101.3, 119.9 (q, ^{3}J = 3.8 Hz), 121.0 (q, ^{3}J = 3.8 Hz), 122.4, 123.4 (q, ^{1}J = 272.2 Hz), 126.2, 128.3, 128.9, 129.3, 130.4, 131.3 (q, ^{2}J = 30.7 Hz), 134.2, 136.8, 138.4, 139.6, 147.6, 150.2, 161.6, 189.1. MS (GC, 70 eV) *m/z* (%) 402 (M^{+}, 30), 367 (100), 290 (63), 262 (73), 145 (20); HRMS (EI): calcd for $C_{21}H_{14}F_3N_2O$ (M^{+}) 402.0719, found 402.0721; IR (ATR, cm^{-1}) $\tilde{\nu}$ 2196 (w), 1593 (m), 1567 (s), 1514 (m), 1490 (w), 1471 (m), 1451 (m), 1392 (m), 1307 (s), 1265 (m), 1222 (m), 1161 (m), 1124 (s), 1098 (s), 1064 (m), 1037 (m), 999 (m), 891 (m), 871 (m), 799 (m), 763 (s), 729 (m), 697 (s), 656 (m), 639 (s).

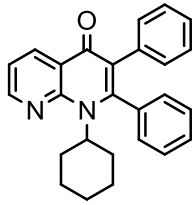
3-bromo-1-cyclohexyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (20).



Starting with 1-cyclohexyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (**5e**) (0.600 g, 1.97 mmol), Br_2 (0.15 mL, 2.96 mmol) and Na_2CO_3 (1.252 g, 11.82 mmol) in THF (30 mL), product **20** was isolated as a white solid (0.680 g, 90 %); mp 253-255 °C; Procedure C. ^{1}H NMR ($CDCl_3$,

250 MHz): δ = 0.73-0.86 (m, 2H, $H_{Cyclohexyl}$), 1.09-1.18 (m, 1H, $H_{Cyclohexyl}$), 1.43-1.48 (m, 1H, $H_{Cyclohexyl}$), 1.59-1.69 (m, 4H, $H_{Cyclohexyl}$), 2.89-2.93 (m, 2H, $H_{Cyclohexyl}$), 3.87 (m, 1H, $H_{Cyclohexyl}$), 7.22-7.32 (m, 3H, H_{Ar}), 7.47-7.54 (m, 3H, H_{Ar}), 8.68 (dd, ^4J = 2.1 Hz, ^3J = 4.3 Hz, 1H, H_{Ar}), 8.74 (dd, ^4J = 2.1 Hz, ^3J = 7.9 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 25.0, 26.6, 30.5, 66.0, 109.9, 120.0, 120.1, 127.3, 129.2, 129.6, 136.4, 136.8, 150.3, 151.2, 154.0, 172.8. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3045 (w), 2997 (w), 2929 (w), 2866 (w), 2842 (w), 1620 (s), 1590 (s), 1575 (m), 1529 (w), 1483 (m), 1444 (w), 1425 (w), 1414 (w), 1383 (m), 1332 (w), 1310 (w), 1264 (w), 1235 (s), 1156 (w), 1128 (m), 1094 (w), 1059 (w), 1046 (m). m/z (%) = 384 ($M\text{-}H^+$, 14, ^{81}Br), 382 ($M\text{-}H^+$, 14, ^{79}Br), 302 (98, ^{81}Br), 300 (100,^{79}Br), 274 (18), 221 (35), 192 (18), 166 (18), 139 (5), 55 (7), 41 (7). Anal. calcd for $C_{20}H_{19}BrN_2O$ (383.28): C, 62.67; H, 5.00; N, 7.31. Found: C, 62.71 ; H, 5.01 ; N, 7.43.

1-cyclohexyl-2,3-diphenyl-1,8-naphthyridin-4(1*H*)-one (21a).



Starting with 3-bromo-1-cyclohexyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (**20**) (0.150 g, 0.39 mmol), $Pd(PPh_3)_4$ (0.023 g, 0.020 mmol), K_2CO_3 (0.108 g, 0.78 mmol) and phenylboronic acid (0.052 g, 0.43 mmol) in DMF (10 mL), product **21a** was isolated as a white solid (0.089 g, 60 %); mp 215-218 °C; Procedure D. ^1H NMR ($CDCl_3$, 250 MHz): δ = 0.74-0.87 (m, 2H, $H_{Cyclohexyl}$), 1.15-1.21 (m, 1H, $H_{Cyclohexyl}$), 1.44-1.48 (m, 1H, $H_{Cyclohexyl}$), 1.65-1.69 (m, 4H, $H_{Cyclohexyl}$), 2.90-3.02 (m, 2H, $H_{Cyclohexyl}$), 3.84-3.91 (m, 1H, $H_{Cyclohexyl}$), 6.91-7.10 (m, 7H, H_{Ar}), 7.17-7.21 (m, 3H, H_{Ar}), 7.26 (dd, ^3J = 4.4 Hz, ^3J = 8.2 Hz, 1H, H_{Ar}), 8.67 (dd, ^4J = 2.1 Hz, ^3J = 4.5 Hz, 1H, H_{Ar}), 8.72 (dd, ^4J = 2.1 Hz, ^3J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 25.2, 26.7, 30.6, 64.3, 119.4, 121.8, 125.2, 126.2, 127.5, 128.2, 128.6, 128.7, 131.2, 135.5, 135.7, 136.1, 150.8, 151.1, 153.7, 176.6. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3056 (w), 3030 (w), 2997 (w), 2930 (w), 2853 (w), 1614 (s), 1587 (s), 1537 (m), 1498 (w), 1484 (m), 1451 (w), 1444 (w), 1426 (w), 1412 (w), 1394 (m), 1279 (m), 1265 (w), 1252 (w), 1225 (w), 1208 (w), 1177 (w), 1147 (w), 1115 (w), 1075 (w),

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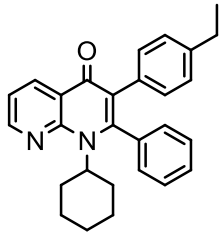
1060 (w), 1043 (w), 1025 (w). m/z (%) = 380 (M^+, 22), 297 (100), 268 (5), 176 (2), 139 (1), 55 (2), 41 (1). HRMS (ESI): calcd for $C_{26}H_{25}N_2O$ ($[M+H]^+$) 381.19614, found 381.19551.

1-cyclohexyl-3-(4-ethylphenyl)-2-phenyl-1,8-naphthyridin-4(1*H*)-one (21b).



Starting with 3-bromo-1-cyclohexyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (**20**) (0.150 g, 0.39 mmol), $Pd(PPh_3)_4$ (0.023 g, 0.020 mmol), K_2CO_3 (0.108 g, 0.78 mmol) and 4-ethylphenylboronic acid (0.065 g, 0.43 mmol) in DMF (10 mL), product **21b** was isolated as a white solid (0.096 g, 60 %); mp 195-198 °C; Procedure D. ^{1}H NMR ($CDCl_3$, 250 MHz): δ = 0.73-0.86 (m, 2H, $H_{Cyclohexyl}$), 1.03-1.08 (t, ^3J = 7.6 Hz, 3H, CH_3), 1.15-1.20 (m, 1H, $H_{Cyclohexyl}$), 1.43-1.47 (m, 1H, $H_{Cyclohexyl}$), 1.65-1.68 (m, 4H, $H_{Cyclohexyl}$), 2.43 (q, ^3J = 7.6 Hz, 2H, CH_2), 2.90-3.01 (m, 2H, $H_{Cyclohexyl}$), 3.81-3.89 (m, 1H, $H_{Cyclohexyl}$), 6.81-6.87 (m, 4H, H_{Ar}); 7.06-7.09 (m, 2H, H_{Ar}), 7.17-7.26 (m, 4H, H_{Ar}), 8.67 (dd, ^4J = 2.1 Hz, ^3J = 4.5 Hz, 1H, H_{Ar}), 8.72 (dd, ^4J = 2.1 Hz, ^3J = 8.0 Hz, 1H, H_{Ar}). ^{13}C NMR ($CDCl_3$, 63 MHz): δ = 15.3, 25.1, 26.7, 28.5, 30.5, 64.2, 119.3, 121.7, 125.2, 127.0, 128.2, 128.4, 128.6, 131.0, 132.7, 135.6, 136.1, 141.8, 150.7, 151.1, 153.6, 176.7. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3054 (w), 3024 (w), 2962 (w), 2869 (w), 2851 (w), 1622 (s), 1589 (s), 1537 (w), 1511 (w), 1484 (m), 1453 (w), 1442 (m), 1407 (w), 1395 (m), 1280 (m), 1265 (m), 1233 (w), 1212 (w), 1180 (w), 1149 (w), 1114 (w), 1059 (w), 1040 (w), 1022 (w). m/z (%) = 408 (M^+, 28), 325 (100), 297 (11), 227 (1), 189 (1), 165 (1), 55 (2), 41 (1). HRMS (ESI): calcd for $C_{28}H_{29}N_2O$ ($[M+H]^+$) 409.22744, found 409.22695.

1-cyclohexyl-2-phenyl-3-(4-(trifluoromethyl)phenyl)-1,8-naphthyridin-4(1*H*)-one (21c).

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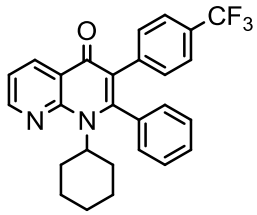

Starting with 3-bromo-1-cyclohexyl-2-phenyl-1,8-naphthyridin-4(1*H*)-one (**20**) (0.150 g, 0.39 mmol), $Pd(PPh_3)_4$ (0.023 g, 0.020 mmol), K_2CO_3 (0.108 g, 0.78 mmol) and 4-(trifluoromethyl)phenylboronic acid (0.082 g, 0.43 mmol) in DMF (10 mL), product **21c** was isolated as a white solid (0.075 g, 43 %); mp 200-203 °C; Procedure D. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 0.74-0.88 (m, 2H, $H_{Cyclohexyl}$), 1.15-1.21 (m, 1H, $H_{Cyclohexyl}$), 1.44-1.49 (m, 1H, $H_{Cyclohexyl}$), 1.66-1.69 (m, 4H, $H_{Cyclohexyl}$), 2.91-2.98 (m, 2H, $H_{Cyclohexyl}$), 3.86-3.88 (m, 1H, $H_{Cyclohexyl}$), 7.04-7.08 (m, 4H, H_{Ar}), 7.21-7.30 (m, 6H, H_{Ar}), 8.69-8.73 (m, 2H, H_{Ar}). ^{19}F ($CDCl_3$, 282 MHz) δ = -62.54 (CF_3). ^{13}C NMR ($CDCl_3$, 63 MHz) δ = 25.1, 26.6, 30.6, 64.5, 119.7, 121.7, 123.8, 124.3 ($^3J_{CF}$ = 3.8 Hz, C_{Ph}-C_{Ph}-CF_3), 124.4 ($^1J_{CF}$ = 271.9 Hz, CF_3), 128.2 ($^2J_{CF}$ = 32.4 Hz, C_{Ph}-CF_3), 128.5, 129.0, 131.6, 134.9, 136.1, 139.7, 139.7, 151.1, 151.1, 153.9, 176.2. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3085 (w), 3060 (w), 2990 (w), 2935 (w), 2854 (w), 1623 (w), 1609 (m), 1587 (s), 1539 (w), 1516 (w), 1485 (m), 1453 (w), 1448 (w), 1430 (m), 1396 (m), 1321 (s), 1283 (m), 1251 (w), 1228 (w), 1178 (w), 1160 (m), 1116 (s), 1105 (s), 1064 (s), 1039 (w), 1020 (w). m/*z* (%) = 448 (M^+, 17), 365 (100), 295 (2), 268 (3), 55 (2), 41 (2). HRMS (ESI): calcd for $C_{27}H_{24}F_3NO$ ($[M+H]^+$) 449.18352, found 449.18382.

References

[1] F. C. Fuchs, G. A. Eller, W. Holzer, *Molecules* **2009**, *14*, 3814-3832.
[2] Compounds were used, but not isolated (no analytical data are given): B. Willy, W. Frank, T. J. J. Müller, *Org. Biomol. Chem.* **2010**, *8*, 90-95.

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(C) UV-Study

The absorption spectra were measured on a Perkin Elmer UV/Vis Spectrometer Lambda 2 in dichloromethane ($c \approx 2.5 * 10^{-5}$ mol/l). The fluorescence spectra were recorded on a Hitachi F-4010 fluorescence spectrometer in dichloromethane ($c = 10^{-4}$ mol/l; excitation wavelength: 350 nm). The solvent was distilled before use.

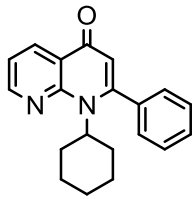
Table 1. Absorption and emission data for of 1,8-naphthyridin-4(1*H*)-ones.

Compound	$\lambda_{a,\,max1}$ /nm (ε /L mol^{-1} cm^{-1})	$\lambda_{a,\,max2}$ /nm (ε /L mol^{-1} cm^{-1})	$\lambda_{a,\,max3}$ /nm (ε /L mol^{-1} cm^{-1})	$\lambda_{e,\,max}$ /nm	Stokes Shift ($\lambda_{e,\,max} - \lambda_{a,\,max3}$ /cm^{-1})
5e	230 (50458)	254 (103142)	348 (43946)	390	3095
20	230 (34092)	260 (81918)	353 (32701)	395	3012
21a	230 (53378)	252 (60787)	353 (26922)	435	5340
21b	230 (51187)	254 (59285)	351 (30534)	410	4100
21c	230 (47339)	256 (54416)	353 (26676)	420	4519

$\lambda_{a,\,max1}$: wavelength absorption maximum 1.
$\lambda_{a,\,max2}$: wavelength absorption maximum 2.
$\lambda_{a,\,max3}$: wavelength absorption maximum 3.
$\lambda_{e,\,max}$: wavelength fluorescence maximum.
ε : extinction coefficient (L mol^{-1} cm^{-1}).

The following diagrams show the normalized absorption and emission spectra of the corresponding compounds.

a) **Compound 5e**



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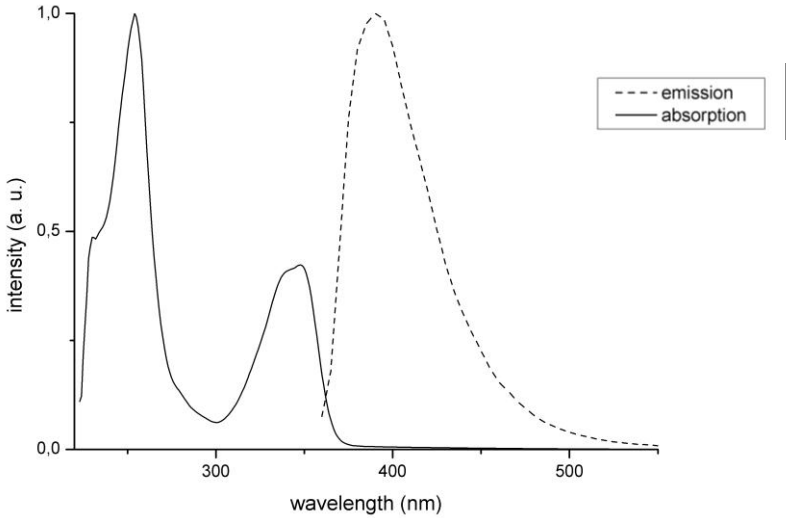
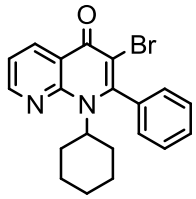


b) **Compound 20**



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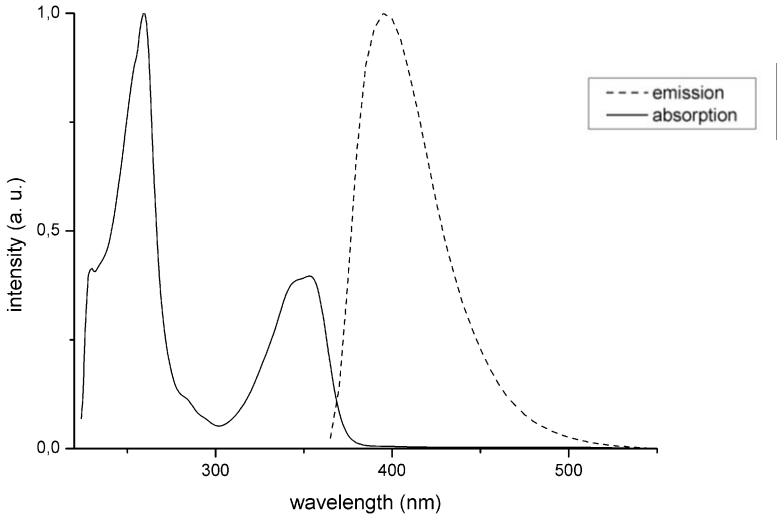

c) **Compound 21a**

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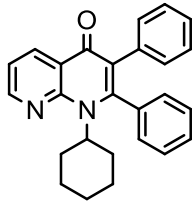

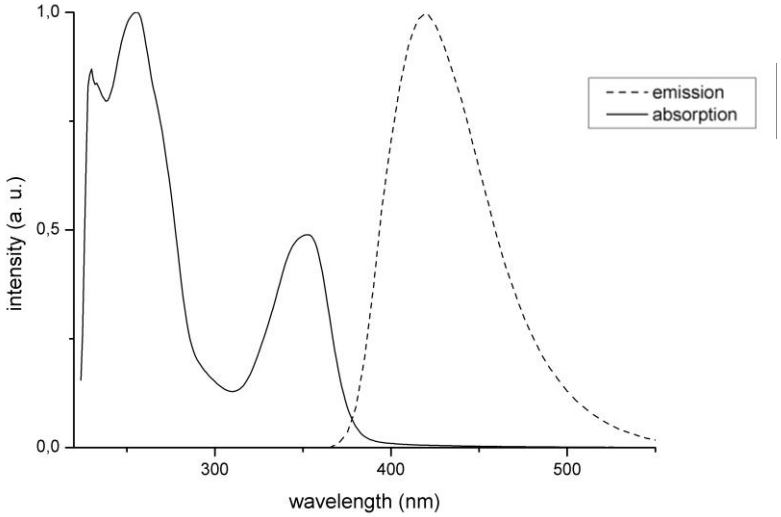

d) **Compound 21b**

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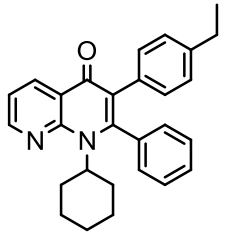

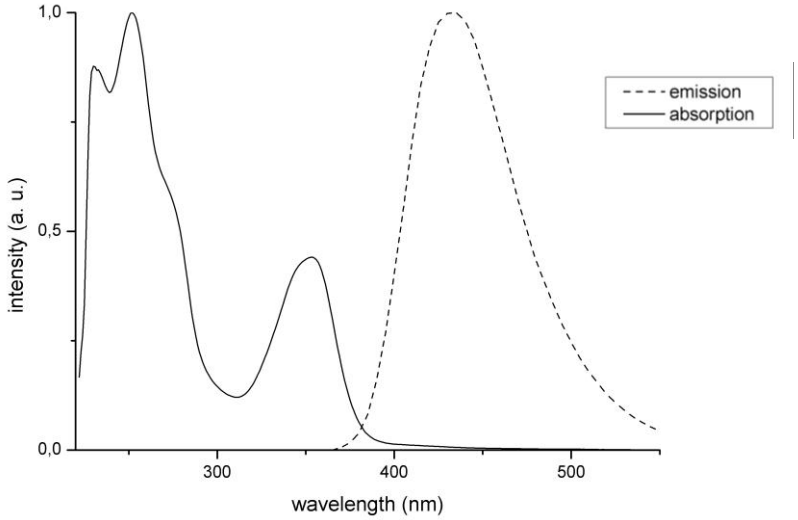

e) **Compound 21c**

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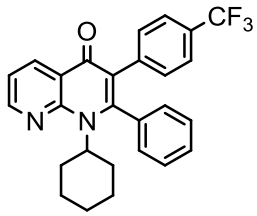

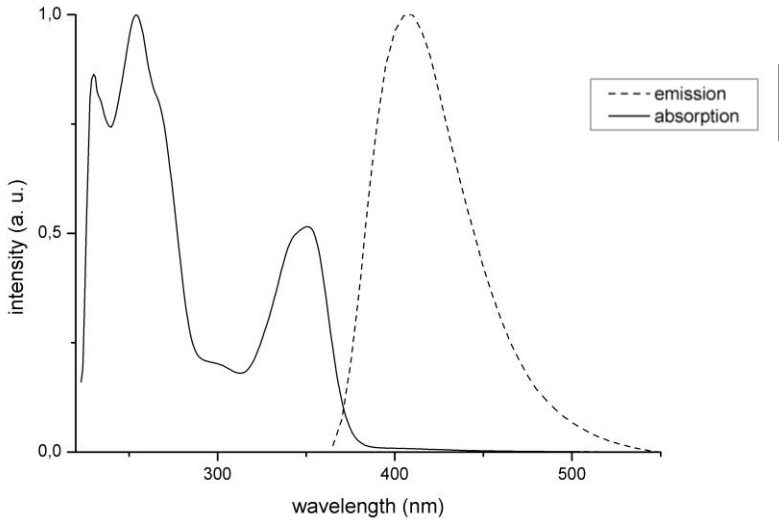

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(D) Copies of MS, ^{1}H and ^{13}C NMR spectra

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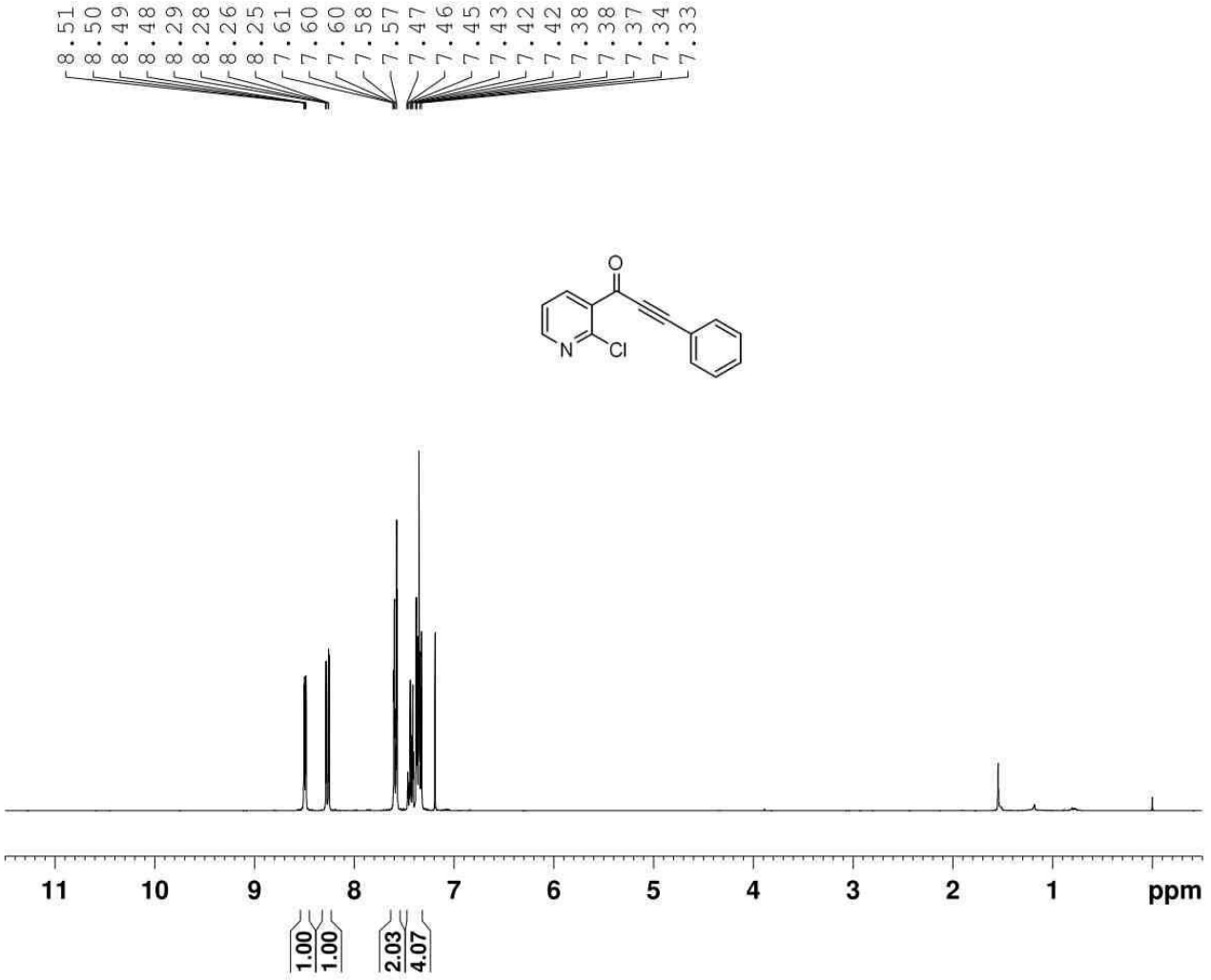

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PC	1.00

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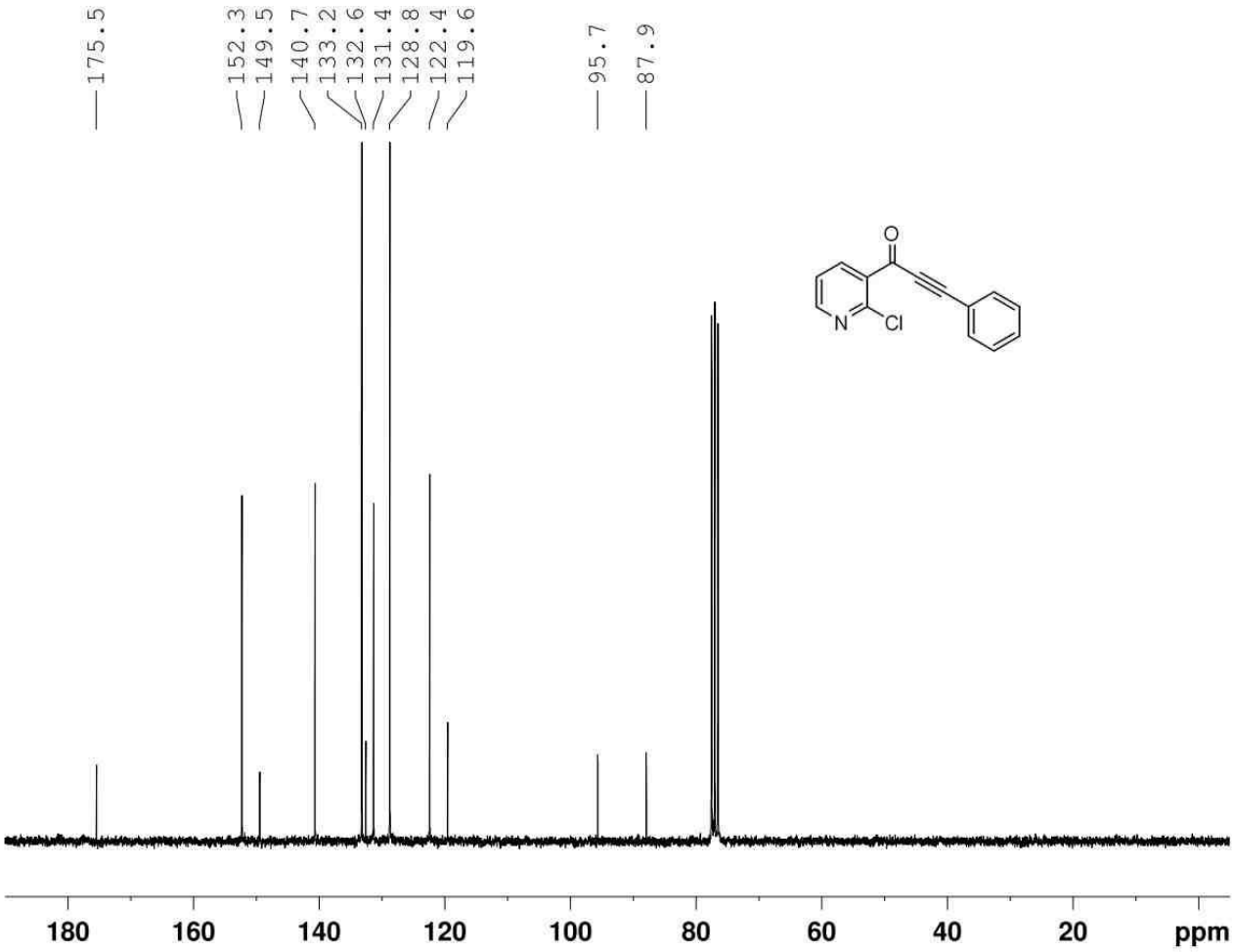

BRUKER

NAME	101019.204
EXPNO	10
PROCNO	1
Date_	20101019
Time	13.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1440
DW	33.333 usec
DE	10.00 usec
TE	297.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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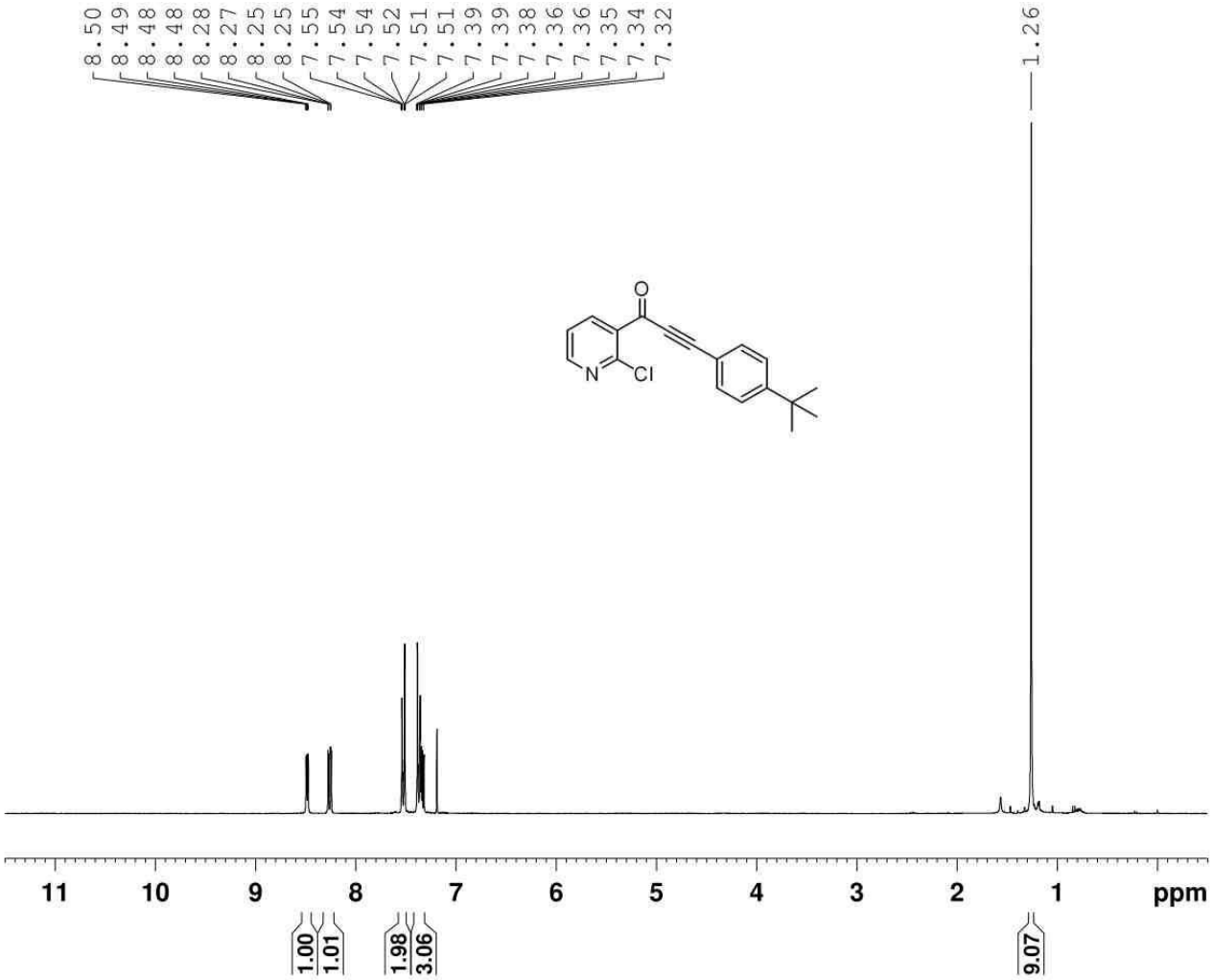

NAME	101029.u326	
EXPNO	10	
PROCNO	1	
Date_	20101029	
Time	13.38	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	114	
DW	80.800	use
DE	10.00	use
TE	296.8	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300286	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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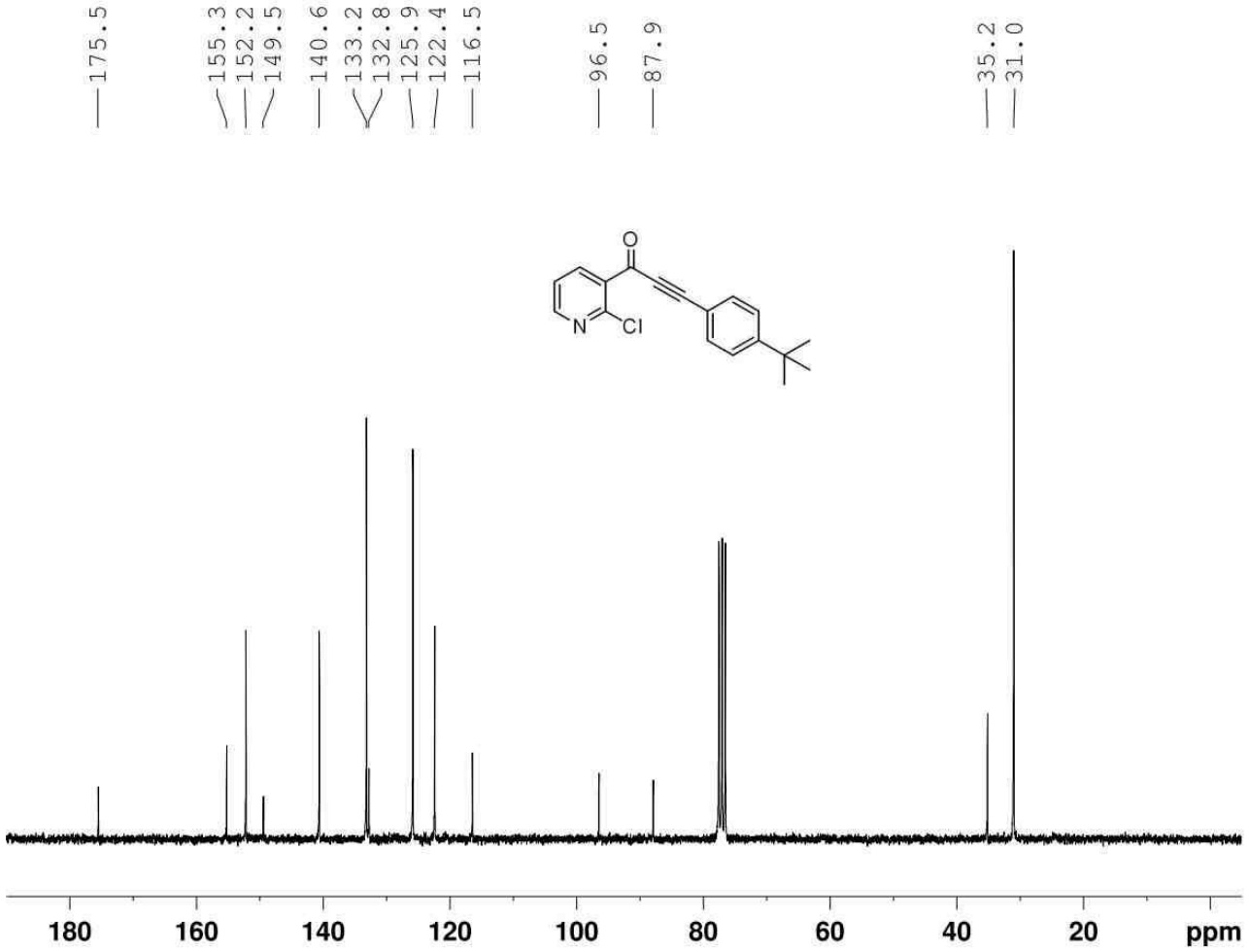

NAME	101101.214
EXPNO	10
PROCNO	1
Date_	20101102
Time	6.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	298.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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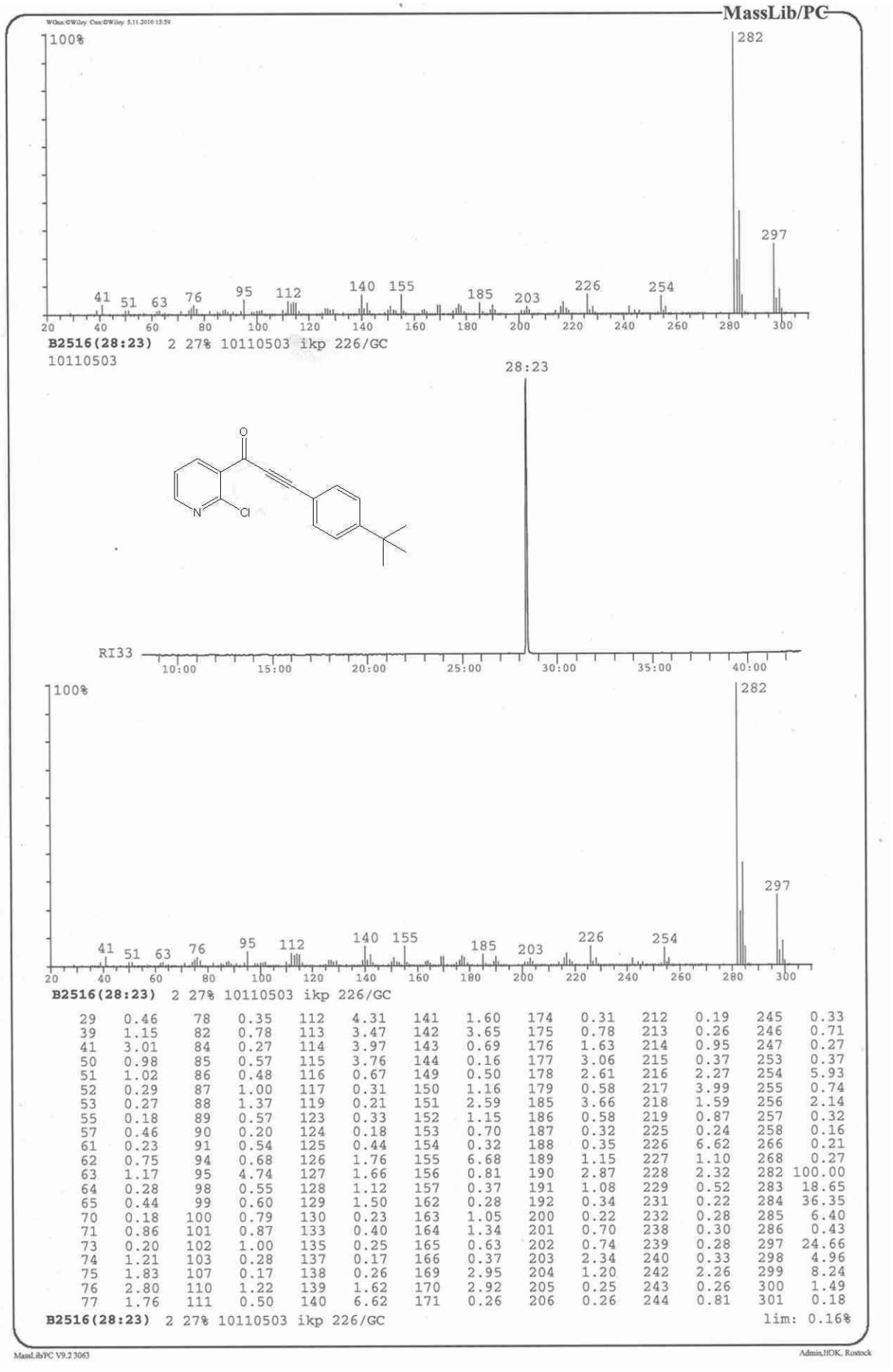

29	0.46	78	0.35	112	4.31	141	1.60	174	0.31	212	0.19	245	0.33
39	1.15	82	0.78	113	3.47	142	3.65	175	0.78	213	0.26	246	0.71
41	3.01	84	0.27	114	3.97	143	0.69	176	1.63	214	0.95	247	0.27
50	0.98	85	0.57	115	3.76	144	0.16	177	3.06	215	0.37	253	0.37
51	1.02	86	0.48	116	0.67	149	0.50	178	2.61	216	2.27	254	5.93
52	0.29	87	1.00	117	0.31	150	1.16	179	0.58	217	3.99	255	0.74
53	0.27	88	1.37	119	0.21	151	2.59	185	3.66	218	1.59	256	2.14
55	0.18	89	0.57	123	0.33	152	1.15	186	0.58	219	0.87	257	0.32
57	0.46	90	0.20	124	0.18	153	0.70	187	0.32	225	0.24	258	0.16
61	0.23	91	0.54	125	0.44	154	0.32	188	0.35	226	6.62	266	0.21
62	0.75	94	0.68	126	1.76	155	6.68	189	1.15	227	1.10	268	0.27
63	1.17	95	4.74	127	1.66	156	0.81	190	2.87	228	2.32	282	100.00
64	0.28	98	0.55	128	1.12	157	0.37	191	1.08	229	0.52	283	18.65
65	0.44	99	0.60	129	1.50	162	0.28	192	0.34	231	0.22	284	36.35
70	0.18	100	0.79	130	0.23	163	1.05	200	0.22	232	0.28	285	6.40
71	0.86	101	0.87	133	0.40	164	1.34	201	0.70	238	0.30	286	0.43
73	0.20	102	1.00	135	0.25	165	0.63	202	0.74	239	0.28	297	24.66
74	1.21	103	0.28	137	0.17	166	0.37	203	2.34	240	0.33	298	4.96
75	1.83	107	0.17	138	0.26	169	2.95	204	1.20	242	2.26	299	8.24
76	2.80	110	1.22	139	1.62	170	2.92	205	0.25	243	0.26	300	1.49
77	1.76	111	0.50	140	6.62	171	0.26	206	0.26	244	0.81	301	0.18

B2516(28:23) 2 27% 10110503 ikp 226/GC lim: 0.16%

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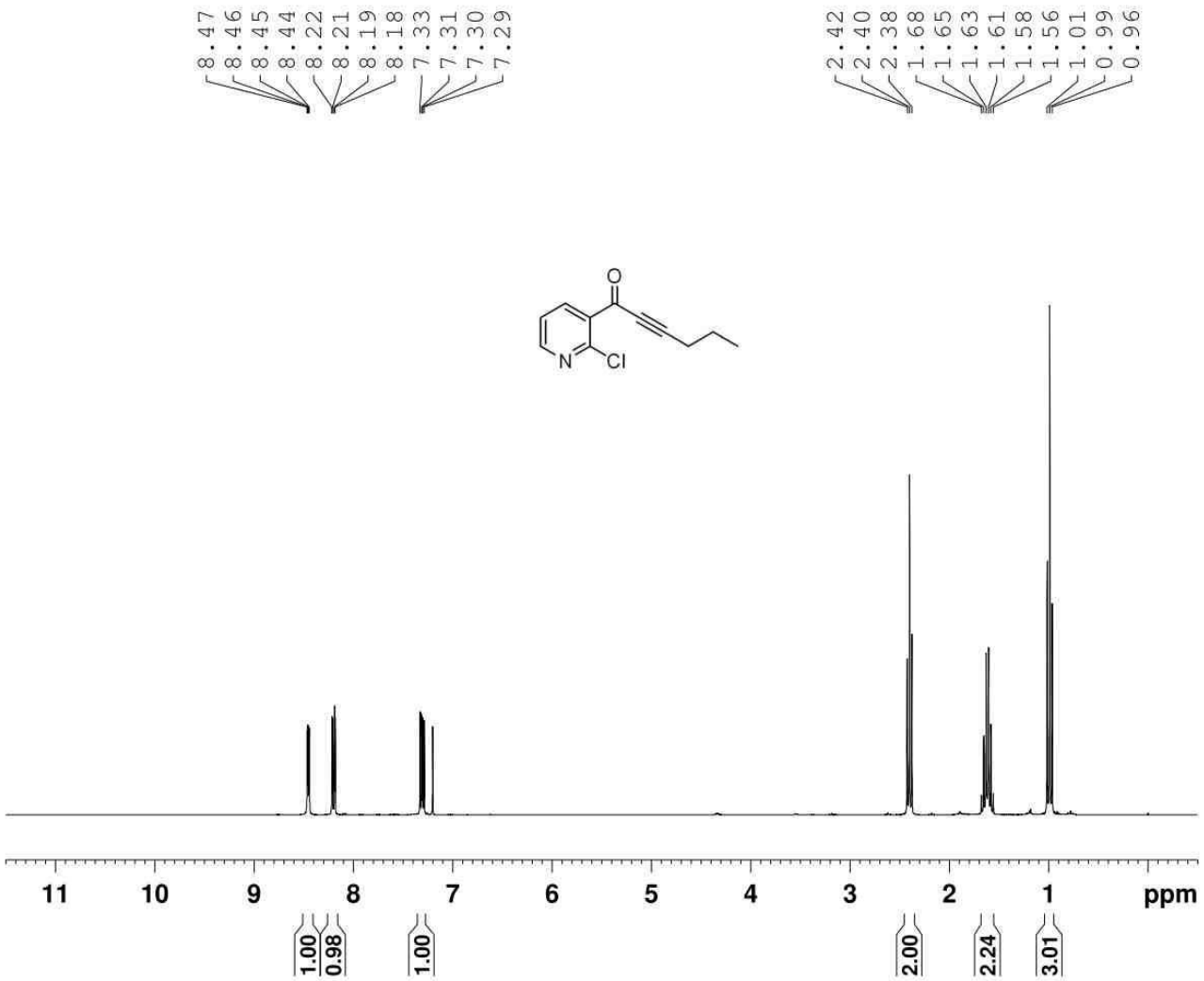

BRUKER

NAME	100730.u332
EXPNO	10
PROCNO	1
Date_	20100731
Time	18.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	128
DW	80.800 use
DE	10.00 use
TE	298.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300250 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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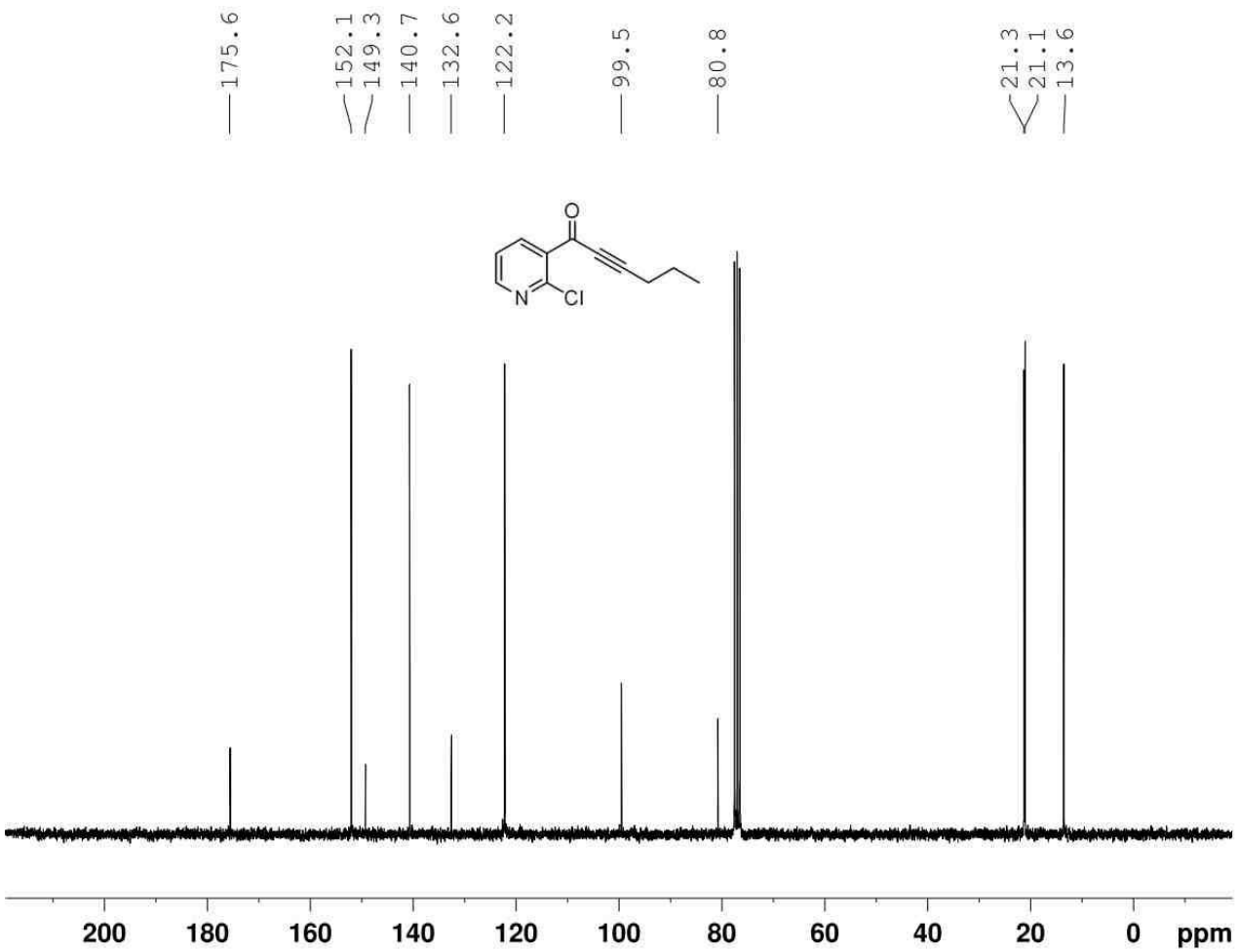

NAME	100811.202
EXPNO	10
PROCNO	1
Date_	20100811
Time	12.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	300.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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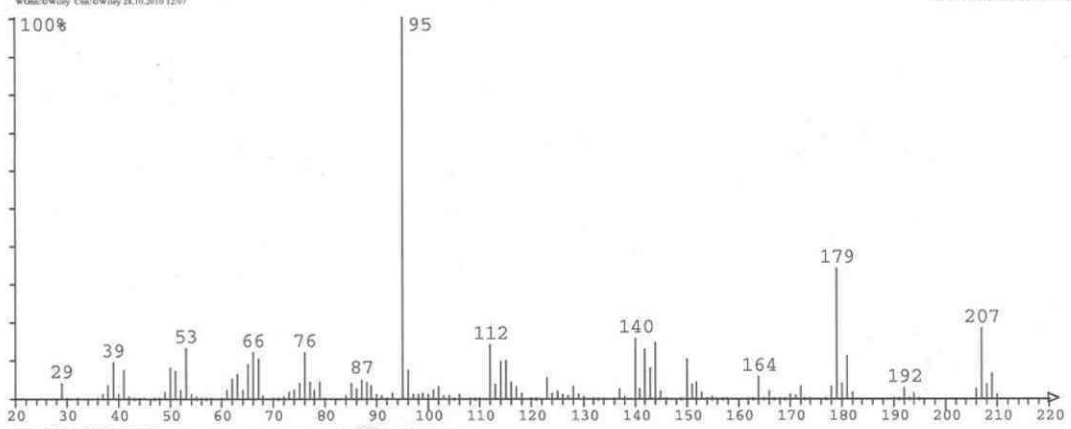
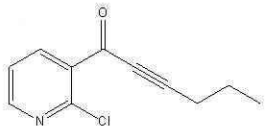
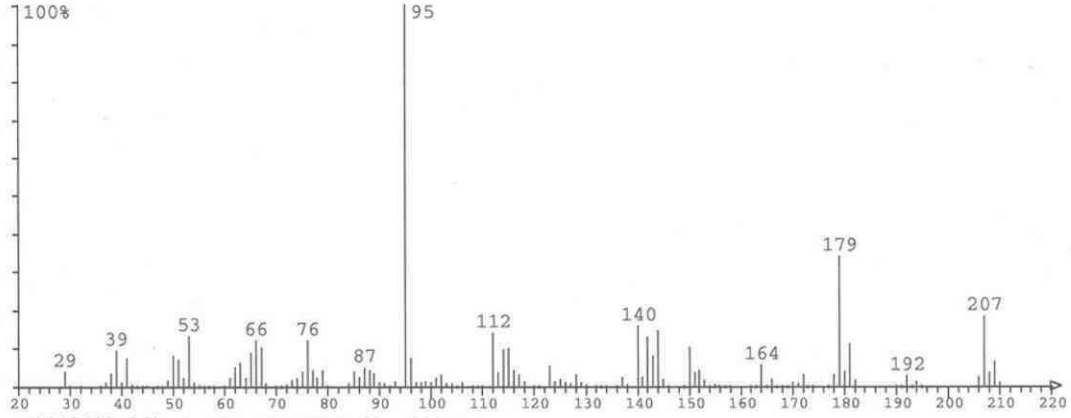


B1840(18:26) 2 19% 10102712 ikp 203/GC

10102712

18:26





B1840(18:26) 2 19% 10102712 ikp 203/GC

29	3.63	55	0.50	78	2.02	103	0.62	128	2.72	154	0.35	180	3.84
30	0.16	56	0.09	79	4.03	104	0.60	129	0.94	155	0.47	181	11.00
32	0.15	57	0.16	80	0.20	105	0.36	130	0.48	156	0.03	182	1.28
36	0.15	58	0.10	84	0.59	106	0.69	132	0.08	157	0.12	190	0.23
37	0.91	60	0.28	85	3.75	108	0.16	133	0.15	158	0.07	191	0.14
38	3.04	61	1.90	86	2.27	109	0.26	134	0.17	162	0.14	192	2.57
39	9.17	62	4.94	87	4.72	110	0.35	136	0.21	163	0.16	193	0.25
40	0.85	63	6.08	88	3.99	112	13.82	137	2.26	164	5.30	194	1.11
41	7.05	64	2.02	89	3.17	113	3.51	138	0.44	165	0.30	195	0.10
42	0.40	65	8.59	90	0.71	114	9.39	140	15.61	166	1.66	206	2.22
43	0.20	66	11.74	91	0.57	115	9.92	141	2.37	167	0.35	207	18.20
44	0.12	67	10.04	92	0.09	116	4.07	142	12.71	168	0.25	208	3.48
45	0.08	68	0.64	93	1.16	117	2.84	143	7.78	169	0.13	209	6.35
47	0.11	70	0.25	95	100.00	118	1.12	144	14.41	170	0.76	210	0.75
48	0.16	71	0.24	96	7.11	120	0.10	145	1.61	171	0.57		
49	1.36	72	0.44	97	0.94	121	0.14	146	0.29	172	2.80		
50	7.74	73	1.41	98	0.73	123	5.20	149	0.20	173	0.33		
51	6.84	74	2.06	99	1.06	124	1.22	150	10.12	174	0.14		
52	1.86	75	3.85	100	0.79	125	1.67	151	3.47	177	0.15		
53	12.93	76	11.81	101	1.95	126	0.91	152	4.10	178	2.81		
54	0.72	77	3.95	102	2.88	127	0.66	153	1.34	179	33.80		

B1840(18:26) 2 19% 10102712 ikp 203/GC

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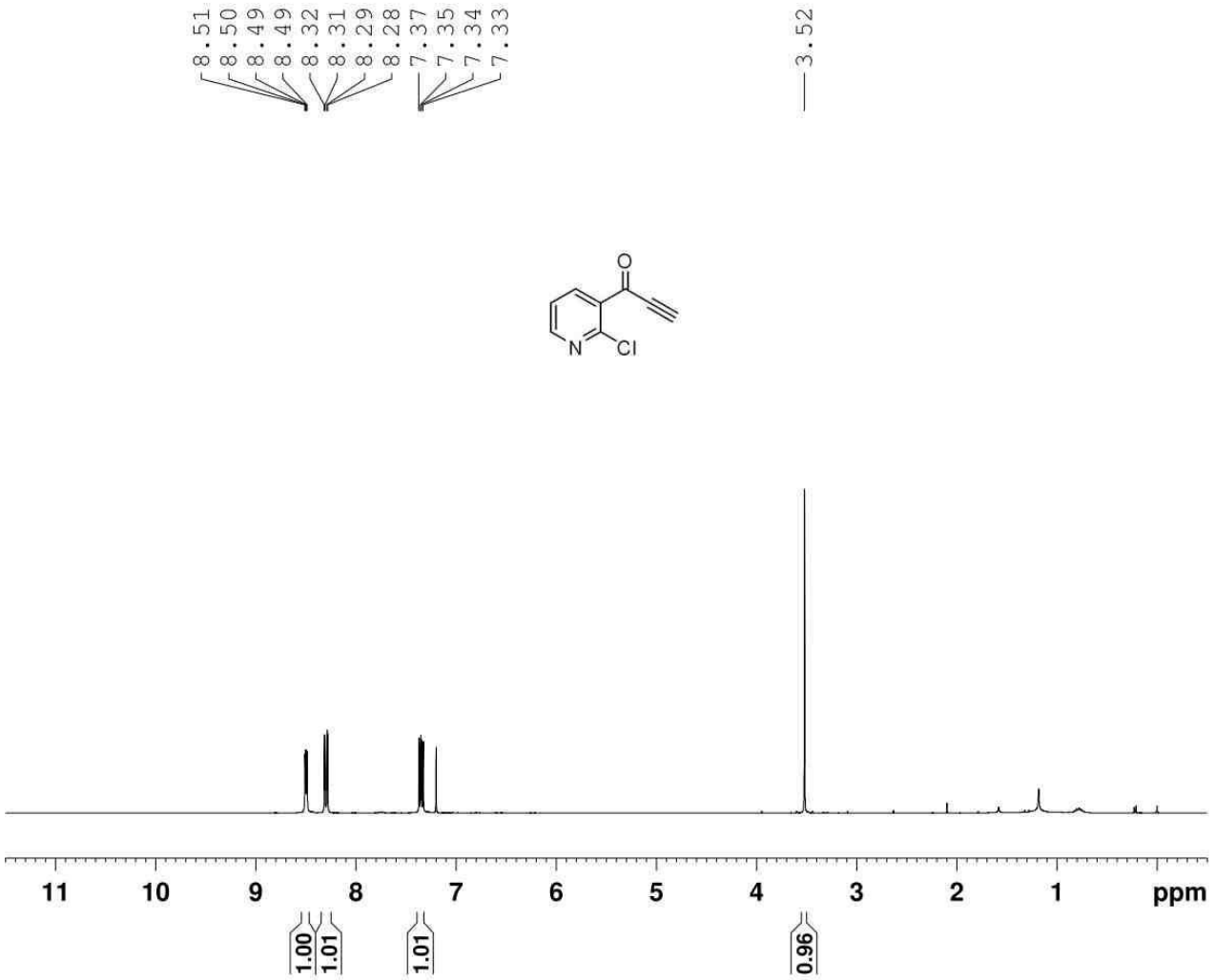

BRUKER

NAME	101203.u305	
EXPNO	10	
PROCNO	1	
Date_	20101203	
Time	8.46	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300256	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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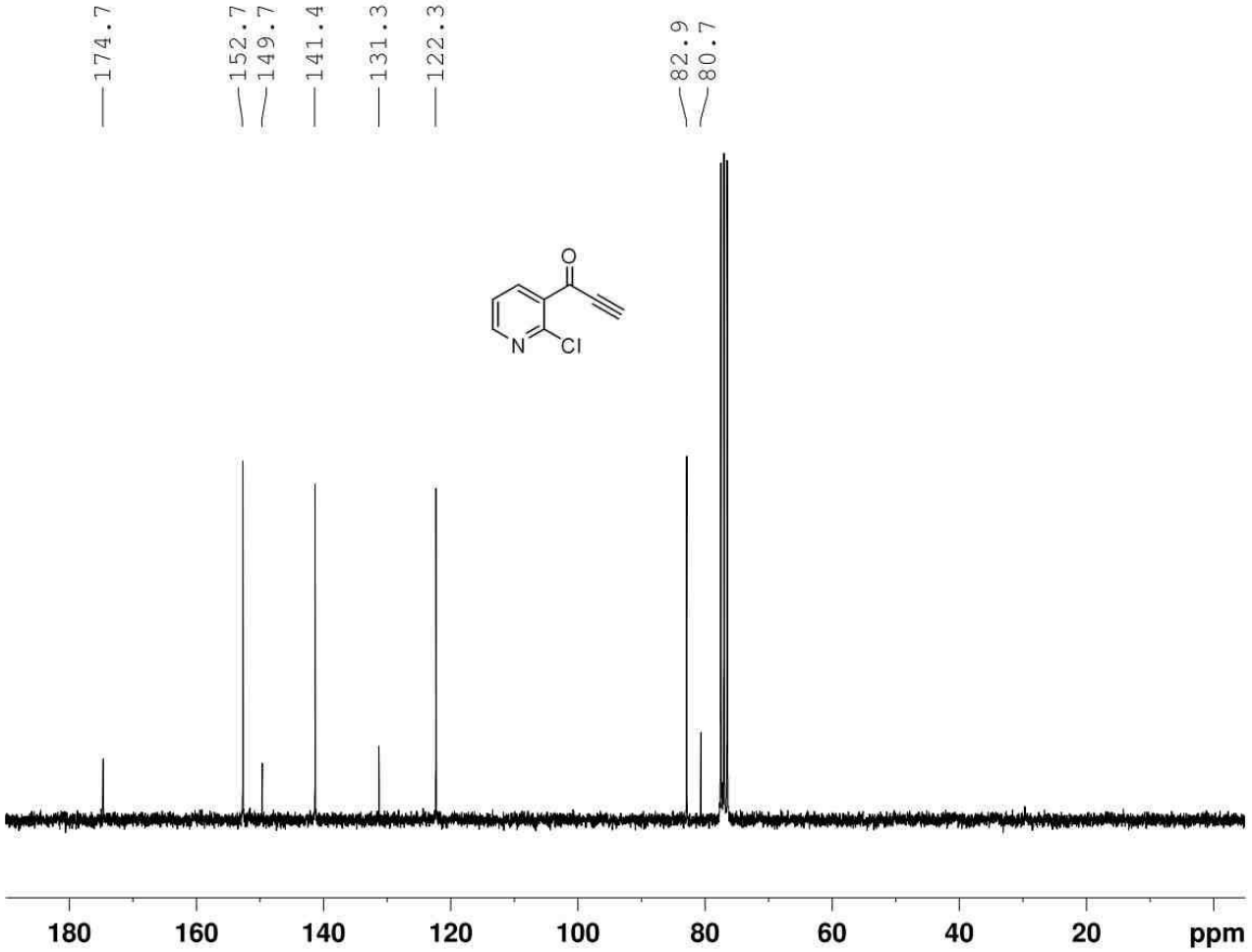

BRUKER

NAME	101203.225
EXPNO	10
PROCNO	1
Date_	20101205
Time	12.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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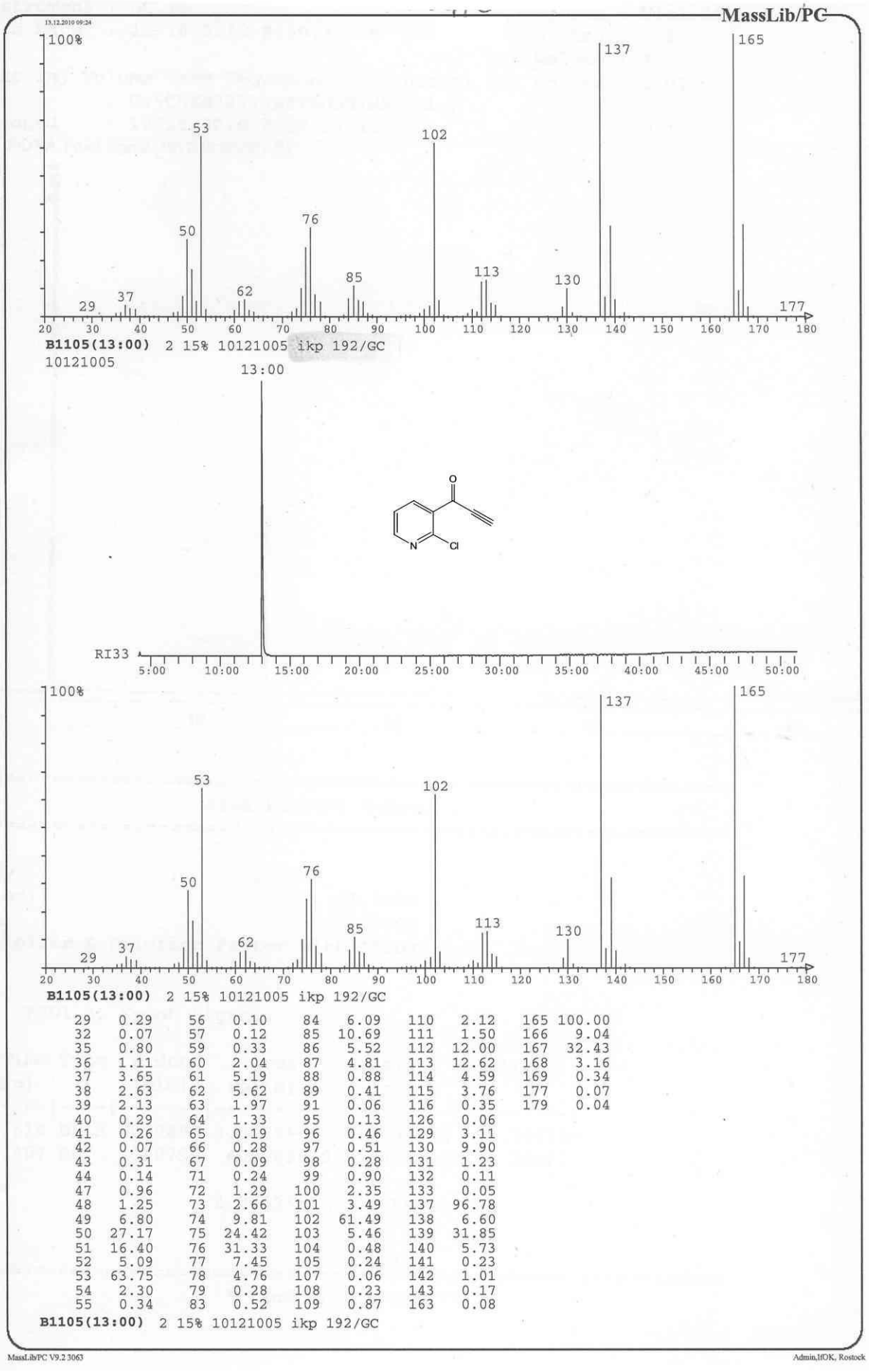

29	0.29	56	0.10	84	6.09	110	2.12	165	100.00
32	0.07	57	0.12	85	10.69	111	1.50	166	9.04
35	0.80	59	0.33	86	5.52	112	12.00	167	32.43
36	1.11	60	2.04	87	4.81	113	12.62	168	3.16
37	3.65	61	5.19	88	0.88	114	4.59	169	0.34
38	2.63	62	5.62	89	0.41	115	3.76	177	0.07
39	2.13	63	1.97	91	0.06	116	0.35	179	0.04
40	0.29	64	1.33	95	0.13	126	0.06		
41	0.26	65	0.19	96	0.46	129	3.11		
42	0.07	66	0.28	97	0.51	130	9.90		
43	0.31	67	0.09	98	0.28	131	1.23		
44	0.14	71	0.24	99	0.90	132	0.11		
47	0.96	72	1.29	100	2.35	133	0.05		
48	1.25	73	2.66	101	3.49	137	96.78		
49	6.80	74	9.81	102	61.49	138	6.60		
50	27.17	75	24.42	103	5.46	139	31.85		
51	16.40	76	31.33	104	0.48	140	5.73		
52	5.09	77	7.45	105	0.24	141	0.23		
53	63.75	78	4.76	107	0.06	142	1.01		
54	2.30	79	0.28	108	0.23	143	0.17		
55	0.34	83	0.52	109	0.87	163	0.08		

B1105(13:00) 2 15% 10121005 ikp 192/GC

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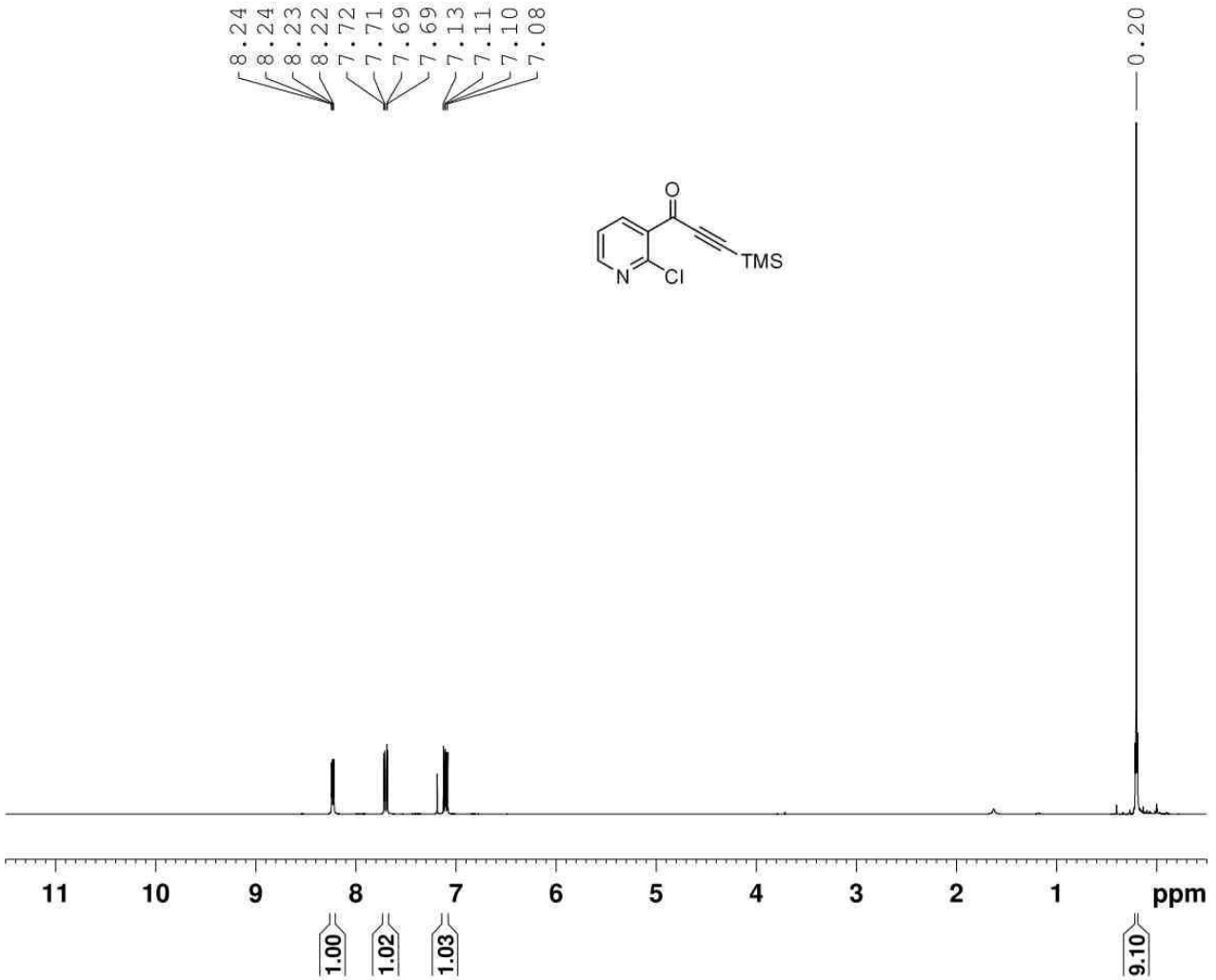

BRUKER

NAME	100706.u313	
EXPNO	10	
PROCNO	1	
Date_	20100706	
Time	11.01	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	101	
DW	80.800	use
DE	10.00	use
TE	298.7	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300295	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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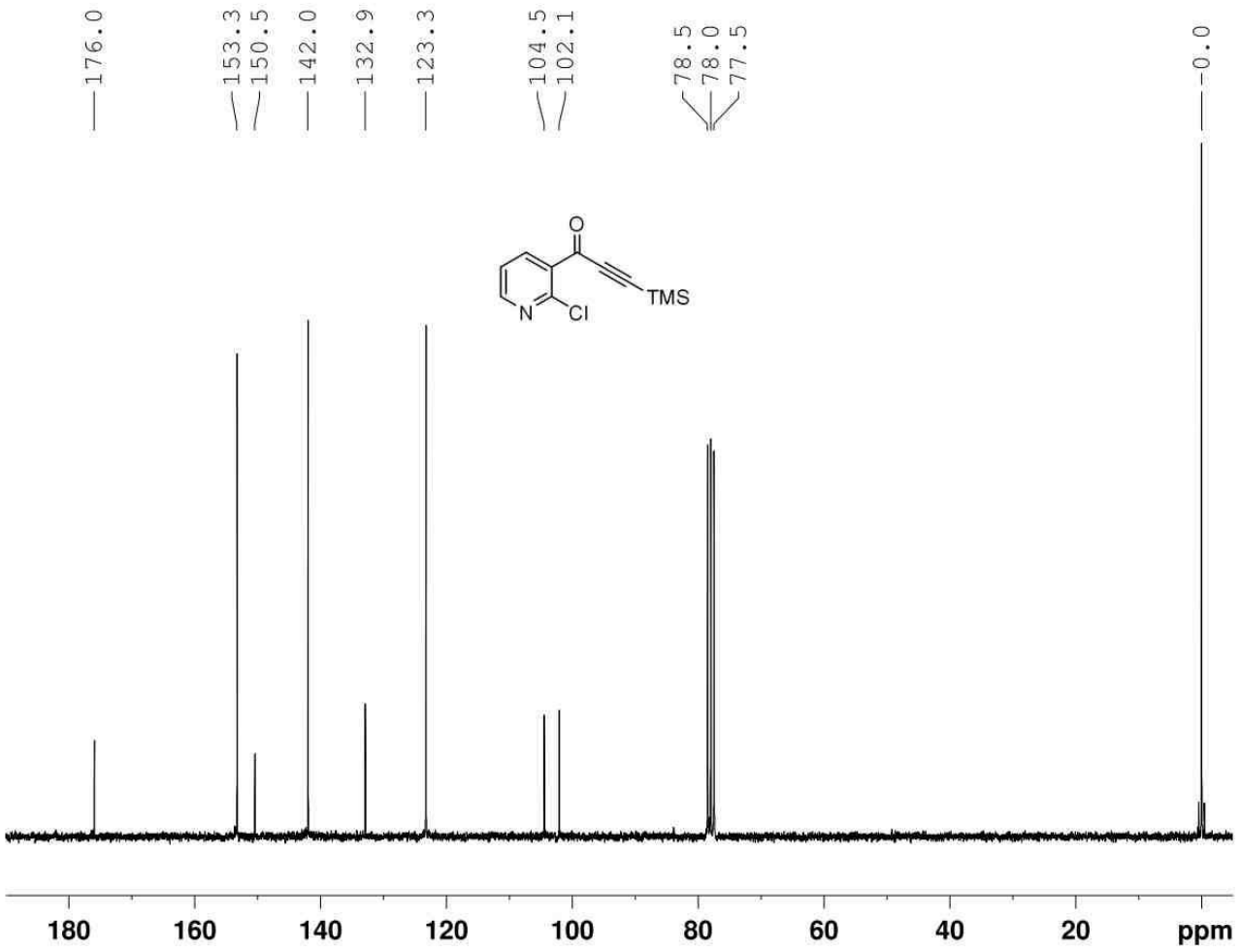

BRUKER

NAME	100706.210
EXPNO	10
PROCNO	1
Date_	20100707
Time	2.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8951794 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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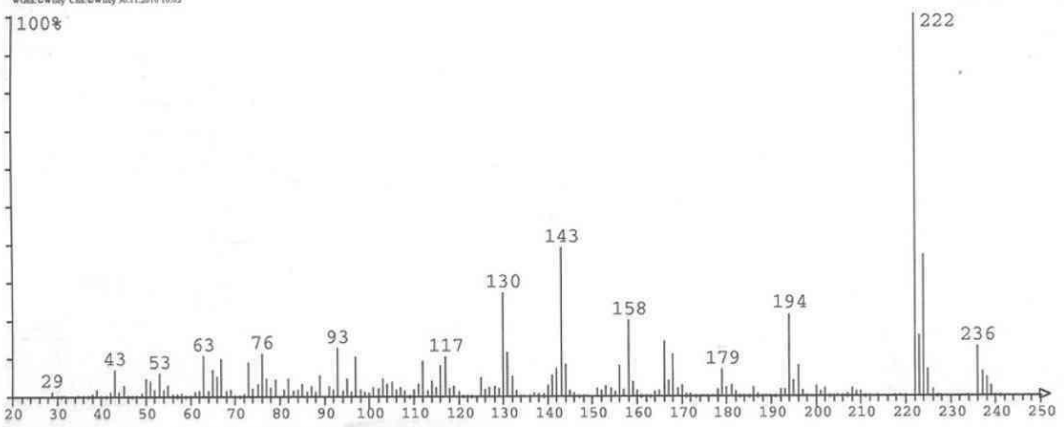
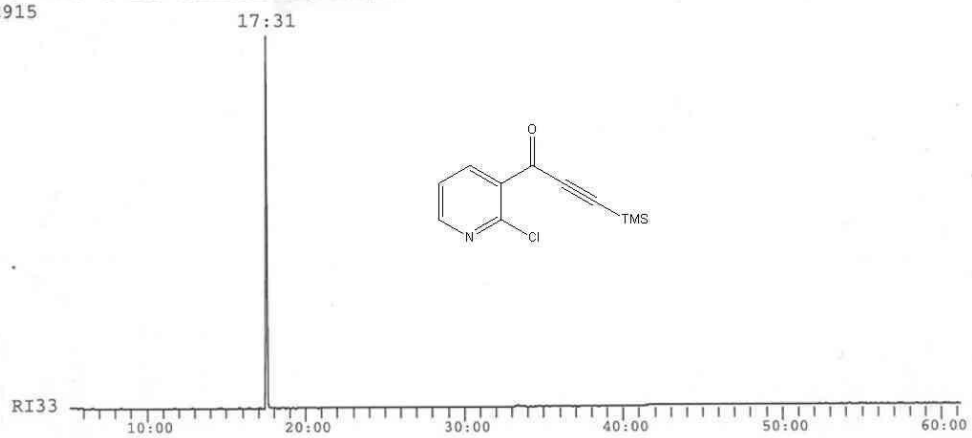
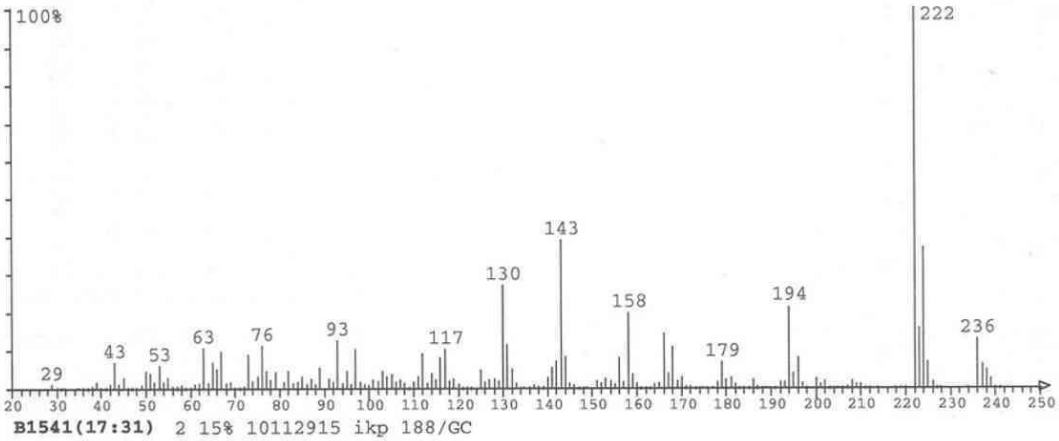


B1541(17:31) 2 15% 10112915 ikp 188/GC

10112915





B1541(17:31) 2 15% 10112915 ikp 188/GC

29	0.73	64	1.12	88	0.81	111	2.70	137	0.59	165	1.22	196	7.77
38	0.48	65	6.75	89	5.29	112	8.99	138	0.38	166	14.03	197	1.03
39	1.29	66	4.78	91	2.13	113	1.07	139	0.52	167	3.64	200	2.20
42	0.89	67	9.44	92	1.35	114	3.76	140	2.45	168	10.73	201	0.78
43	6.71	68	1.13	93	12.44	115	1.99	141	5.24	169	1.74	202	1.55
44	0.83	69	1.36	94	1.23	116	7.66	142	6.99	170	2.43	207	0.37
45	2.64	72	0.39	95	4.21	117	10.06	143	38.73	171	0.48	208	1.68
49	0.61	73	8.65	96	0.67	118	1.63	144	8.10	172	0.46	209	0.80
50	4.29	74	1.73	97	10.10	119	2.32	145	0.95	178	1.30	210	0.71
51	3.80	75	2.73	98	1.26	120	0.71	146	0.53	179	6.72	211	0.33
52	1.29	76	10.89	99	0.78	121	0.34	151	1.72	180	1.82	222	100.00
53	5.69	77	4.36	100	0.64	125	4.55	152	1.18	181	2.56	223	15.53
54	1.49	78	2.00	101	1.88	126	1.24	153	2.23	182	0.70	224	36.67
55	2.53	79	3.97	102	1.68	127	2.09	154	1.72	183	0.32	225	6.49
56	0.40	81	1.53	103	4.37	128	2.38	155	0.93	186	2.00	226	1.43
57	0.45	82	4.32	104	2.74	129	1.65	156	7.80	187	0.47	236	12.70
58	0.56	83	1.12	105	3.41	130	26.82	157	1.53	188	0.29	237	5.90
59	0.36	84	1.26	106	1.46	131	11.38	158	19.57	192	1.34	238	4.72
61	0.68	85	2.81	107	1.98	132	4.92	159	3.45	193	1.35	239	2.19
62	1.21	86	0.89	108	1.14	133	1.03	160	1.11	194	21.23	240	0.35
63	10.31	87	2.16	110	1.25	134	0.28	164	0.72	195	3.65		

B1541(17:31) 2 15% 10112915 ikp 188/GC lim: 0.28%

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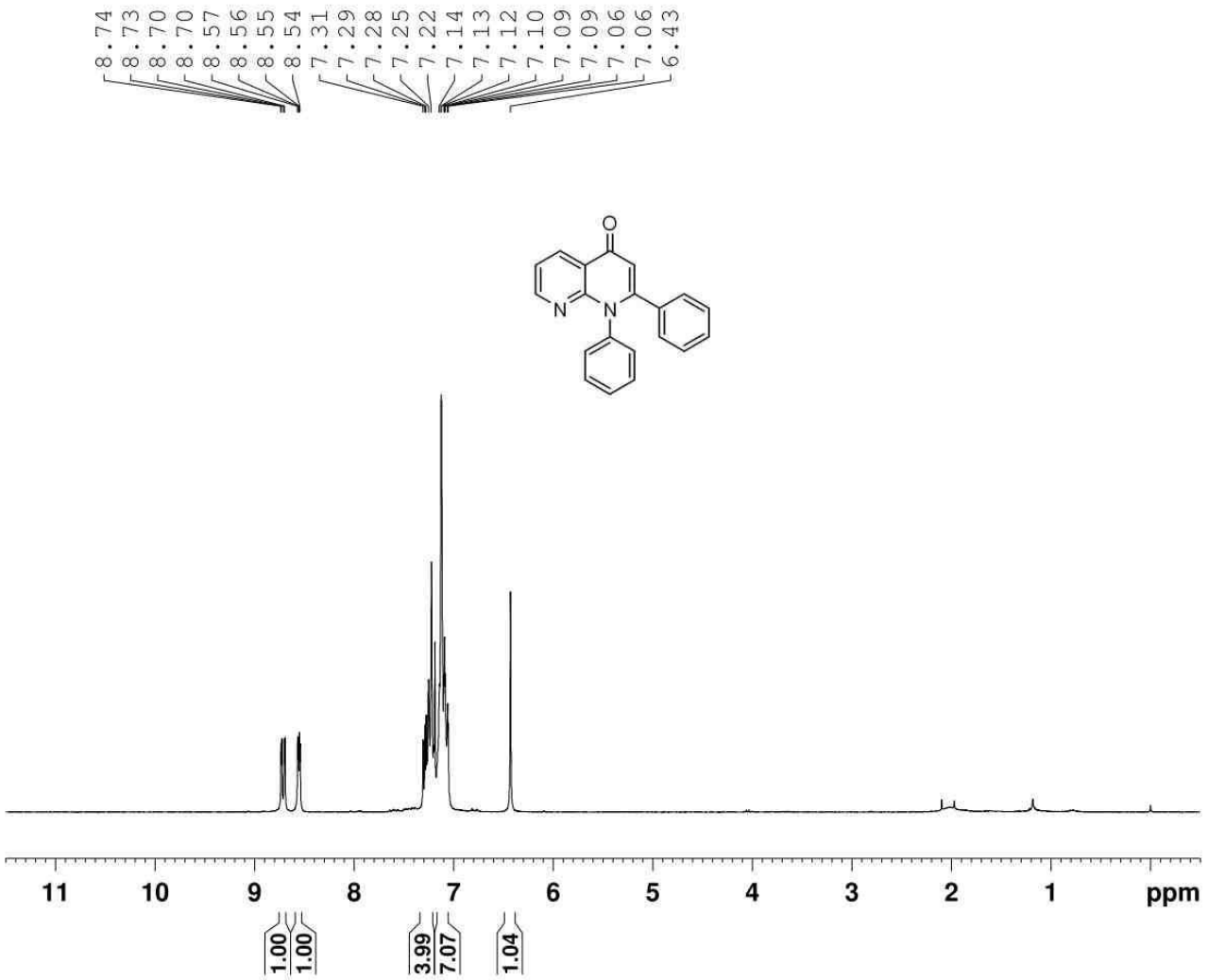

NAME	101021.201
EXPNO	10
PROCNO	1
Date_	20101021
Time	8.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	5165.289 Hz
FIDRES	0.078816 Hz
AQ	6.3439350 sec
RG	645
DW	96.800 use
DE	10.00 use
TE	296.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	-2.50 dB
SFO1	250.1315447 MHz
SI	32768
SF	250.1300180 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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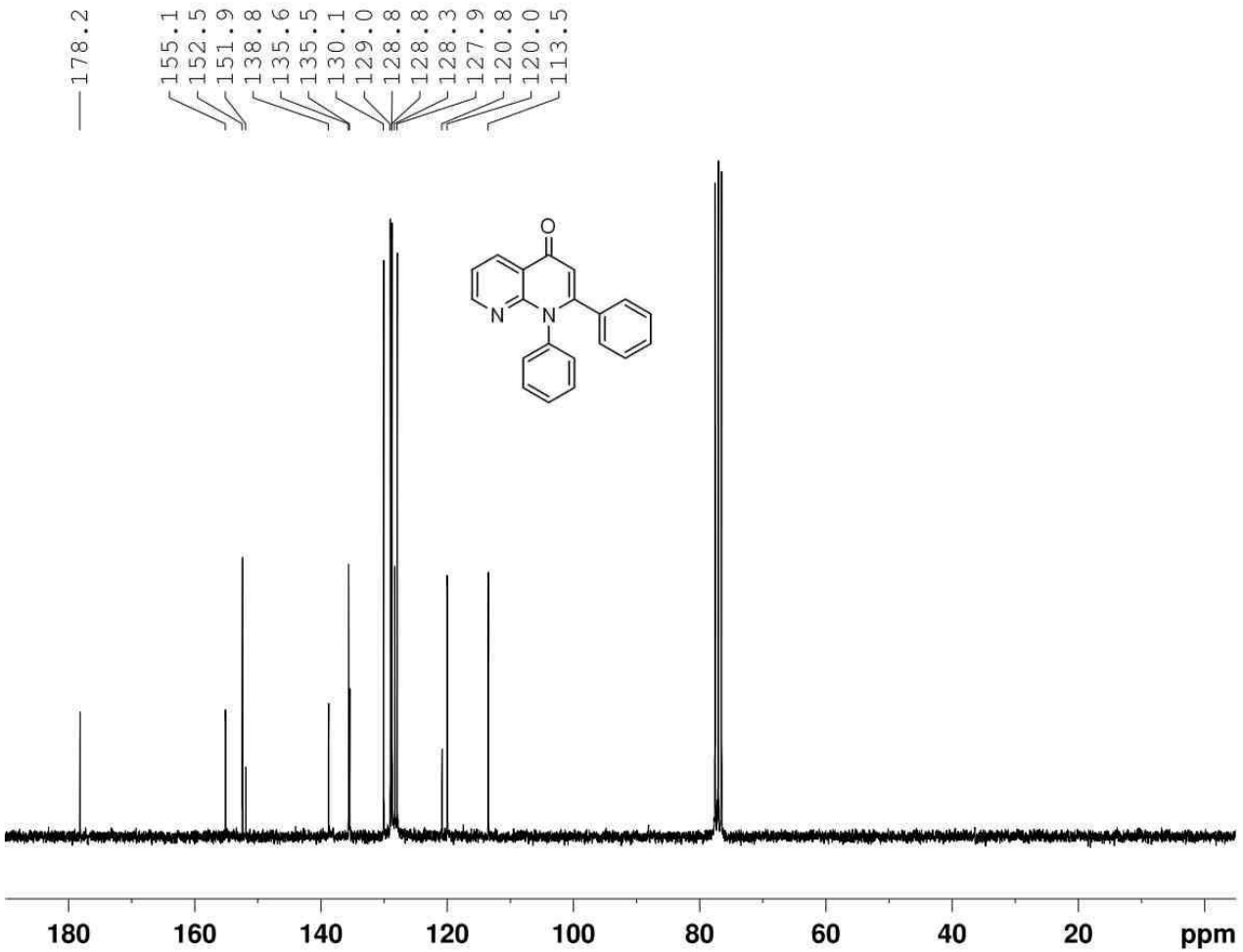

BRUKER

NAME	101217.216	
EXPNO	11	
PROCNO	1	
Date_	20101217	
Time	22.16	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	15000.000	Hz
FIDRES	0.228882	Hz
AQ	2.1845834	sec
RG	2050	
DW	33.333	usec
DE	10.00	usec
TE	296.2	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	-1.00	dB
SFO1	62.9015280	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	70.00	usec
PL12	15.00	dB
PL13	15.00	dB
PL2	-2.50	dB
SFO2	250.1310005	MHz
SI	32768	
SF	62.8952390	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

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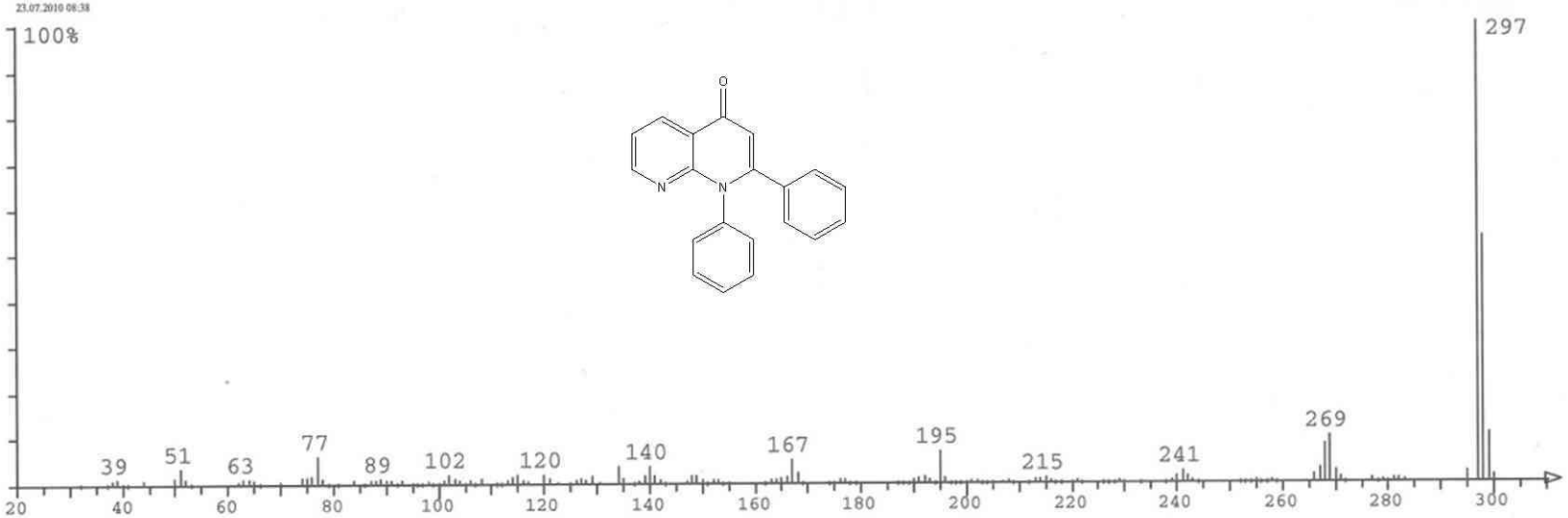

B3344(33:04) 2 35% 10072213 ikp 166/GC

32	0.12	81	0.16	108	0.83	147	0.32	187	0.16	216	0.32	257	0.12
38	0.37	84	0.50	111	0.12	148	1.33	188	0.25	217	0.22	258	0.36
39	0.72	86	0.20	113	0.54	149	1.30	189	0.19	218	0.13	266	1.32
40	0.19	87	0.44	114	1.03	150	0.63	190	0.41	221	0.29	267	2.77
41	0.12	88	0.59	115	1.65	151	0.28	191	0.83	226	0.21	268	7.92
44	0.43	89	0.92	116	0.48	152	0.55	192	0.99	227	0.20	269	9.75
50	1.01	90	0.51	117	0.36	153	0.59	193	0.58	228	0.25	270	2.21
51	3.01	91	0.41	120	1.77	154	0.13	194	0.25	229	0.32	271	0.68
52	0.68	92	0.23	121	0.69	162	0.13	195	6.66	230	0.19	272	0.25
53	0.13	93	0.49	126	0.45	163	0.51	196	0.73	233	0.12	277	0.48
62	0.35	96	0.26	127	0.82	164	0.48	199	0.11	238	0.22	278	0.15
63	0.88	97	0.14	128	0.52	165	0.93	200	0.20	239	0.31	279	0.31
64	0.71	98	0.34	129	1.25	166	1.02	201	0.34	240	1.03	281	0.48
65	0.39	100	0.16	134	3.27	167	4.84	202	0.31	241	2.12	282	0.39
66	0.13	101	0.54	135	0.74	168	1.90	203	0.26	242	1.15	283	0.31
70	0.34	102	1.75	138	0.33	169	0.20	204	0.15	243	0.35	295	2.07
74	1.01	103	0.95	139	1.44	175	0.26	205	0.27	244	0.15	297	100.00
75	1.02	104	0.55	140	3.30	176	0.49	208	0.32	252	0.27	298	53.32
76	1.29	105	0.15	141	1.48	177	0.41	213	0.40	253	0.24	299	10.36
77	5.60	106	0.57	142	0.58	178	0.27	214	0.62	254	0.15	300	1.07
78	0.87	107	0.18	143	0.18	179	0.19	215	0.66	255	0.36		

B3344(33:04) 2 35% 10072213 ikp 166/GC lim: 0.11%

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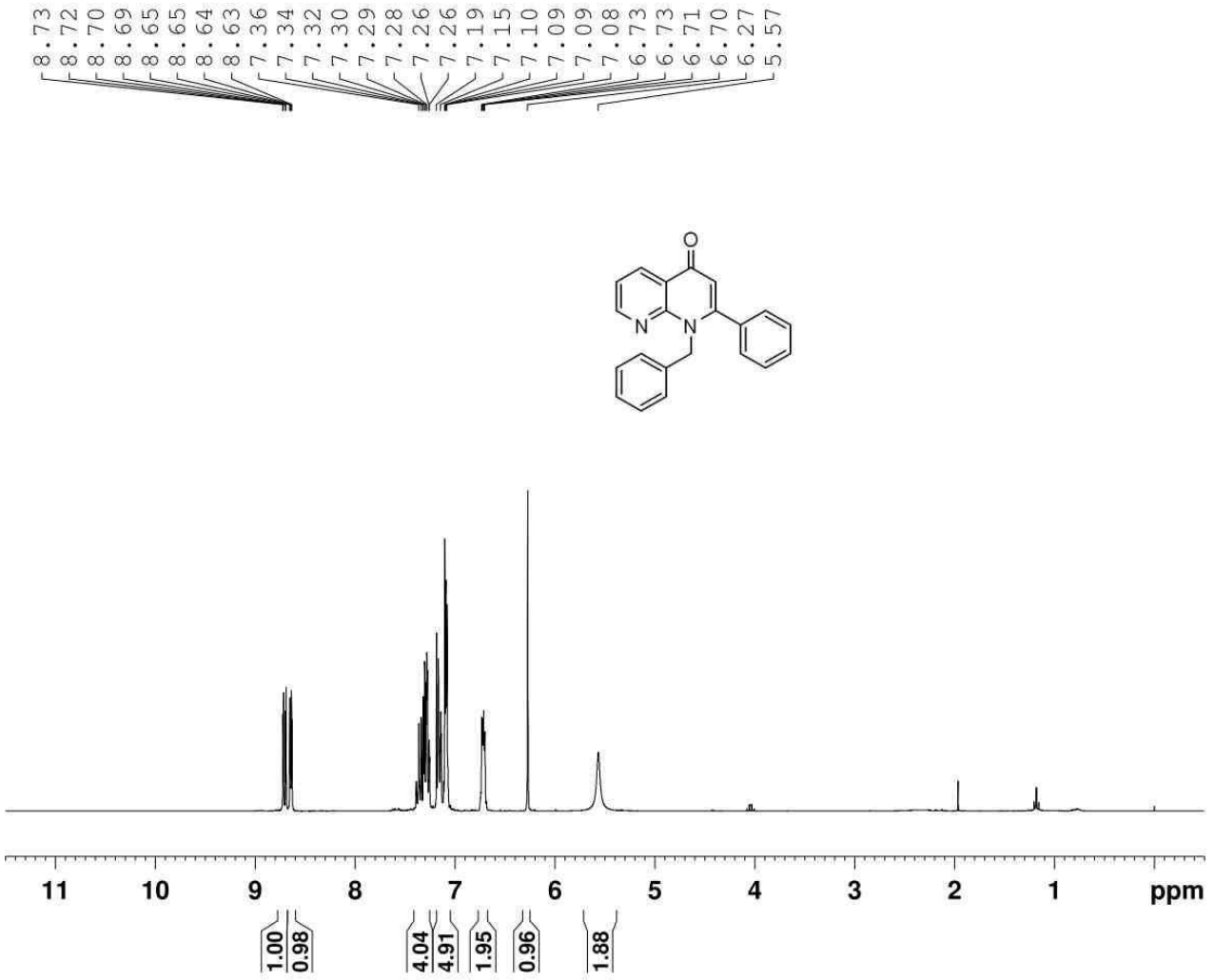

NAME	101008.u315	
EXPNO	10	
PROCNO	1	
Date_	20101008	
Time	11.49	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	128	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300300	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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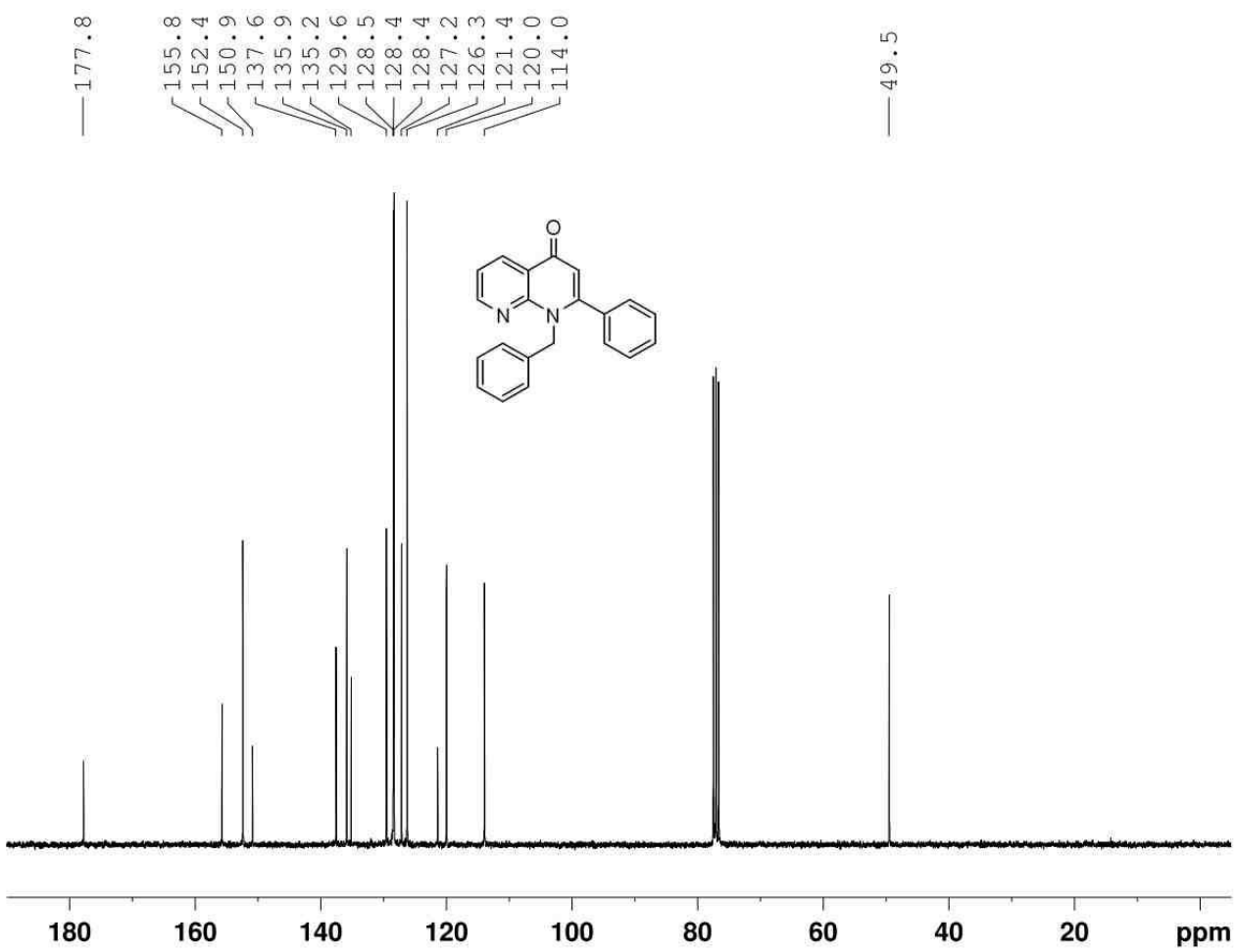

BRUKER

NAME	101008.u315
EXPNO	11
PROCNO	1
Date_	20101009
Time	14.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1200
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	299.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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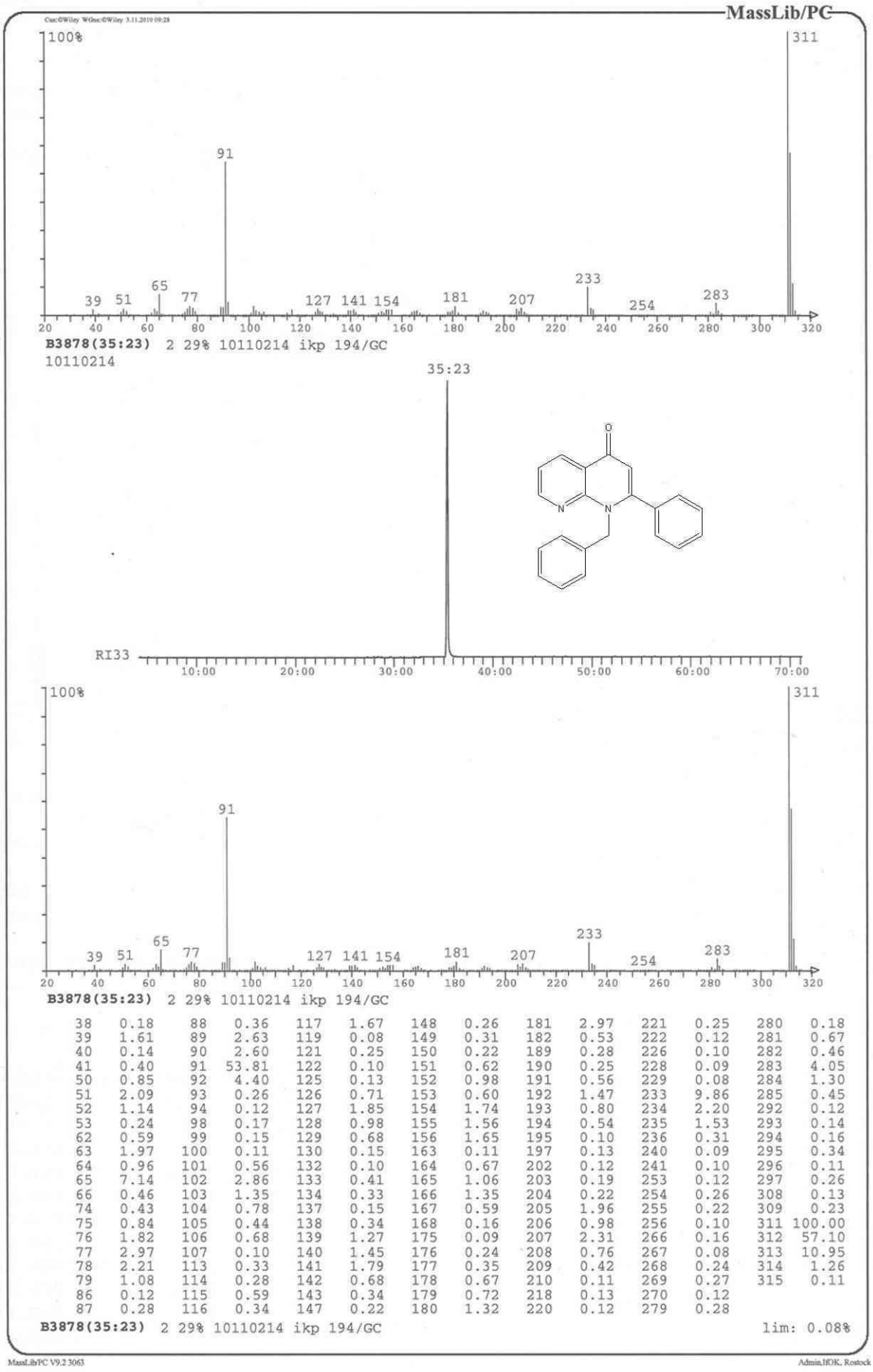

38	0.18	88	0.36	117	1.67	148	0.26	181	2.97	221	0.25	280	0.18
39	1.61	89	2.63	119	0.08	149	0.31	182	0.53	222	0.12	281	0.67
40	0.14	90	2.60	121	0.25	150	0.22	189	0.28	226	0.10	282	0.46
41	0.40	91	53.81	122	0.10	151	0.62	190	0.25	228	0.09	283	4.05
50	0.85	92	4.40	125	0.13	152	0.98	191	0.56	229	0.08	284	1.30
51	2.09	93	0.26	126	0.71	153	0.60	192	1.47	233	9.86	285	0.45
52	1.14	94	0.12	127	1.85	154	1.74	193	0.80	234	2.20	292	0.12
53	0.24	98	0.17	128	0.98	155	1.56	194	0.54	235	1.53	293	0.14
62	0.59	99	0.15	129	0.68	156	1.65	195	0.10	236	0.31	294	0.16
63	1.97	100	0.11	130	0.15	163	0.11	197	0.13	240	0.09	295	0.34
64	0.96	101	0.56	132	0.10	164	0.67	202	0.12	241	0.10	296	0.11
65	7.14	102	2.86	133	0.41	165	1.06	203	0.19	253	0.12	297	0.26
66	0.46	103	1.35	134	0.33	166	1.35	204	0.22	254	0.26	308	0.13
74	0.43	104	0.78	137	0.15	167	0.59	205	1.96	255	0.22	309	0.23
75	0.84	105	0.44	138	0.34	168	0.16	206	0.98	256	0.10	311	100.00
76	1.82	106	0.68	139	1.27	175	0.09	207	2.31	266	0.16	312	57.10
77	2.97	107	0.10	140	1.45	176	0.24	208	0.76	267	0.08	313	10.95
78	2.21	113	0.33	141	1.79	177	0.35	209	0.42	268	0.24	314	1.26
79	1.08	114	0.28	142	0.68	178	0.67	210	0.11	269	0.27	315	0.11
86	0.12	115	0.59	143	0.34	179	0.72	218	0.13	270	0.12		
87	0.28	116	0.34	147	0.22	180	1.32	220	0.12	279	0.28		

B3878(35:23) 2 29% 10110214 ikp 194/GC lim: 0.08%

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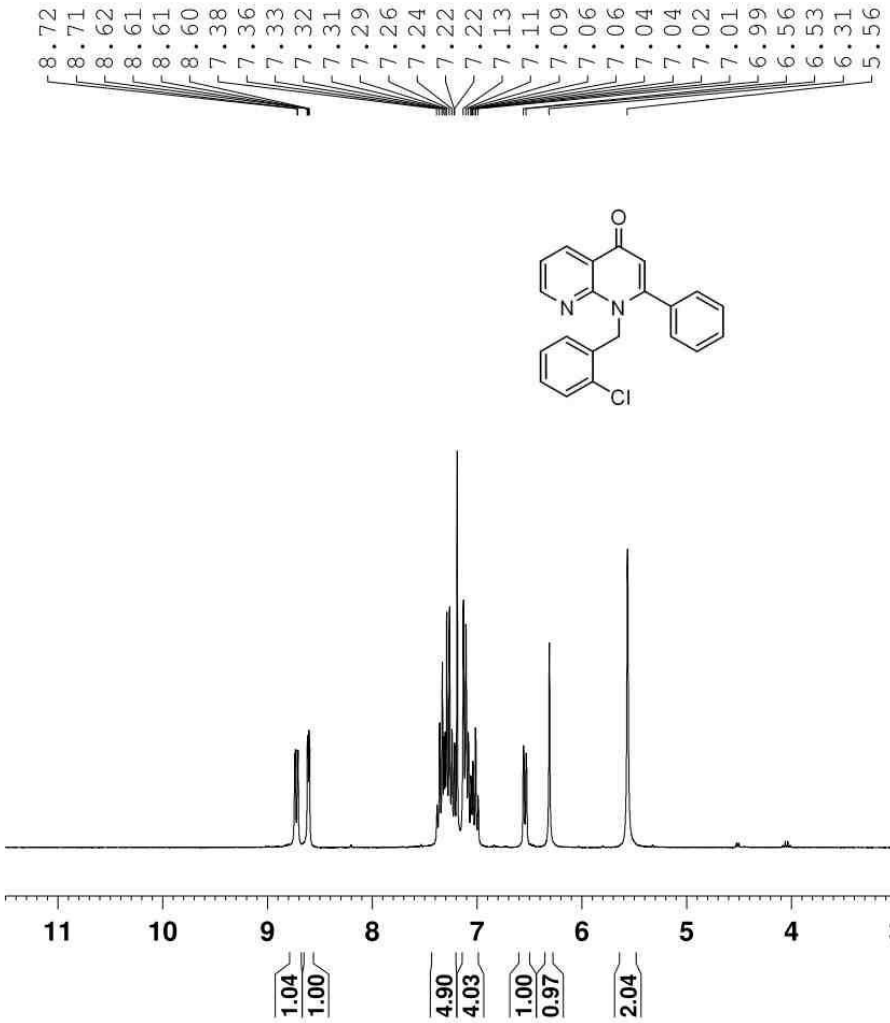

BRUKER

NAME	110104.u315	
EXPNO	10	
PROCNO	1	
Date_	20110104	
Time	14.00	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300295	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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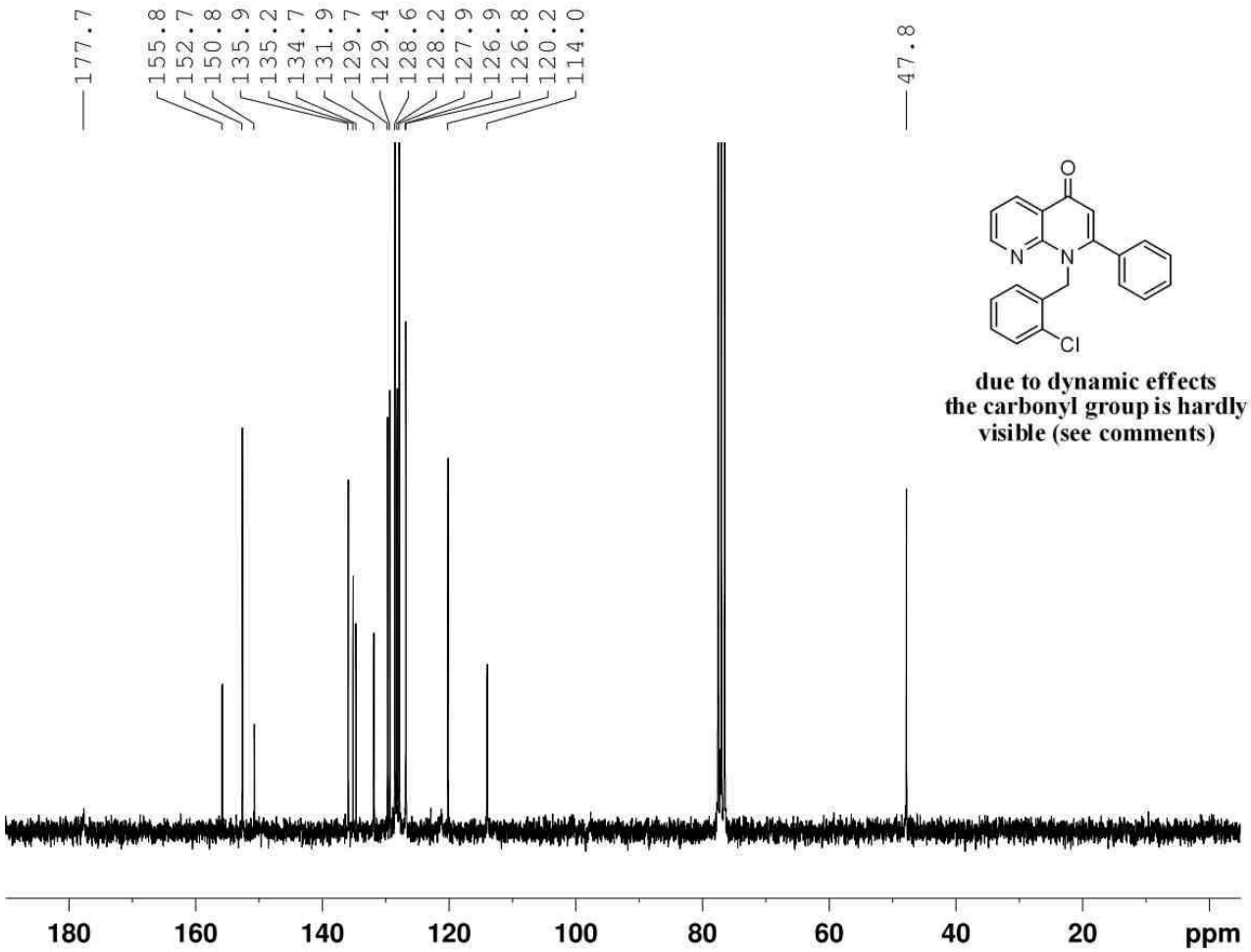

due to dynamic effects the carbonyl group is hardly visible (see comments)

NAME	110106.204	
EXPNO	11	
PROCNO	1	
Date_	20110106	
Time	16.22	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	15000.000	Hz
FIDRES	0.228882	Hz
AQ	2.1845834	sec
RG	2050	
DW	33.333	usec
DE	10.00	usec
TE	297.9	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	-1.00	dB
SFO1	62.9015280	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	70.00	usec
PL12	15.00	dB
PL13	15.00	dB
PL2	-2.50	dB
SFO2	250.1310005	MHz
SI	32768	
SF	62.8952390	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

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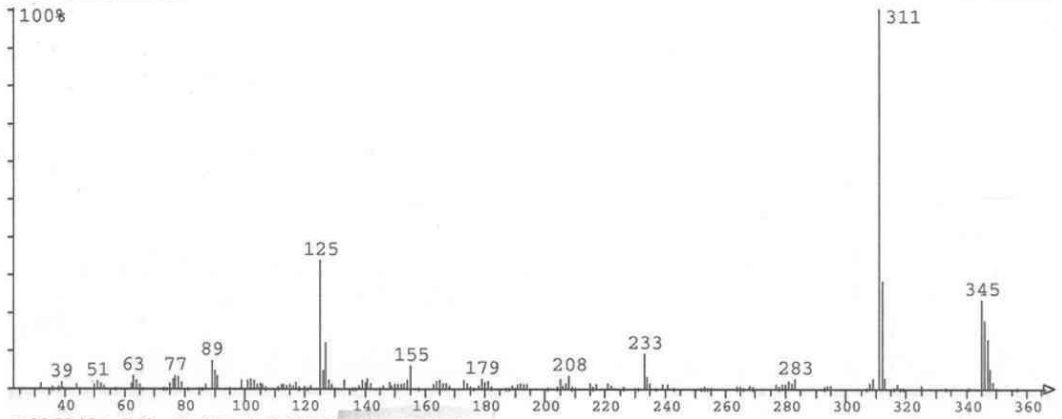
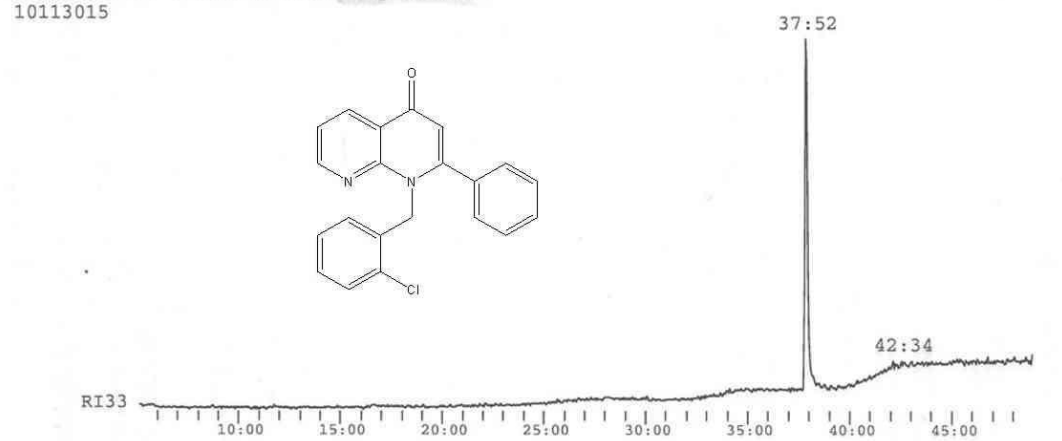
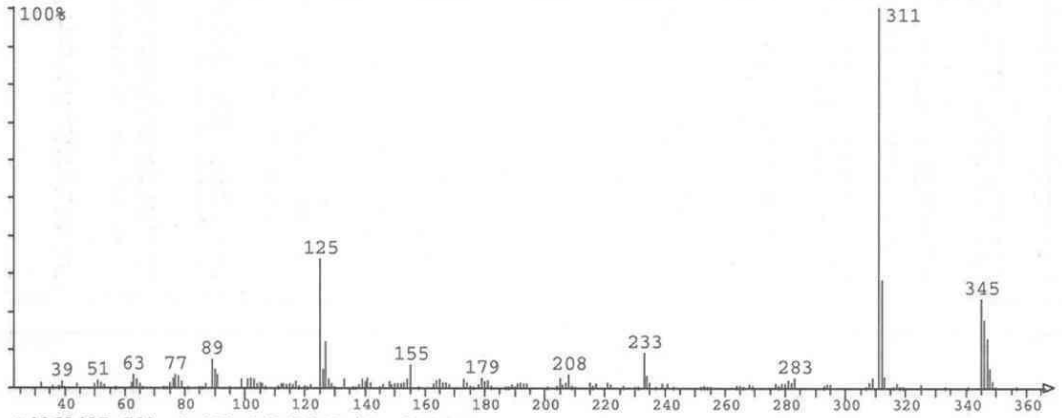


B4062(37:52) 2 25% 10113015 ikp 241/GC

10113015





B4062(37:52) 2 25% 10113015 ikp 241/GC

32	1.22	86	0.31	118	0.46	152	0.91	189	0.61	233	8.81	283	2.18
36	0.37	87	0.83	120	0.45	153	1.21	190	0.36	234	2.89	293	0.37
38	0.38	89	7.28	122	0.59	154	1.99	191	0.79	235	1.23	294	0.54
39	1.37	90	4.48	125	33.56	155	5.75	192	1.14	237	0.36	295	0.62
44	0.81	91	3.22	126	4.50	158	0.34	193	0.72	239	0.89	307	0.35
50	0.68	95	0.29	127	11.85	163	0.70	194	0.86	241	0.86	308	1.11
51	1.60	99	1.84	128	1.98	164	1.53	201	0.36	243	0.27	309	2.31
52	1.17	101	1.90	129	0.91	165	2.02	204	0.43	252	0.31	311	100.00
53	0.59	102	2.31	133	2.10	166	1.08	205	2.19	253	0.44	312	28.04
57	0.29	103	1.99	136	0.33	167	1.14	206	0.65	255	0.30	313	2.65
62	0.97	104	0.86	137	0.31	168	0.56	207	1.18	264	0.47	316	0.35
63	3.08	105	1.23	138	0.56	173	2.01	208	3.03	265	0.50	317	0.69
64	1.82	106	0.78	139	1.88	174	0.96	209	0.48	266	0.28	318	0.34
65	0.86	107	0.51	140	1.33	175	0.43	210	0.28	268	0.64	319	0.29
66	0.36	111	0.47	141	2.21	176	0.34	215	1.01	269	0.52	325	0.59
75	0.97	112	0.71	142	0.99	178	0.55	216	0.45	277	0.85	345	23.02
76	2.26	113	0.94	146	0.65	179	2.33	217	0.69	278	0.42	346	17.75
77	3.05	114	0.56	148	1.46	180	1.39	221	1.16	279	0.86	347	12.77
78	2.80	115	0.68	149	0.60	181	1.56	222	0.54	280	0.76	348	4.75
79	1.42	116	0.58	150	0.75	182	0.39	226	0.38	281	1.76	349	1.32
81	0.34	117	1.31	151	0.91	188	0.34	230	0.30	282	1.19	357	0.33

B4062(37:52) 2 25% 10113015 ikp 241/GC lim: 0.27%

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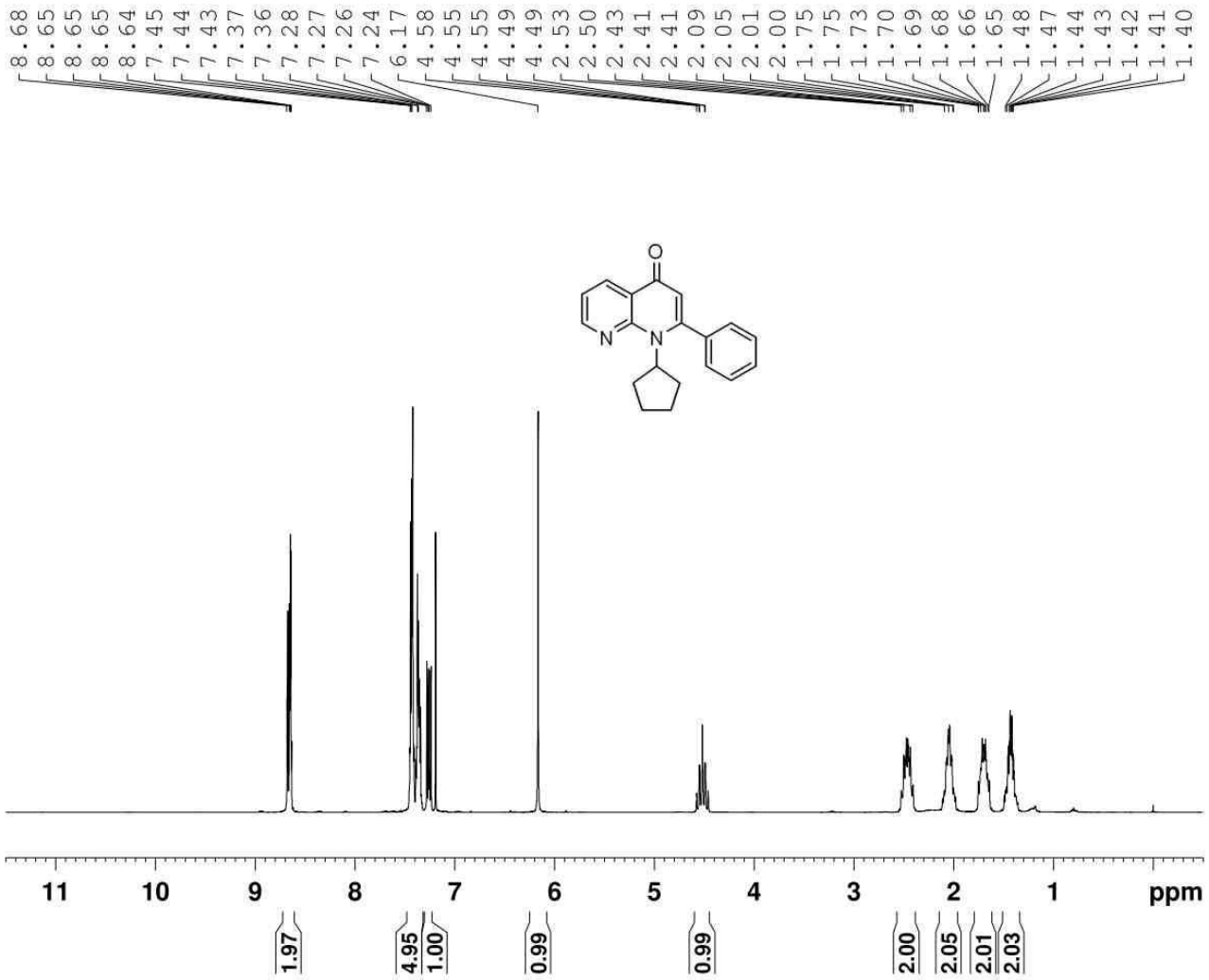

NAME	100719.u322
EXPNO	10
PROCNO	1
Date_	20100719
Time	13.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	128
DW	80.800 use
DE	10.00 use
TE	299.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300281 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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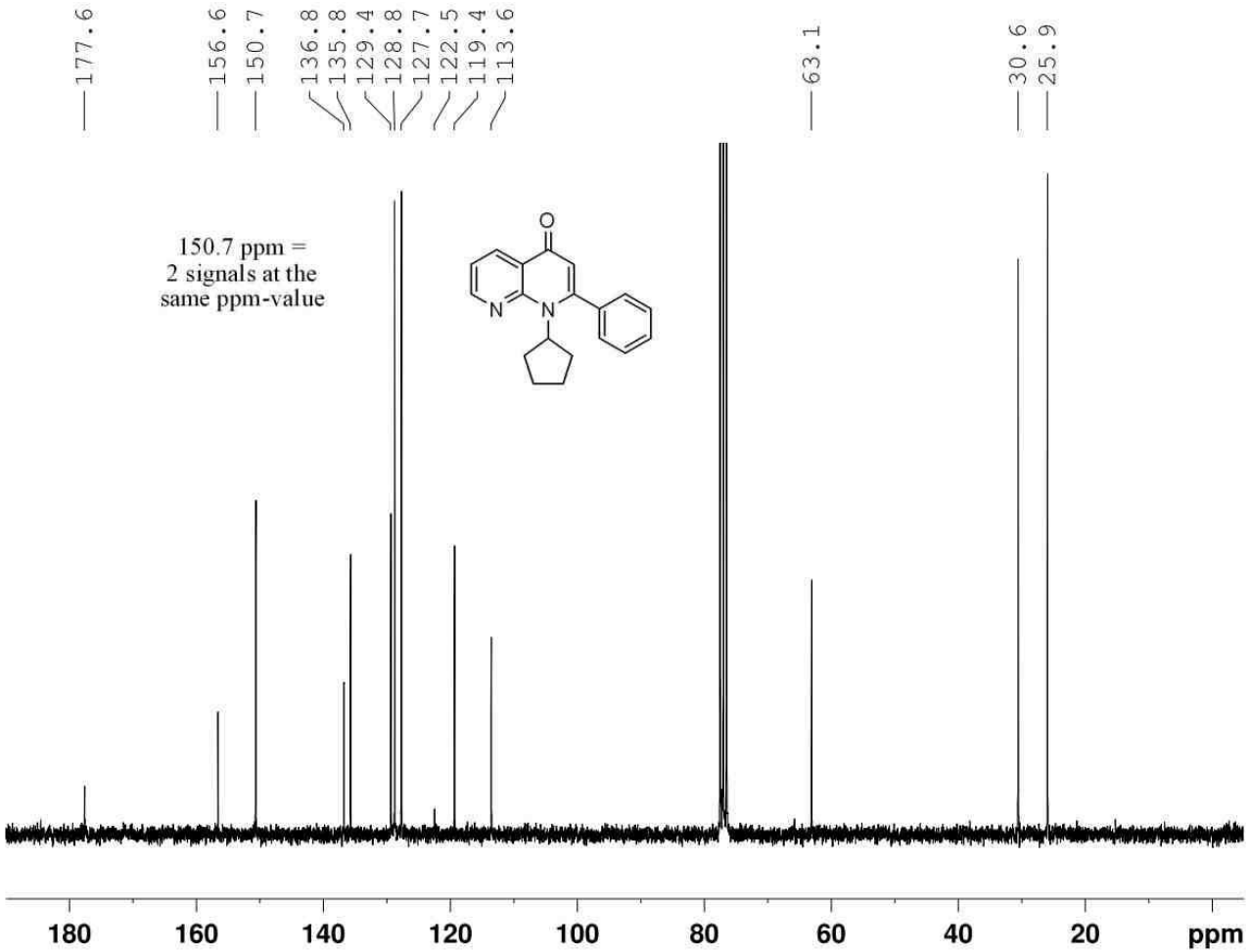

NAME	100720.205
EXPNO	10
PROCNO	1
Date_	20100720
Time	23.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	299.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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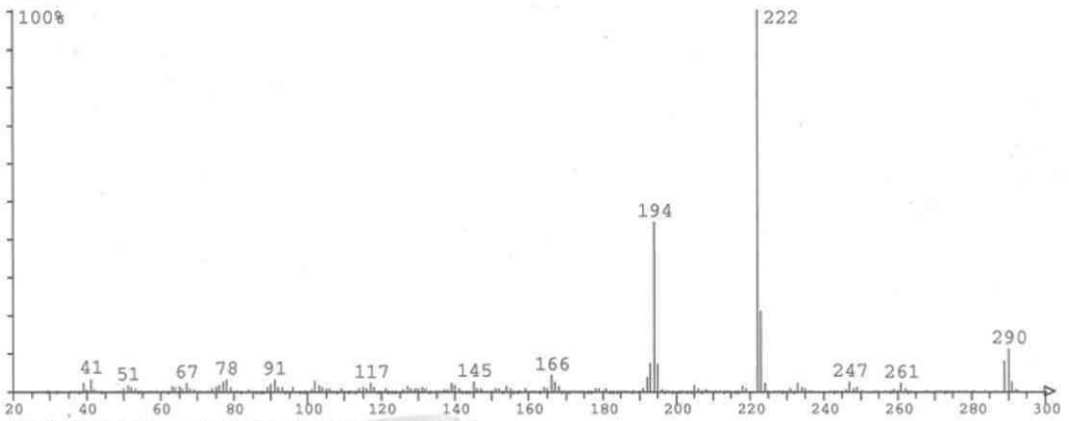
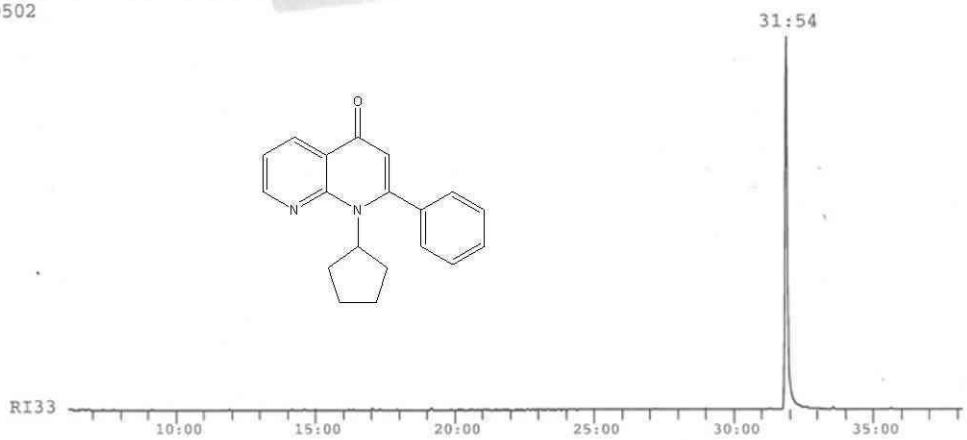
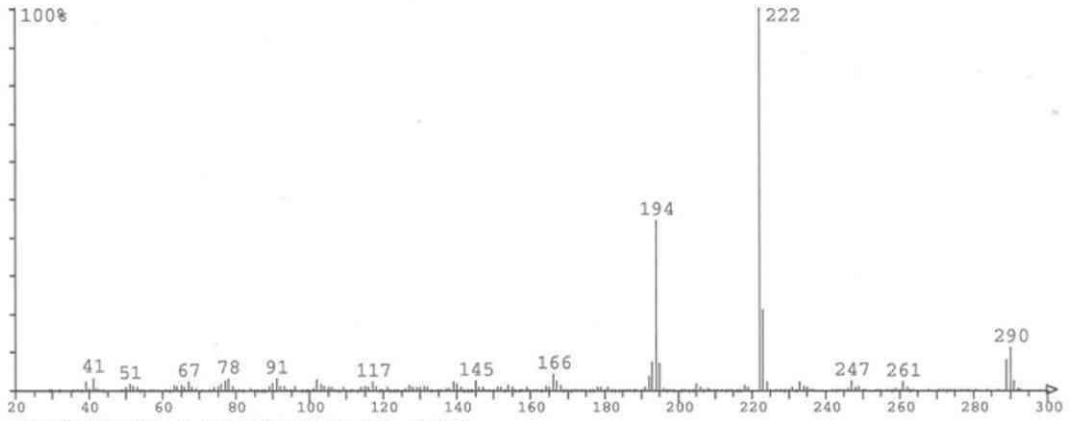
MassLib/PC



B3200(31:54) 2 33% 10070502 ikp 169/GC

10070502





B3200(31:54) 2 33% 10070502 ikp 169/GC

32	0.12	75	0.74	104	0.87	131	0.87	157	0.16	196	0.30	245	0.13
38	0.28	76	1.34	105	0.46	132	0.46	159	0.48	203	0.15	246	0.36
39	2.11	77	2.14	106	0.50	133	0.19	164	0.87	204	0.14	247	2.20
40	0.31	78	2.86	108	0.12	137	0.30	165	0.54	205	1.48	248	0.38
41	2.97	79	0.83	109	0.46	138	0.32	166	4.05	206	0.55	249	0.88
42	0.32	80	0.14	110	0.27	139	2.09	167	2.30	207	0.20	250	0.23
44	0.11	84	0.34	113	0.28	140	1.51	168	0.96	208	0.30	258	0.20
50	0.61	85	0.12	114	0.50	141	0.53	169	0.17	213	0.21	259	0.35
51	1.26	86	0.13	115	0.74	142	0.24	171	0.13	217	0.21	260	0.27
52	0.77	87	0.22	116	0.62	143	0.20	177	0.26	218	1.00	261	1.93
53	0.64	88	0.26	117	1.84	144	0.17	178	0.37	219	0.39	262	0.64
54	0.20	89	0.77	118	0.73	145	2.21	179	0.45	222	100.00	263	0.16
62	0.26	90	1.65	119	0.24	146	0.37	180	0.25	223	20.95	273	0.17
63	1.05	91	2.78	121	0.46	147	0.46	181	0.39	224	1.90	289	7.64
64	0.90	92	0.68	123	0.27	150	0.17	185	0.22	225	0.19	290	10.88
65	1.13	93	0.78	124	0.28	151	0.37	190	0.28	231	0.45	291	2.23
66	0.51	96	0.69	126	0.33	152	0.61	191	0.62	232	0.21	292	0.32
67	1.89	99	0.13	127	1.07	153	0.28	192	3.50	233	1.84		
68	0.55	101	0.34	128	0.45	154	1.00	193	7.31	234	0.92		
69	0.35	102	2.45	129	0.60	155	0.55	194	44.25	235	0.48		
74	0.44	103	1.26	130	0.54	156	0.13	195	6.87	243	0.17		

B3200(31:54) 2 33% 10070502 ikp 169/GC lim: 0.11%

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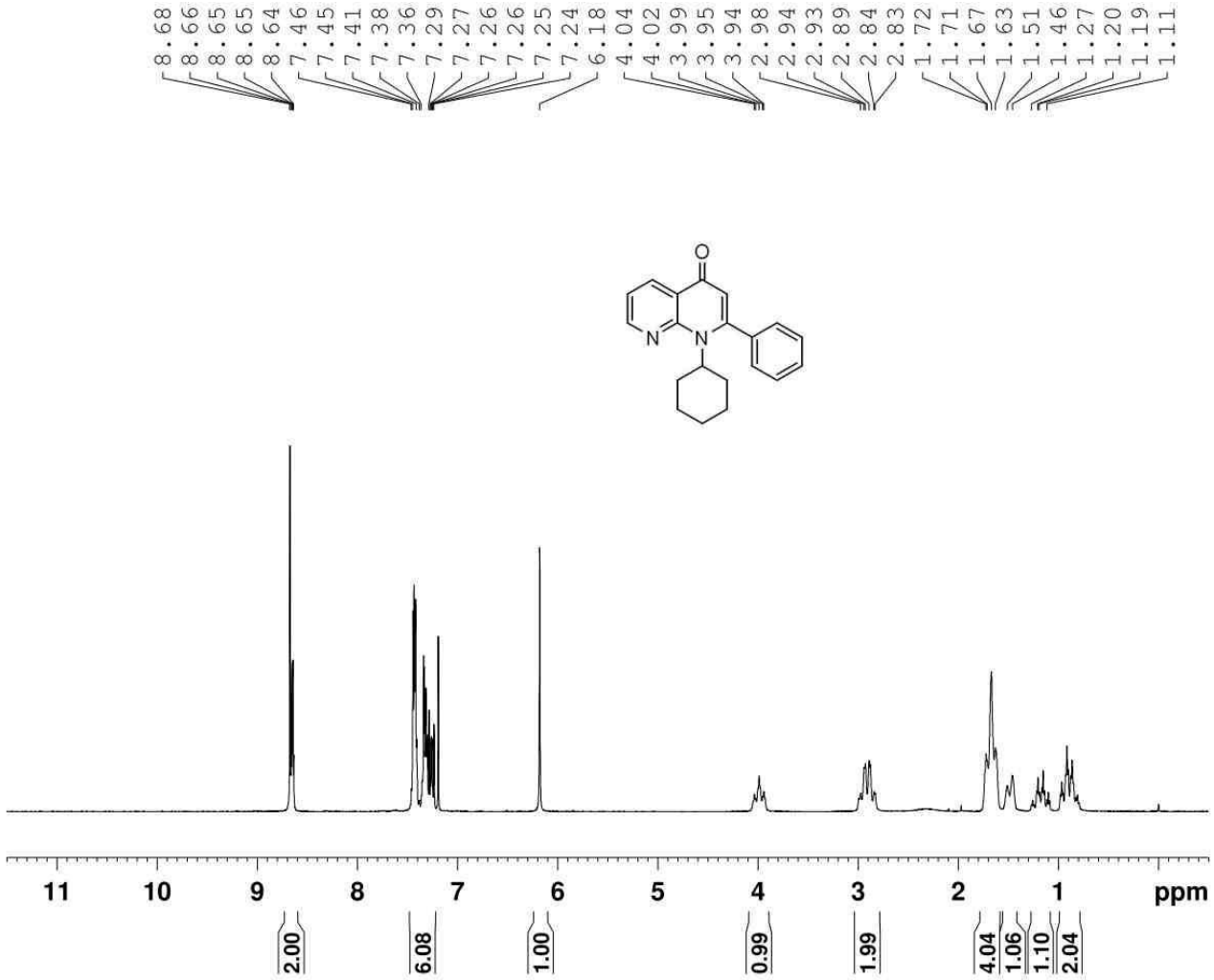

NAME	101027.206
EXPNO	10
PROCNO	1
Date_	20101027
Time	11.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	5165.289 Hz
FIDRES	0.078816 Hz
AQ	6.3439350 sec
RG	575
DW	96.800 use
DE	10.00 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	1H
P1	10.00 use
PL1	-2.50 dB
SFO1	250.1315447 MHz
SI	32768
SF	250.1300170 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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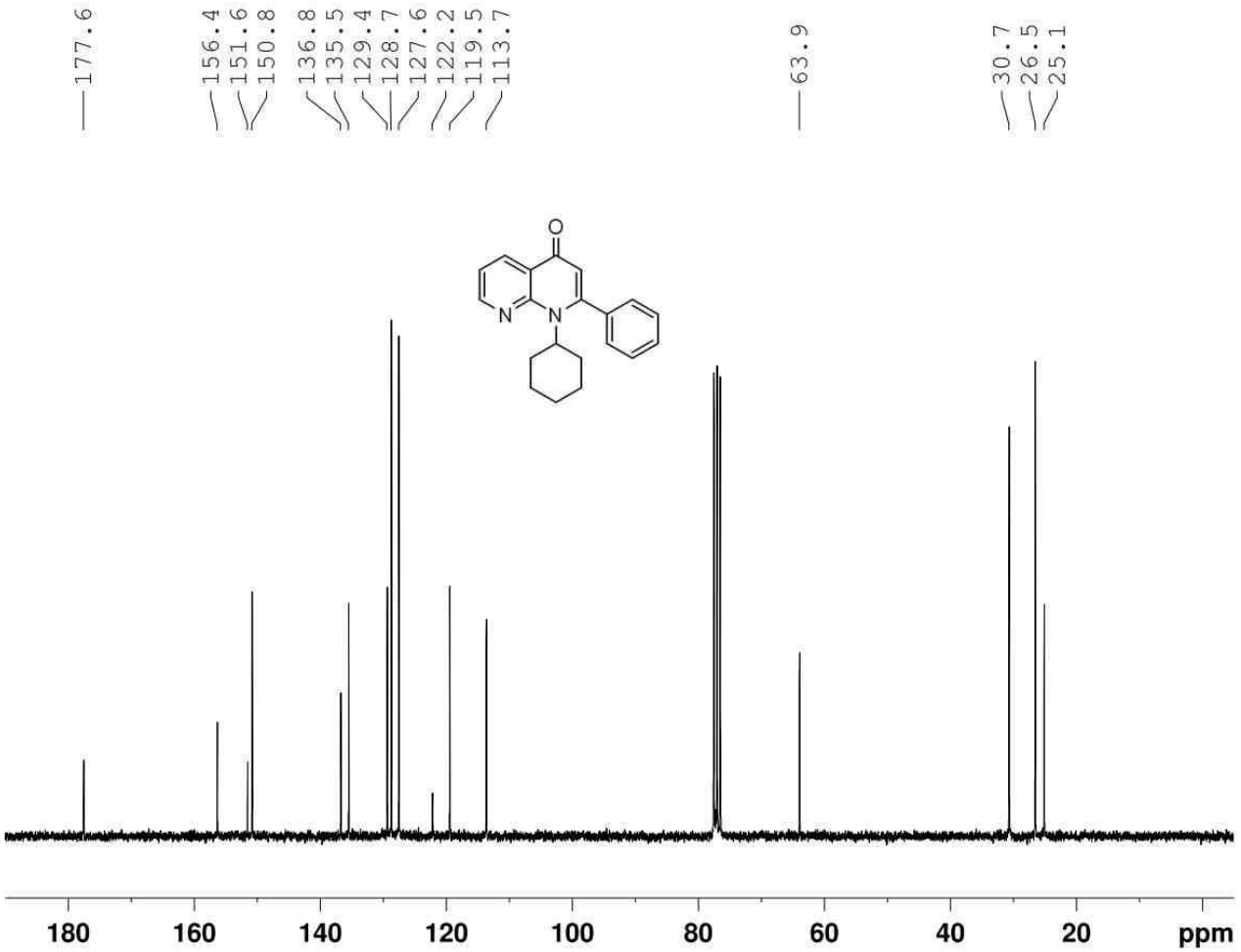
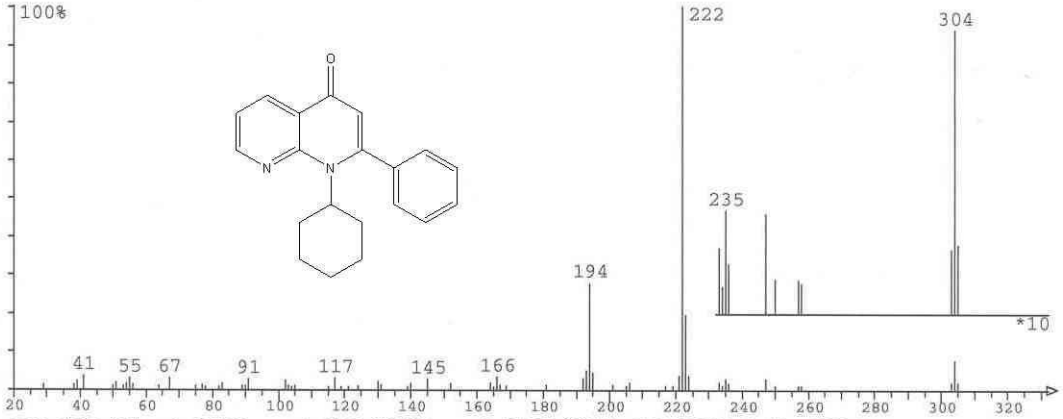


NAME	101028.212
EXPNO	10
PROCNO	1
Date_	20101028
Time	12.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



R3: 227 40% m(3617) - m(575-2298) - m(6476-8824) 10102514 * ikp 224/GC

29	0.95	103	0.90	193	4.98	304	7.40
38	0.98	104	0.63	194	27.63	305	1.77
39	2.04	105	0.76	195	4.37		
41	3.52	115	0.58	201	0.98		
50	0.92	117	2.79	205	0.91		
51	1.71	119	0.57	206	1.76		
53	0.83	121	0.63	217	0.77		
54	1.26	124	0.74	219	0.70		
55	2.86	130	2.11	221	3.51		
56	1.09	131	1.05	222	100.00		
64	0.93	139	0.65	223	19.27		
67	2.91	140	1.24	224	3.35		
75	0.67	145	2.54	233	1.68		
77	1.06	152	1.34	234	0.66		
78	0.58	164	1.61	235	2.66		
82	0.65	165	0.59	236	1.28		
83	1.32	166	3.03	247	2.57		
89	0.67	167	1.23	250	0.86		
90	0.68	169	0.79	257	0.83		
91	2.52	181	1.06	258	0.76		
102	2.13	192	2.75	303	1.64		

R3: 227 40% m(3617) - m(575-2298) - m(6476-8824) 10102514 * ikp 224/GC

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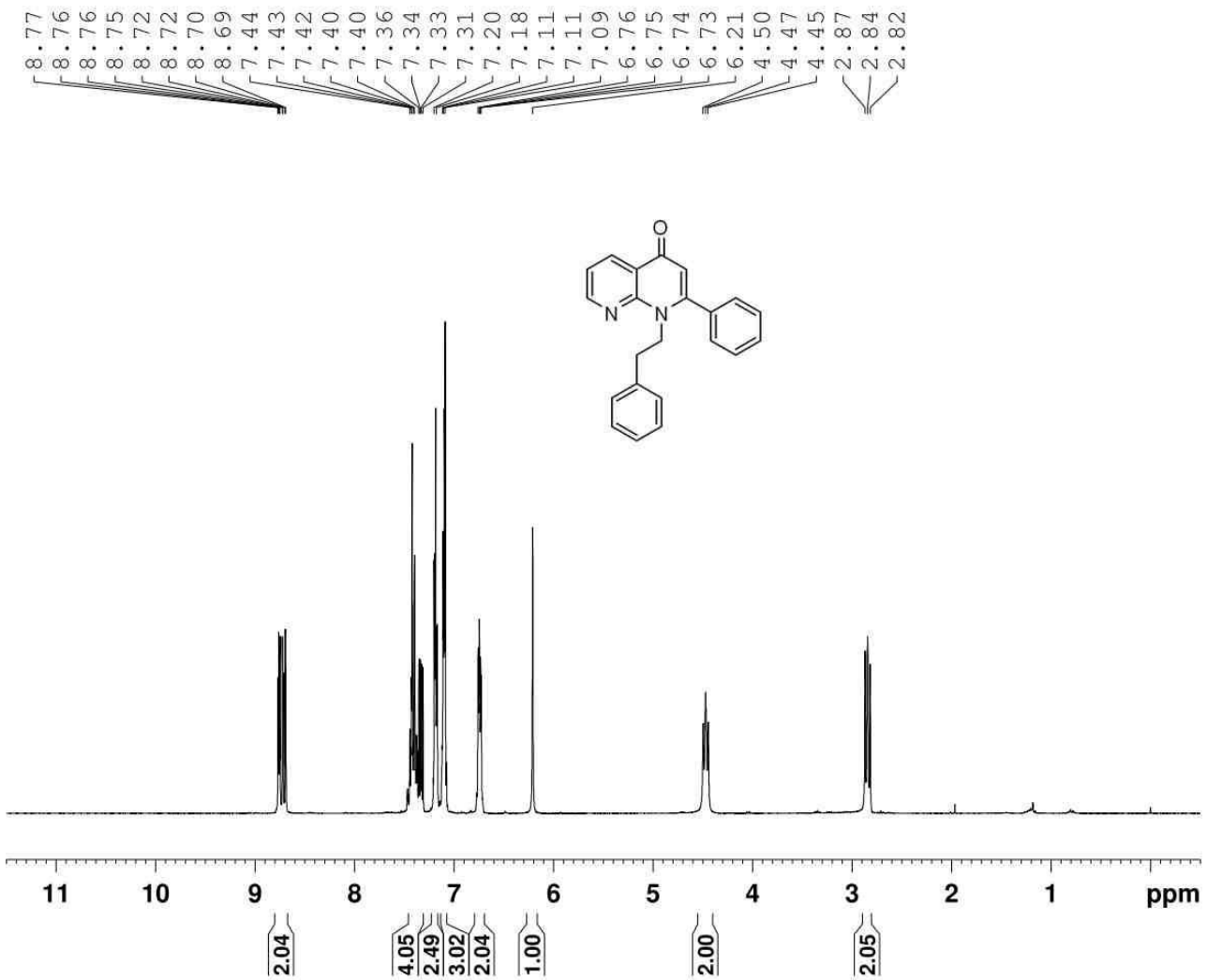

NAME	100719.u321
EXPNO	10
PROCNO	1
Date_	20100719
Time	13.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	128
DW	80.800 use
DE	10.00 use
TE	299.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300302 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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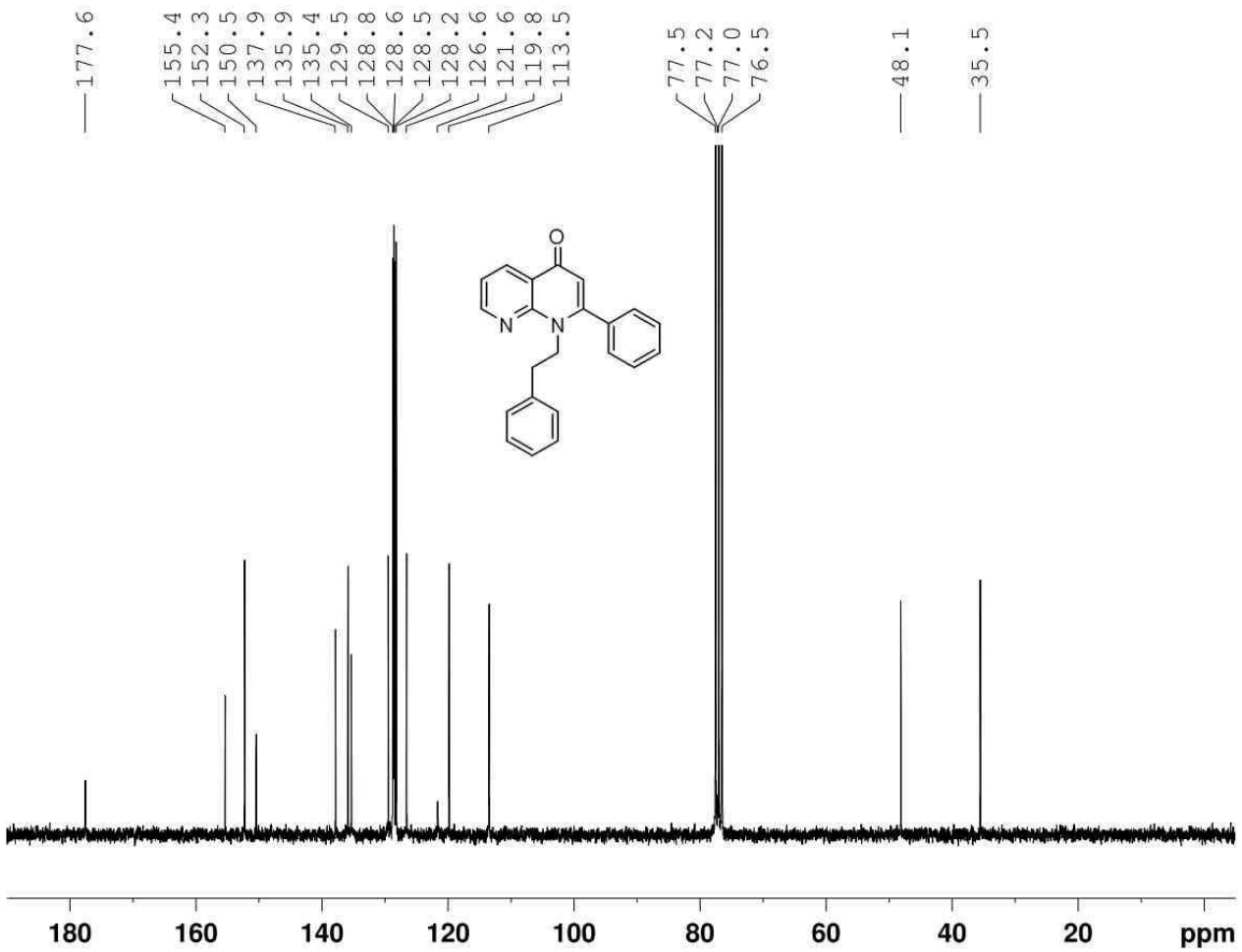

NAME	101014.201	
EXPNO	10	
PROCNO	1	
Date_	20101014	
Time	10.33	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	15000.000	Hz
FIDRES	0.228882	Hz
AQ	2.1845834	sec
RG	2050	
DW	33.333	usec
DE	10.00	usec
TE	297.3	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	-1.00	dB
SFO1	62.9015280	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	70.00	usec
PL12	15.00	dB
PL13	15.00	dB
PL2	-2.50	dB
SFO2	250.1310005	MHz
SI	32768	
SF	62.8952390	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

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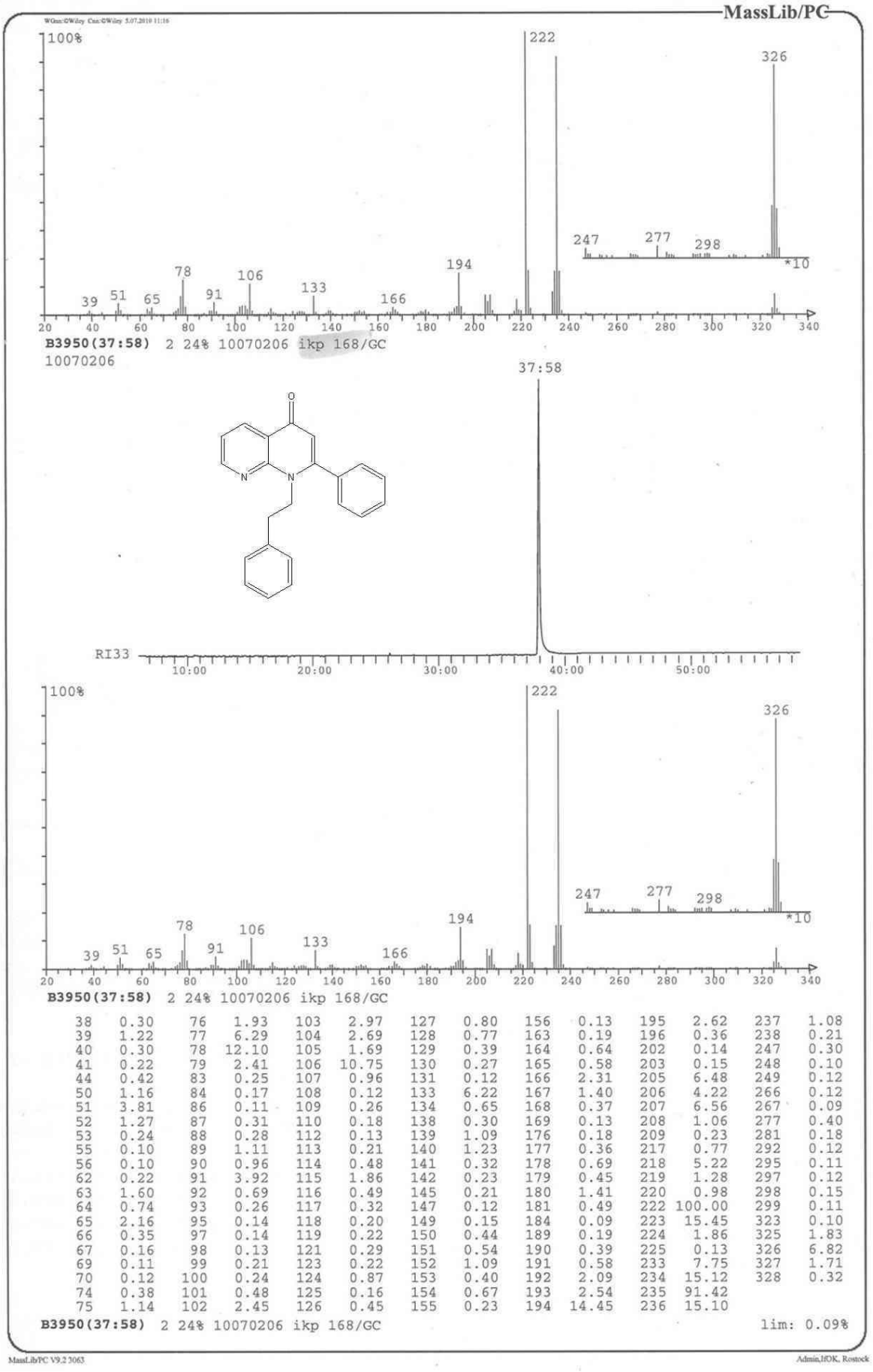

38	0.30	76	1.93	103	2.97	127	0.80	156	0.13	195	2.62	237	1.08
39	1.22	77	6.29	104	2.69	128	0.77	163	0.19	196	0.36	238	0.21
40	0.30	78	12.10	105	1.69	129	0.39	164	0.64	202	0.14	247	0.30
41	0.22	79	2.41	106	10.75	130	0.27	165	0.58	203	0.15	248	0.10
44	0.42	83	0.25	107	0.96	131	0.12	166	2.31	205	6.48	249	0.12
50	1.16	84	0.17	108	0.12	133	6.22	167	1.40	206	4.22	266	0.12
51	3.81	86	0.11	109	0.26	134	0.65	168	0.37	207	6.56	267	0.09
52	1.27	87	0.31	110	0.18	138	0.30	169	0.13	208	1.06	277	0.40
53	0.24	88	0.28	112	0.13	139	1.09	176	0.18	209	0.23	281	0.18
55	0.10	89	1.11	113	0.21	140	1.23	177	0.36	217	0.77	292	0.12
56	0.10	90	0.96	114	0.48	141	0.32	178	0.69	218	5.22	295	0.11
62	0.22	91	3.92	115	1.86	142	0.23	179	0.45	219	1.28	297	0.12
63	1.60	92	0.69	116	0.49	145	0.21	180	1.41	220	0.98	298	0.15
64	0.74	93	0.26	117	0.32	147	0.12	181	0.49	222	100.00	299	0.11
65	2.16	95	0.14	118	0.20	149	0.15	184	0.09	223	15.45	323	0.10
66	0.35	97	0.14	119	0.22	150	0.44	189	0.19	224	1.86	325	1.83
67	0.16	98	0.13	121	0.29	151	0.54	190	0.39	225	0.13	326	6.82
69	0.11	99	0.21	123	0.22	152	1.09	191	0.58	233	7.75	327	1.71
70	0.12	100	0.24	124	0.87	153	0.40	192	2.09	234	15.12	328	0.32
74	0.38	101	0.48	125	0.16	154	0.67	193	2.54	235	91.42		
75	1.14	102	2.45	126	0.45	155	0.23	194	14.45	236	15.10		

B3950(37:58) 2 24% 10070206 ikp 168/GC lim: 0.09%

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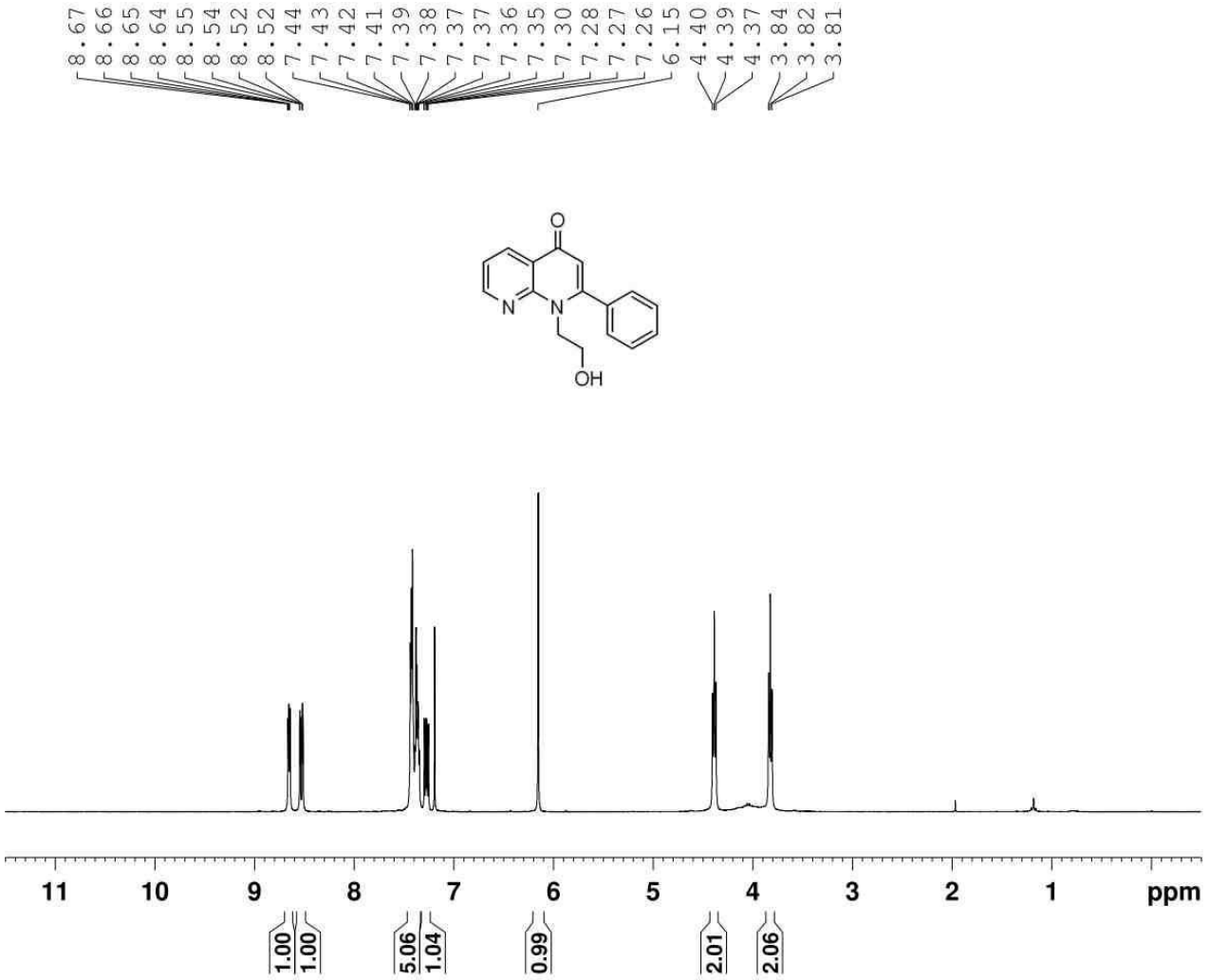

BRUKER

NAME	101115.u328	
EXPNO	10	
PROCNO	1	
Date_	20101115	
Time	14.42	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 =======		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300282	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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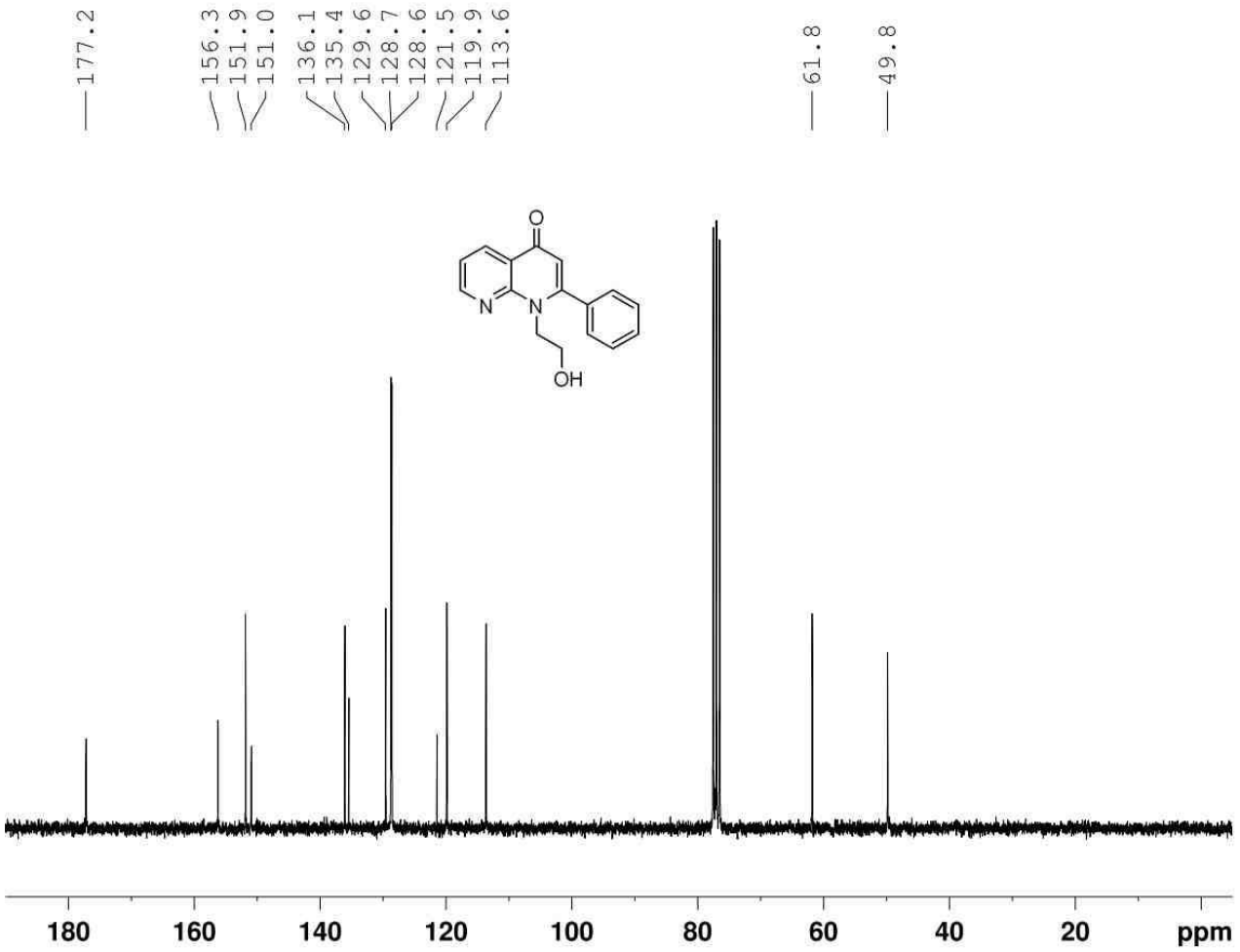

BRUKER

NAME	101116.212
EXPNO	10
PROCNO	1
Date_	20101117
Time	4.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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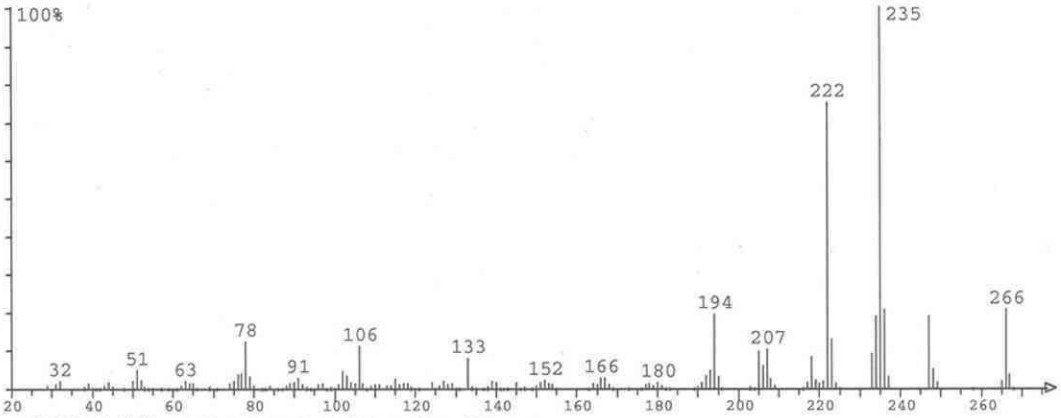
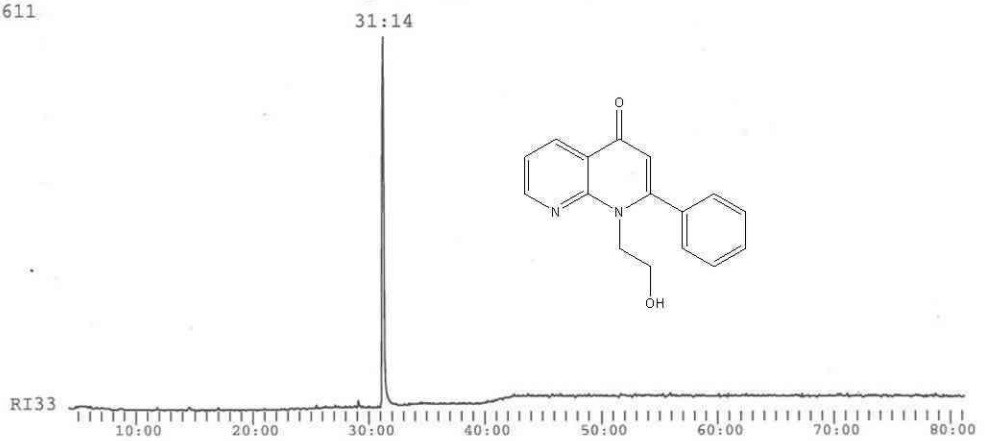
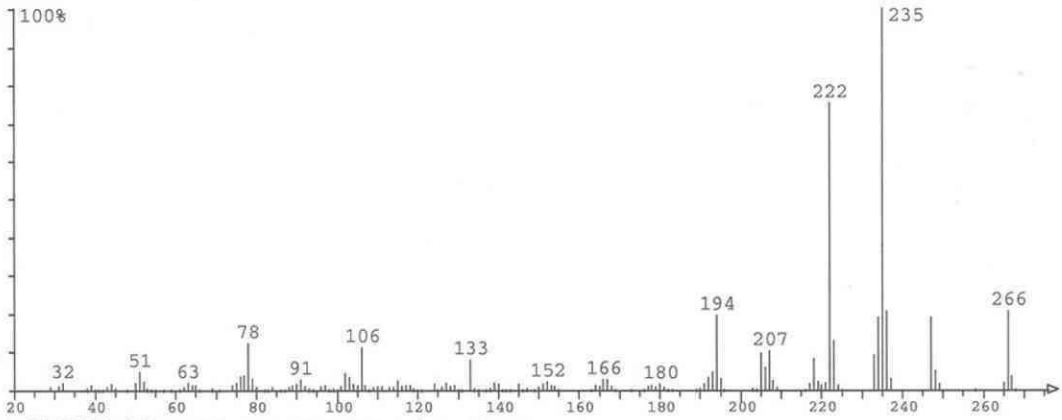


3364(31:14) 1123 20% 10111611 * ikp 227/GC

10111611





3364(31:14) 1123 20% 10111611 * ikp 227/GC

29	0.64	65	1.09	96	0.90	119	0.42	145	1.28	179	0.65	218	8.15
31	0.94	66	0.25	97	1.05	120	0.29	146	0.17	180	1.37	219	1.85
32	1.61	69	0.39	98	0.34	121	0.30	147	0.44	181	0.64	220	1.04
38	0.52	74	1.05	99	0.52	124	1.25	149	0.18	182	0.32	221	1.74
39	1.06	75	1.65	100	0.22	125	0.23	150	0.65	183	0.18	222	75.07
40	0.32	76	3.38	101	0.78	126	0.56	151	1.49	190	0.42	223	12.70
43	0.55	77	3.82	102	4.36	127	1.64	152	1.89	191	1.31	224	1.09
44	1.36	78	11.99	103	3.08	128	0.88	153	1.00	192	3.21	225	0.23
45	0.41	79	2.69	104	1.41	129	1.02	154	0.83	193	4.54	233	8.80
48	0.18	80	0.61	105	0.95	130	0.24	155	0.17	194	19.28	234	18.67
50	1.66	83	0.26	106	11.05	131	0.30	163	0.17	195	2.75	235	100.00
51	4.46	84	0.61	107	1.23	133	7.71	164	1.06	196	0.23	236	20.55
52	1.99	86	0.27	109	0.64	134	0.44	165	0.66	203	0.37	237	2.96
53	0.48	87	0.31	110	0.85	135	0.32	166	2.59	204	0.24	247	18.69
54	0.22	88	0.58	111	0.68	137	0.26	167	2.45	205	9.60	248	5.01
57	0.19	89	1.14	113	0.60	138	0.41	168	0.76	206	5.60	249	1.31
59	0.20	90	1.31	114	0.56	139	1.80	169	0.19	207	10.15	265	1.65
61	0.21	91	2.53	115	2.36	140	1.34	173	0.31	208	2.18	266	20.55
62	0.58	92	0.89	116	0.94	141	0.30	176	0.19	209	0.60	267	3.47
63	1.75	93	0.46	117	1.20	142	0.22	177	0.70	216	0.28	268	0.31
64	1.18	94	0.36	118	1.10	143	0.18	178	1.10	217	1.28		

3364(31:14) 1123 20% 10111611 * ikp 227/GC lim: 0.17%

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Admin,IfOK, Rostock

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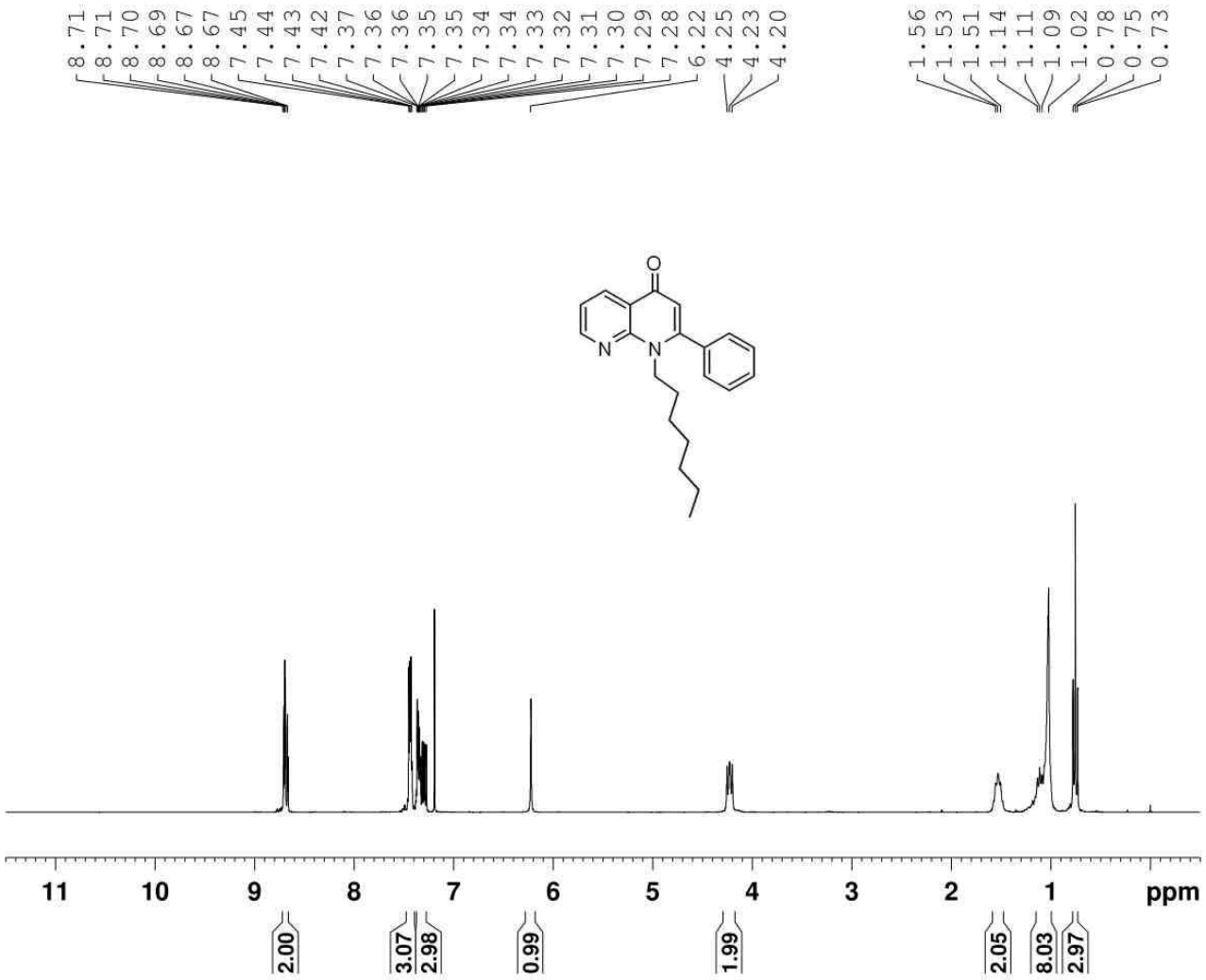

BRUKER

NAME	101207.u342	
EXPNO	10	
PROCNO	1	
Date_	20101207	
Time	15.02	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	128	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300276	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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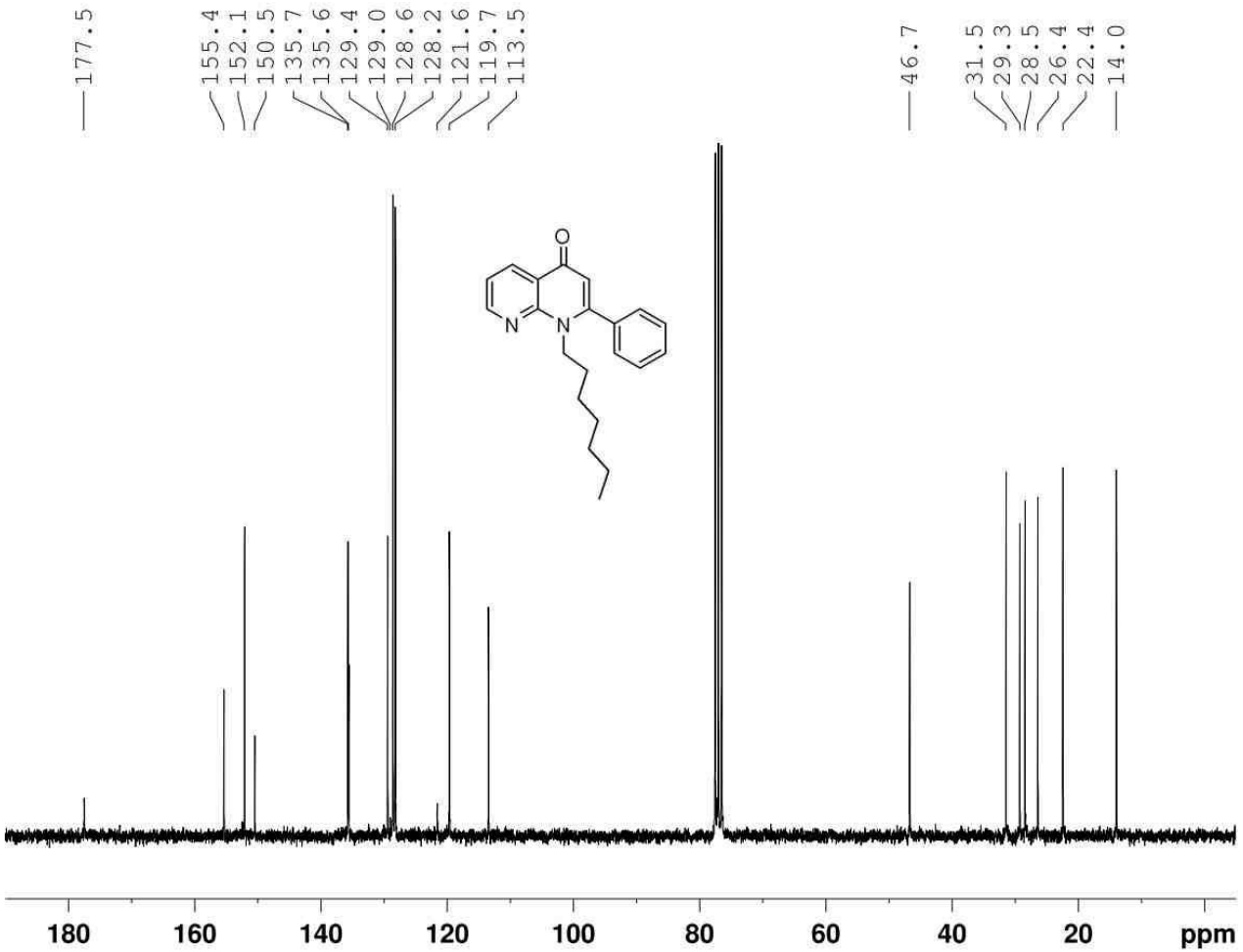

NAME	101208.209
EXPNO	10
PROCNO	1
Date_	20101209
Time	1.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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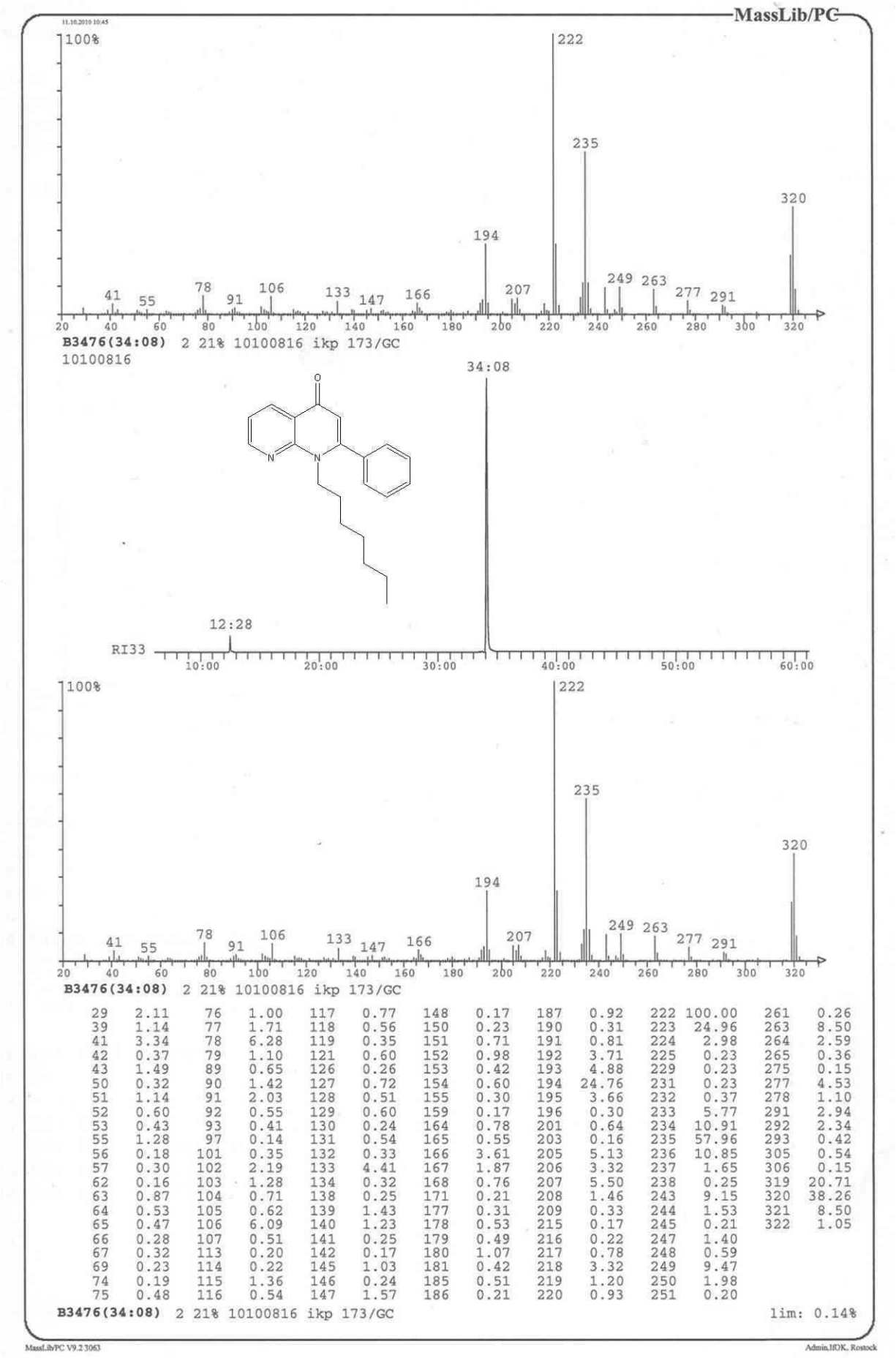

29	2.11	76	1.00	117	0.77	148	0.17	187	0.92	222	100.00	261	0.26
39	1.14	77	1.71	118	0.56	150	0.23	190	0.31	223	24.96	263	8.50
41	3.34	78	6.28	119	0.35	151	0.71	191	0.81	224	2.98	264	2.59
42	0.37	79	1.10	121	0.60	152	0.98	192	3.71	225	0.23	265	0.36
43	1.49	89	0.65	126	0.26	153	0.42	193	4.88	229	0.23	275	0.15
50	0.32	90	1.42	127	0.72	154	0.60	194	24.76	231	0.23	277	4.53
51	1.14	91	2.03	128	0.51	155	0.30	195	3.66	232	0.37	278	1.10
52	0.60	92	0.55	129	0.60	159	0.17	196	0.30	233	5.77	291	2.94
53	0.43	93	0.41	130	0.24	164	0.78	201	0.64	234	10.91	292	2.34
55	1.28	97	0.14	131	0.54	165	0.55	203	0.16	235	57.96	293	0.42
56	0.18	101	0.35	132	0.33	166	3.61	205	5.13	236	10.85	305	0.54
57	0.30	102	2.19	133	4.41	167	1.87	206	3.32	237	1.65	306	0.15
62	0.16	103	1.28	134	0.32	168	0.76	207	5.50	238	0.25	319	20.71
63	0.87	104	0.71	138	0.25	171	0.21	208	1.46	243	9.15	320	38.26
64	0.53	105	0.62	139	1.43	177	0.31	209	0.33	244	1.53	321	8.50
65	0.47	106	6.09	140	1.23	178	0.53	215	0.17	245	0.21	322	1.05
66	0.28	107	0.51	141	0.25	179	0.49	216	0.22	247	1.40		
67	0.32	113	0.20	142	0.17	180	1.07	217	0.78	248	0.59		
69	0.23	114	0.22	145	1.03	181	0.42	218	3.32	249	9.47		
74	0.19	115	1.36	146	0.24	185	0.51	219	1.20	250	1.98		
75	0.48	116	0.54	147	1.57	186	0.21	220	0.93	251	0.20		

B3476(34:08) 2 21% 10100816 ikp 173/GC lim: 0.14%

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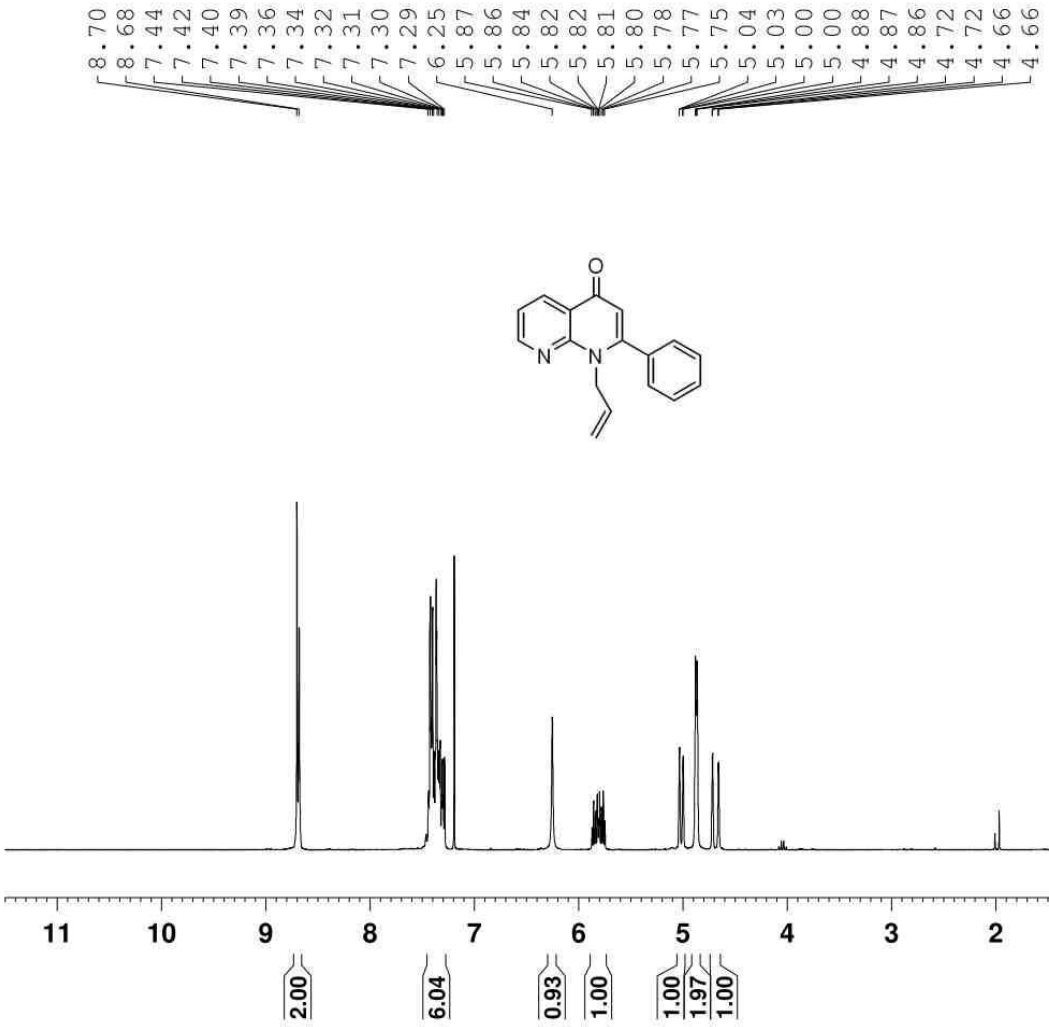

NAME	110209.u318	
EXPNO	10	
PROCNO	1	
Date_	20110209	
Time	11.08	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDC13	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	161	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300276	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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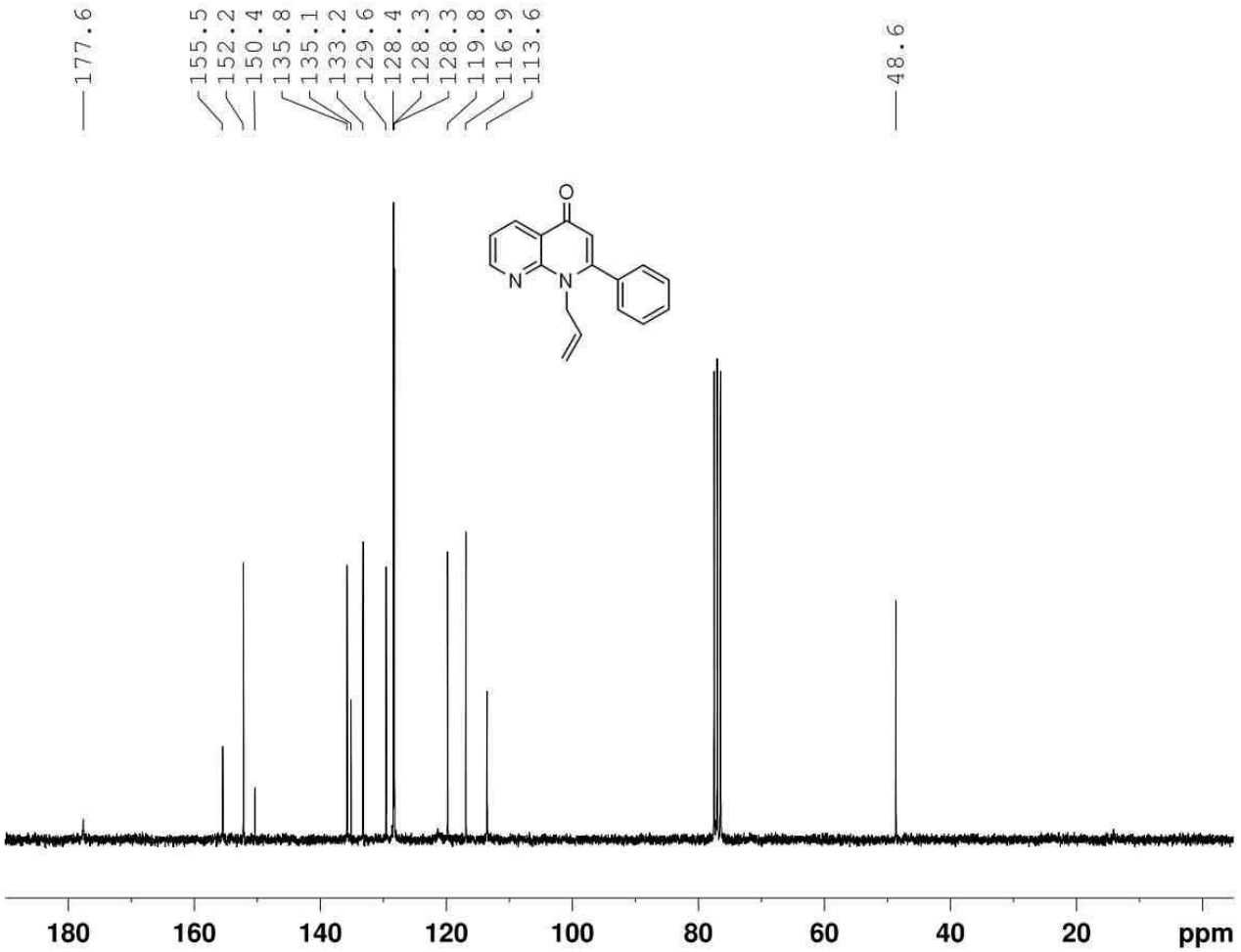
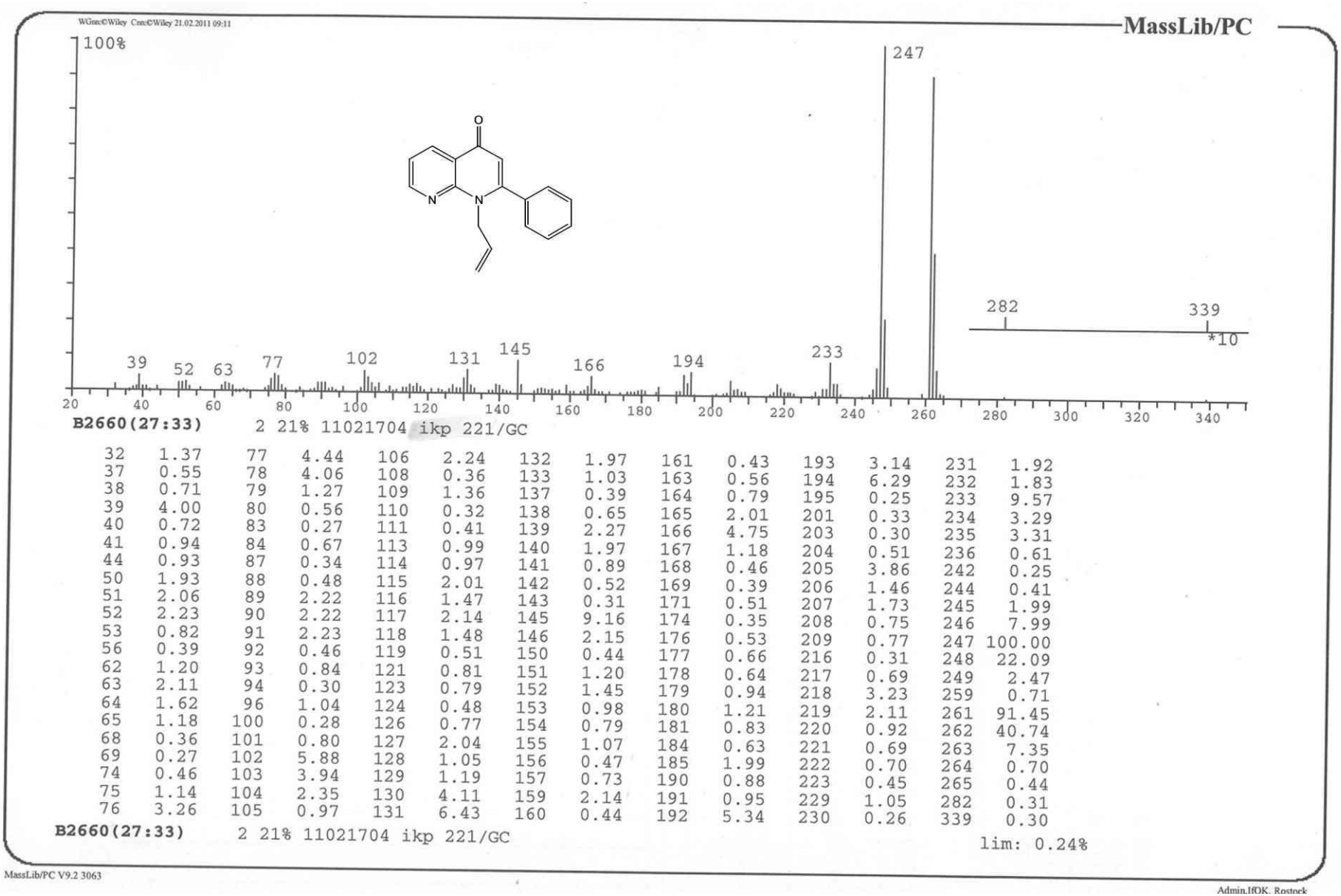


NAME	110210.201
EXPNO	10
PROCNO	1
Date_	20110210
Time	12.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952420 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



B2660(27:33) 2 21% 11021704 ikp 221/GC

32	1.37	77	4.44	106	2.24	132	1.97	161	0.43	193	3.14	231	1.92
37	0.55	78	4.06	108	0.36	133	1.03	163	0.56	194	6.29	232	1.83
38	0.71	79	1.27	109	1.36	137	0.39	164	0.79	195	0.25	233	9.57
39	4.00	80	0.56	110	0.32	138	0.65	165	2.01	201	0.33	234	3.29
40	0.72	83	0.27	111	0.41	139	2.27	166	4.75	203	0.30	235	3.31
41	0.94	84	0.67	113	0.99	140	1.97	167	1.18	204	0.51	236	0.61
44	0.93	87	0.34	114	0.97	141	0.89	168	0.46	205	3.86	242	0.25
50	1.93	88	0.48	115	2.01	142	0.52	169	0.39	206	1.46	244	0.41
51	2.06	89	2.22	116	1.47	143	0.31	171	0.51	207	1.73	245	1.99
52	2.23	90	2.22	117	2.14	145	9.16	174	0.35	208	0.75	246	7.99
53	0.82	91	2.23	118	1.48	146	2.15	176	0.53	209	0.77	247	100.00
56	0.39	92	0.46	119	0.51	150	0.44	177	0.66	216	0.31	248	22.09
62	1.20	93	0.84	121	0.81	151	1.20	178	0.64	217	0.69	249	2.47
63	2.11	94	0.30	123	0.79	152	1.45	179	0.94	218	3.23	259	0.71
64	1.62	96	1.04	124	0.48	153	0.98	180	1.21	219	2.11	261	91.45
65	1.18	100	0.28	126	0.77	154	0.79	181	0.83	220	0.92	262	40.74
68	0.36	101	0.80	127	2.04	155	1.07	184	0.63	221	0.69	263	7.35
69	0.27	102	5.88	128	1.05	156	0.47	185	1.99	222	0.70	264	0.70
74	0.46	103	3.94	129	1.19	157	0.73	190	0.88	223	0.45	265	0.44
75	1.14	104	2.35	130	4.11	159	2.14	191	0.95	229	1.05	282	0.31
76	3.26	105	0.97	131	6.43	160	0.44	192	5.34	230	0.26	339	0.30

B2660(27:33) 2 21% 11021704 ikp 221/GC lim: 0.24%

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Admin.IfOK. Rostock

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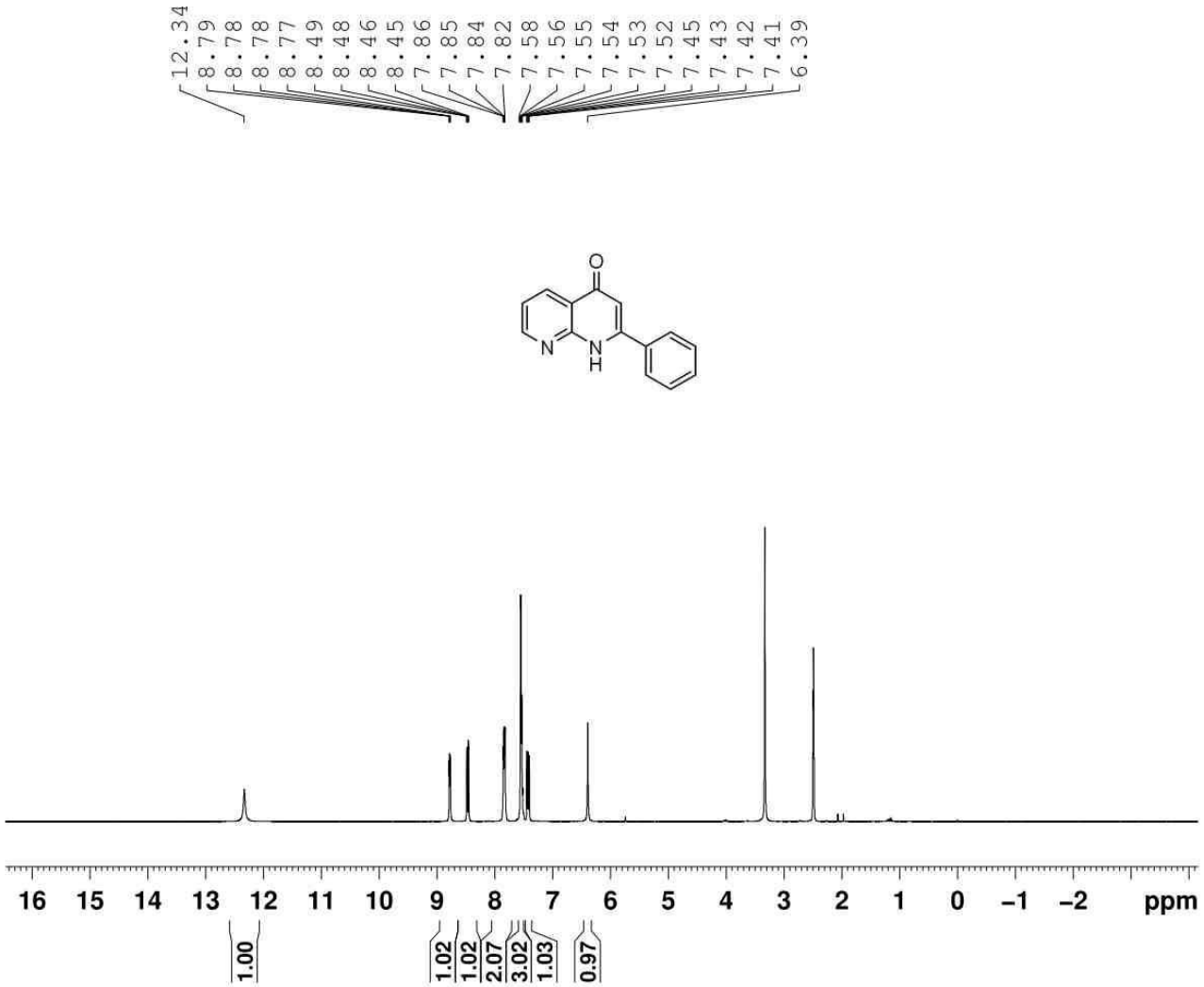

NAME	101207.u341
EXPNO	10
PROCNO	1
Date_	20101207
Time	14.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	128
DW	80.800 use
DE	10.00 use
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300082 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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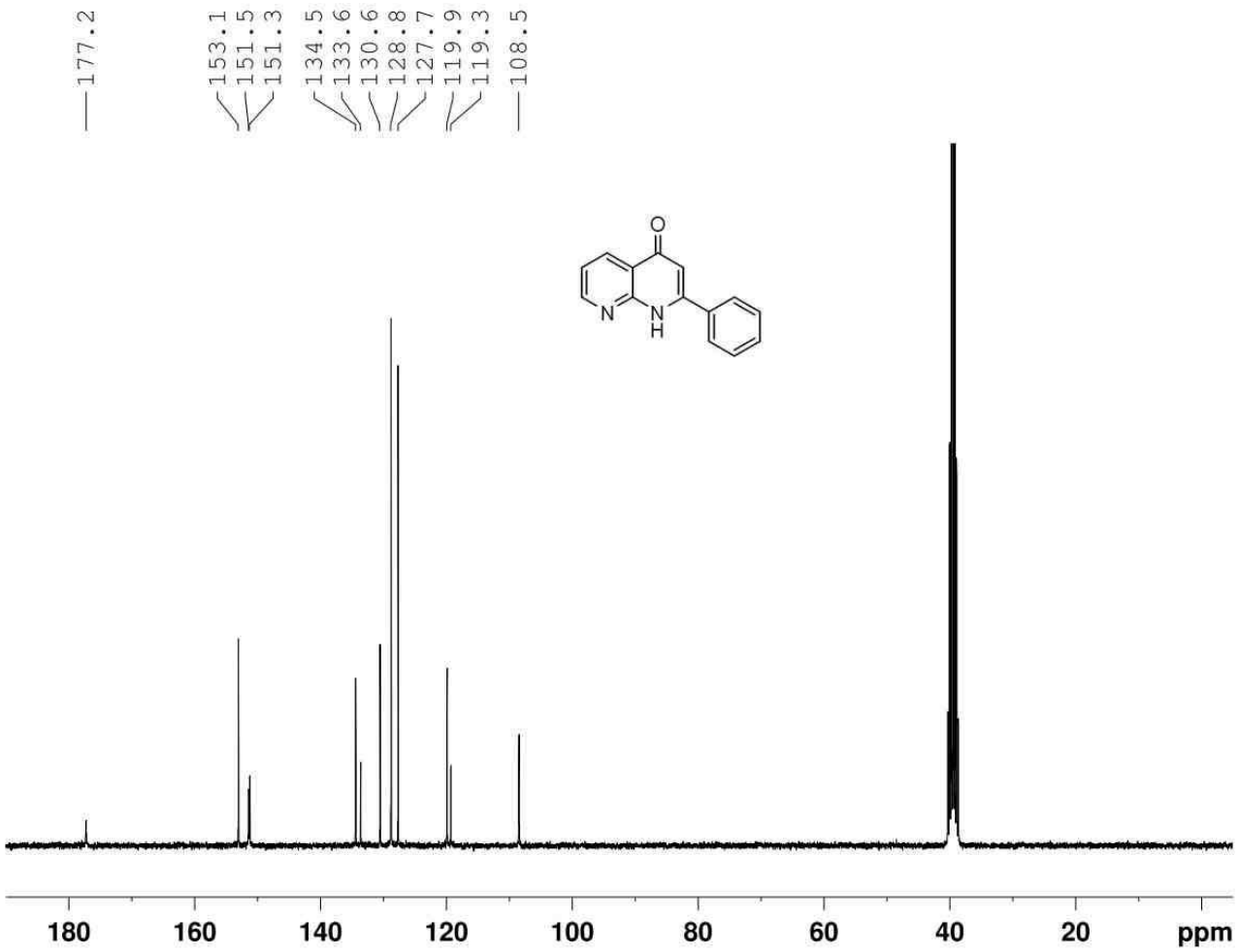

BRUKER

NAME	101209.u326
EXPNO	11
PROCNO	1
Date_	20101209
Time	23.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	296.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677867 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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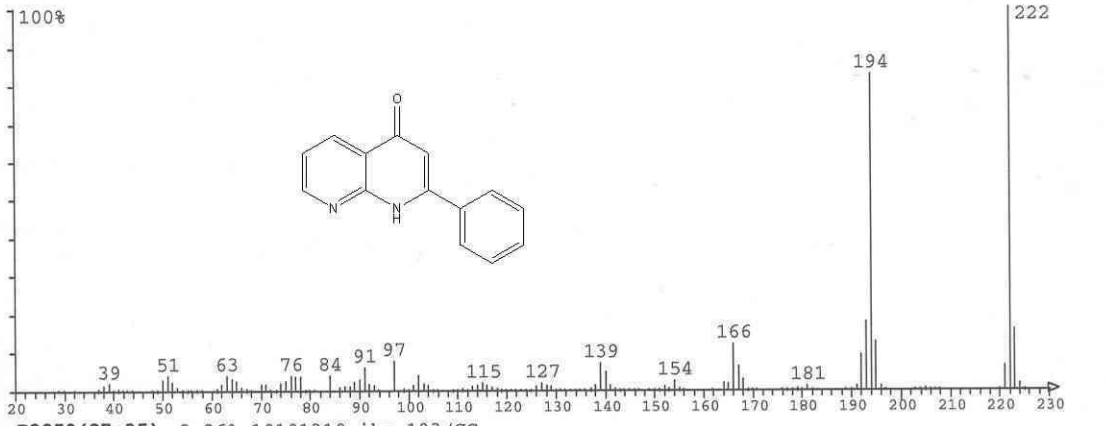

B2850(27:35) 2 26% 10101310 ikp 193/GC

29	0.03	58	0.06	84	3.71	111	0.41	132	0.01	154	2.11	191	0.93
30	0.02	61	0.46	86	0.55	112	0.22	133	0.02	155	0.51	192	8.97
32	0.09	62	1.38	87	0.73	113	0.68	134	0.05	156	0.13	193	17.60
37	0.38	63	3.74	88	0.81	114	1.19	135	0.03	162	0.03	194	82.56
38	1.05	64	2.97	89	2.10	115	1.65	136	0.02	164	1.80	195	12.52
39	1.78	65	2.16	90	2.56	116	1.17	137	0.47	165	1.45	196	0.77
40	0.29	66	0.56	91	5.59	117	0.55	138	0.96	166	11.83	197	0.06
41	0.44	67	0.43	92	1.44	118	0.46	139	6.86	167	6.14	203	0.04
42	0.04	68	0.31	93	1.06	119	0.24	140	4.57	168	2.51	204	0.04
43	0.05	70	1.27	94	0.06	120	0.06	141	0.97	169	0.20	205	0.40
44	0.04	71	1.26	97	7.51	121	0.02	142	0.45	170	0.04	206	0.12
48	0.02	72	0.05	99	0.40	122	0.06	143	0.35	171	0.03	207	0.06
49	0.20	73	0.13	100	0.31	123	0.07	144	0.03	176	0.07	208	0.02
50	2.40	74	1.66	101	1.08	124	0.03	145	0.05	177	0.08	220	0.37
51	3.78	75	2.33	102	3.62	125	0.21	146	0.02	178	0.10	221	5.90
52	1.92	76	3.74	103	1.31	126	0.84	147	0.04	179	0.44	222	100.00
53	0.58	77	3.51	104	0.96	127	1.75	149	0.06	180	0.13	223	15.70
54	0.09	78	3.36	105	0.18	128	0.96	150	0.23	181	0.73	224	1.36
55	0.08	79	0.34	106	0.03	129	0.93	151	0.34	182	0.08	225	0.12
56	0.07	80	0.02	109	0.08	130	0.22	152	0.67	189	0.03		
57	0.10	81	0.06	110	0.15	131	0.06	153	0.51	190	0.13		

B2850(27:35) 2 26% 10101310 ikp 193/GC

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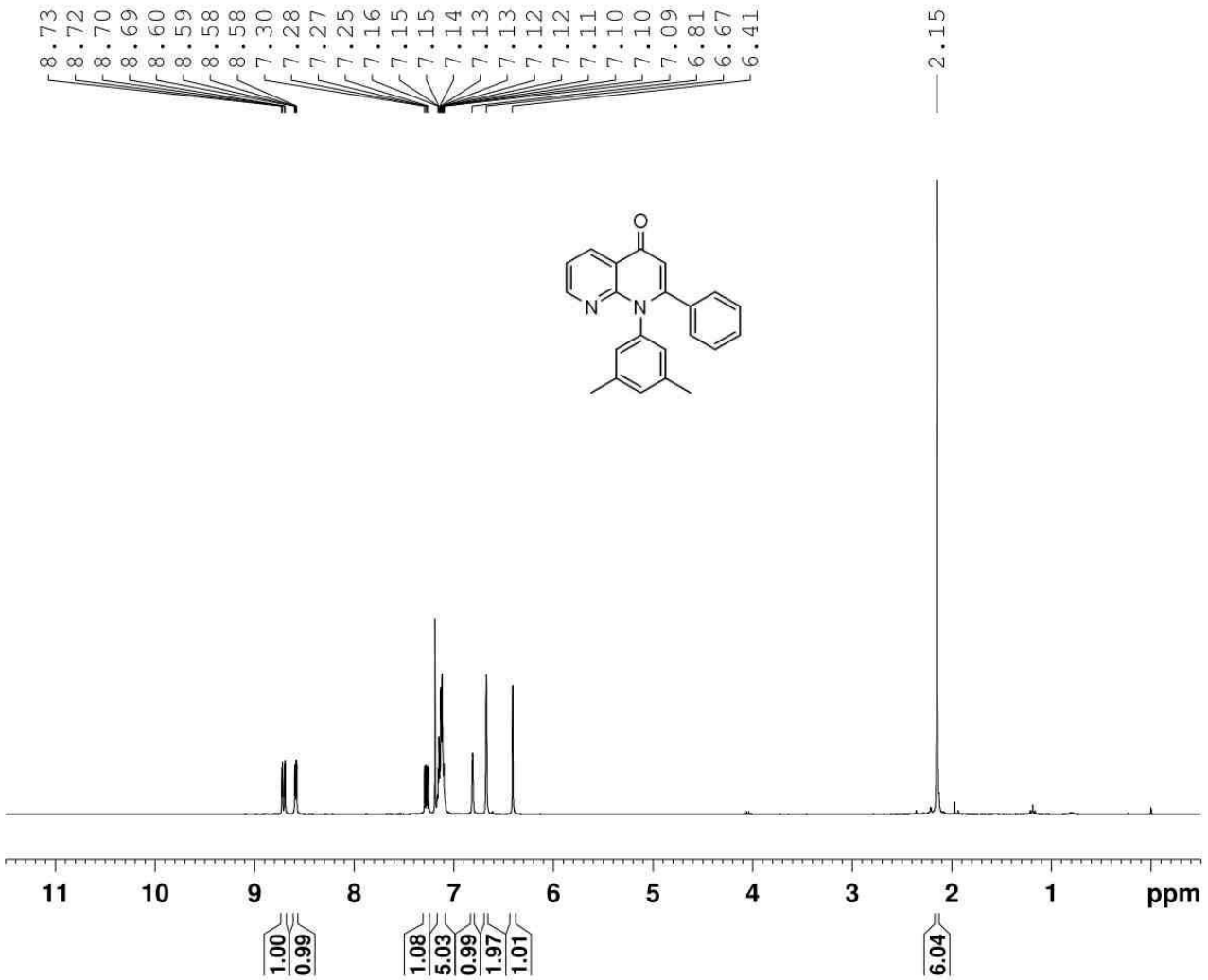

NAME	101207.u344	
EXPNO	10	
PROCNO	1	
Date_	20101207	
Time	15.14	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	256	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300293	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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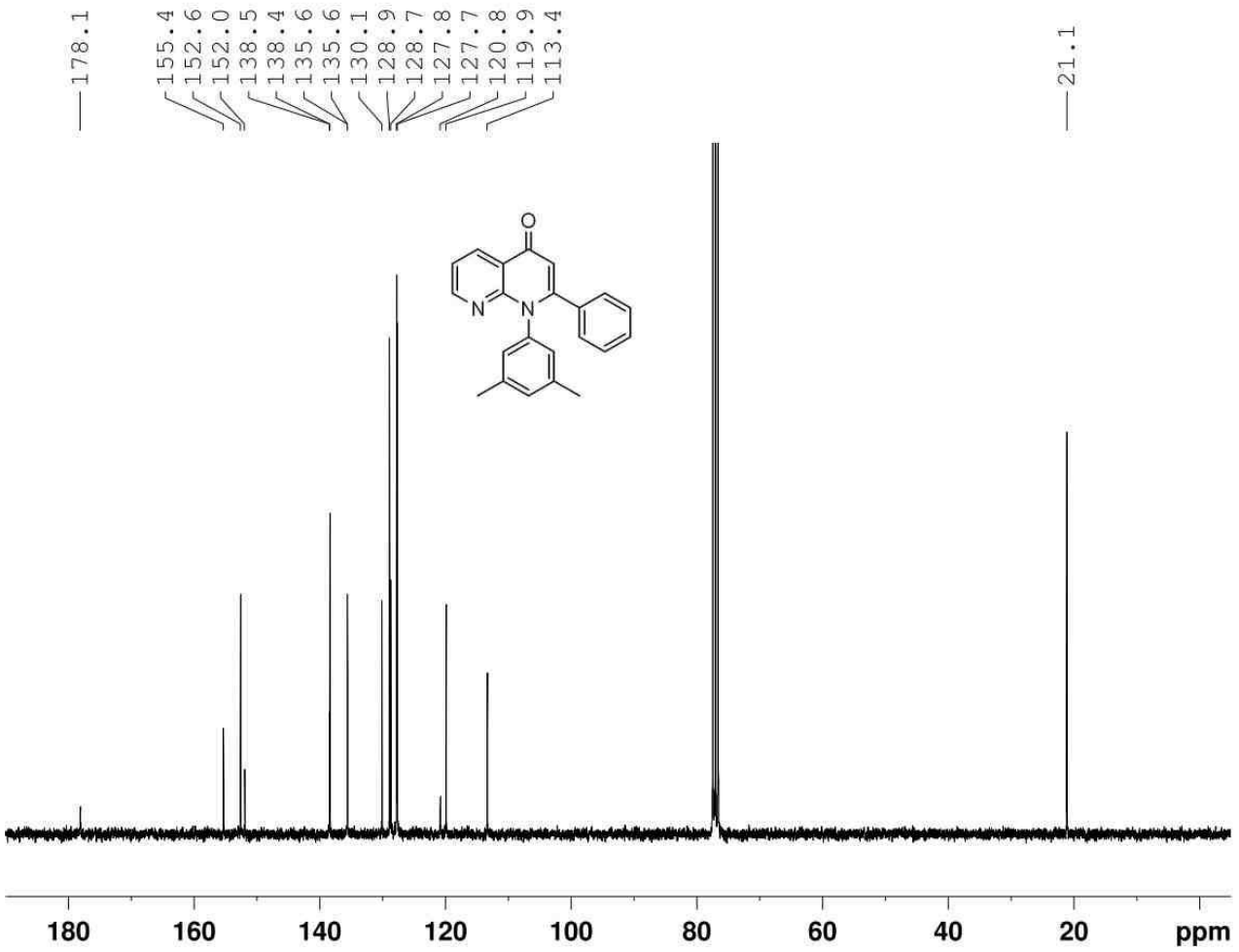

BRUKER

NAME	101209.u325
EXPNO	11
PROCNO	1
Date_	20101209
Time	22.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	296.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

WGms:©Wiley Cms:©Wiley 28.10.2010 14:05

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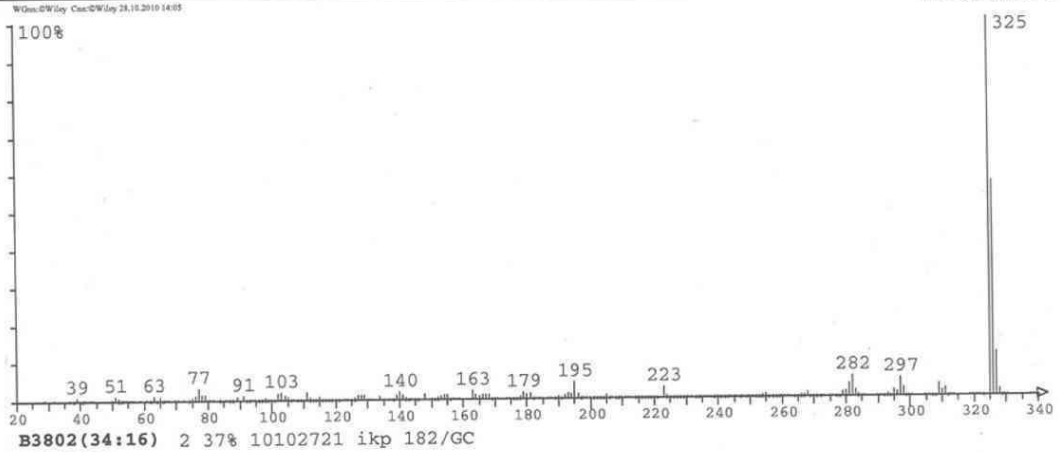
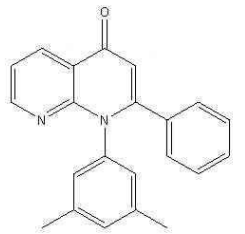
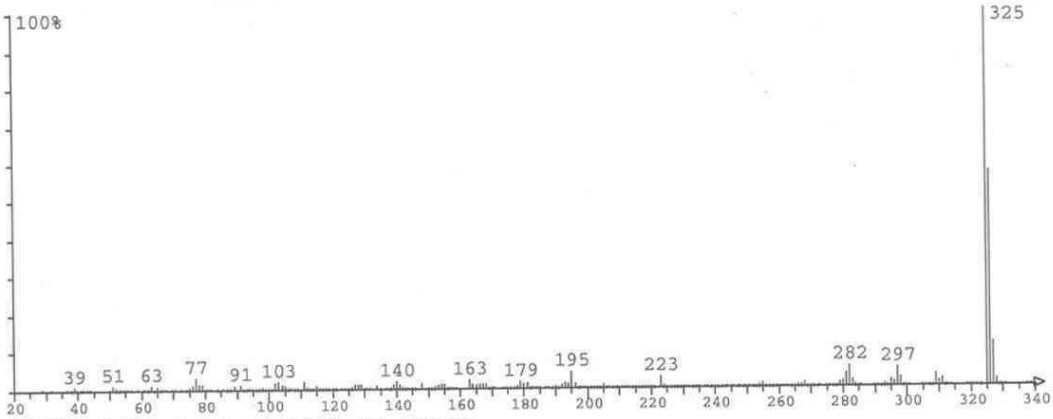


B3802(34:16) 2 37% 10102721 ikp 182/GC

10102721

34:16





B3802(34:16) 2 37% 10102721 ikp 182/GC

39	0.53	98	0.50	138	0.15	168	0.92	204	0.22	253	0.22	294	0.36
50	0.31	100	0.14	139	0.81	169	0.22	205	0.53	254	0.49	295	1.25
51	0.78	101	0.32	140	1.66	176	0.16	206	0.23	255	0.59	296	0.68
52	0.42	102	1.53	141	0.90	177	0.23	209	0.23	256	0.26	297	4.54
53	0.34	103	1.78	142	0.47	178	0.51	215	0.19	257	0.21	298	2.02
63	0.74	104	0.71	143	0.30	179	1.27	216	0.14	258	0.16	299	0.26
64	0.34	105	0.52	145	0.15	180	0.91	218	0.28	266	0.44	307	0.21
65	0.53	111	1.58	146	0.19	181	1.20	219	0.19	267	0.50	308	0.35
74	0.18	112	0.49	148	1.11	182	0.19	220	0.13	268	0.89	309	2.75
75	0.44	113	0.20	150	0.18	189	0.30	221	0.27	269	0.34	310	1.15
76	0.80	114	0.29	151	0.34	190	0.39	223	2.50	270	0.19	311	1.57
77	2.83	115	0.61	152	0.50	191	0.35	224	0.44	271	0.22	312	0.30
78	1.03	116	0.35	153	0.60	192	0.62	228	0.14	279	0.82	323	0.36
79	1.07	117	0.20	154	0.78	193	0.96	229	0.20	280	1.18	325	100.00
84	0.15	121	0.27	155	0.87	194	0.83	233	0.27	281	3.16	326	56.71
87	0.17	126	0.41	156	0.26	195	3.99	240	0.25	282	5.02	327	11.18
88	0.15	127	0.81	163	1.83	196	0.68	241	0.23	283	1.52	328	1.32
89	0.54	128	0.76	164	0.72	197	0.14	242	0.35	284	0.37		
91	0.91	129	0.84	165	0.64	201	0.17	243	0.15	285	0.18		
93	0.13	130	0.20	166	0.70	202	0.22	249	0.18	292	0.19		
97	0.17	134	0.66	167	0.67	203	0.26	252	0.20	293	0.38		

B3802(34:16) 2 37% 10102721 ikp 182/GC

lim: 0.13%

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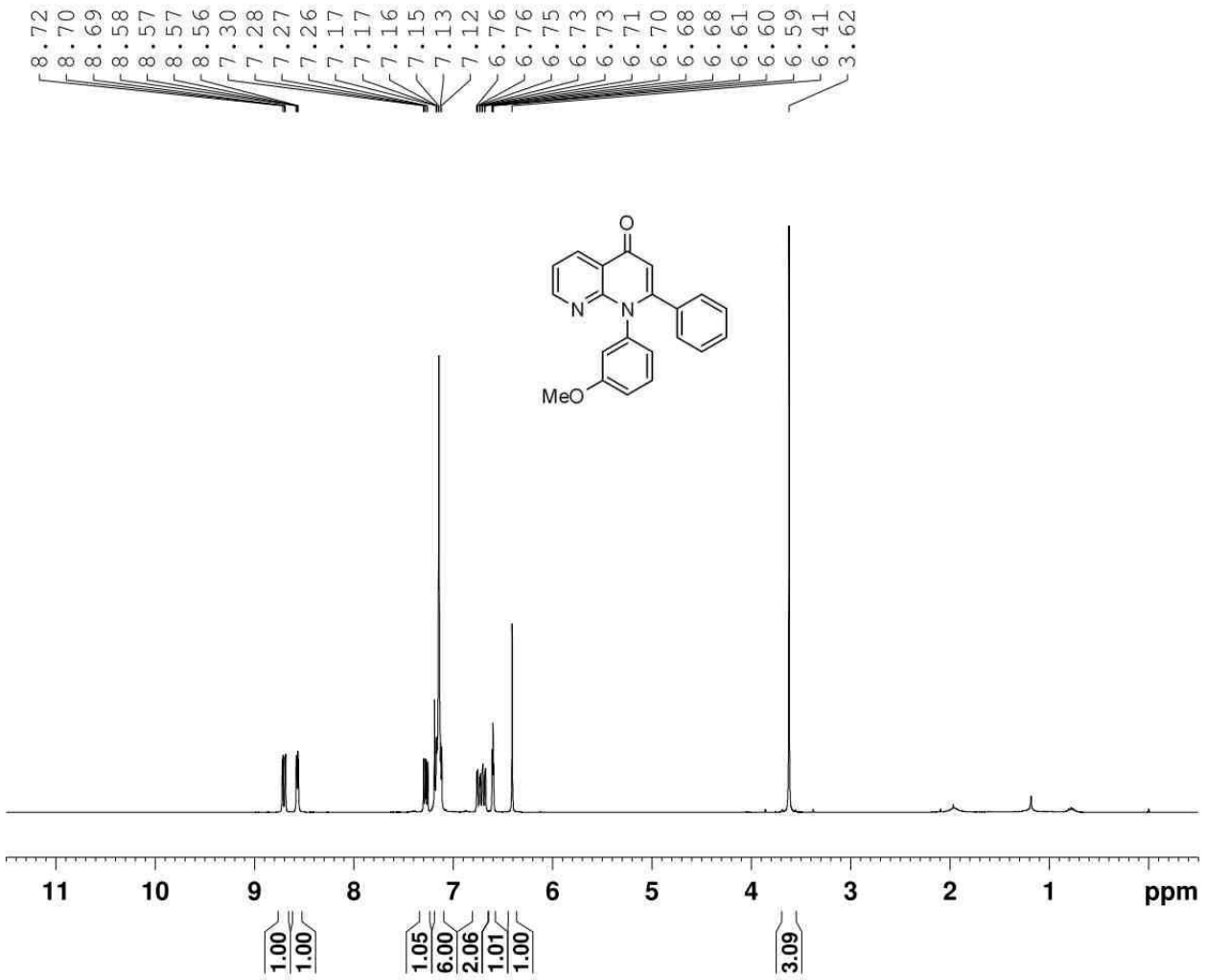

NAME	101007.u317	
EXPNO	10	
PROCNO	1	
Date_	20101007	
Time	13.31	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300295	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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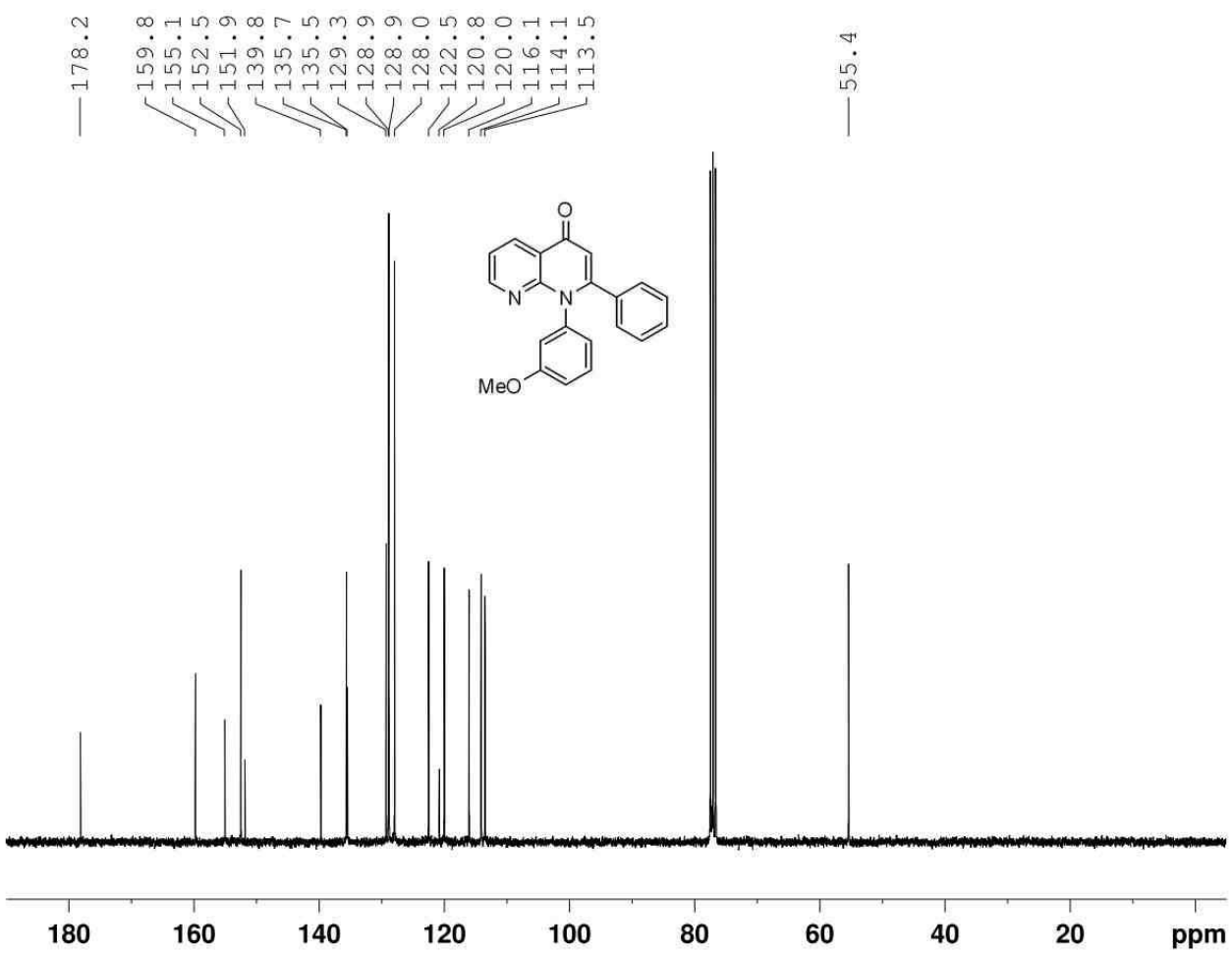

BRUKER

NAME	101007.u317
EXPNO	11
PROCNO	1
Date_	20101007
Time	22.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1200
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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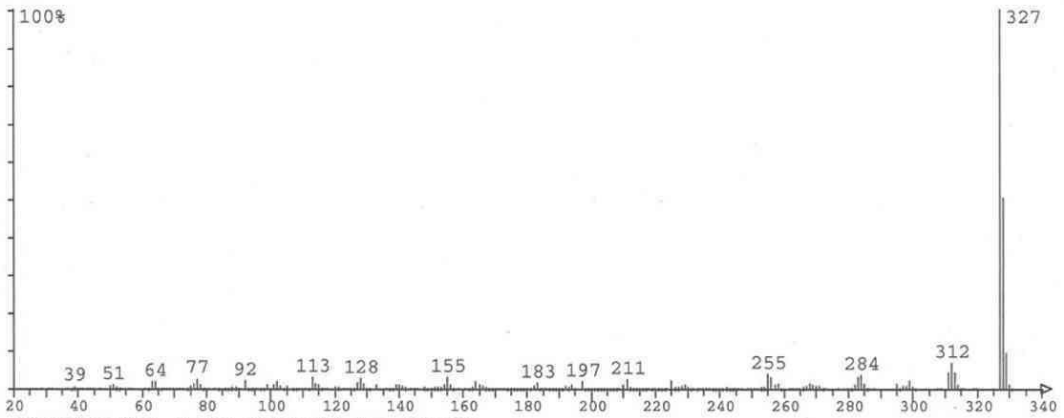
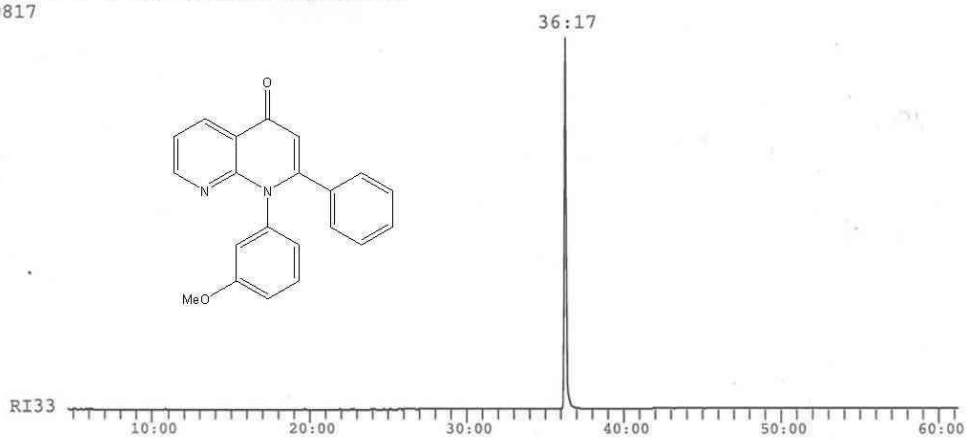
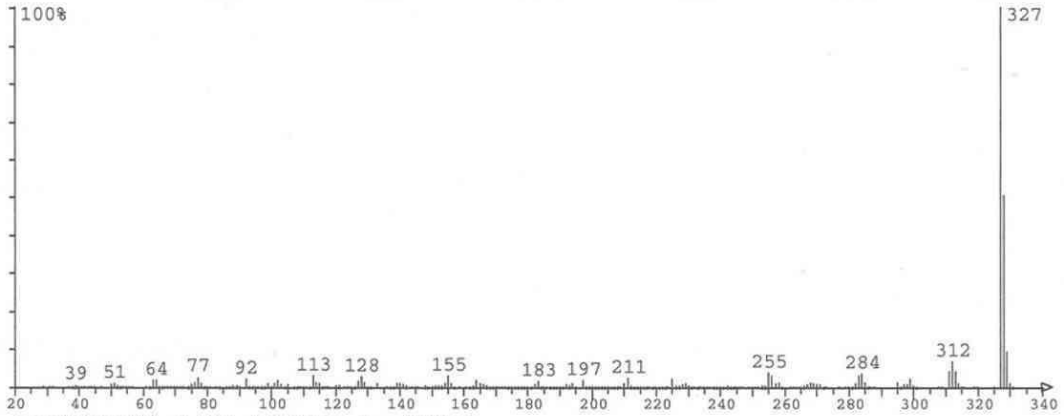


B3929(36:17) 2 36% 10100817 ikp 198/GC

10100817





B3929(36:17) 2 36% 10100817 ikp 198/GC

38	0.16	98	0.13	130	0.27	166	0.59	197	1.72	230	0.39	283	2.71
39	0.48	99	0.73	133	0.86	167	0.52	198	0.27	233	0.14	284	3.35
50	0.53	100	0.25	138	0.18	168	0.26	201	0.24	240	0.30	285	1.09
51	0.84	101	0.94	139	0.71	169	0.31	202	0.20	241	0.26	286	0.24
52	0.39	102	1.77	140	0.90	170	0.25	203	0.28	242	0.41	295	1.24
53	0.15	103	0.66	141	0.53	175	0.19	204	0.16	243	0.33	296	0.35
62	0.22	104	0.14	142	0.48	176	0.28	205	0.19	253	0.51	297	0.57
63	1.53	105	0.53	145	0.14	177	0.31	206	0.15	254	0.39	298	0.55
64	1.64	107	0.25	148	0.48	178	0.24	208	0.24	255	3.73	299	2.01
65	0.35	108	0.15	149	0.29	179	0.35	210	0.84	256	2.87	300	0.49
74	0.29	112	0.18	150	0.28	180	0.20	211	2.35	257	0.77	311	4.02
75	0.65	113	2.80	151	0.37	182	0.54	212	0.39	258	1.07	312	6.47
76	1.21	114	0.98	152	0.47	183	1.38	214	0.17	259	0.25	313	4.09
77	2.38	115	0.78	153	0.41	184	0.16	216	0.20	266	0.45	314	0.81
78	0.75	116	0.22	154	0.91	189	0.14	219	0.13	267	0.62	325	0.16
87	0.24	120	0.49	155	2.82	190	0.21	223	0.16	268	1.04	327	100.00
88	0.39	121	0.37	156	0.76	191	0.18	225	1.87	269	0.82	328	50.33
89	0.51	126	0.32	157	0.22	192	0.57	226	0.44	270	0.54	329	9.25
90	0.35	127	1.39	163	0.46	193	0.40	227	0.49	271	0.60	330	0.94
92	1.86	128	2.56	164	1.71	194	0.69	228	0.61	272	0.15		
93	0.22	129	1.23	165	0.67	195	0.32	229	0.87	282	0.78		

B3929(36:17) 2 36% 10100817 ikp 198/GC lim: 0.13%

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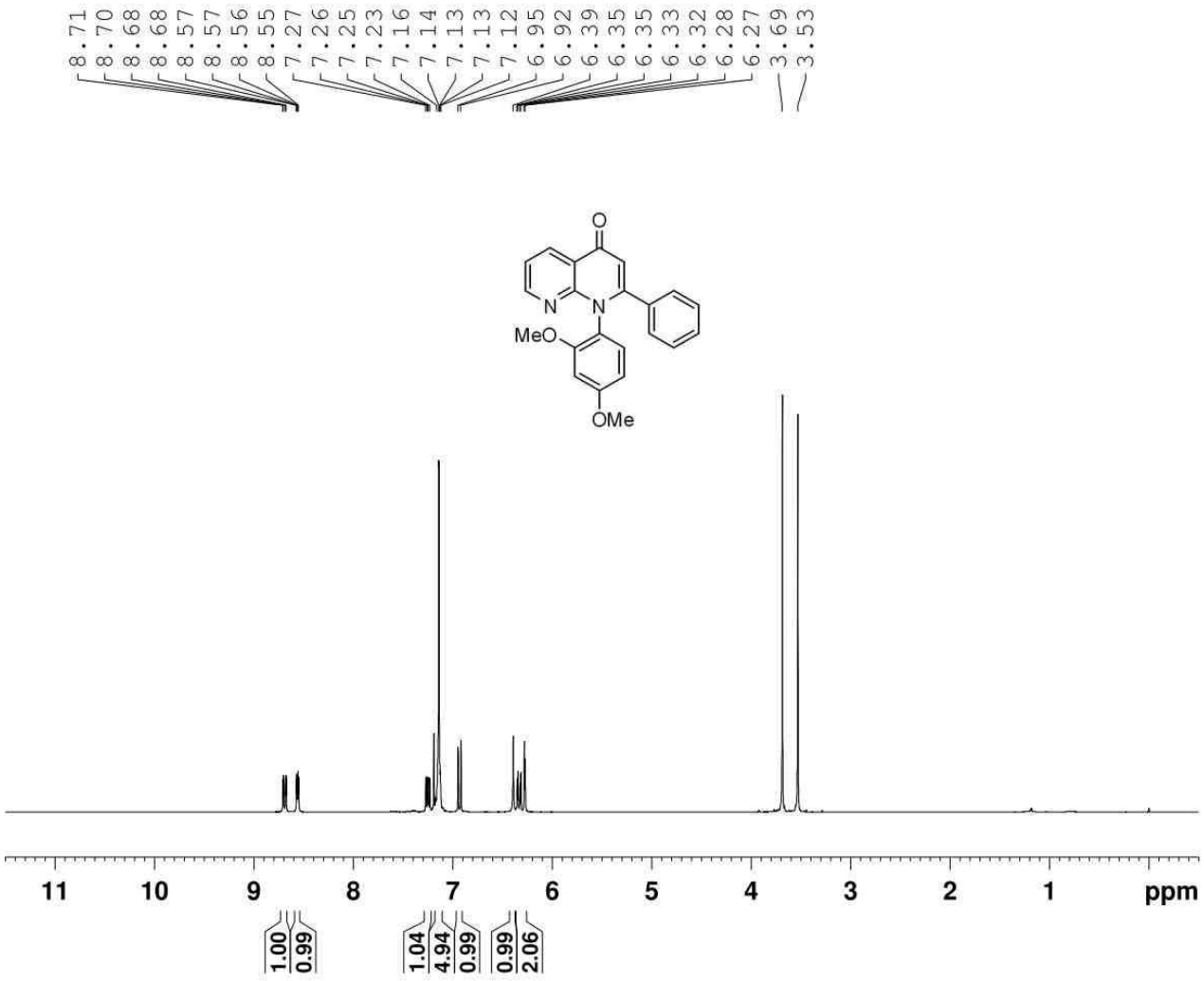

NAME	101207.u309	
EXPNO	10	
PROCNO	1	
Date_	20101207	
Time	9.31	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDC13	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	128	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300287	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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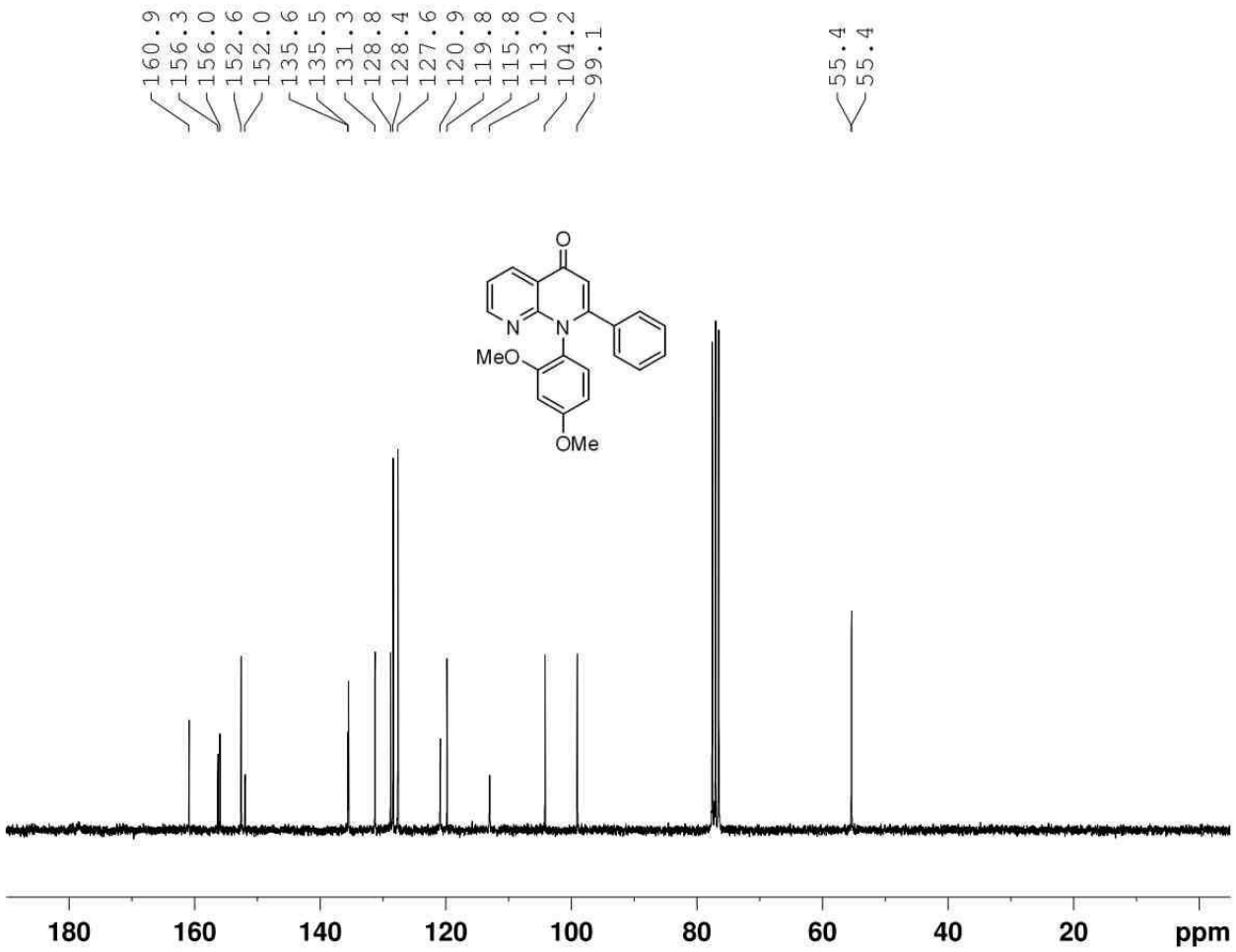

NAME	101208.210
EXPNO	10
PROCNO	1
Date_	20101209
Time	2.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	297.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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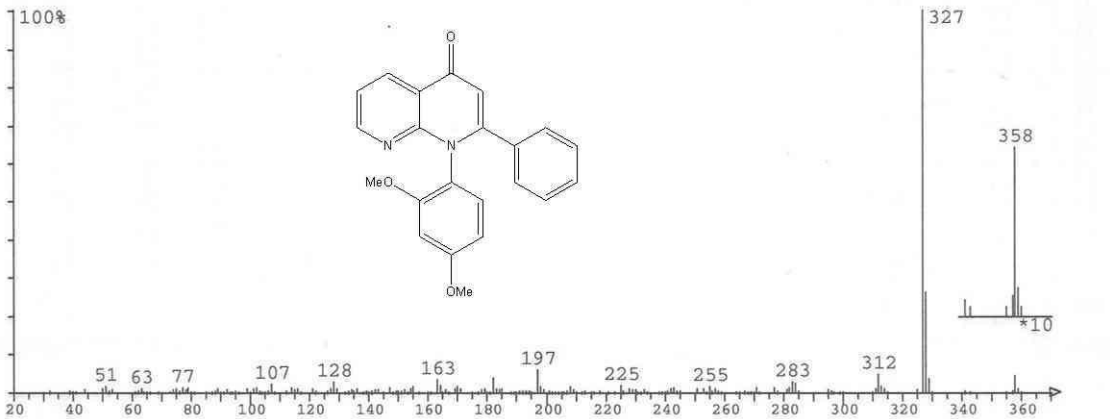

B4205(39:01) 2 40% 10113012 ikp 225/GC

32	0.44	90	0.29	129	0.91	164	1.62	198	1.41	243	1.06	285	0.45
39	0.40	91	0.34	133	0.45	165	0.28	199	0.57	244	0.47	295	0.59
40	0.31	92	0.58	134	0.65	166	0.54	201	0.51	245	0.47	296	0.48
41	0.26	93	0.27	135	0.40	167	0.31	202	0.30	251	0.79	311	0.90
44	0.58	95	0.39	136	0.86	169	0.72	204	0.30	253	0.76	312	4.58
50	0.67	96	0.30	139	0.37	170	1.40	205	0.31	254	0.27	313	1.46
51	1.24	99	0.89	141	0.40	171	0.69	207	0.39	255	1.29	314	0.69
52	0.44	101	0.73	142	0.58	178	0.59	208	1.40	256	0.47	315	0.27
53	0.53	102	1.09	143	0.57	179	0.72	209	0.60	257	0.81	325	0.62
62	0.46	103	0.42	145	0.29	180	0.36	213	0.38	258	0.48	327	100.00
63	0.75	106	0.52	147	1.05	182	3.68	215	0.32	259	0.29	328	26.05
69	0.31	107	2.05	148	0.34	183	0.84	218	0.46	267	0.38	329	3.33
74	0.54	112	0.39	149	0.49	184	0.66	225	1.58	270	0.29	330	0.34
75	0.78	114	1.02	150	0.39	185	0.75	226	0.45	271	1.21	341	0.41
76	0.50	115	0.63	151	0.46	190	0.33	228	0.84	272	0.35	357	0.51
77	1.20	116	0.71	152	0.54	191	0.44	229	0.65	277	1.07	358	4.40
78	0.59	121	0.85	153	0.32	192	0.43	230	0.58	278	0.41	359	0.73
79	1.08	122	0.49	154	0.94	193	0.40	233	0.66	281	0.62		
80	0.26	126	0.50	155	1.30	194	0.39	240	0.29	282	1.03		
88	0.46	127	0.94	161	0.28	195	0.28	241	0.49	283	2.44		
89	0.92	128	2.63	163	3.20	197	5.73	242	0.81	284	2.33		

B4205(39:01) 2 40% 10113012 ikp 225/GC lim: 0.26%

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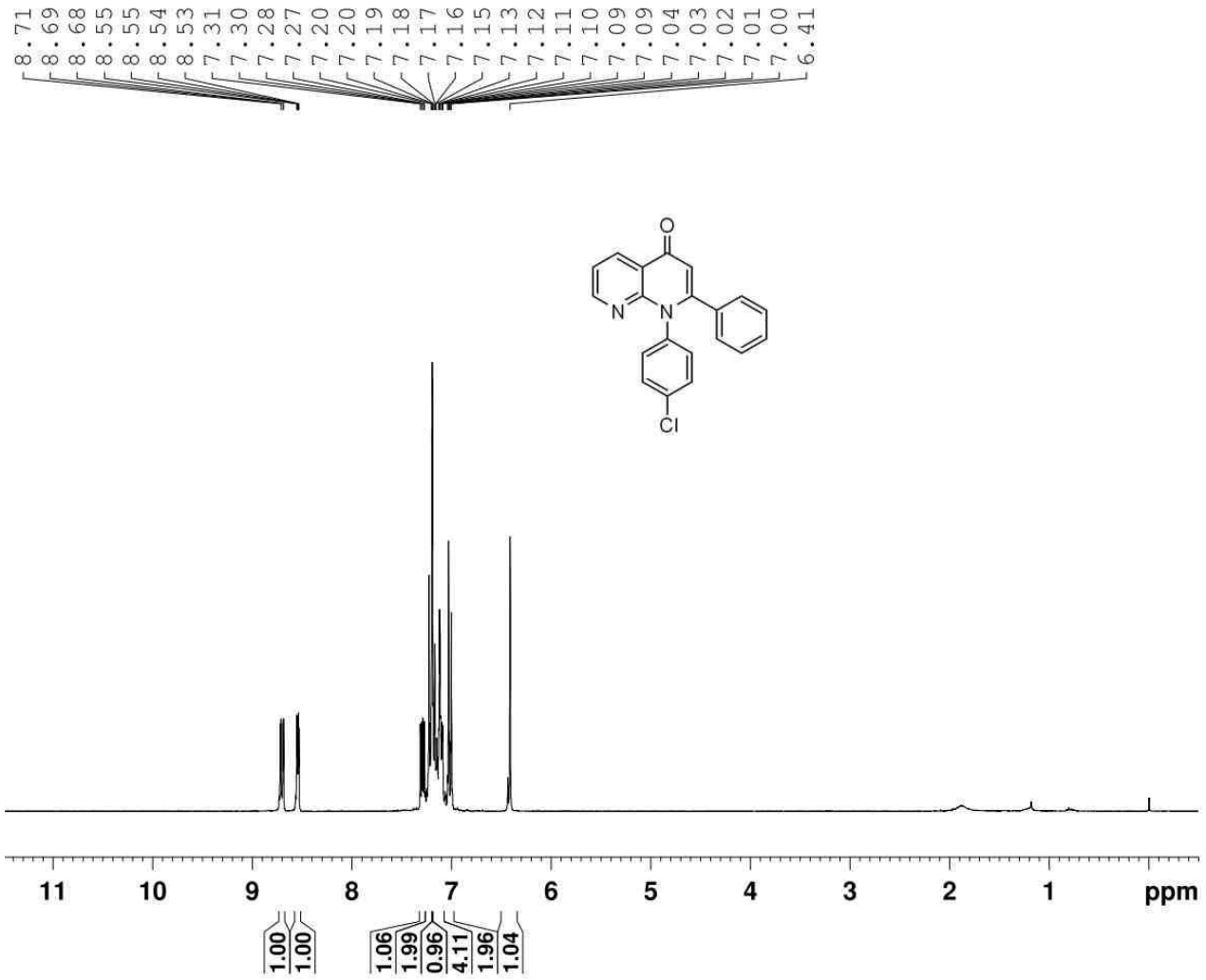

NAME	100719.u325	
EXPNO	10	
PROCNO	1	
Date_	20100719	
Time	13.38	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDC13	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	256	
DW	80.800	use
DE	10.00	use
TE	299.3	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300292	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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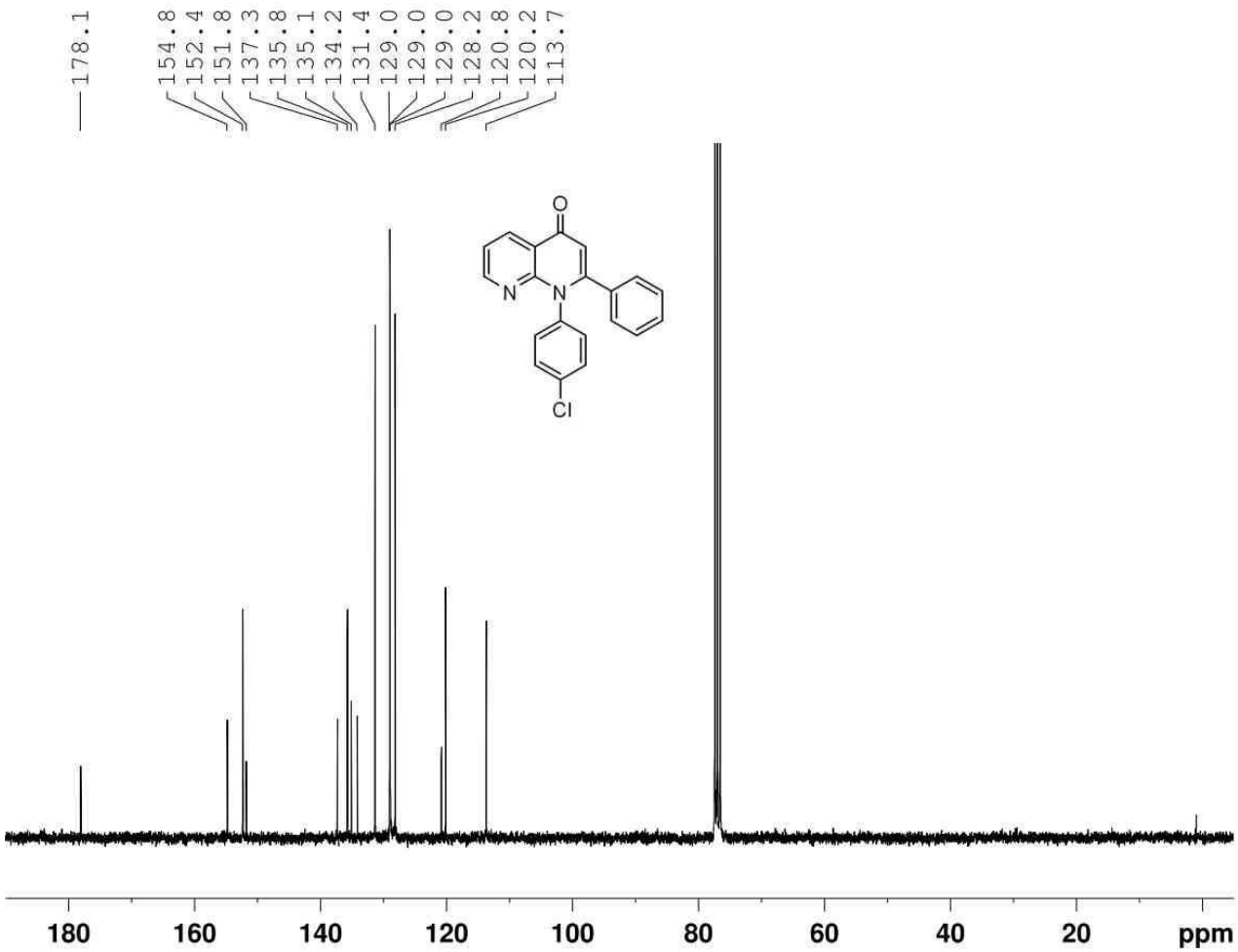

NAME	101022.u323
EXPNO	10
PROCNO	1
Date_	20101024
Time	21.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1600
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677524 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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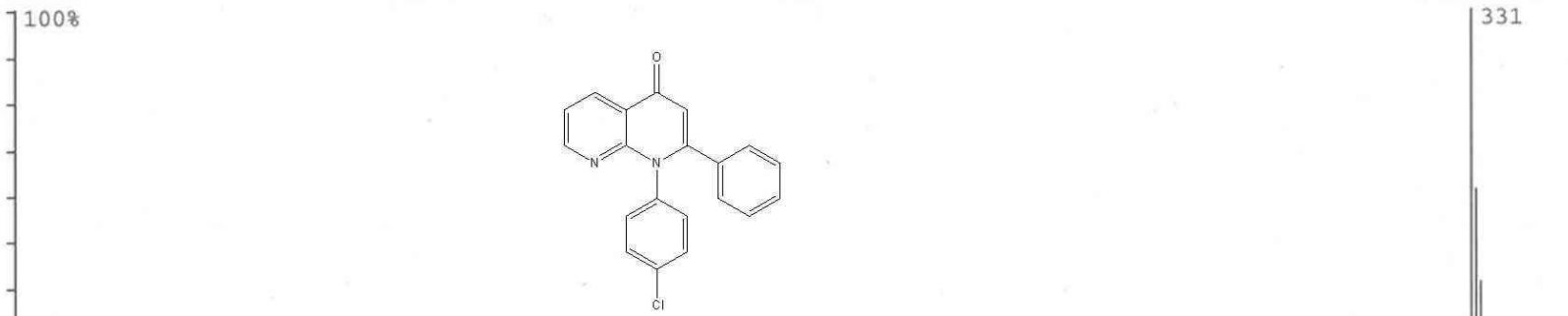

B3702(35:57) 2 24% 10072218 ikp 175/GC

38	0.25	90	0.64	115	1.13	150	0.64	195	0.86	238	0.46	296	3.26
39	1.04	92	0.29	116	0.50	151	1.06	199	0.38	239	0.67	297	3.49
50	1.38	93	0.64	119	1.06	152	1.37	201	5.28	240	1.61	298	1.24
51	1.87	94	0.37	120	0.98	153	0.62	202	2.06	241	1.27	299	0.38
52	0.56	95	0.57	121	0.89	163	0.56	203	1.72	242	1.24	301	0.34
62	0.72	97	0.64	123	0.34	164	1.22	204	0.76	243	0.34	302	1.52
63	1.58	98	0.40	125	0.31	165	0.92	205	0.24	252	0.29	303	5.78
64	0.68	99	0.48	126	0.46	166	3.74	212	0.34	253	0.26	304	1.82
65	0.54	100	0.49	127	0.66	167	3.71	213	0.39	258	0.32	305	2.39
73	0.24	101	0.85	128	0.27	168	0.27	214	0.68	265	0.80	306	0.69
74	1.15	102	3.17	129	2.09	174	0.88	215	0.69	266	3.80	329	0.42
75	4.78	103	1.04	130	0.48	175	0.67	216	0.31	267	4.59	331	100.00
76	2.73	104	0.28	134	4.81	176	1.25	217	0.28	268	15.06	332	61.14
77	1.31	106	0.50	137	0.39	177	0.97	221	0.24	269	3.57	333	41.27
78	0.64	107	0.99	138	0.88	178	0.37	226	0.25	270	0.71	334	20.34
83	0.34	108	0.24	139	2.47	179	0.24	227	0.26	271	0.33	335	3.95
85	0.52	110	0.31	140	3.81	188	0.46	228	0.41	275	0.40	336	0.59
86	0.44	111	3.37	141	0.79	190	0.58	229	5.59	276	0.29	341	0.23
87	0.84	112	0.83	147	0.37	191	0.64	230	0.79	278	0.30		
88	0.51	113	2.19	148	1.76	192	0.84	231	1.95	289	0.23		
89	1.24	114	1.00	149	1.42	193	0.35	232	0.33	295	9.26		

B3702(35:57) 2 24% 10072218 ikp 175/GC lim: 0.23%

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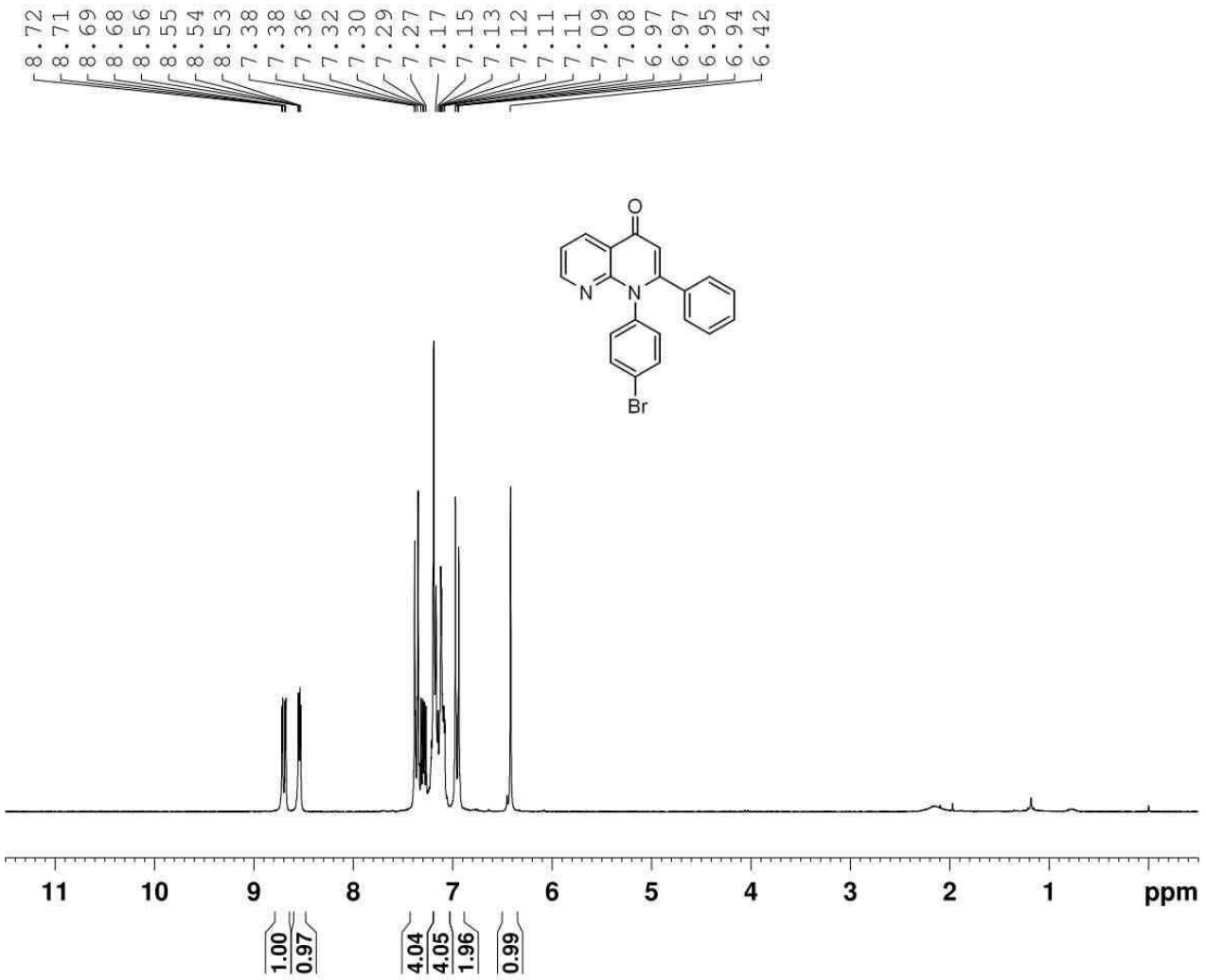

BRUKER

NAME	101021.202	
EXPNO	10	
PROCNO	1	
Date_	20101021	
Time	8.18	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	5165.289	Hz
FIDRES	0.078816	Hz
AQ	6.3439350	sec
RG	645	
DW	96.800	use
DE	10.00	use
TE	296.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	-2.50	dB
SFO1	250.1315447	MHz
SI	32768	
SF	250.1300176	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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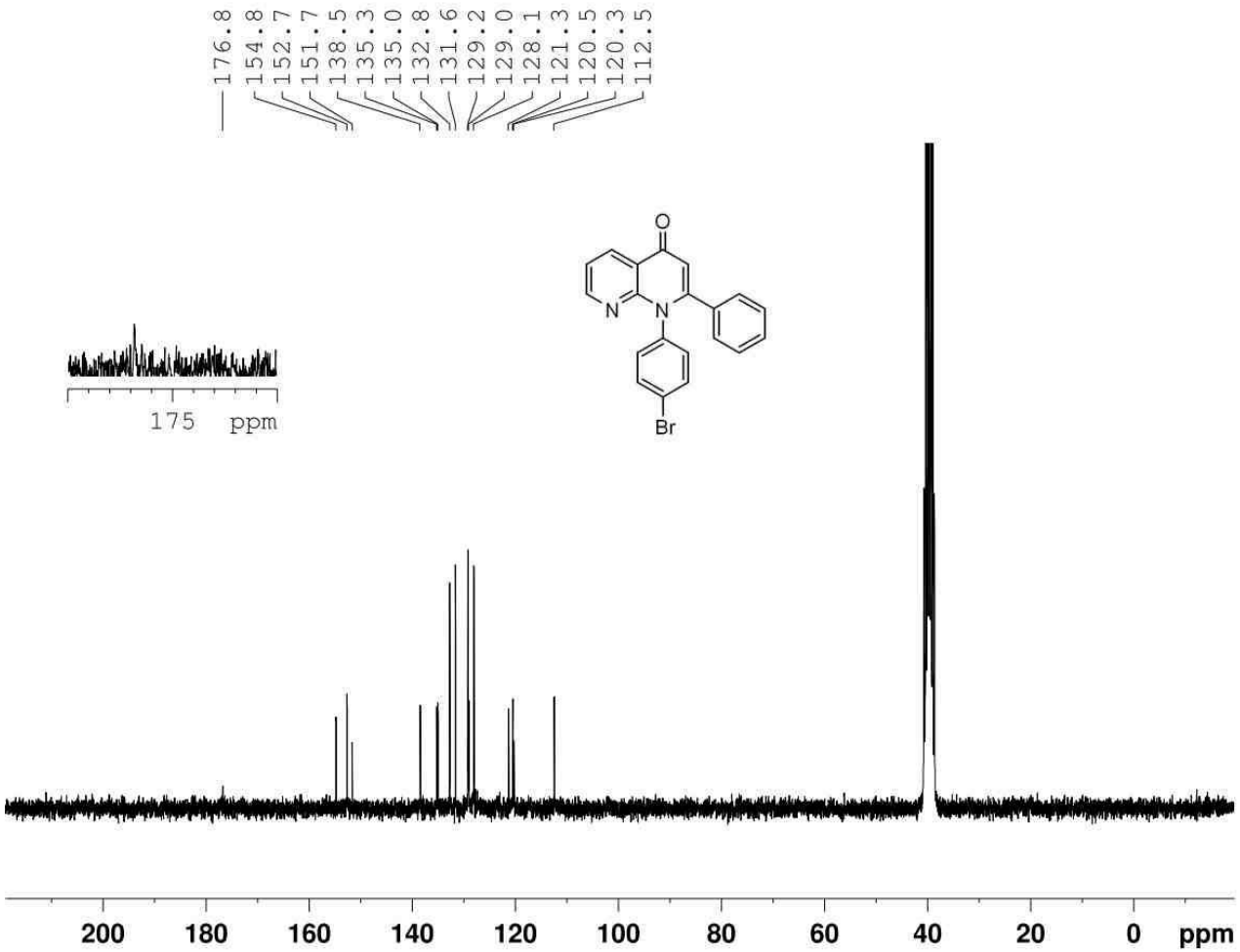

NAME	110211.230
EXPNO	10
PROCNO	1
Date_	20110213
Time	18.23
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1440
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952581 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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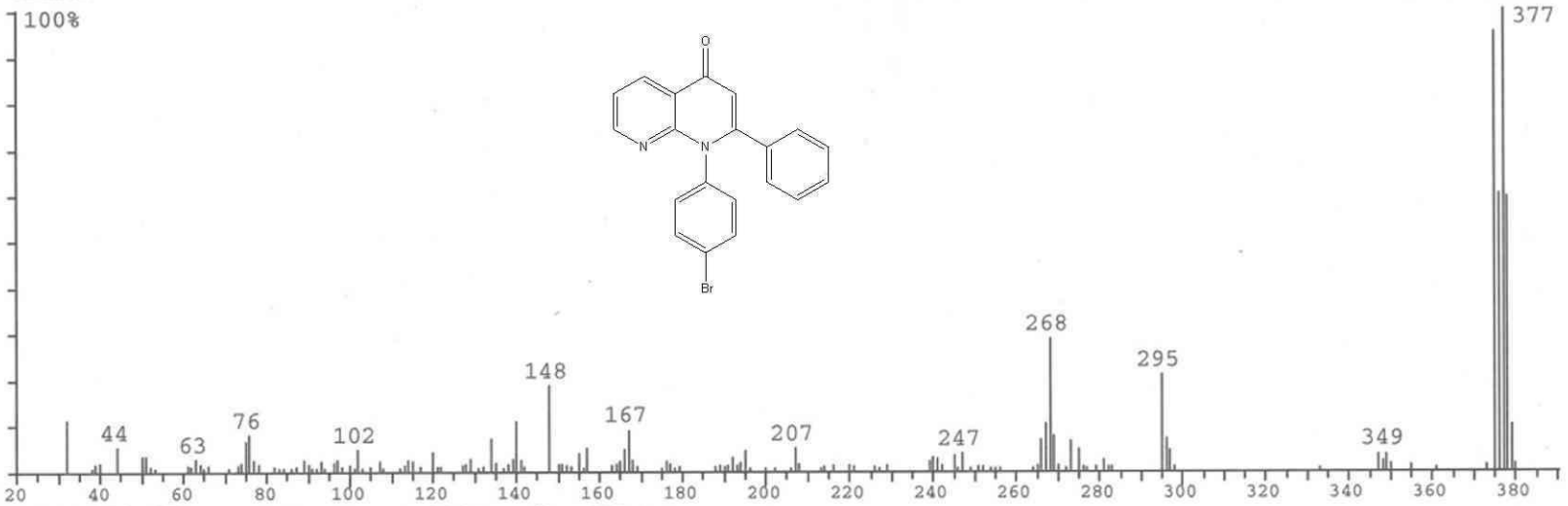

3983(38:13) 329 14% 10072207 * ikp 170/GC

32	10.88	78	1.40	114	2.21	152	1.13	192	2.93	246	0.52	283	0.94
38	0.56	82	0.87	115	1.84	153	0.74	193	1.11	247	3.71	295	20.93
39	1.25	84	0.53	117	0.72	155	3.61	194	1.62	249	0.62	296	6.79
40	1.68	87	0.92	120	3.91	156	0.60	195	4.24	251	0.79	297	4.26
44	5.03	89	2.16	121	0.74	157	4.75	196	0.55	252	0.90	298	0.70
50	3.01	90	1.29	122	0.93	163	1.15	202	0.60	255	0.55	333	0.52
51	3.08	91	0.64	127	1.14	164	1.35	207	4.83	256	0.56	347	3.32
52	0.84	92	0.58	128	1.36	165	2.08	208	1.50	264	0.64	348	2.01
53	0.53	93	1.84	129	2.51	166	4.44	213	0.59	265	1.12	349	3.55
61	1.00	96	1.56	132	0.78	167	8.78	214	0.70	266	6.74	350	1.42
62	0.94	97	2.35	134	6.87	168	2.14	216	1.22	267	10.06	355	1.03
63	2.53	98	0.90	135	1.76	169	0.78	220	0.98	268	28.57	373	1.04
64	1.51	100	1.15	137	0.49	175	0.52	221	0.78	269	7.59	375	95.17
65	0.61	101	0.64	138	1.31	176	1.99	226	0.76	270	1.02	376	60.13
66	1.01	102	4.64	139	2.43	177	1.27	227	0.53	272	0.63	377	100.00
71	0.52	103	0.66	140	10.79	178	0.65	229	1.12	273	6.37	378	59.28
73	0.95	105	0.69	141	2.36	179	0.76	239	1.85	275	4.67	379	9.89
74	1.65	107	2.08	142	0.70	188	0.72	240	2.76	276	0.93	380	1.27
75	6.29	108	0.60	148	18.60	189	0.97	241	2.69	279	0.69		
76	7.70	112	0.65	150	1.24	190	0.73	242	1.16	281	2.35		
77	2.24	113	1.22	151	1.53	191	1.23	245	2.99	282	0.82		

3983(38:13) 329 14% 10072207 * ikp 170/GC lim: 0.48%

MassLib/PC V9.2 3063

Admin,IfOK, Rostock

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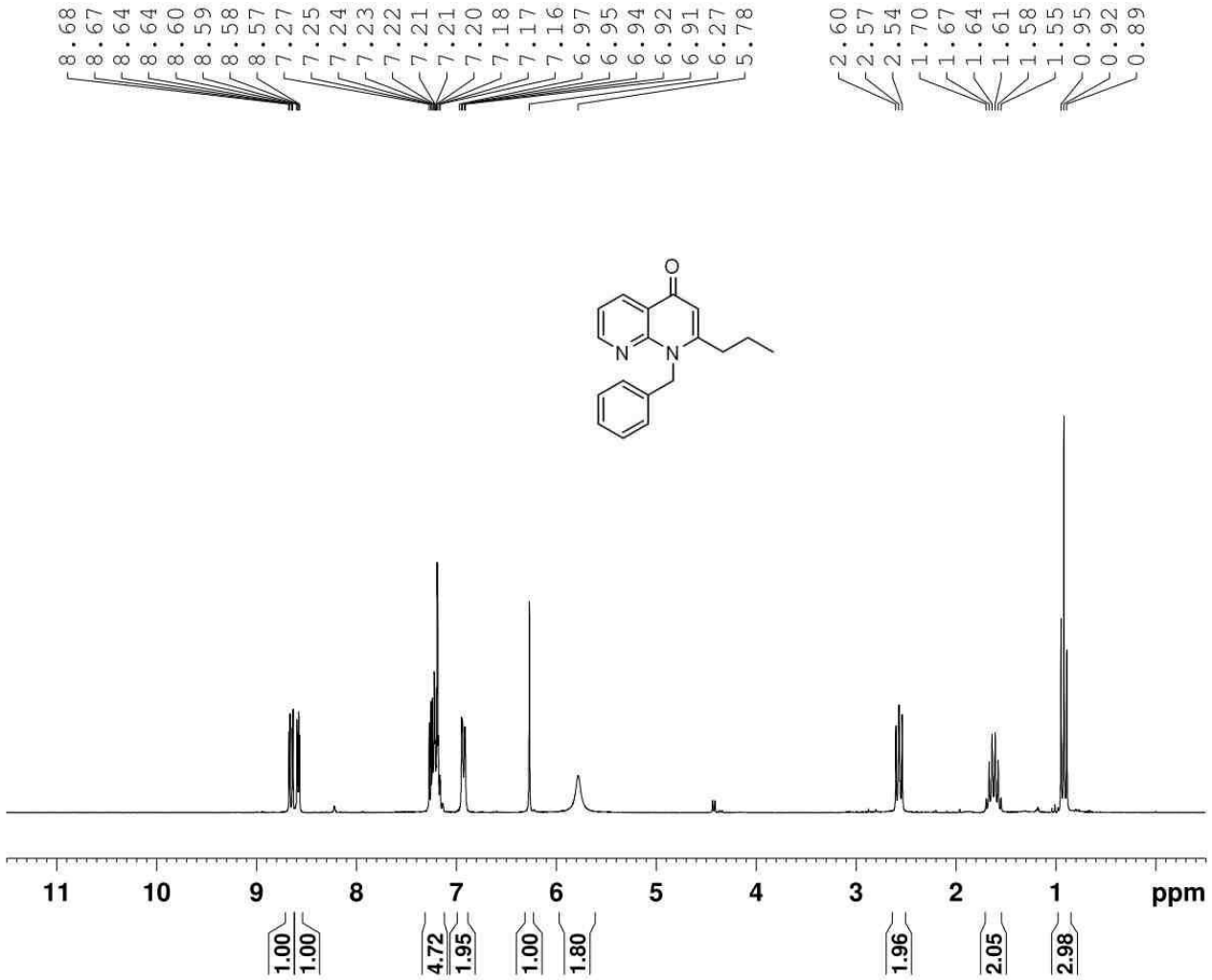

NAME	110113.210
EXPNO	10
PROCNO	1
Date_	20110113
Time	11.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	5165.289 Hz
FIDRES	0.078816 Hz
AQ	6.3439350 sec
RG	1620
DW	96.800 use
DE	10.00 use
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	-2.50 dB
SFO1	250.1315447 MHz
SI	32768
SF	250.1300173 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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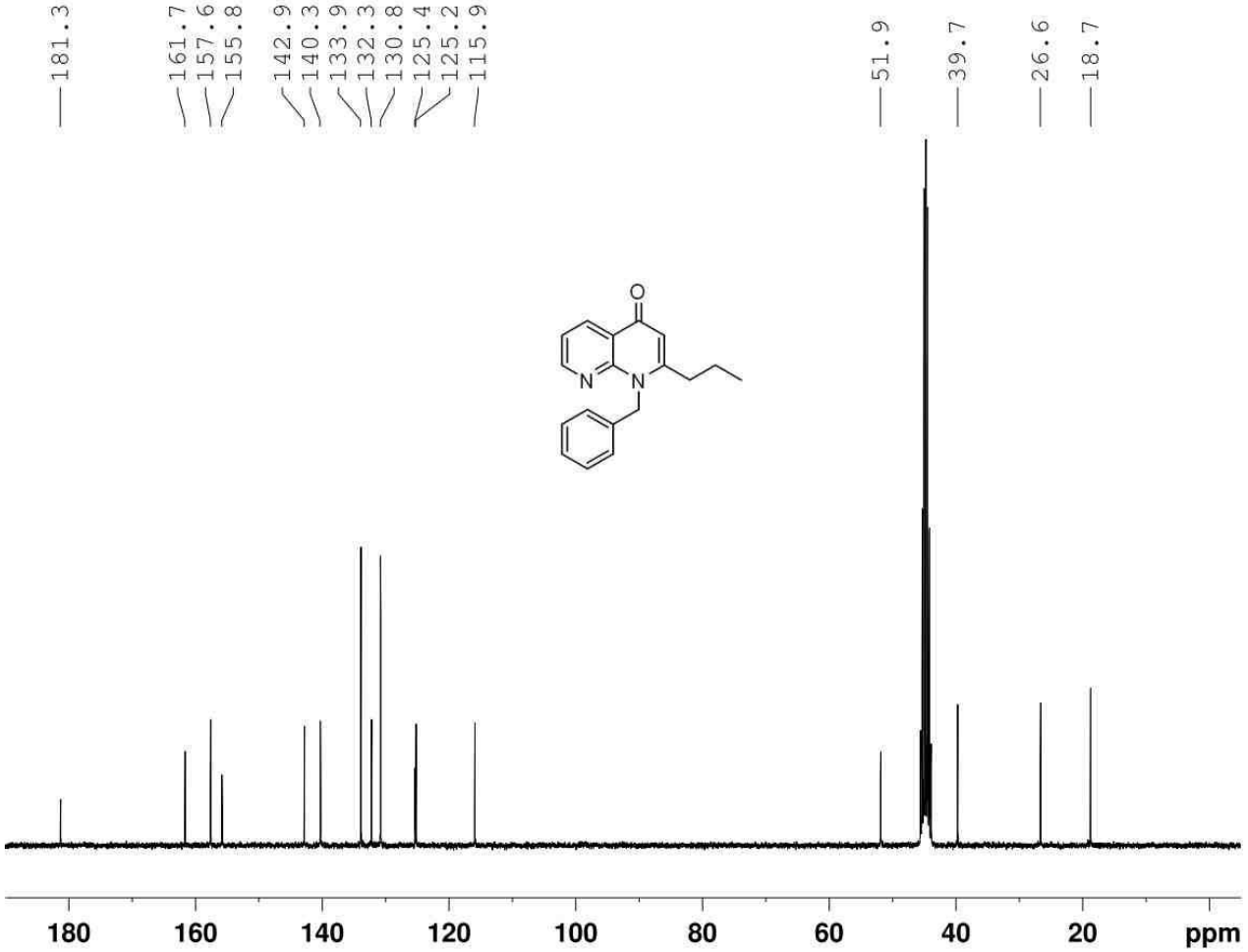

NAME	110211.u320
EXPNO	11
PROCNO	1
Date_	20110211
Time	19.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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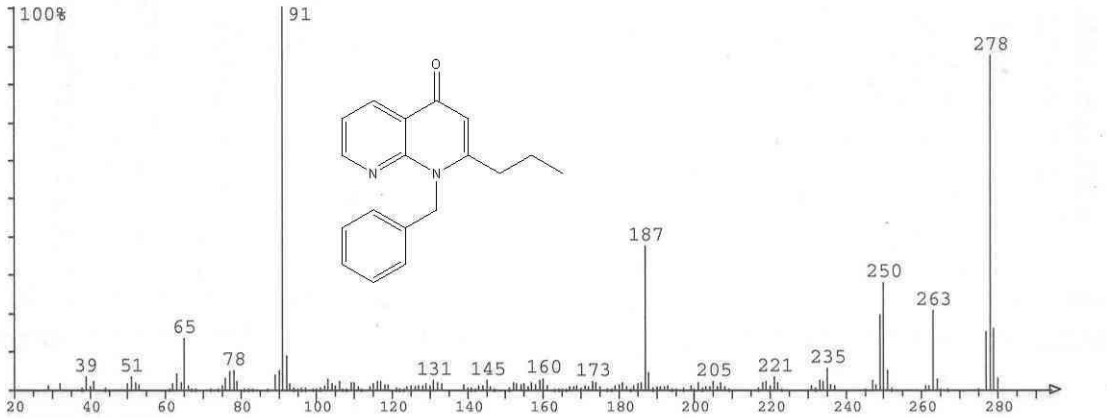

B3093(30:03) 2 19% 10113010 ikp 206/GC

29	0.72	77	4.61	110	1.66	140	0.45	168	0.63	193	0.85	234	1.96
32	1.40	78	4.94	111	0.53	141	0.47	169	0.74	197	0.37	235	5.48
38	0.41	79	1.99	114	0.54	142	0.33	170	0.37	199	0.93	236	1.17
39	3.20	87	0.27	115	1.36	143	0.83	171	0.76	201	1.71	237	0.75
40	0.53	89	3.73	116	1.88	144	0.84	172	0.65	202	0.47	247	2.17
41	1.97	90	4.92	117	1.92	145	2.29	173	2.04	203	0.63	248	1.23
44	0.51	91	100.00	118	0.97	146	0.54	174	1.69	204	0.57	249	19.27
50	1.44	92	8.76	119	1.12	147	0.36	175	0.61	205	1.95	250	27.81
51	3.02	93	1.38	121	0.41	151	0.38	179	0.91	206	0.63	251	4.80
52	1.61	94	0.37	122	0.27	152	1.58	180	0.98	207	1.66	252	0.50
53	0.96	95	0.29	124	0.60	153	1.37	181	1.75	208	0.54	261	0.68
62	1.40	96	0.39	125	0.81	154	1.24	182	0.64	217	0.47	262	0.68
63	4.12	97	0.44	126	0.64	155	1.31	184	0.83	218	1.68	263	20.46
64	1.70	99	0.27	127	0.87	156	0.53	185	1.28	219	1.99	264	2.52
65	13.15	101	0.41	128	0.75	157	1.69	186	1.71	220	0.79	277	15.02
66	0.95	102	0.92	129	1.40	158	1.18	187	37.38	221	3.05	278	87.28
67	0.31	103	2.44	130	0.81	159	2.30	188	4.36	222	1.68	279	15.77
72	0.32	104	1.27	131	2.18	160	2.67	189	0.43	223	0.29	280	2.69
74	0.27	105	0.89	132	1.55	161	0.70	190	0.55	231	0.68		
75	0.79	106	2.10	133	1.41	166	0.33	191	0.55	232	0.39		
76	2.90	109	1.61	139	1.24	167	0.64	192	0.57	233	2.25		

B3093(30:03) 2 19% 10113010 ikp 206/GC lim: 0.26%

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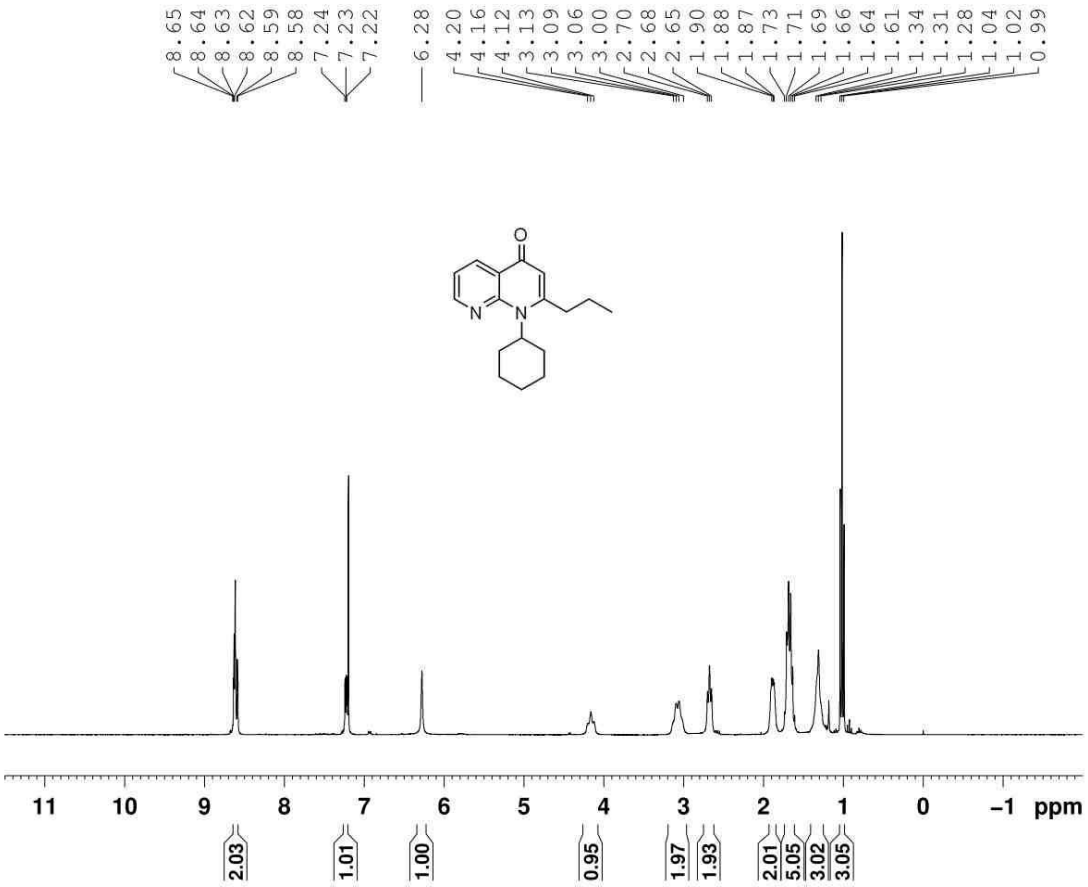

BRUKER

NAME	110210.u332
EXPNO	10
PROCNO	1
Date_	20110210
Time	13.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	128
DW	80.800 use
DE	10.00 use
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300262 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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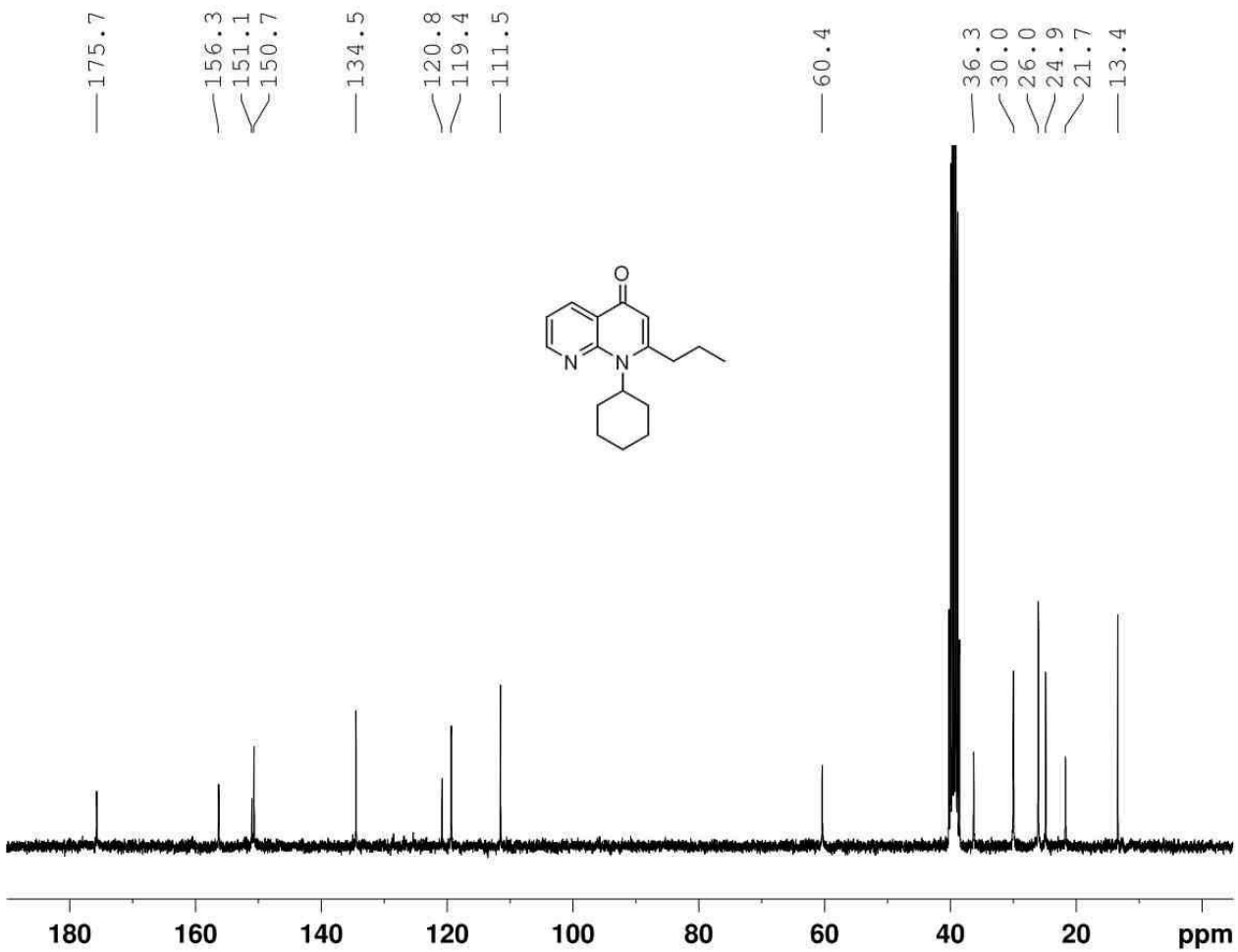

BRUKER

NAME	110211.u321
EXPNO	11
PROCNO	1
Date_	20110211
Time	21.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4681542 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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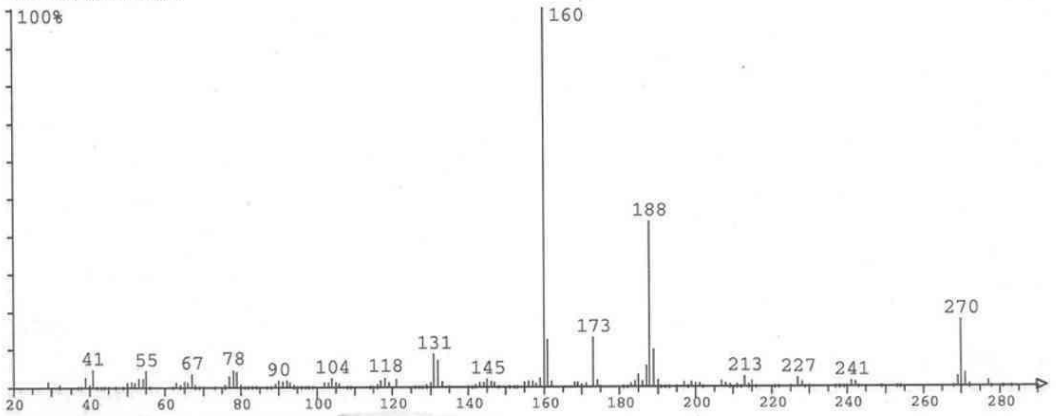
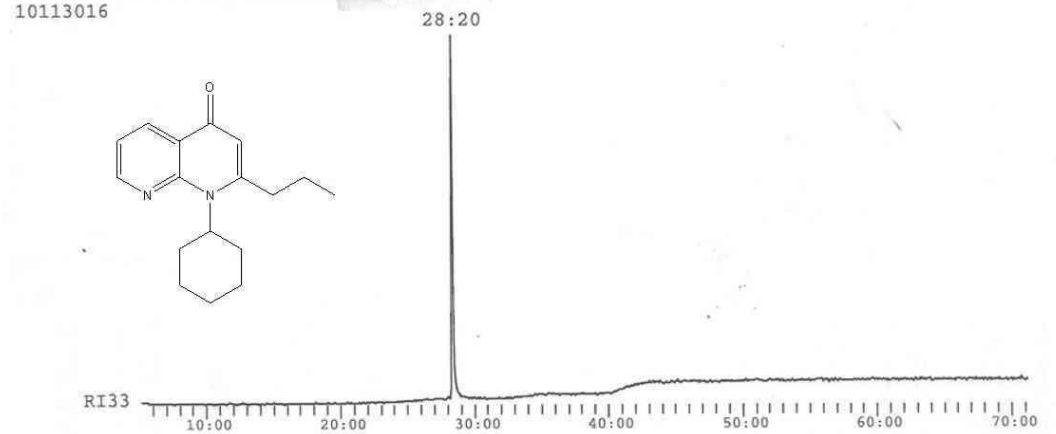
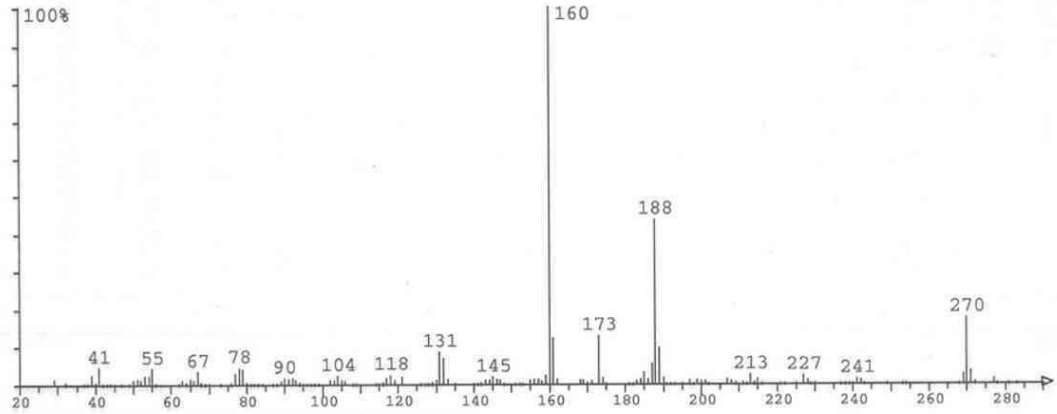


B2880(28:20) 2 31% 10113016 ikp 207/GC

10113016





B2880(28:20) 2 31% 10113016 ikp 207/GC

29	1.12	65	1.16	96	0.19	133	1.16	168	0.91	198	0.32	241	1.00
32	0.41	66	0.74	97	0.20	135	0.14	169	0.82	199	0.94	242	0.69
38	0.36	67	3.21	99	0.14	140	0.16	170	0.52	200	0.64	243	0.16
39	2.13	68	0.44	102	0.79	141	0.17	171	0.60	201	0.54	253	0.16
40	0.52	69	0.18	103	0.81	142	0.44	173	12.61	202	0.22	254	0.15
41	4.16	76	0.51	104	1.95	143	0.78	174	1.39	207	1.11	268	0.24
42	0.23	77	2.59	105	0.66	144	0.81	175	0.34	208	0.58	269	2.30
43	0.19	78	4.13	106	0.53	145	1.59	181	0.17	209	0.41	270	17.27
44	0.25	79	3.79	108	0.15	146	1.07	182	0.32	211	0.51	271	3.05
45	0.14	80	0.38	115	0.29	147	0.94	183	0.53	212	0.36	272	0.52
47	0.15	81	0.31	116	0.44	148	0.16	184	0.96	213	2.25	277	1.01
50	0.66	82	0.37	117	1.30	152	0.16	185	2.76	214	0.39	278	0.25
51	1.10	83	0.29	118	2.08	153	0.18	186	1.05	215	1.11	281	0.26
52	0.73	88	0.16	119	0.75	155	0.82	187	5.19	225	0.32	283	0.14
53	1.93	89	0.56	121	1.58	156	0.95	188	43.50	227	1.90		
54	1.89	90	1.29	127	0.13	157	1.16	189	9.46	228	0.66		
55	3.98	91	1.05	128	0.18	158	0.59	190	1.32	229	0.34		
56	0.20	92	1.28	129	0.42	159	1.82	191	0.32	230	0.14		
62	0.16	93	0.88	130	0.81	160	100.00	193	0.21	238	0.26		
63	0.73	94	0.45	131	8.37	161	12.03	195	0.13	239	0.15		
64	0.48	95	0.19	132	6.50	162	1.10	197	0.66	240	0.15		

B2880(28:20) 2 31% 10113016 ikp 207/GC lim: 0.13%

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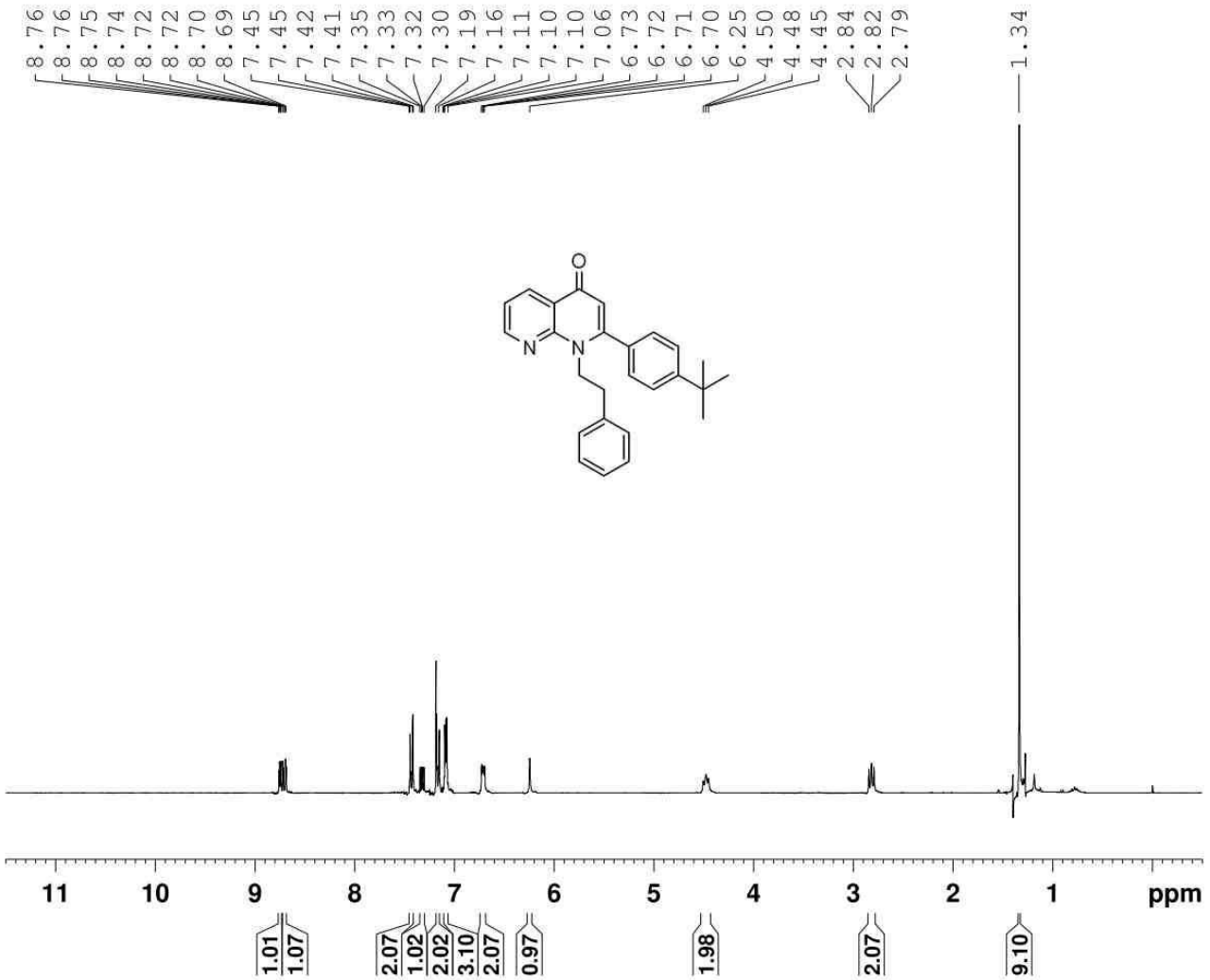

BRUKER

NAME	101123.u335	
EXPNO	10	
PROCNO	1	
Date_	20101123	
Time	15.41	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300295	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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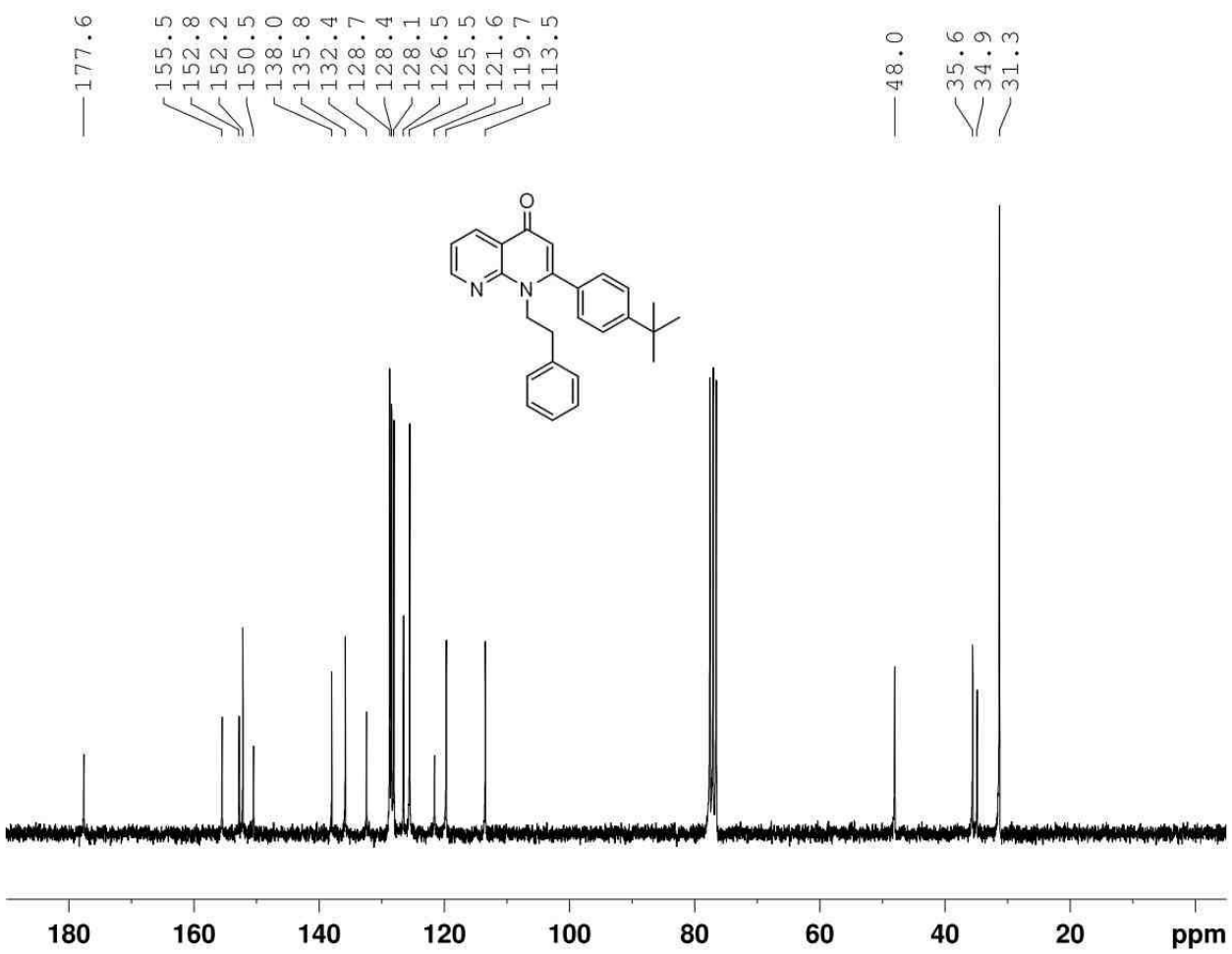

BRUKER

NAME	101116.213
EXPNO	10
PROCNO	1
Date_	20101117
Time	6.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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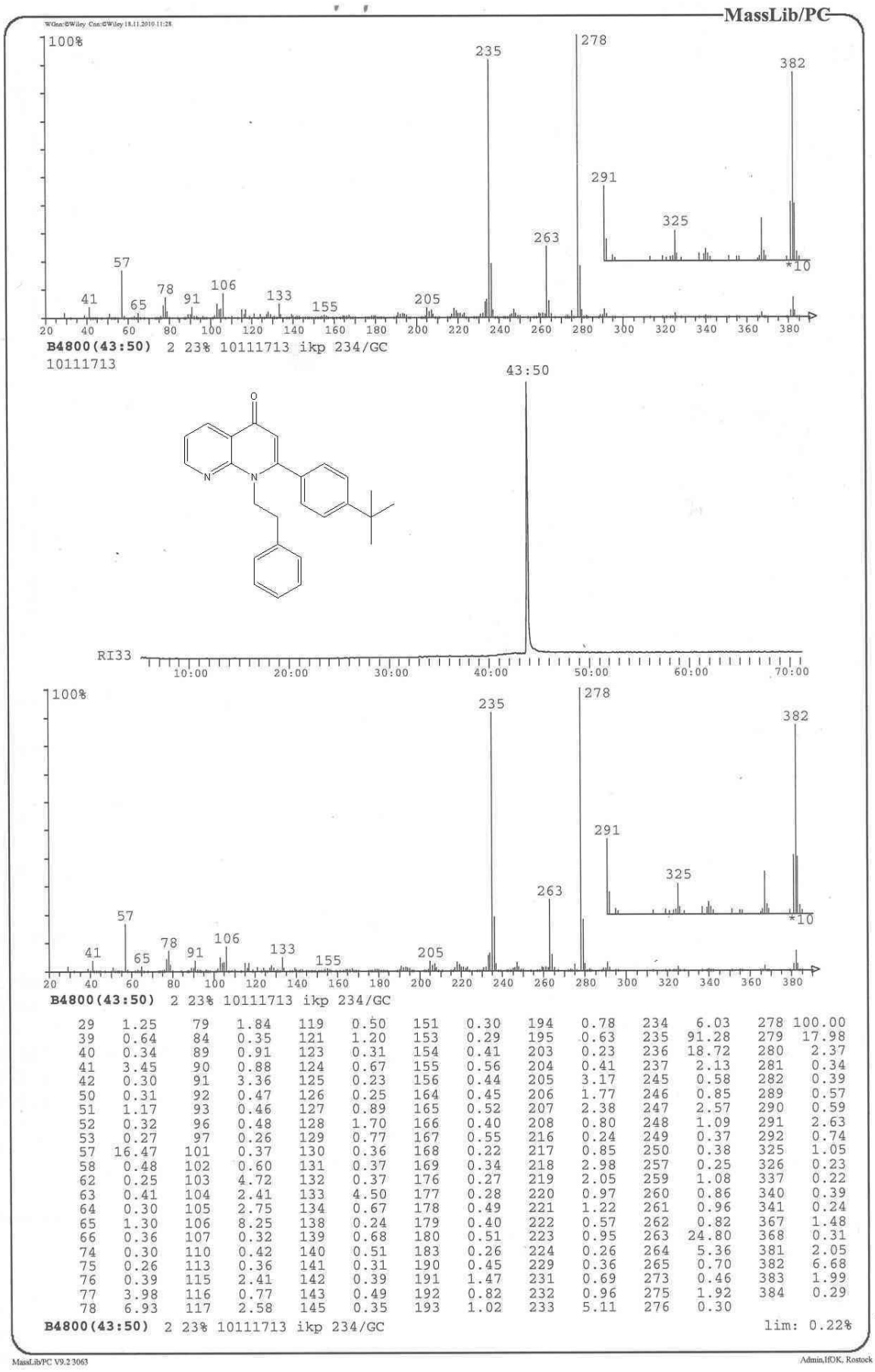

29	1.25	79	1.84	119	0.50	151	0.30	194	0.78	234	6.03	278	100.00
39	0.64	84	0.35	121	1.20	153	0.29	195	0.63	235	91.28	279	17.98
40	0.34	89	0.91	123	0.31	154	0.41	203	0.23	236	18.72	280	2.37
41	3.45	90	0.88	124	0.67	155	0.56	204	0.41	237	2.13	281	0.34
42	0.30	91	3.36	125	0.23	156	0.44	205	3.17	245	0.58	282	0.39
50	0.31	92	0.47	126	0.25	164	0.45	206	1.77	246	0.85	289	0.57
51	1.17	93	0.46	127	0.89	165	0.52	207	2.38	247	2.57	290	0.59
52	0.32	96	0.48	128	1.70	166	0.40	208	0.80	248	1.09	291	2.63
53	0.27	97	0.26	129	0.77	167	0.55	216	0.24	249	0.37	292	0.74
57	16.47	101	0.37	130	0.36	168	0.22	217	0.85	250	0.38	325	1.05
58	0.48	102	0.60	131	0.37	169	0.34	218	2.98	257	0.25	326	0.23
62	0.25	103	4.72	132	0.37	176	0.27	219	2.05	259	1.08	337	0.22
63	0.41	104	2.41	133	4.50	177	0.28	220	0.97	260	0.86	340	0.39
64	0.30	105	2.75	134	0.67	178	0.49	221	1.22	261	0.96	341	0.24
65	1.30	106	8.25	138	0.24	179	0.40	222	0.57	262	0.82	367	1.48
66	0.36	107	0.32	139	0.68	180	0.51	223	0.95	263	24.80	368	0.31
74	0.30	110	0.42	140	0.51	183	0.26	224	0.26	264	5.36	381	2.05
75	0.26	113	0.36	141	0.31	190	0.45	229	0.36	265	0.70	382	6.68
76	0.39	115	2.41	142	0.39	191	1.47	231	0.69	273	0.46	383	1.99
77	3.98	116	0.77	143	0.49	192	0.82	232	0.96	275	1.92	384	0.29
78	6.93	117	2.58	145	0.35	193	1.02	233	5.11	276	0.30		

B4800(43:50) 2 23% 10111713 ikp 234/GC lim: 0.22%

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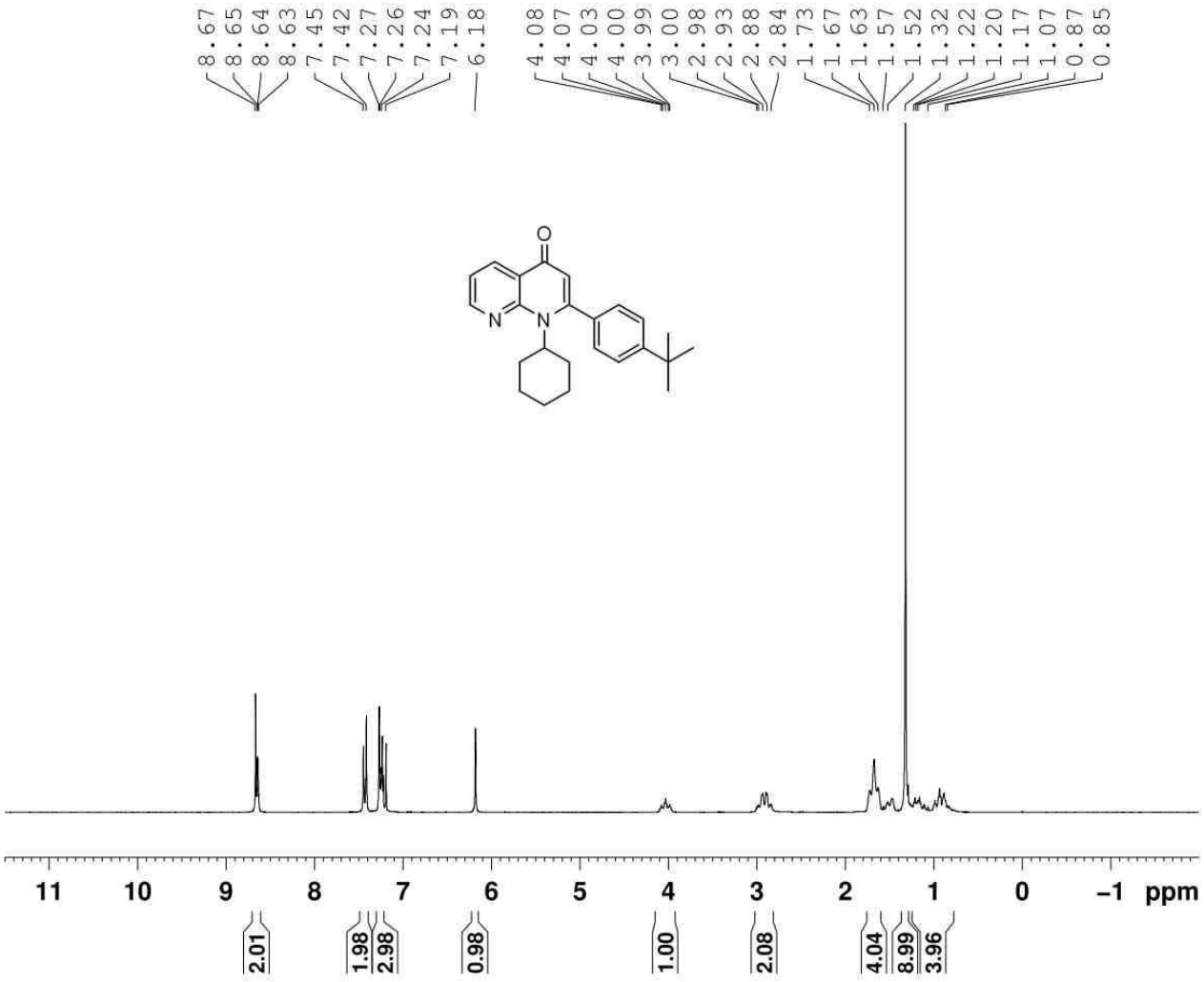

NAME	101112.202
EXPNO	10
PROCNO	1
Date_	20101112
Time	8.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	5165.289 Hz
FIDRES	0.078816 Hz
AQ	6.3439350 sec
RG	512
DW	96.800 use
DE	10.00 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	-2.50 dB
SFO1	250.1315447 MHz
SI	32768
SF	250.1300174 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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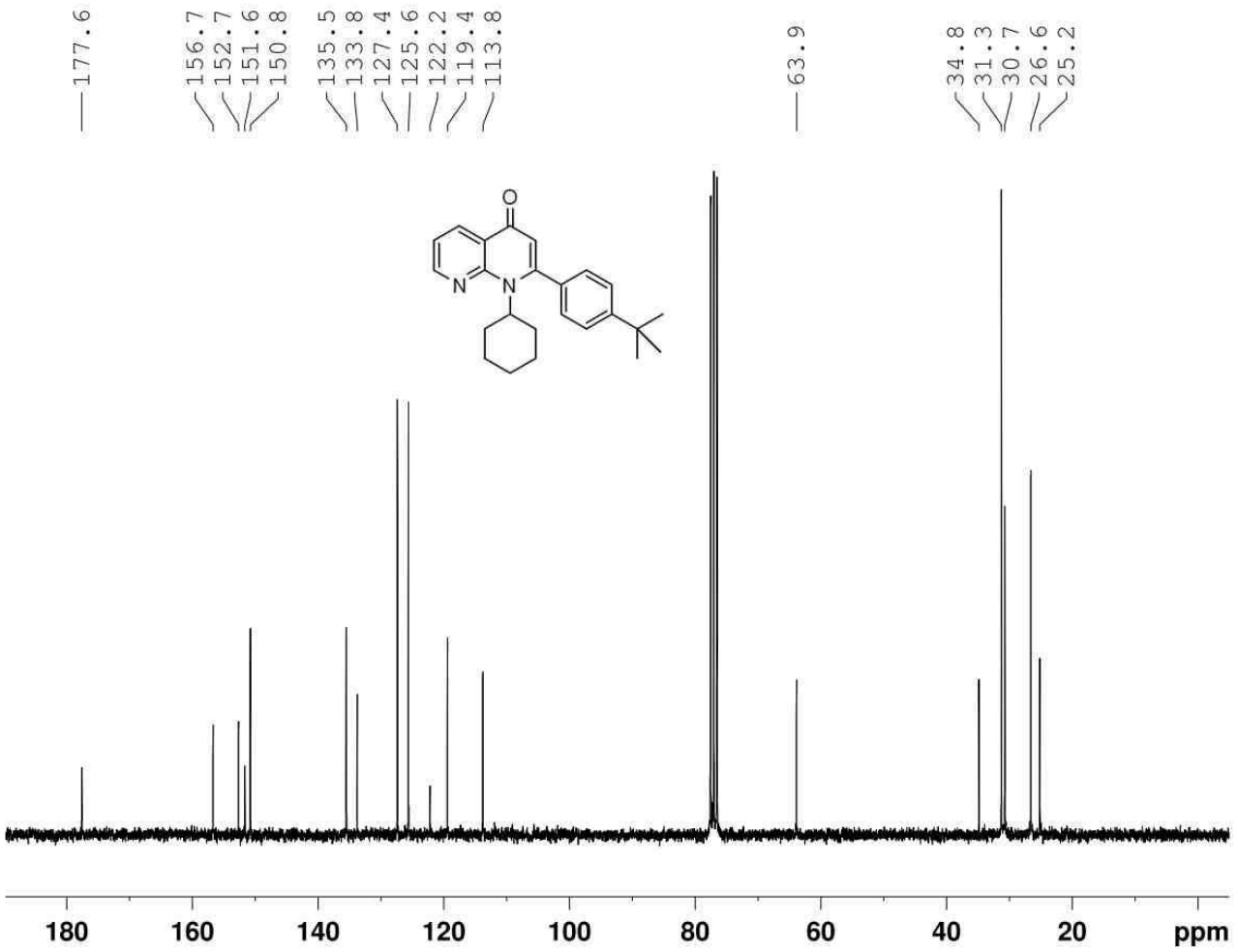

NAME	101112.202
EXPNO	11
PROCNO	1
Date_	20101112
Time	15.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1440
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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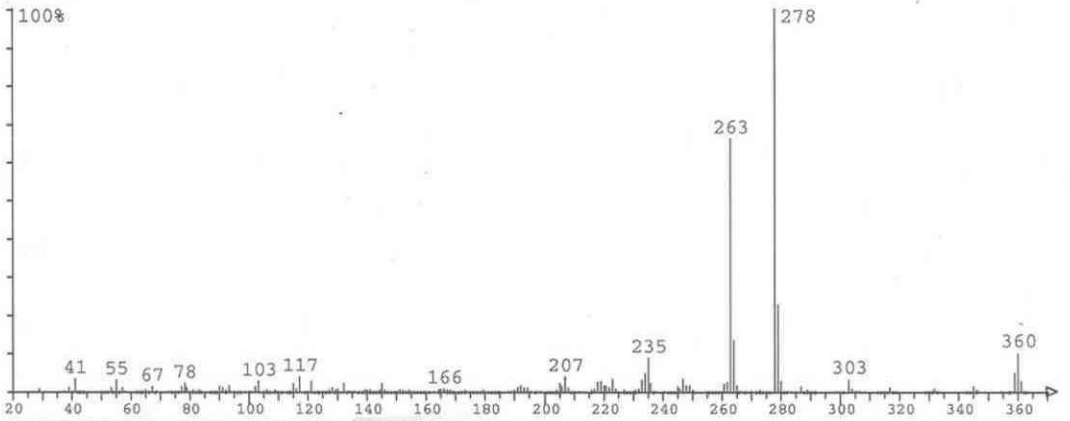
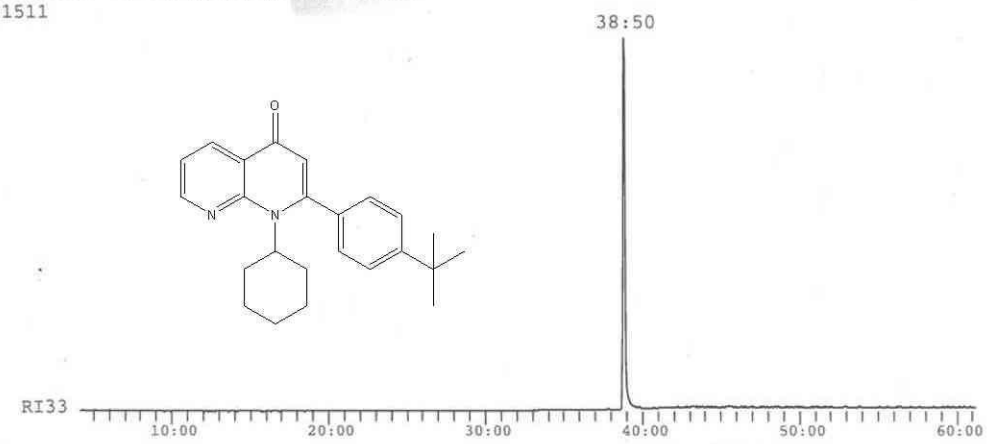
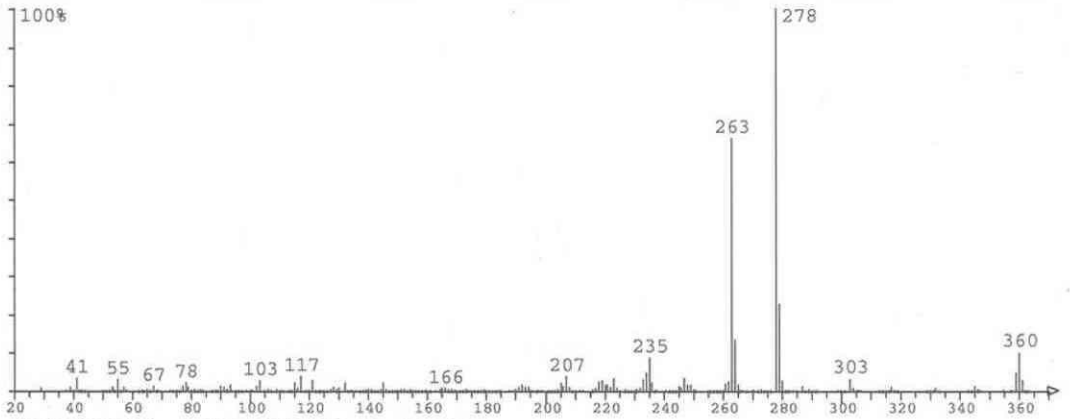
MassLib/PC



B4307(38:50) 2 28% 10111511 ikp 235/GC
10111511





B4307(38:50) 2 28% 10111511 ikp 235/GC

29	0.58	81	0.51	127	0.44	159	0.26	204	0.42	236	2.08	281	0.22
39	0.75	82	0.24	128	0.90	164	0.44	205	1.98	237	0.30	287	1.06
41	3.08	83	0.50	129	0.43	165	0.54	206	1.21	245	1.06	288	0.26
43	0.25	88	0.20	130	0.55	166	0.62	207	3.70	246	0.60	289	0.41
50	0.20	89	0.22	132	2.10	167	0.47	208	0.69	247	3.01	301	0.22
51	0.32	90	1.03	133	0.30	168	0.37	216	0.42	248	1.45	303	2.96
52	0.21	91	0.76	139	0.42	171	0.21	217	0.63	249	1.37	304	0.58
53	0.69	92	0.42	140	0.49	172	0.36	218	2.14	250	0.44	305	0.22
54	0.34	93	1.27	141	0.46	173	0.40	219	2.45	259	0.32	317	0.83
55	2.83	97	0.21	142	0.28	177	0.22	220	1.36	260	0.36	318	0.27
57	0.83	102	0.96	143	0.32	178	0.27	221	1.32	261	1.62	331	0.29
63	0.35	103	2.59	144	0.49	179	0.40	222	0.87	262	2.38	332	0.52
64	0.27	106	0.45	145	1.94	180	0.33	223	3.07	263	66.12	343	0.37
65	0.38	109	0.46	146	0.45	181	0.24	224	0.54	264	13.38	345	1.12
66	0.31	114	0.22	147	0.33	184	0.21	227	0.50	265	1.30	346	0.39
67	1.07	115	2.01	151	0.39	190	0.45	229	0.28	273	0.47	359	4.67
75	0.19	116	0.61	152	0.39	191	0.74	231	0.47	275	0.27	360	9.94
76	0.21	117	3.59	154	0.40	192	1.48	232	0.60	276	0.28	361	2.65
77	1.06	121	2.47	155	0.27	193	0.95	233	2.71	278	100.00	362	0.31
78	1.88	122	0.27	156	0.25	194	0.92	234	4.68	279	22.61		
79	0.81	125	0.32	158	0.25	195	0.20	235	8.58	280	2.64		

B4307(38:50) 2 28% 10111511 ikp 235/GC lim: 0.19%

MassLib/PC V9.2 3063 Admin,IfOK, Rostock

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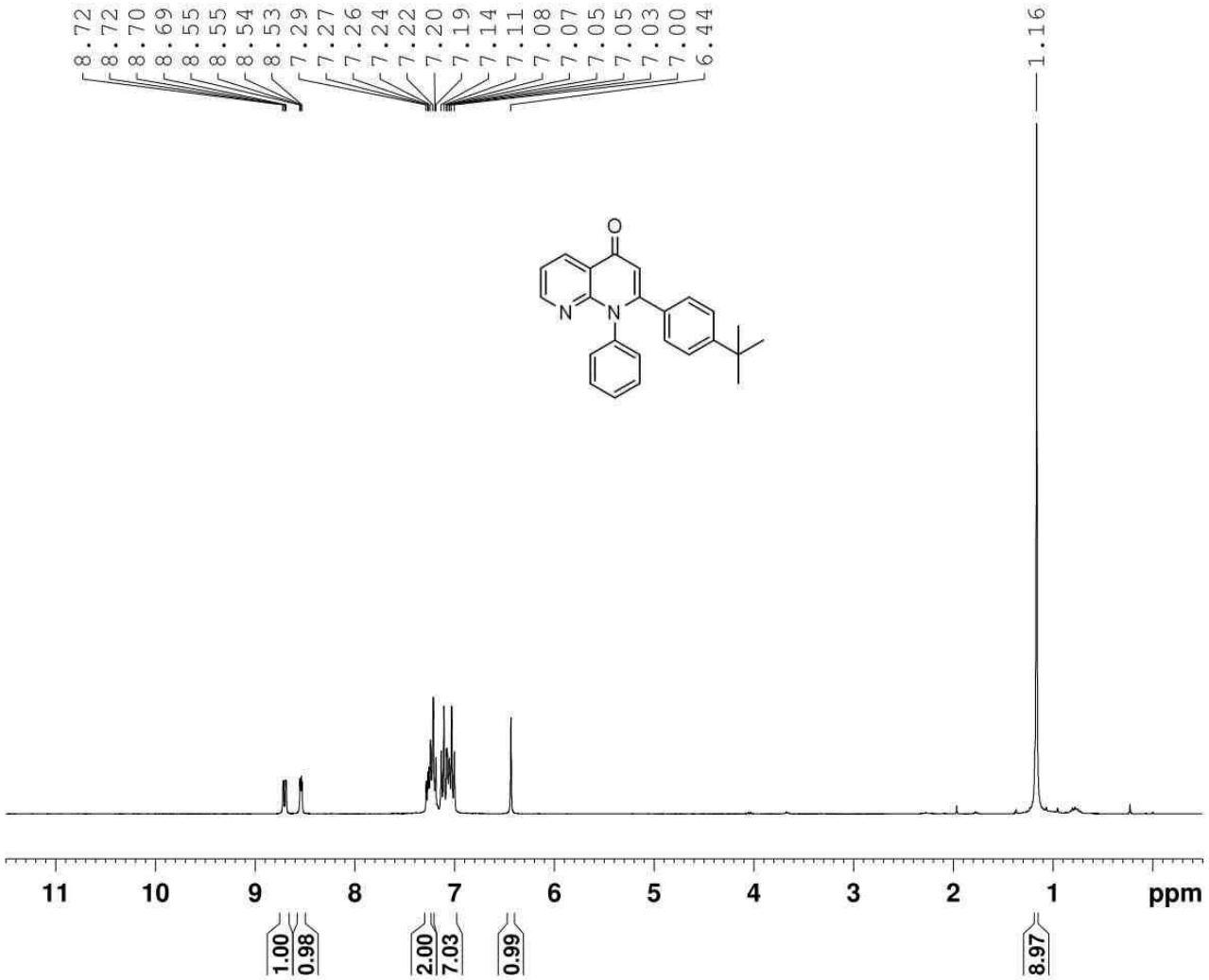

NAME	101202.u301
EXPNO	10
PROCNO	1
Date_	20101202
Time	8.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	114
DW	80.800 use
DE	10.00 use
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300297 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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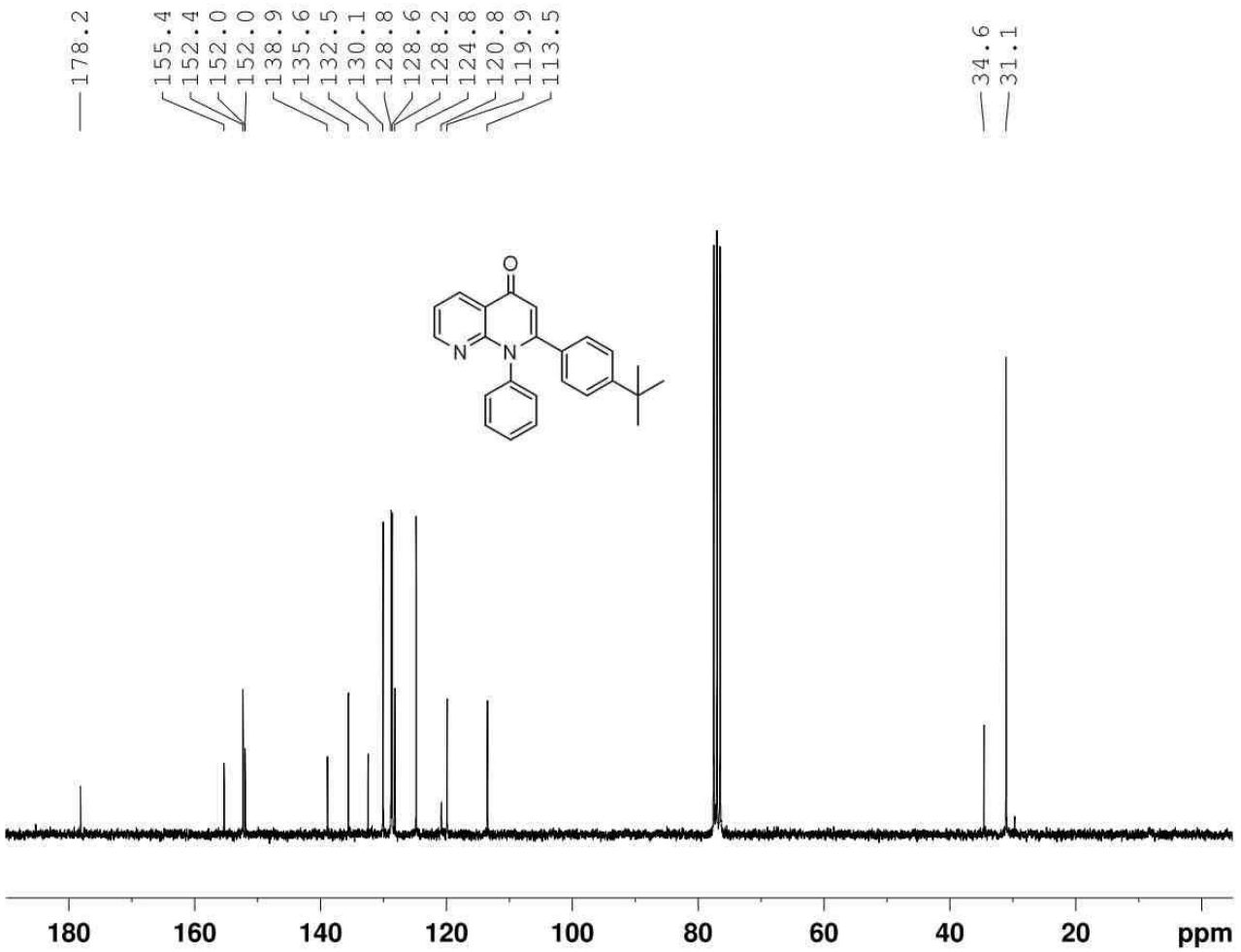

BRUKER

NAME	101203.212
EXPNO	10
PROCNO	1
Date_	20101204
Time	11.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1400
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1620
DW	33.333 usec
DE	10.00 usec
TE	297.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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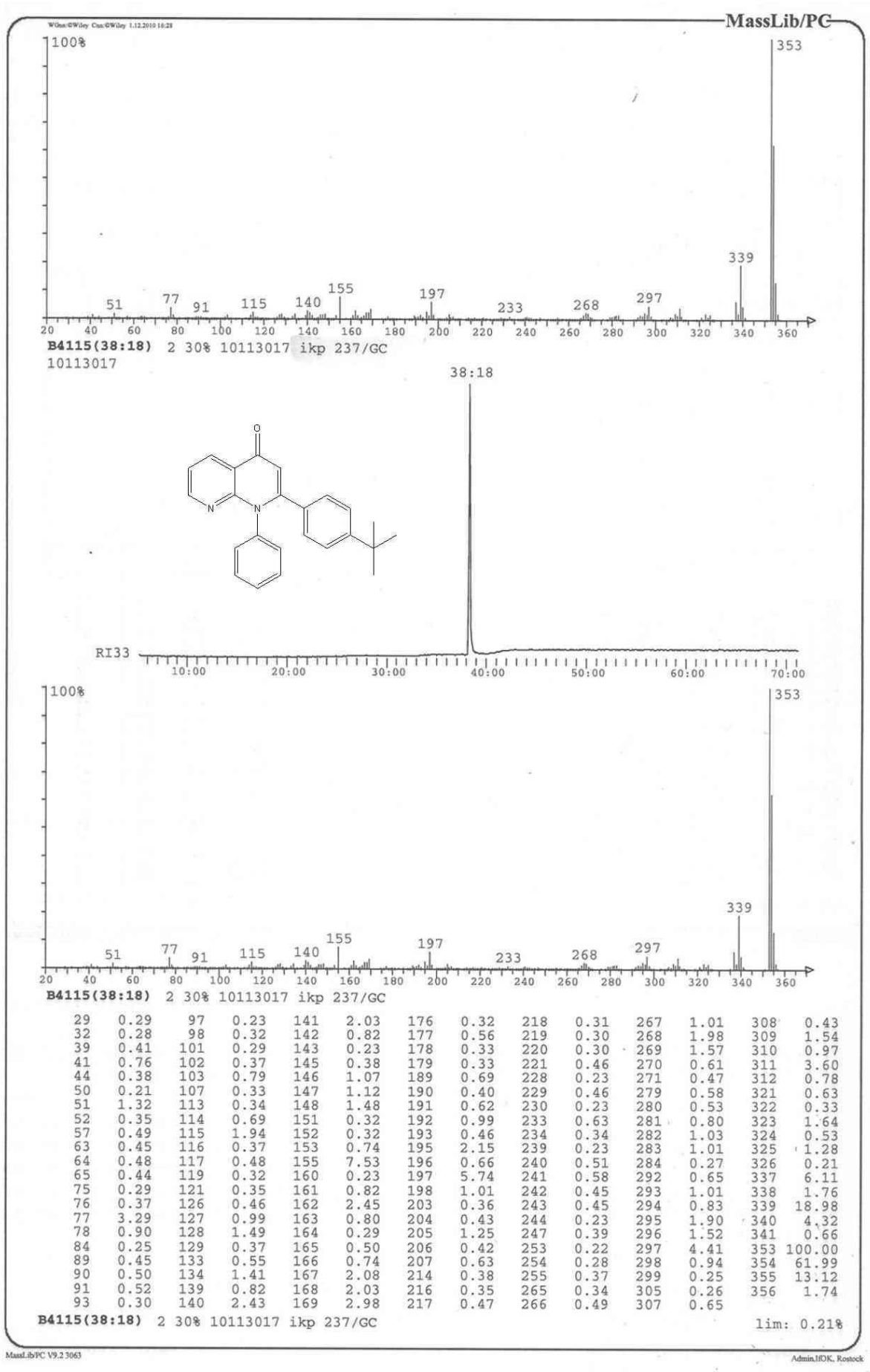

29	0.29	97	0.23	141	2.03	176	0.32	218	0.31	267	1.01	308	0.43
32	0.28	98	0.32	142	0.82	177	0.56	219	0.30	268	1.98	309	1.54
39	0.41	101	0.29	143	0.23	178	0.33	220	0.30	269	1.57	310	0.97
41	0.76	102	0.37	145	0.38	179	0.33	221	0.46	270	0.61	311	3.60
44	0.38	103	0.79	146	1.07	189	0.69	228	0.23	271	0.47	312	0.78
50	0.21	107	0.33	147	1.12	190	0.40	229	0.46	279	0.58	321	0.63
51	1.32	113	0.34	148	1.48	191	0.62	230	0.23	280	0.53	322	0.33
52	0.35	114	0.69	151	0.32	192	0.99	233	0.63	281	0.80	323	1.64
57	0.49	115	1.94	152	0.32	193	0.46	234	0.34	282	1.03	324	0.53
63	0.45	116	0.37	153	0.74	195	2.15	239	0.23	283	1.01	325	1.28
64	0.48	117	0.48	155	7.53	196	0.66	240	0.51	284	0.27	326	0.21
65	0.44	119	0.32	160	0.23	197	5.74	241	0.58	292	0.65	337	6.11
75	0.29	121	0.35	161	0.82	198	1.01	242	0.45	293	1.01	338	1.76
76	0.37	126	0.46	162	2.45	203	0.36	243	0.45	294	0.83	339	18.98
77	3.29	127	0.99	163	0.80	204	0.43	244	0.23	295	1.90	340	4.32
78	0.90	128	1.49	164	0.29	205	1.25	247	0.39	296	1.52	341	0.66
84	0.25	129	0.37	165	0.50	206	0.42	253	0.22	297	4.41	353	100.00
89	0.45	133	0.55	166	0.74	207	0.63	254	0.28	298	0.94	354	61.99
90	0.50	134	1.41	167	2.08	214	0.38	255	0.37	299	0.25	355	13.12
91	0.52	139	0.82	168	2.03	216	0.35	265	0.34	305	0.26	356	1.74
93	0.30	140	2.43	169	2.98	217	0.47	266	0.49	307	0.65		

B4115(38:18) 2 30% 10113017 ikp 237/GC lim: 0.21%

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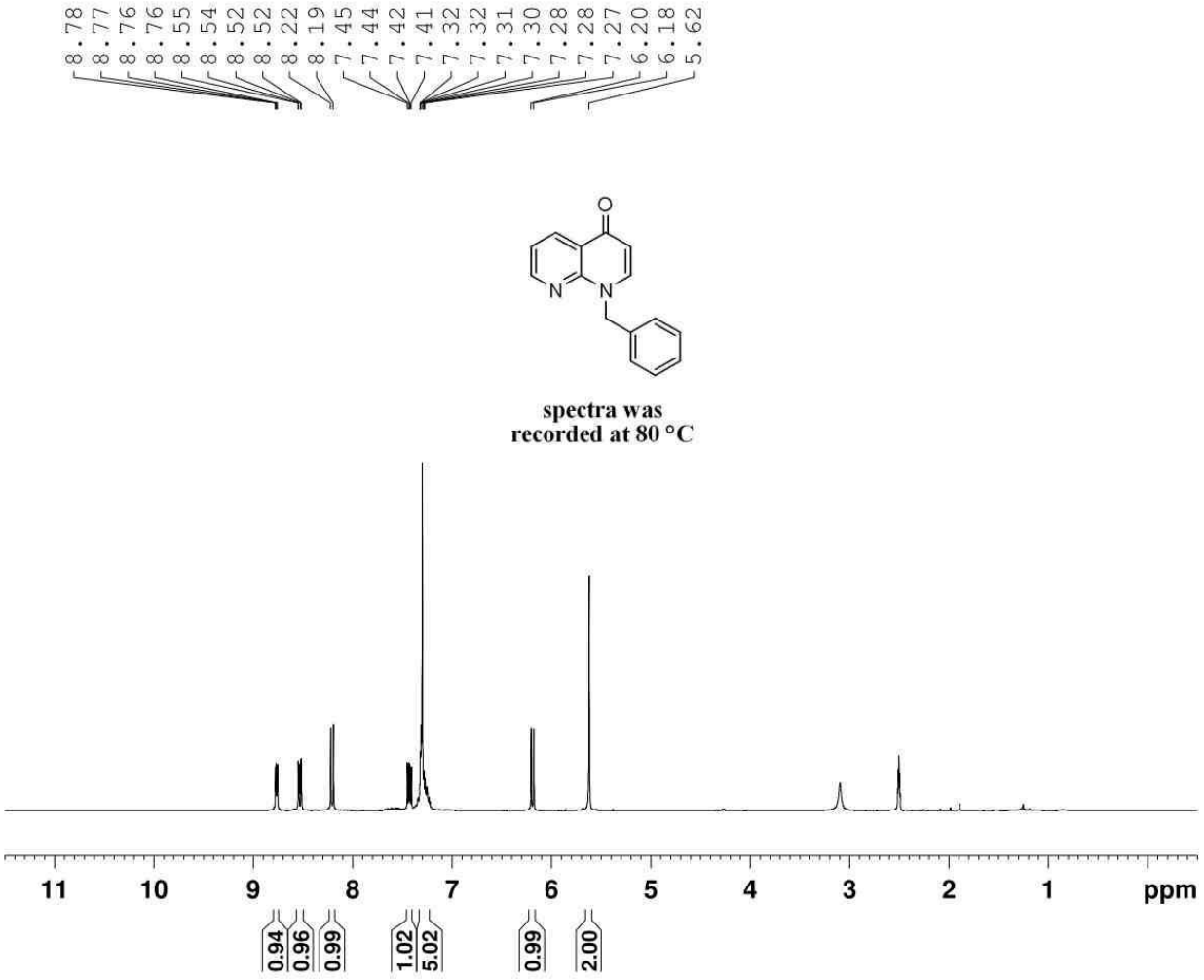

NAME	110201.u319	
EXPNO	10	
PROCNO	1	
Date_	20110201	
Time	15.01	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	101	
DW	80.800	use
DE	10.00	use
TE	353.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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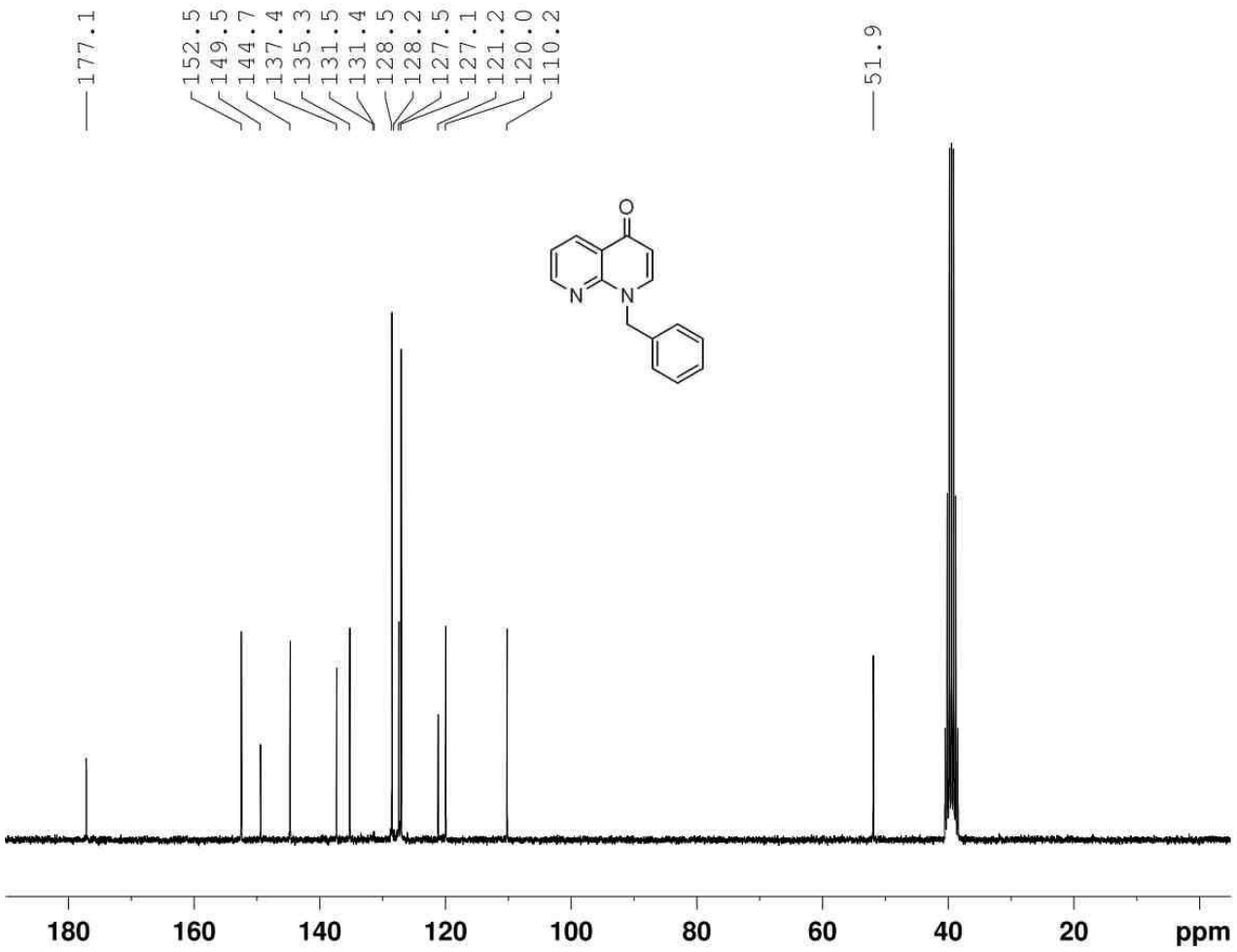
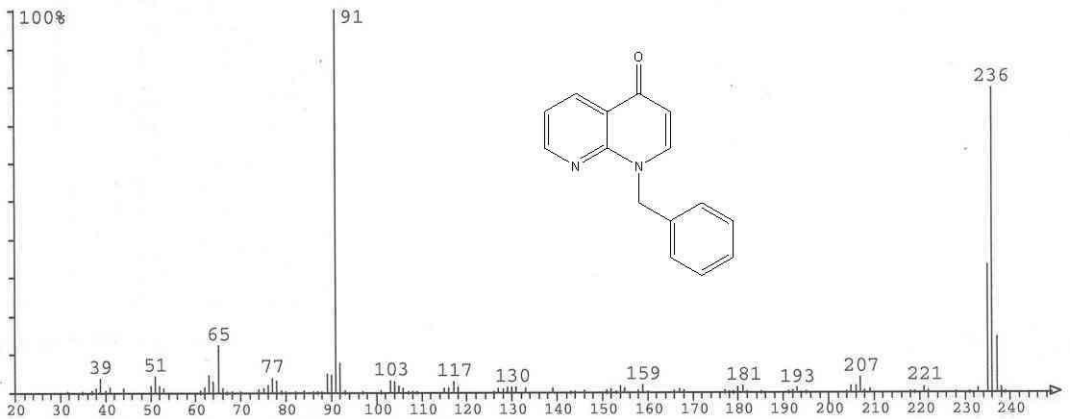


BRUKER

NAME	110204.213	
EXPNO	10	
PROCNO	1	
Date_	20110206	
Time	20.09	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	DMSO	
NS	1024	
DS	4	
SWH	15000.000	Hz
FIDRES	0.228882	Hz
AQ	2.1845834	sec
RG	2050	
DW	33.333	usec
DE	10.00	usec
TE	297.7	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	-1.00	dB
SFO1	62.9015280	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	70.00	usec
PL12	15.00	dB
PL13	15.00	dB
PL2	-2.50	dB
SFO2	250.1310005	MHz
SI	32768	
SF	62.8952704	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



B2670(26:38) 2 29% 10113011 ikp 238/GC

32	0.05	74	0.65	105	1.51	152	0.66	204	0.22
35	0.18	75	0.87	106	0.75	153	0.27	205	1.50
37	0.39	76	1.80	107	0.33	154	1.26	206	1.32
38	0.86	77	3.54	108	0.23	155	0.72	207	3.71
39	3.34	78	2.89	109	0.30	158	0.38	208	0.39
40	0.39	79	0.44	115	0.85	159	1.54	209	0.58
41	1.15	80	0.31	116	0.67	160	0.34	218	0.29
44	0.69	82	0.20	117	2.48	166	0.42	219	0.35
50	1.39	84	0.41	118	1.03	167	0.58	221	1.22
51	3.96	86	0.18	126	0.29	168	0.52	222	0.52
52	1.48	87	0.26	127	0.69	177	0.46	228	0.19
53	0.72	88	0.34	128	0.59	178	0.26	231	0.24
61	0.48	89	4.51	129	1.08	179	0.32	233	0.84
62	1.10	90	4.32	130	1.20	180	1.05	235	33.02
63	4.25	91	100.00	131	1.17	181	1.42	236	79.49
64	2.48	92	7.61	133	0.85	182	0.28	237	14.26
65	12.19	93	0.39	139	0.87	185	0.18	238	1.09
66	0.79	97	0.27	143	0.20	191	0.24	239	0.32
67	0.19	101	0.38	144	0.20	192	0.45	249	0.21
68	0.24	103	2.78	146	0.45	193	0.80		
70	0.21	104	2.42	151	0.43	195	0.24		

B2670(26:38) 2 29% 10113011 ikp 238/GC

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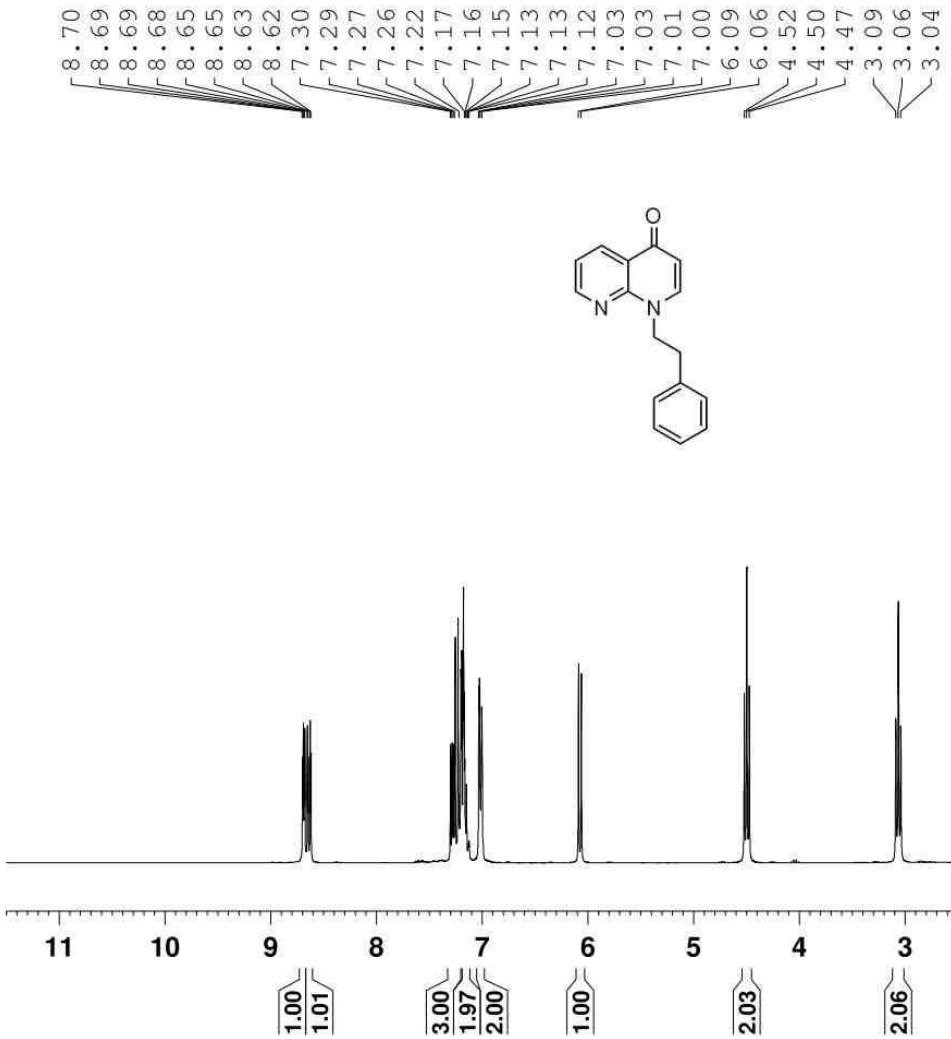

NAME	101210.u336	
EXPNO	10	
PROCNO	1	
Date_	20101210	
Time	14.23	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	114	
DW	80.800	use
DE	10.00	use
TE	296.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300287	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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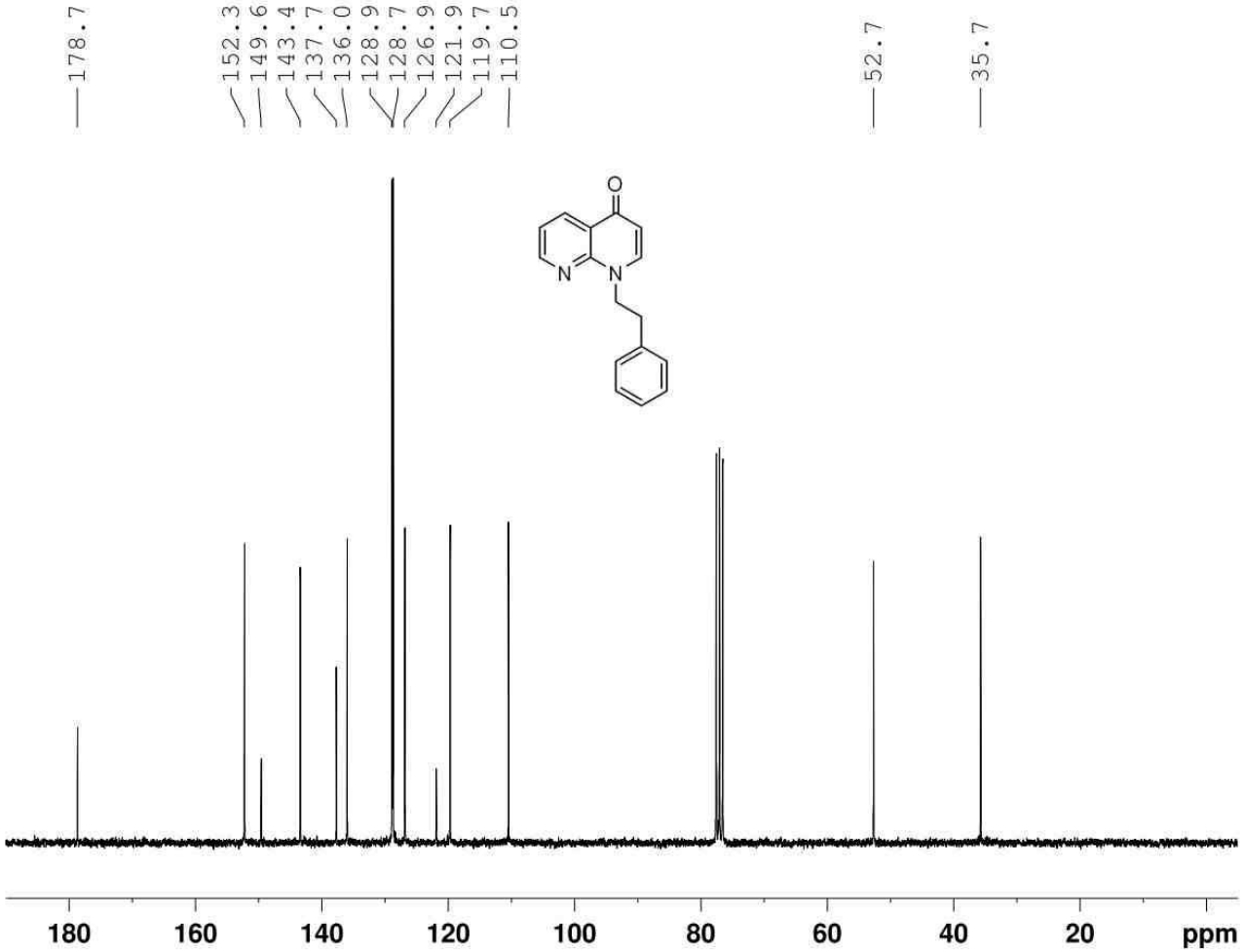

BRUKER

NAME	101213.211
EXPNO	10
PROCNO	1
Date_	20101214
Time	2.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1620
DW	33.333 usec
DE	10.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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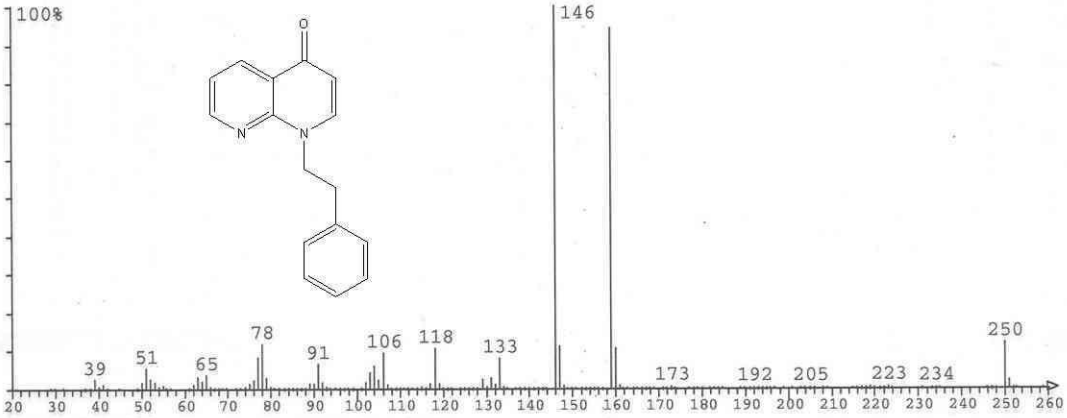

B2782(27:32) 2 28% 10113014 ikp 240/GC

29	0.05	65	3.52	87	0.17	111	0.06	135	0.05	164	0.08	206	0.14
32	0.05	66	0.48	88	0.15	113	0.08	138	0.05	165	0.06	208	0.08
37	0.27	67	0.30	89	1.05	114	0.16	139	0.15	166	0.19	217	0.12
38	0.33	68	0.18	90	1.22	115	0.40	140	0.11	167	0.18	218	0.26
39	2.28	69	0.07	91	6.35	116	0.36	141	0.13	171	0.28	219	0.37
40	0.38	70	0.06	92	1.29	117	1.12	142	0.09	172	0.05	220	0.11
41	0.69	72	0.04	93	0.43	118	10.42	143	0.14	173	0.43	221	0.34
42	0.10	73	0.06	96	0.12	119	1.19	144	0.07	177	0.05	222	0.27
49	0.11	74	0.42	97	0.08	120	0.06	146	100.00	178	0.14	223	0.41
50	1.50	75	0.96	98	0.08	121	0.13	147	11.00	179	0.07	224	0.07
51	5.23	76	1.85	99	0.09	124	0.15	148	0.66	180	0.10	231	0.12
52	2.14	77	8.05	101	0.19	125	0.15	149	0.04	183	0.04	233	0.17
53	1.35	78	11.43	102	1.38	126	0.11	152	0.22	190	0.07	234	0.30
54	0.41	79	2.56	103	3.96	127	0.16	153	0.10	191	0.17	247	0.22
55	0.53	80	0.43	104	5.60	128	0.24	154	0.08	192	0.32	248	0.21
56	0.05	81	0.07	105	1.93	129	2.12	155	0.11	193	0.24	250	11.74
57	0.06	82	0.36	106	9.20	130	0.47	157	0.13	194	0.09	251	2.07
61	0.13	83	0.13	107	0.73	131	2.59	159	94.25	195	0.08	252	0.27
62	0.70	84	0.17	108	0.05	132	0.85	160	10.25	199	0.05		
63	2.72	85	0.10	109	0.14	133	7.76	161	0.55	204	0.06		
64	1.74	86	0.10	110	0.12	134	0.45	162	0.06	205	0.23		

B2782(27:32) 2 28% 10113014 ikp 240/GC lim: 0.04%

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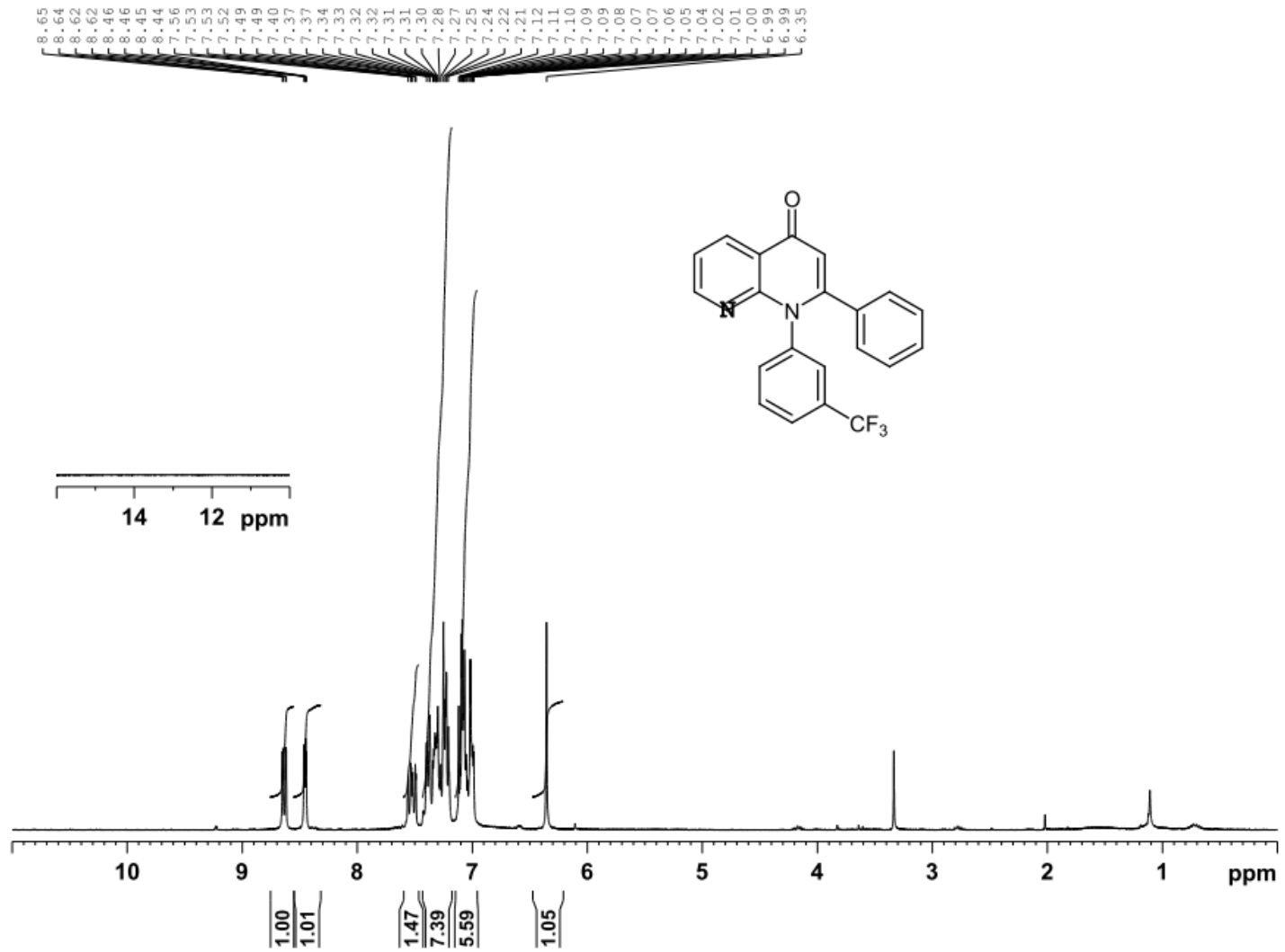
Mkrtchyan, R 629, CDCl3, 1H



Current Data Parameters

NAME	120209.u323 sm 629
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20120209
Time	16.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	181
DW	80.800 usec
DE	10.00 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 =======

NUC1	1H
P1	10.00 usec
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz

F2 - Processing parameters

SI	32768
SF	300.1300515 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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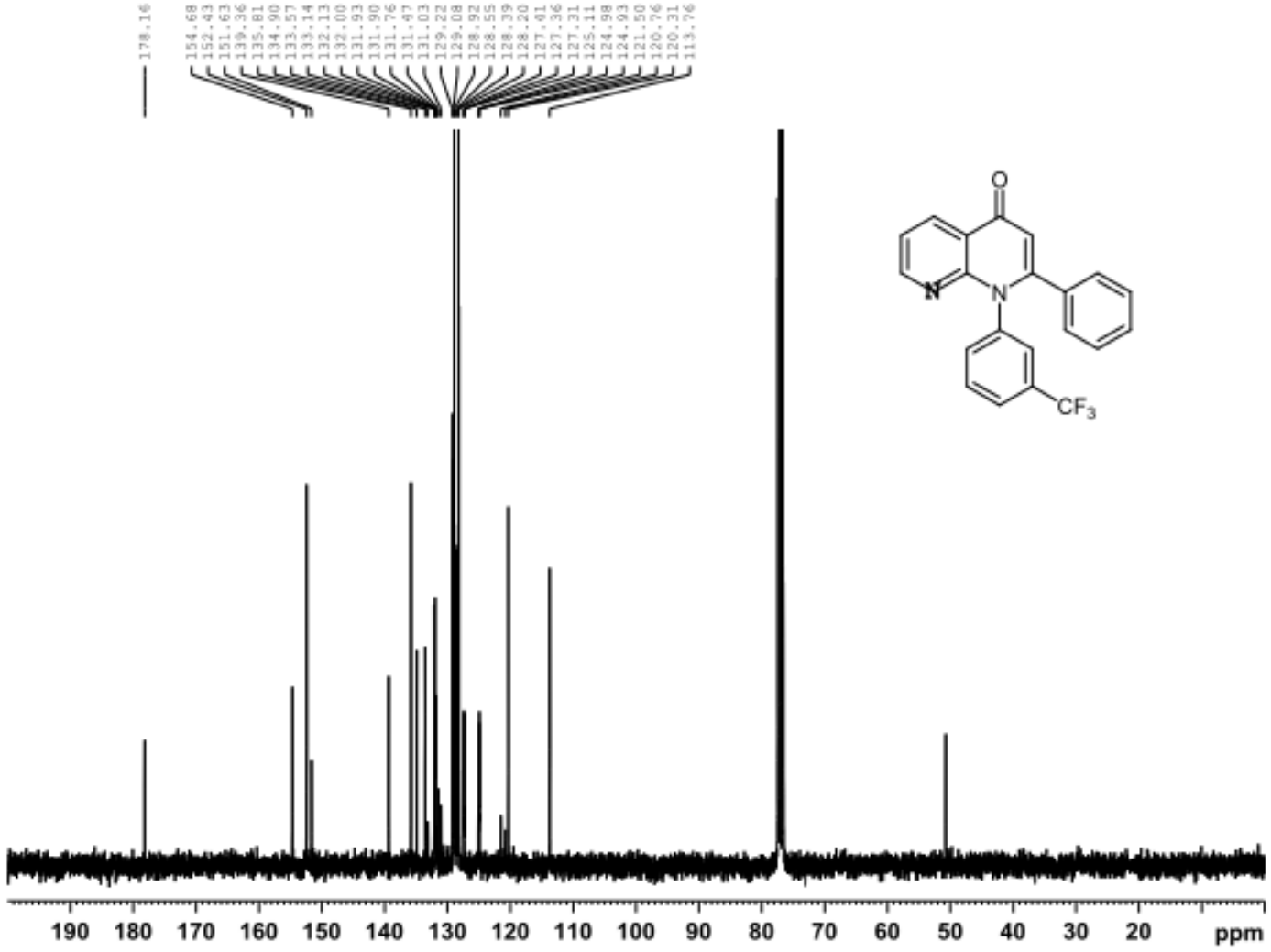
Mkrtchyan, R 629, CDCl3, 13C



BRUKER

Current Data Parameters
NAME 120210.a332 r 629 C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120211
Time 6.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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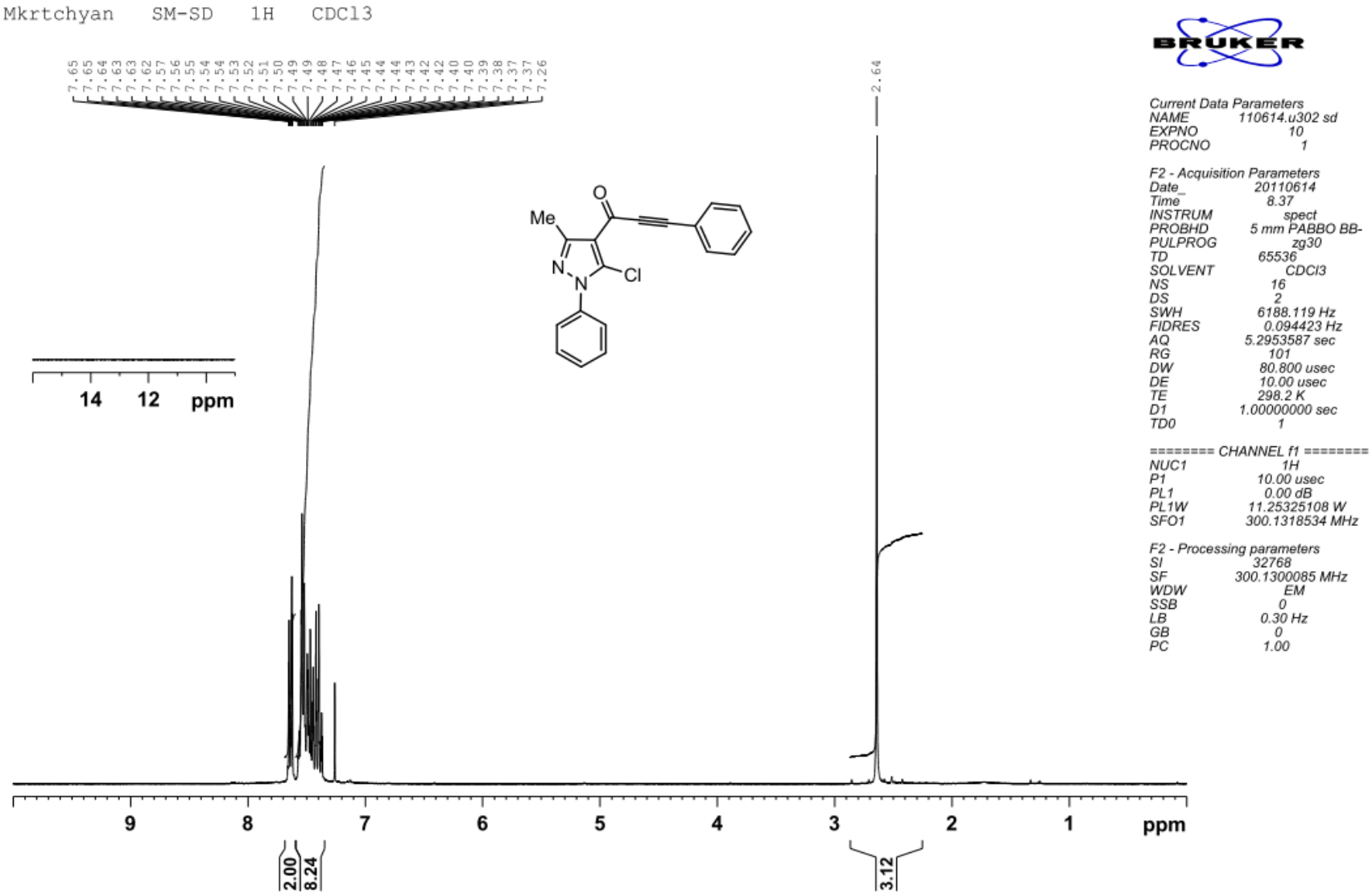

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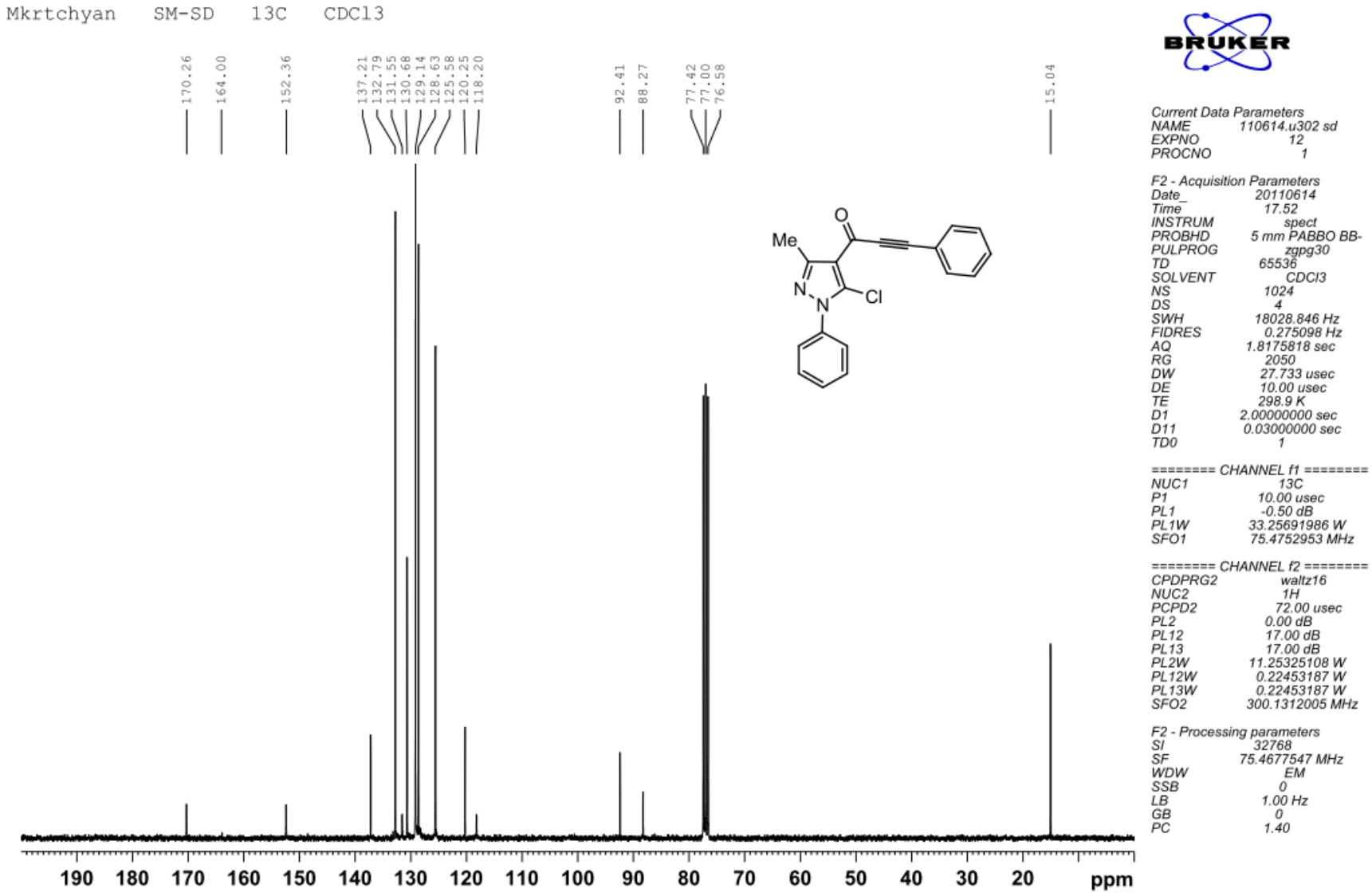

BRUKER

Current Data Parameters

NAME	110614.u302 sd
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20110614
Time	17.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677547 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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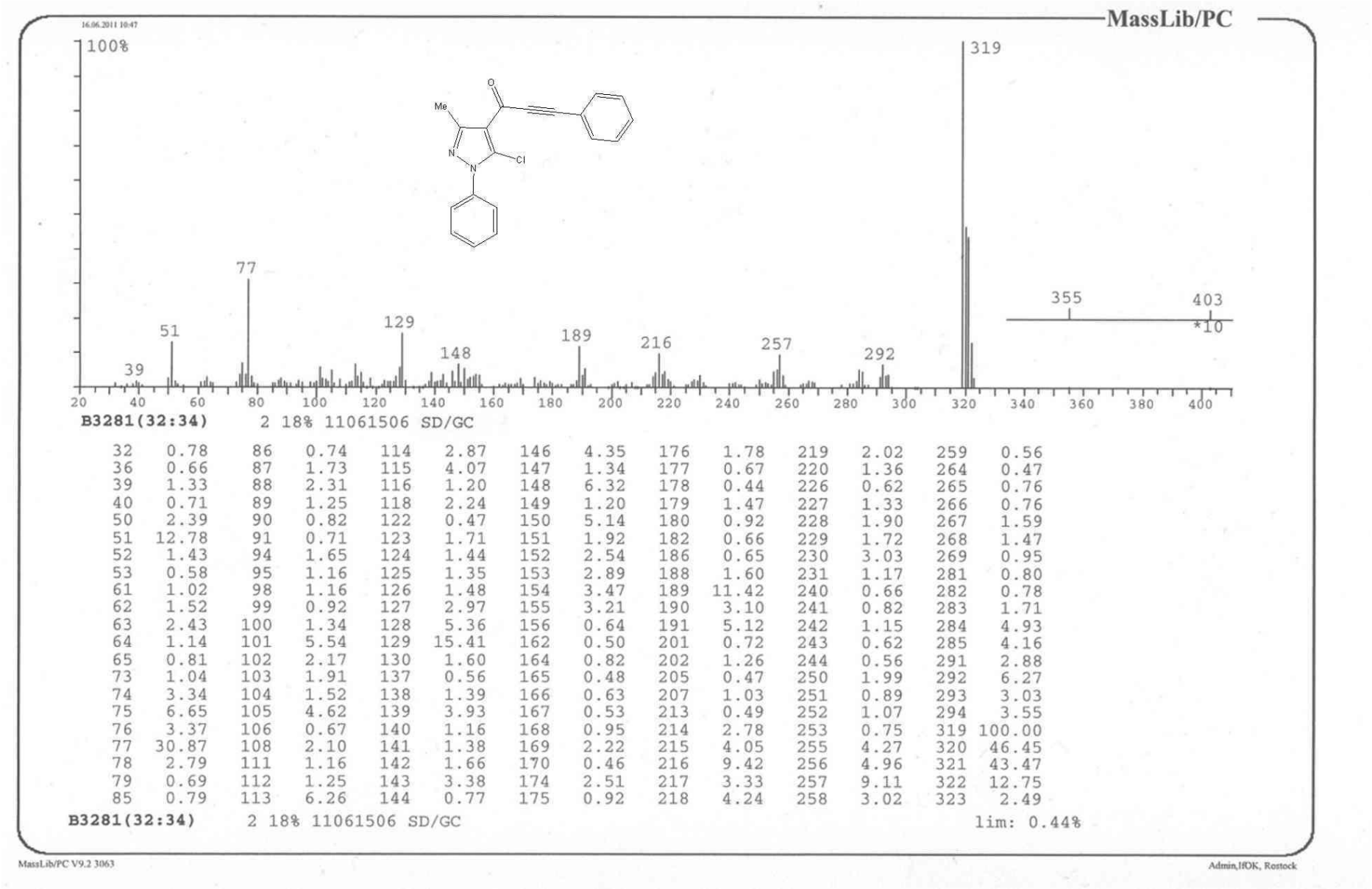

B3281(32:34) 2 18% 11061506 SD/GC

32	0.78	86	0.74	114	2.87	146	4.35	176	1.78	219	2.02	259	0.56
36	0.66	87	1.73	115	4.07	147	1.34	177	0.67	220	1.36	264	0.47
39	1.33	88	2.31	116	1.20	148	6.32	178	0.44	226	0.62	265	0.76
40	0.71	89	1.25	118	2.24	149	1.20	179	1.47	227	1.33	266	0.76
50	2.39	90	0.82	122	0.47	150	5.14	180	0.92	228	1.90	267	1.59
51	12.78	91	0.71	123	1.71	151	1.92	182	0.66	229	1.72	268	1.47
52	1.43	94	1.65	124	1.44	152	2.54	186	0.65	230	3.03	269	0.95
53	0.58	95	1.16	125	1.35	153	2.89	188	1.60	231	1.17	281	0.80
61	1.02	98	1.16	126	1.48	154	3.47	189	11.42	240	0.66	282	0.78
62	1.52	99	0.92	127	2.97	155	3.21	190	3.10	241	0.82	283	1.71
63	2.43	100	1.34	128	5.36	156	0.64	191	5.12	242	1.15	284	4.93
64	1.14	101	5.54	129	15.41	162	0.50	201	0.72	243	0.62	285	4.16
65	0.81	102	2.17	130	1.60	164	0.82	202	1.26	244	0.56	291	2.88
73	1.04	103	1.91	137	0.56	165	0.48	205	0.47	250	1.99	292	6.27
74	3.34	104	1.52	138	1.39	166	0.63	207	1.03	251	0.89	293	3.03
75	6.65	105	4.62	139	3.93	167	0.53	213	0.49	252	1.07	294	3.55
76	3.37	106	0.67	140	1.16	168	0.95	214	2.78	253	0.75	319	100.00
77	30.87	108	2.10	141	1.38	169	2.22	215	4.05	255	4.27	320	46.45
78	2.79	111	1.16	142	1.66	170	0.46	216	9.42	256	4.96	321	43.47
79	0.69	112	1.25	143	3.38	174	2.51	217	3.33	257	9.11	322	12.75
85	0.79	113	6.26	144	0.77	175	0.92	218	4.24	258	3.02	323	2.49

B3281(32:34) 2 18% 11061506 SD/GC lim: 0.44%

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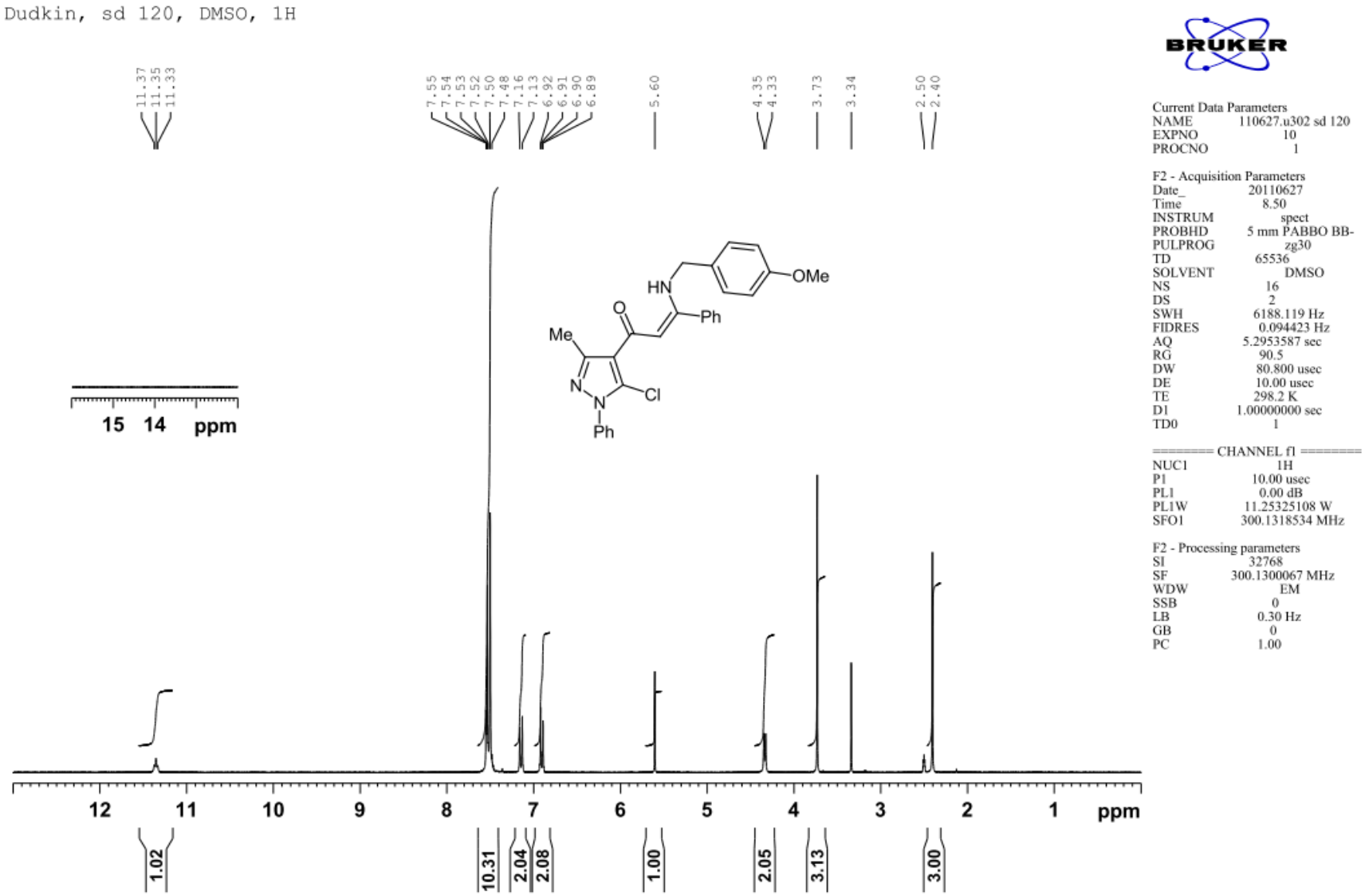

Current Data Parameters

NAME	110627.u302 sd 120
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20110627
Time	8.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	90.5
DW	80.800 usec
DE	10.00 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz

F2 - Processing parameters

SI	32768
SF	300.1300067 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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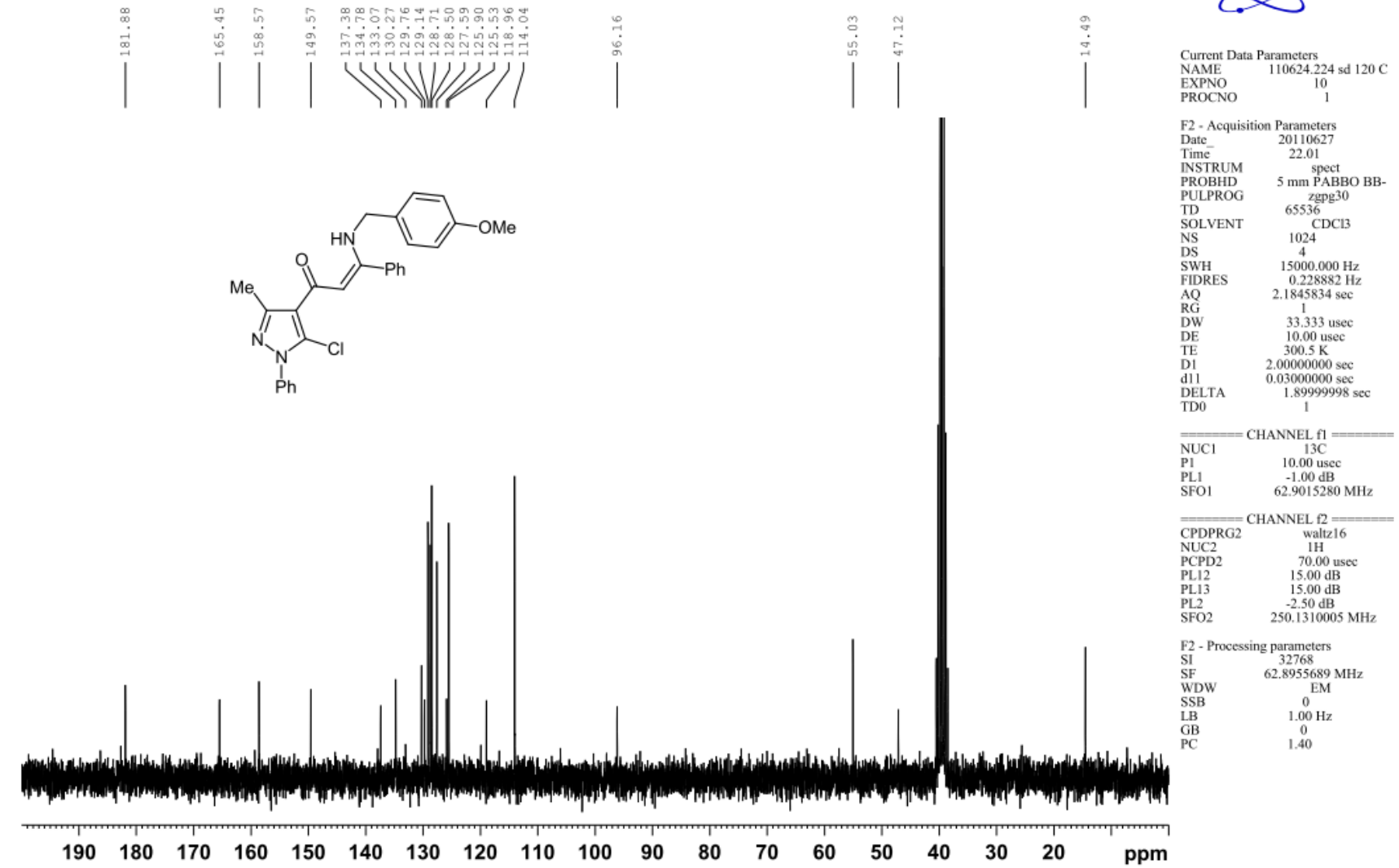
Dudkin, sd 120, CDCl3, 13C



Current Data Parameters
NAME 110624.224 sd 120 C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110627
Time 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 1
DW 33.333 usec
DE 10.00 usec
TE 300.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8955689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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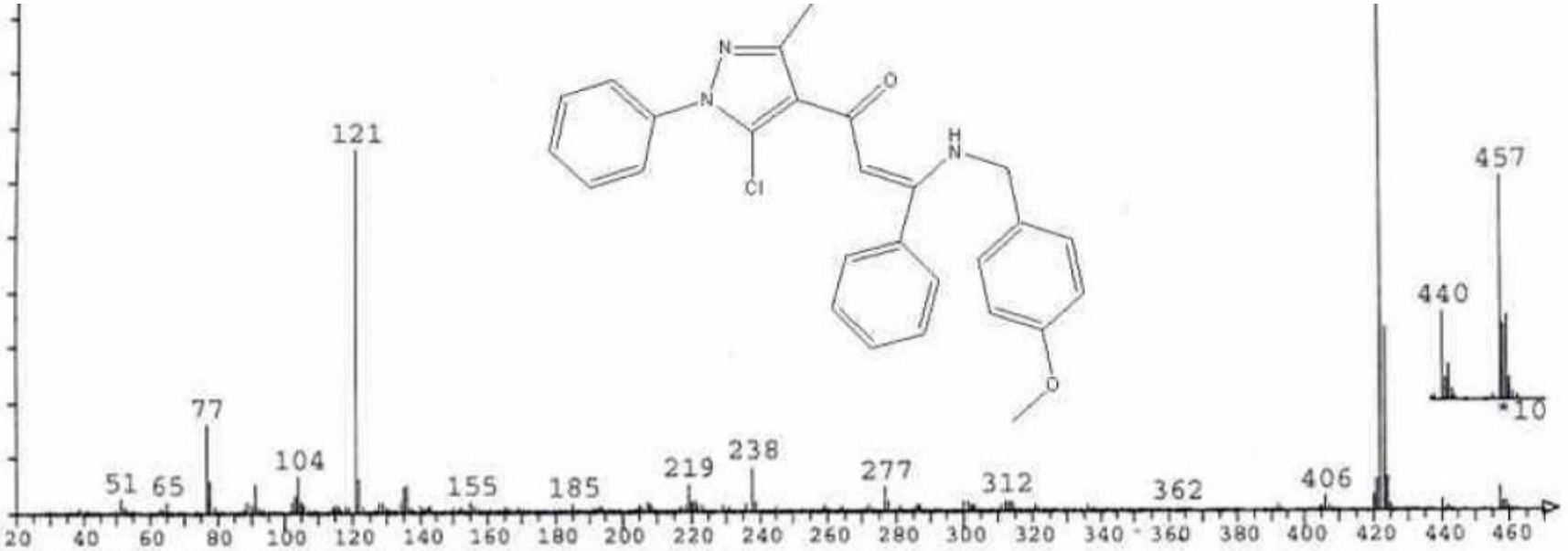

7025(61:47) 8156 248 11063020 * sd 120/GC

39	0.61	103	2.73	133	0.40	167	0.47	219	4.47	278	1.52	404	0.50
41	0.42	104	6.28	134	1.34	168	0.36	220	1.26	281	0.55	405	0.57
50	0.40	105	1.81	135	4.34	169	0.63	221	1.79	285	0.44	406	2.24
51	2.32	106	1.03	136	4.58	178	0.37	222	0.69	286	0.90	407	0.58
52	0.71	107	0.50	137	0.61	185	1.12	223	0.68	287	0.90	420	2.52
53	0.38	108	0.34	138	0.48	191	0.38	229	0.90	288	0.35	421	5.53
55	0.51	109	0.50	139	0.33	192	0.45	230	0.35	300	1.41	422	100.00
63	0.64	114	0.56	140	0.92	193	0.58	231	0.58	301	1.33	423	32.98
64	0.47	115	1.20	141	0.48	194	0.52	236	1.22	302	0.69	424	5.84
65	1.63	116	0.76	142	0.58	196	0.46	238	7.60	303	0.76	425	0.86
77	15.62	117	0.51	143	0.79	197	0.34	239	1.41	311	0.88	440	1.55
78	5.51	118	0.73	144	0.36	204	0.50	243	0.35	312	1.52	441	0.36
79	0.73	119	0.61	150	0.63	205	0.78	244	0.35	313	1.43	442	0.61
88	0.38	121	65.38	151	0.37	206	0.57	245	0.61	314	1.36	457	4.03
89	1.63	122	5.85	152	0.54	207	1.49	259	0.70	315	0.51	458	1.33
90	0.98	123	0.83	155	1.35	208	0.79	260	0.47	321	0.68	459	1.50
91	4.95	127	0.47	156	0.69	209	0.40	264	0.64	322	0.39	460	0.38
92	0.58	128	1.36	157	0.46	211	0.36	271	0.45	323	0.44		
93	0.43	129	1.39	161	0.45	216	0.35	272	0.83	336	0.56		
94	0.39	130	0.54	165	0.64	217	0.58	273	0.51	338	0.39		
102	1.71	131	0.40	166	0.37	218	0.65	277	3.87	392	0.67		

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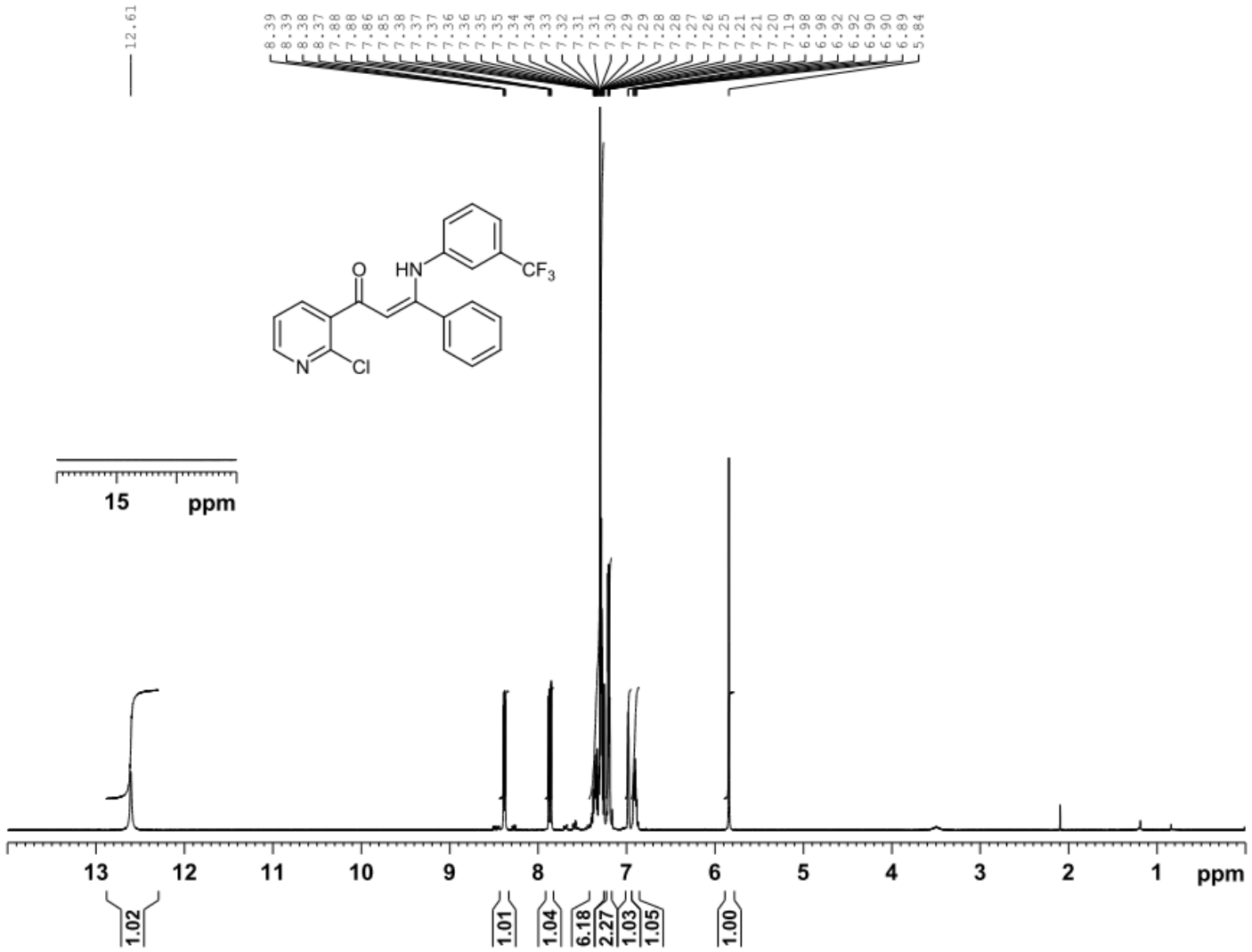
Dudkin, sd 267, CDCl3, 1H



BRUKER

Current Data Parameters
NAME 110708.u311 sd 267
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110708
Time 11.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300273 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Dudkin, sd 267, CDCl3, 13C

189.06

161.61
150.18
147.56
139.58
138.36
136.77
134.23
131.94
131.50
131.07
130.64
130.42
129.32
128.85
128.26
126.22
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121.10
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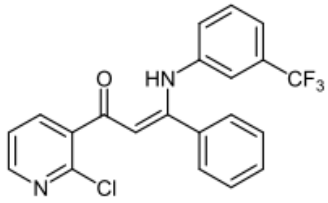
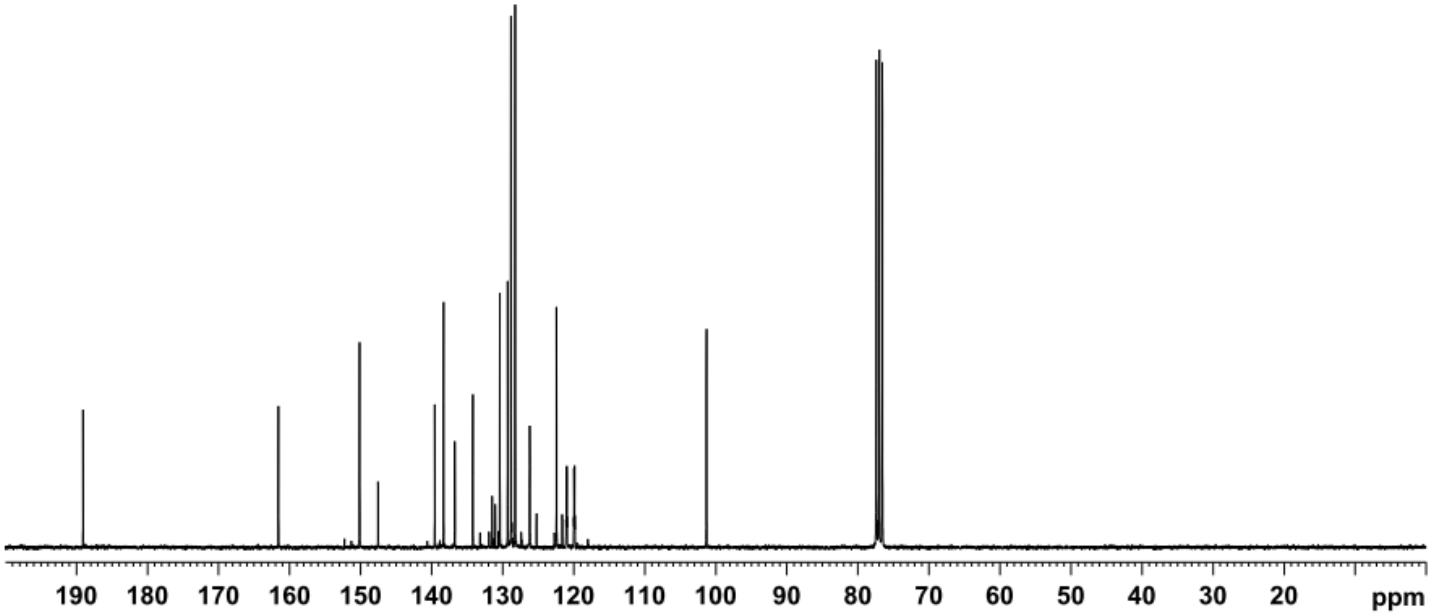
119.86
101.33





BRUKER

Current Data Parameters

NAME	110708.u311 sd 267
EXPNO	13
PROCNO	1

F2 - Acquisition Parameters

Date_	20110709
Time	16.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3072
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677530 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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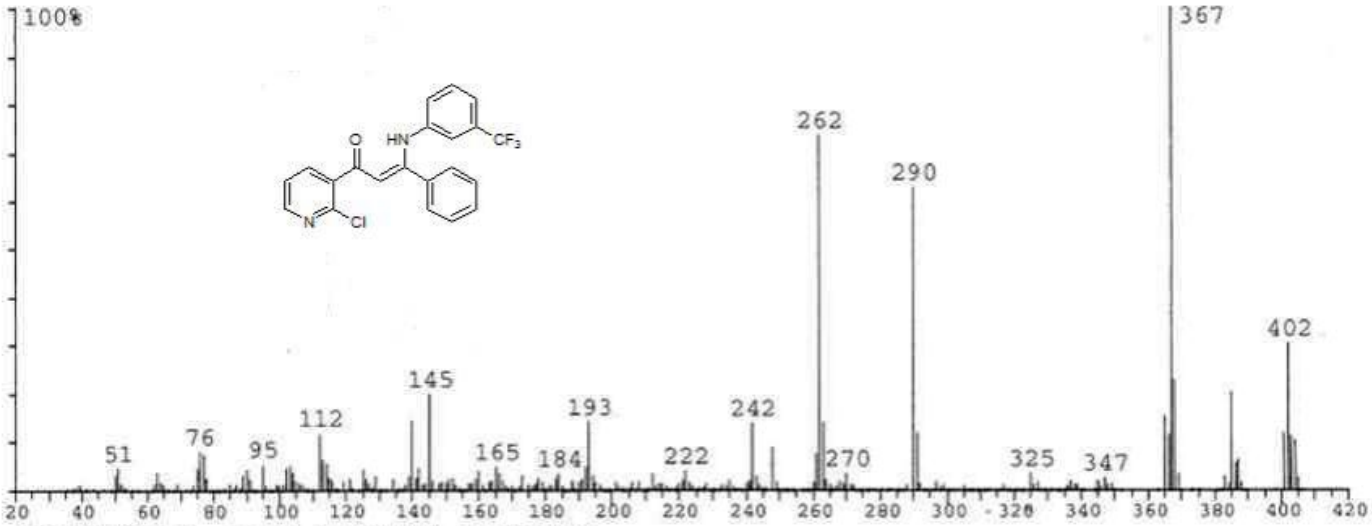

B3406(32:34) 2 13% 11071110 sd 267/GC

39	0.91	101	0.91	140	14.17	166	3.00	212	3.14	262	73.24	339	0.75
50	2.73	102	4.40	141	2.20	167	1.61	214	1.20	263	13.89	345	1.80
51	4.22	103	4.80	142	4.27	173	2.97	215	1.02	264	1.95	347	2.17
52	1.16	104	3.38	143	0.82	175	0.86	220	1.02	265	0.77	348	0.71
62	1.01	105	1.62	144	1.01	177	1.23	221	1.67	268	1.58	349	0.96
63	3.29	106	1.17	145	19.64	178	2.12	222	3.73	269	1.19	365	15.04
64	1.26	107	0.74	146	1.80	179	1.51	223	1.37	270	3.08	366	11.39
65	0.85	112	11.37	148	1.18	182	0.72	228	1.01	271	0.81	367	100.00
69	0.99	113	6.15	149	1.39	183	2.17	233	0.68	272	0.87	368	22.54
74	0.88	114	5.03	150	1.04	184	3.20	234	0.66	288	0.79	369	3.07
75	4.21	115	2.33	151	2.01	188	1.79	235	1.63	290	62.52	383	2.52
76	7.82	116	1.78	152	2.19	190	1.29	236	0.65	291	11.43	384	1.19
77	7.32	119	1.47	153	0.73	191	1.92	240	1.09	292	1.09	385	19.83
78	2.28	121	1.97	157	1.19	192	4.48	241	1.68	297	1.42	386	5.16
85	1.19	125	3.89	158	1.07	193	13.75	242	13.55	299	0.90	387	5.99
87	0.87	126	2.08	159	1.93	194	2.75	243	2.46	317	0.72	388	1.42
89	2.87	127	1.23	160	3.64	195	1.28	244	0.82	325	3.15	401	11.52
90	3.92	129	2.45	161	0.90	196	0.74	248	8.53	326	0.89	402	30.05
91	1.98	134	2.08	163	1.25	201	1.28	249	1.44	327	1.31	403	11.03
95	5.00	138	0.81	164	1.79	206	1.43	260	1.38	337	1.60	404	10.02
99	0.86	139	2.61	165	4.64	208	1.44	261	7.30	338	0.81	405	2.27

B3406(32:34) 2 13% 11071110 sd 267/GC lim: 0.65%

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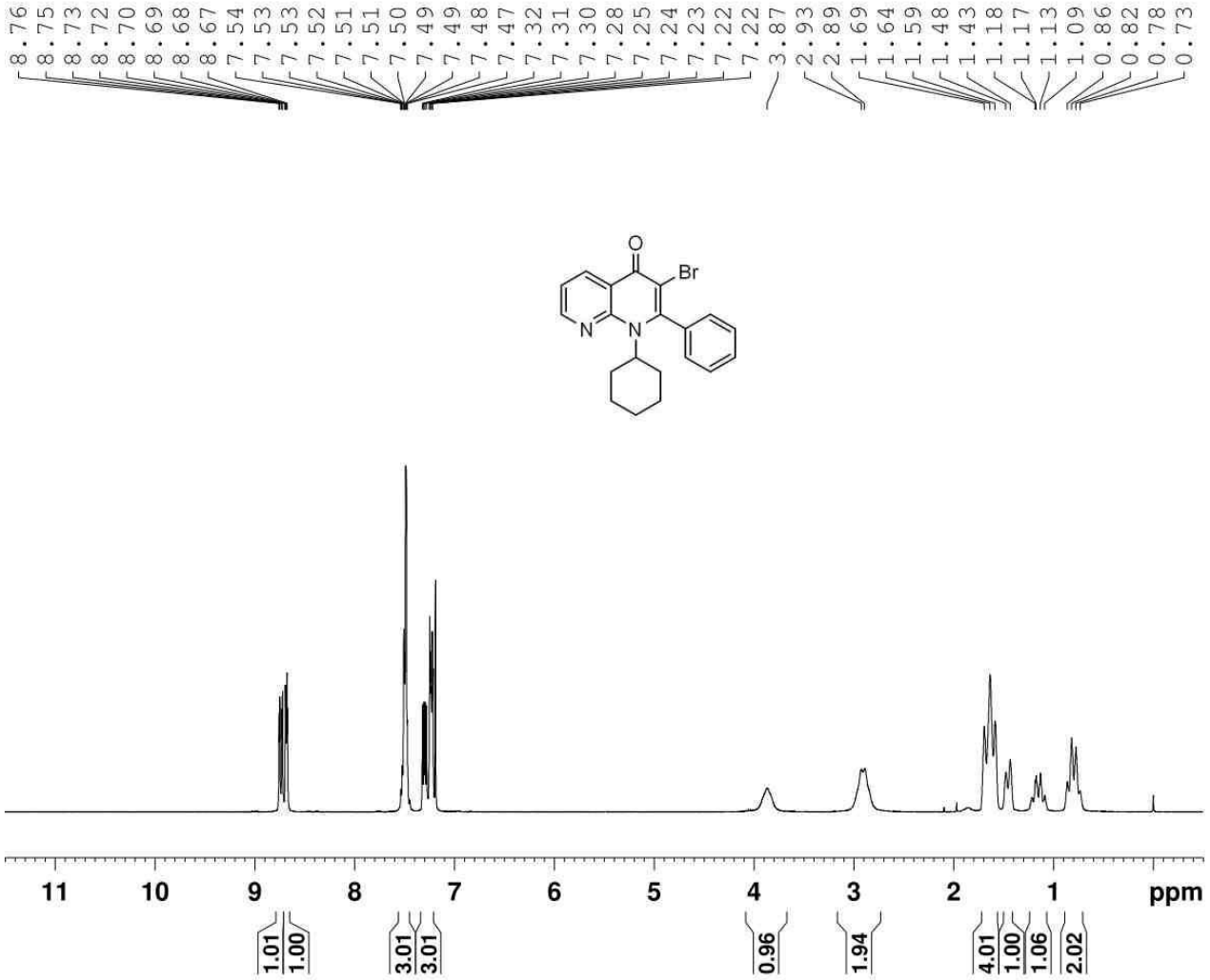

BRUKER

NAME	110113.u321	
EXPNO	10	
PROCNO	1	
Date_	20110113	
Time	11.55	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300287	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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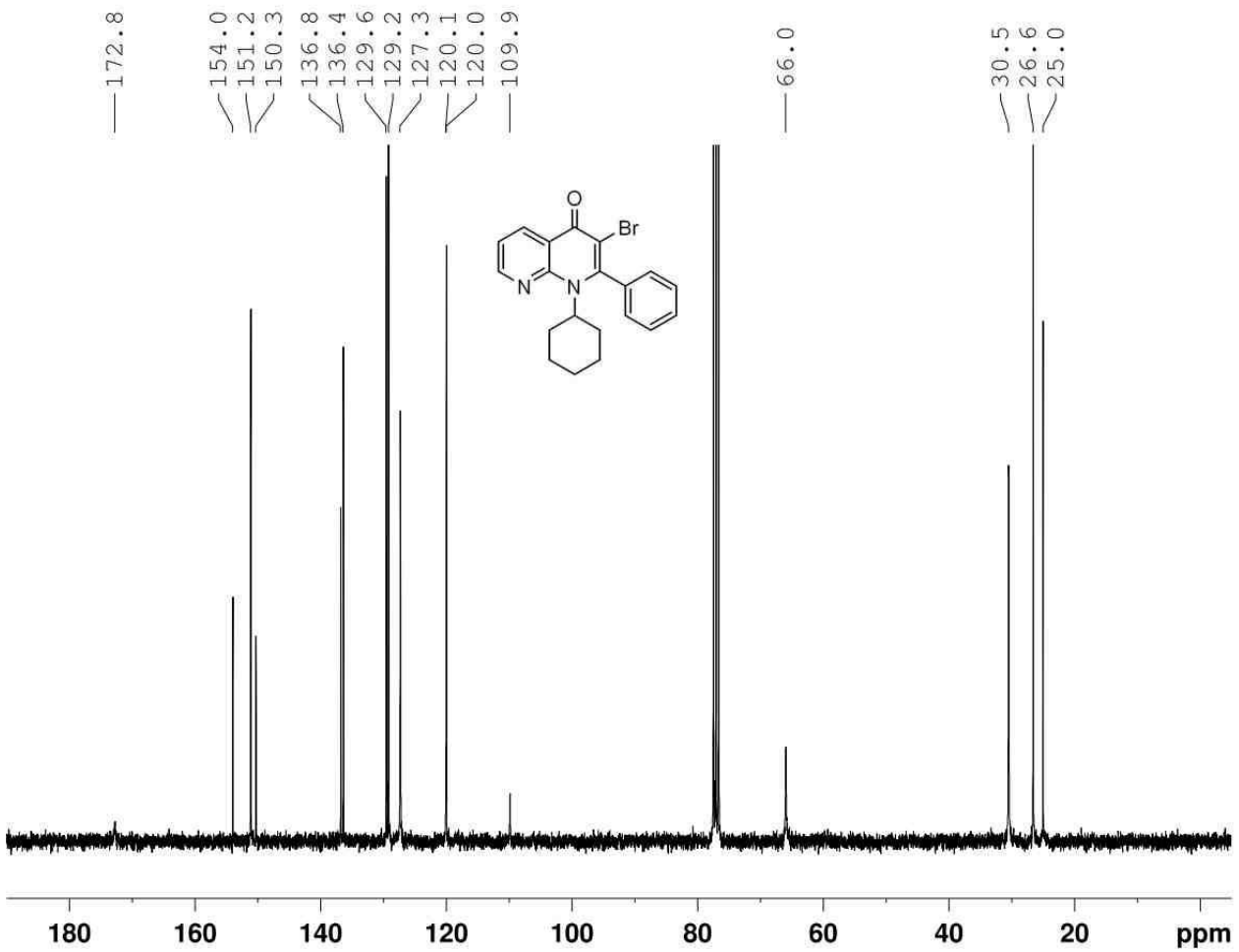

BRUKER

NAME	110114.u340	
EXPNO	10	
PROCNO	1	
Date_	20110116	
Time	23.58	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	18028.846	Hz
FIDRES	0.275098	Hz
AQ	1.8175818	sec
RG	2050	
DW	27.733	usec
DE	10.00	usec
TE	298.2	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	-0.50	dB
PL1W	33.25691986	W
SFO1	75.4752953	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	72.00	usec
PL2	0.00	dB
PL12	17.00	dB
PL13	17.00	dB
PL2W	11.25325108	W
PL12W	0.22453187	W
PL13W	0.22453187	W
SFO2	300.1312005	MHz
SI	32768	
SF	75.4677490	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

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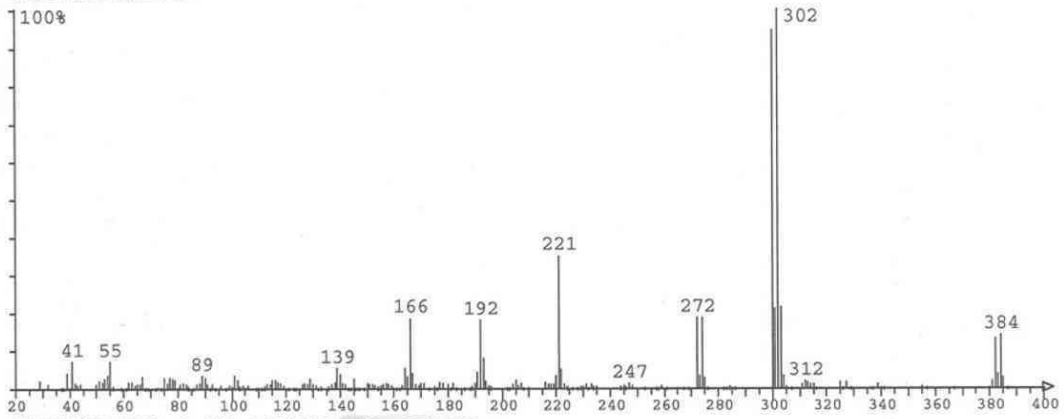
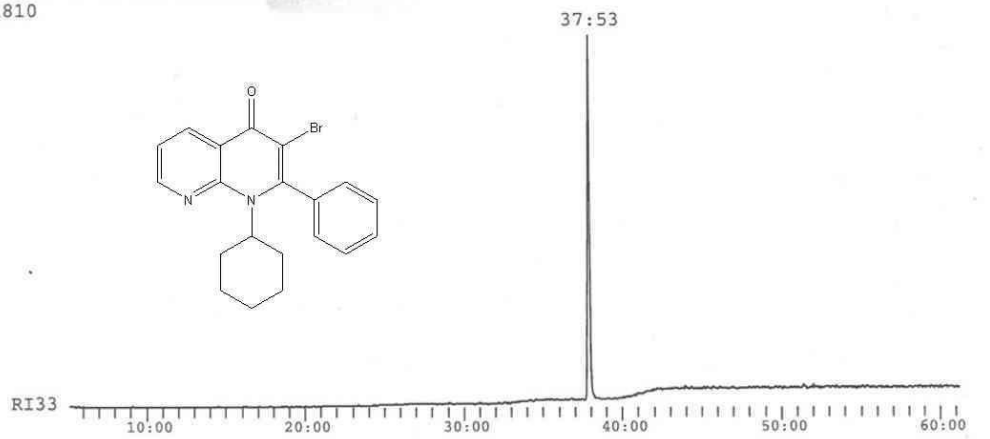
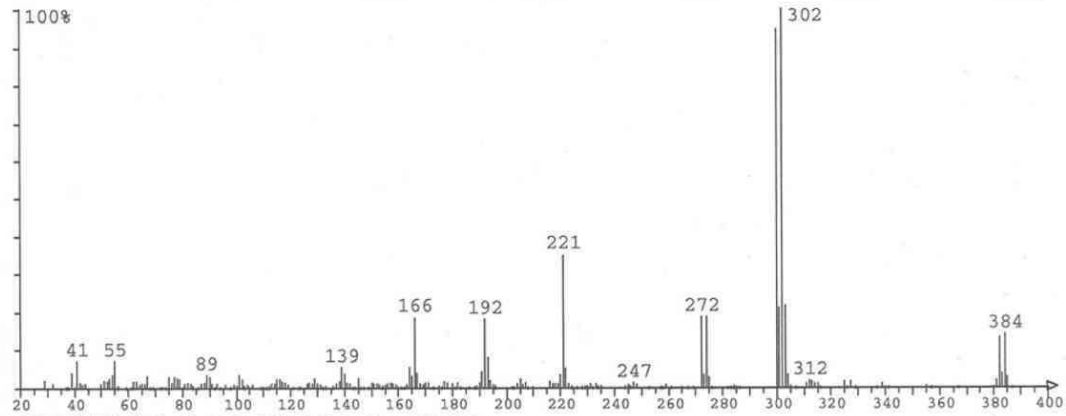
MassLib/PC



B4065(37:53) 2 17% 11011810 ikp 272/GC

11011810





B4065(37:53) 2 17% 11011810 ikp 272/GC

29	1.76	76	1.18	112	0.47	145	2.21	177	1.45	221	34.89	300	94.55
32	0.78	77	2.60	113	0.90	150	1.03	178	1.15	222	4.97	301	20.70
39	3.83	78	2.17	114	0.89	151	0.75	180	0.77	223	0.83	302	100.00
41	6.84	79	1.85	115	2.00	152	0.84	182	0.99	224	0.47	303	21.30
42	1.04	81	0.70	116	2.11	153	0.62	189	0.46	229	0.43	304	3.16
43	0.59	82	1.06	117	1.45	154	0.47	190	0.98	230	0.45	305	0.52
44	0.75	83	0.75	118	1.22	155	0.55	191	4.13	231	0.73	311	0.74
50	0.90	87	0.71	119	0.55	156	0.77	192	17.86	233	0.70	312	1.53
51	1.59	88	1.13	126	0.80	157	1.12	193	7.73	234	0.48	313	1.27
52	1.26	89	3.12	127	1.03	158	0.79	194	1.54	235	0.46	314	0.79
53	2.12	90	2.68	128	0.80	159	0.54	195	0.61	244	0.51	315	0.74
54	3.00	91	0.69	129	2.29	163	0.52	196	0.47	245	0.59	325	1.31
55	6.84	93	0.79	130	0.66	164	5.09	204	0.94	246	0.44	327	1.32
56	0.52	96	0.54	131	0.63	165	2.74	205	1.94	247	1.00	339	0.80
62	1.32	99	0.57	136	0.39	166	18.36	206	0.62	248	0.56	355	0.39
63	1.37	100	0.44	137	0.70	167	3.64	207	1.14	259	0.56	381	1.73
64	0.57	101	3.01	138	1.52	168	0.82	216	1.31	272	18.45	382	13.12
65	0.92	102	2.00	139	5.22	169	0.56	217	0.76	273	3.23	383	3.48
66	0.75	103	0.52	140	3.55	170	1.01	218	0.80	274	18.44	384	13.93
67	2.76	104	0.61	141	1.09	171	1.05	219	0.81	275	2.48	385	2.52
75	2.43	106	0.59	142	0.84	175	0.39	220	3.01	284	0.40		

B4065(37:53) 2 17% 11011810 ikp 272/GC lim: 0.38%

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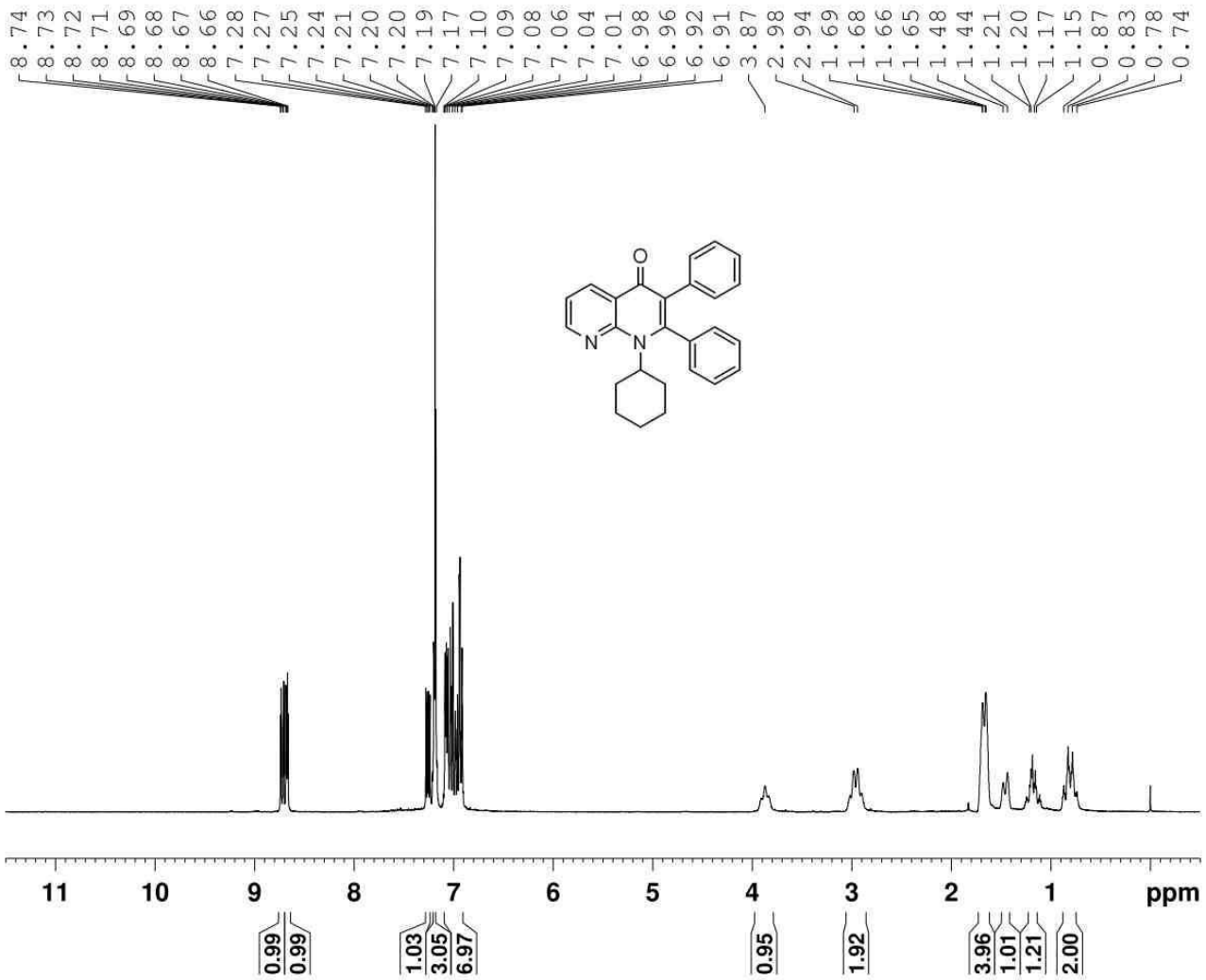


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NAME            110211.u322
EXPNO                    10
PROCNO                    1
Date_              20110211
Time                  11.00
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT             CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      161
DW                   80.800 use
DE                   10.00 use
TE                   298.2 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   10.00 use
PL1                   0.00 dB
PL1W           11.25325108 W
SFO1           300.1318534 MHz
SI                    32768
SF             300.1300296 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
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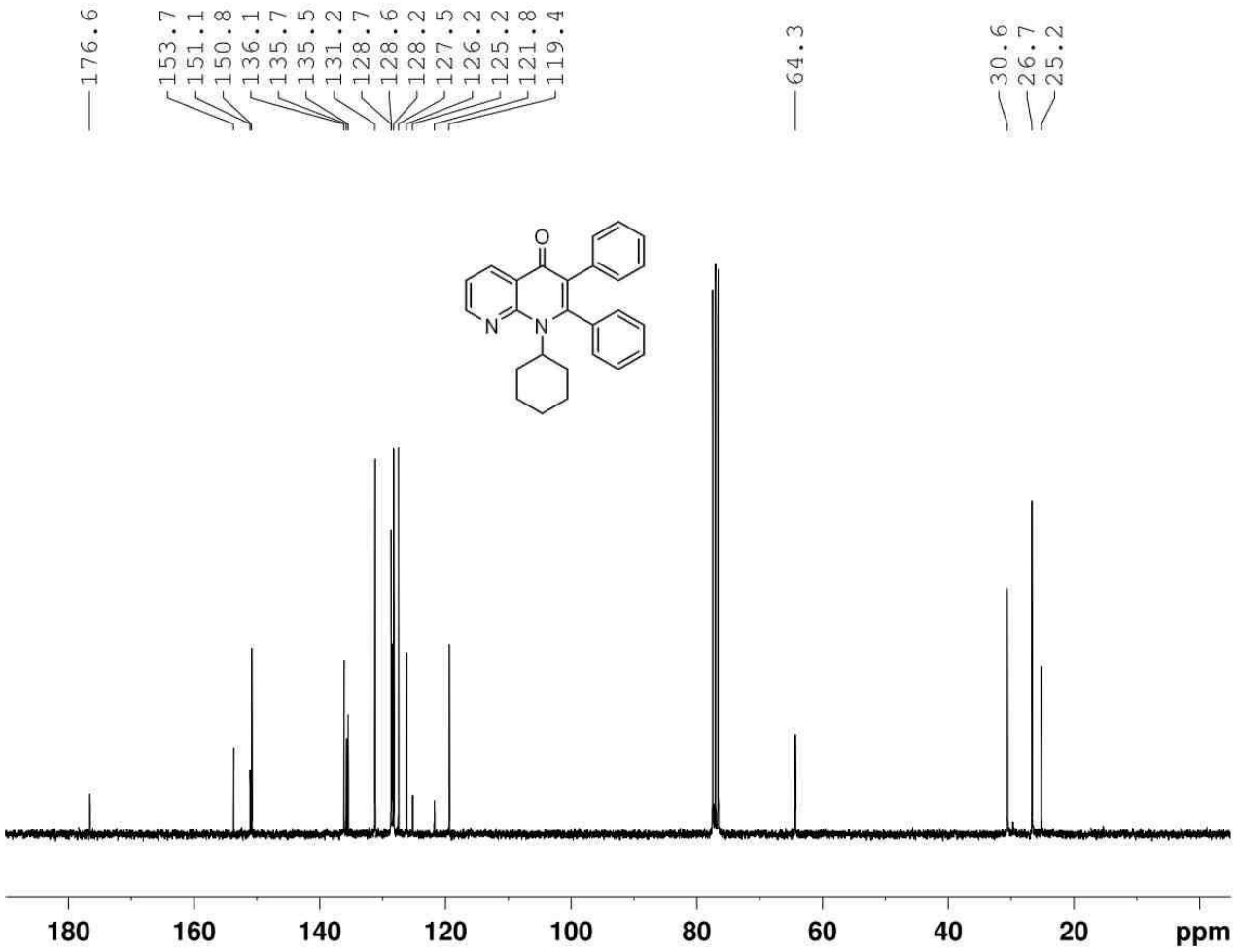

BRUKER

NAME	110211.u322
EXPNO	11
PROCNO	1
Date_	20110211
Time	22.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	27.733 usec
DE	10.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25325108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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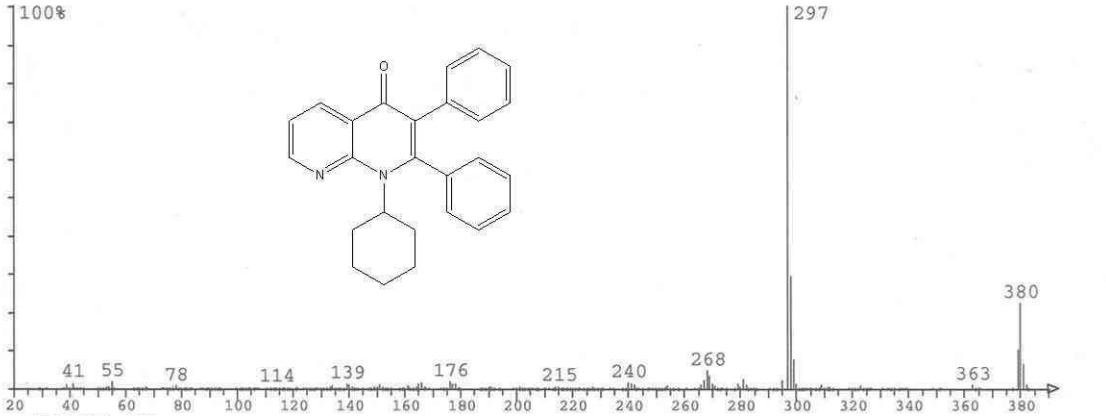

B4354(41:13) 2 40% 11020722 ikp 287/GC

29	0.28	89	0.20	145	0.35	179	0.23	228	0.20	272	0.29	322	0.16
39	0.74	91	0.15	147	0.26	187	0.15	229	0.25	279	1.00	323	0.54
41	1.22	93	0.15	148	0.28	188	0.18	231	0.13	280	0.40	324	0.20
50	0.18	101	0.14	149	0.43	189	0.19	238	0.16	281	2.17	325	0.19
51	0.26	103	0.13	150	0.45	190	0.38	240	1.26	282	0.76	335	0.27
52	0.17	104	0.19	151	0.74	191	0.37	241	1.23	283	0.15	337	0.17
53	0.45	113	0.25	152	0.50	192	0.24	242	0.68	292	0.15	351	0.25
54	0.47	114	0.29	153	0.19	200	0.17	243	0.13	295	2.04	363	0.86
55	1.63	115	0.24	158	0.16	201	0.44	247	0.17	297	100.00	364	0.33
56	0.15	116	0.14	161	0.53	203	0.28	251	0.29	298	29.24	365	0.24
63	0.15	117	0.14	162	0.14	205	0.20	252	0.23	299	7.57	377	0.19
64	0.17	121	0.18	163	0.16	207	0.24	253	0.40	300	1.11	379	10.19
65	0.17	126	0.29	164	0.52	213	0.36	254	0.53	301	0.31	380	22.19
66	0.17	127	0.27	165	0.99	214	0.44	255	0.20	302	0.25	381	6.23
67	0.46	128	0.24	166	1.31	215	0.51	265	0.24	307	0.20	382	0.88
76	0.14	133	0.41	167	0.38	217	0.15	266	0.92	308	0.19	383	0.15
77	0.50	134	0.58	174	0.15	218	0.19	267	1.84	309	0.68		
78	0.60	139	1.04	175	0.35	219	0.25	268	4.58	310	0.23		
79	0.31	140	0.85	176	1.71	220	0.14	269	3.21	311	0.45		
82	0.26	141	0.37	177	1.17	226	0.28	270	1.03	312	0.38		
83	0.17	142	0.17	178	0.98	227	0.49	271	0.56	321	0.28		

B4354(41:13) 2 40% 11020722 ikp 287/GC lim: 0.13%

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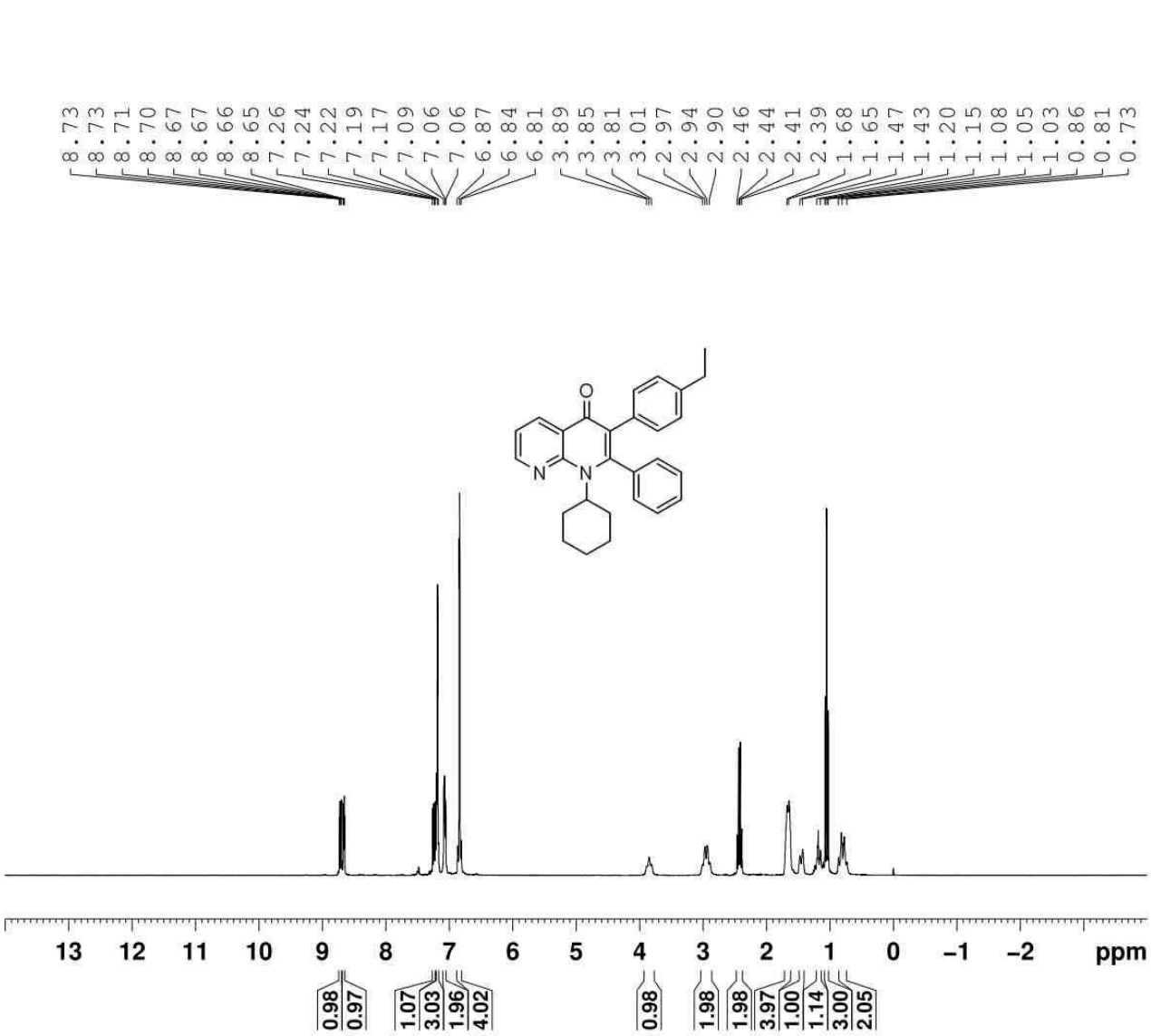

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PROCNO	1	
Date_	20110209	
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PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	6188.119	Hz
FIDRES	0.094423	Hz
AQ	5.2953587	sec
RG	144	
DW	80.800	use
DE	10.00	use
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 =======		
NUC1	1H	
P1	10.00	use
PL1	0.00	dB
PL1W	11.25325108	W
SFO1	300.1318534	MHz
SI	32768	
SF	300.1300301	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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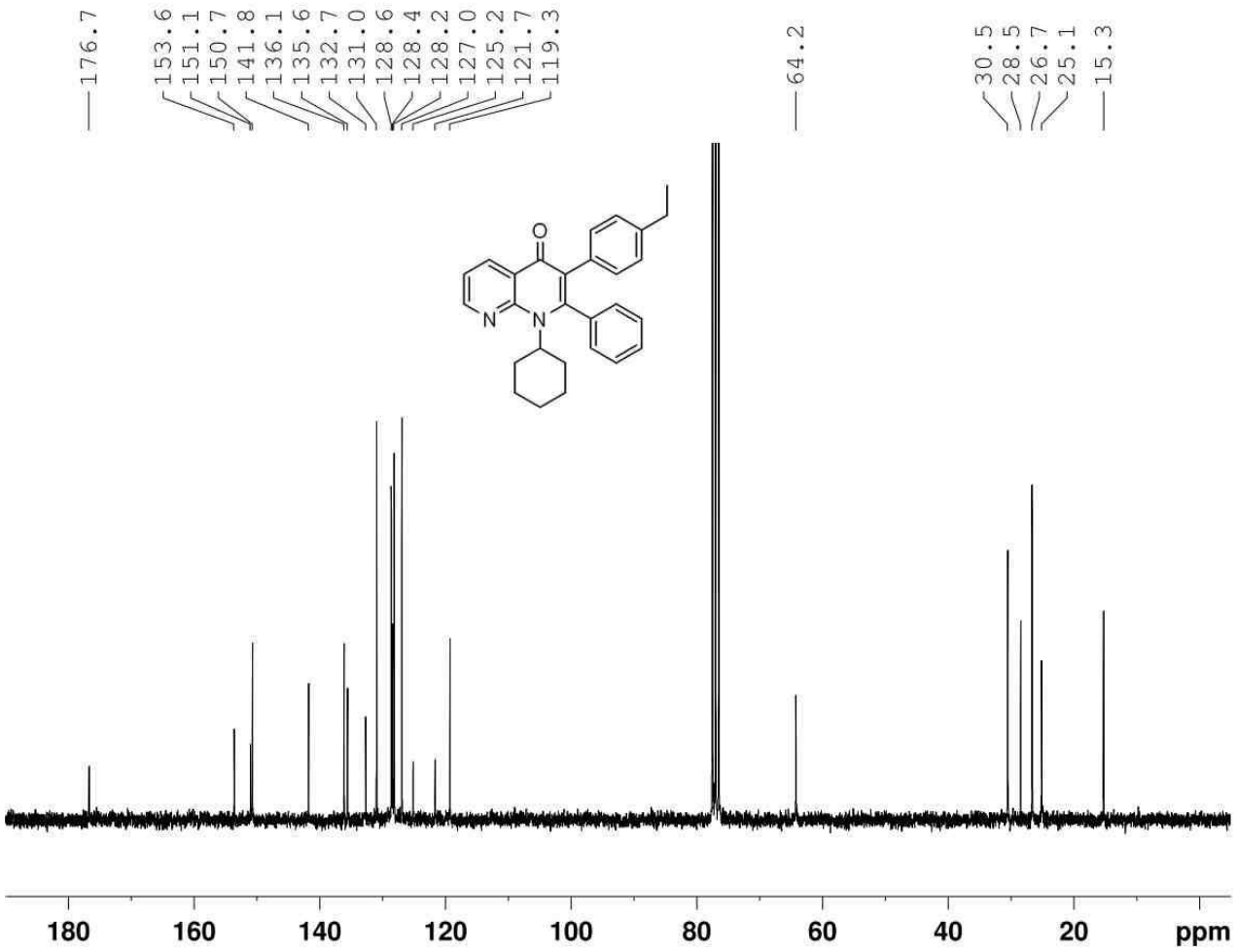

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EXPNO	10	
PROCNO	1	
Date_	20110210	
Time	13.21	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	800	
DS	4	
SWH	15000.000	Hz
FIDRES	0.228882	Hz
AQ	2.1845834	sec
RG	2050	
DW	33.333	usec
DE	10.00	usec
TE	298.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	-1.00	dB
SFO1	62.9015280	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	70.00	usec
PL12	15.00	dB
PL13	15.00	dB
PL2	-2.50	dB
SFO2	250.1310005	MHz
SI	32768	
SF	62.8952390	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

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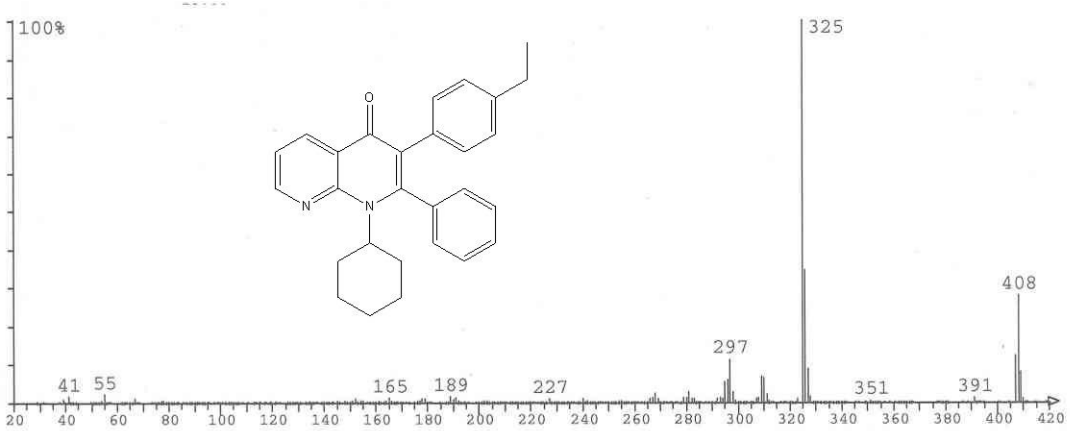

B4755(44:27) 2 33% 11020719 ikp 285/GC

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39	0.57	131	0.16	167	0.20	217	0.17	268	2.30	305	0.27	351	0.40
41	1.35	133	0.17	168	0.22	218	0.25	269	0.78	306	0.15	353	0.19
53	0.37	134	0.18	176	0.47	227	0.80	270	0.33	307	0.95	379	0.22
54	0.44	139	0.27	177	0.49	228	0.19	271	0.27	308	1.08	391	1.19
55	1.99	140	0.37	178	0.67	230	0.28	278	0.22	309	6.51	392	0.34
67	0.83	141	0.29	179	0.67	232	0.15	279	1.11	310	6.32	407	12.16
77	0.46	145	0.38	189	1.46	233	0.24	280	0.98	311	1.89	408	27.78
78	0.49	146	0.22	190	0.65	238	0.17	281	2.47	312	0.43	409	7.67
79	0.34	148	0.41	191	1.11	239	0.19	282	0.93	321	0.30	410	0.84
81	0.20	149	0.20	192	0.45	240	0.67	283	0.71	322	0.15		
82	0.25	150	0.17	194	0.34	241	0.31	284	0.31	323	0.92		
83	0.24	151	0.40	201	0.18	242	0.37	291	0.15	325	100.00		
89	0.15	152	0.73	202	0.51	246	0.14	292	0.69	326	34.46		
91	0.18	153	0.22	203	0.42	252	0.22	293	1.24	327	8.73		
103	0.15	154	0.45	204	0.30	253	0.33	294	0.82	328	1.31		
115	0.23	155	0.47	205	0.29	254	0.40	295	5.03	329	0.30		
117	0.19	161	0.50	206	0.19	255	0.39	296	5.64	330	0.15		
121	0.18	163	0.26	207	0.36	259	0.16	297	11.08	337	0.21		
126	0.27	164	0.51	213	0.17	265	0.18	298	2.54	339	0.30		
127	0.22	165	1.06	214	0.20	266	0.72	299	0.37	340	0.31		

B4755(44:27) 2 33% 11020719 ikp 285/GC lim: 0.14%

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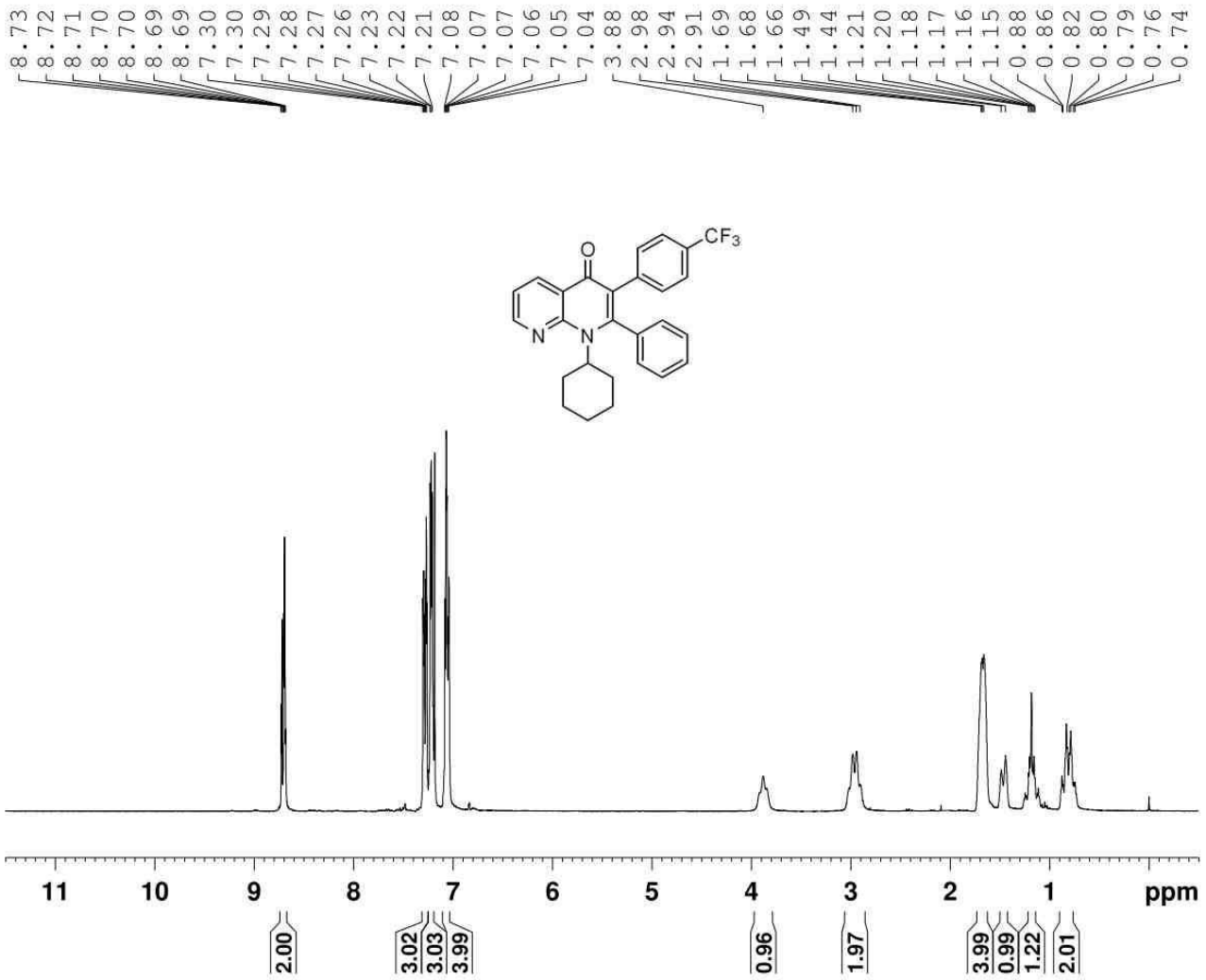

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PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	128
DW	80.800 use
DE	10.00 use
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 use
PL1	0.00 dB
PL1W	11.25325108 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300302 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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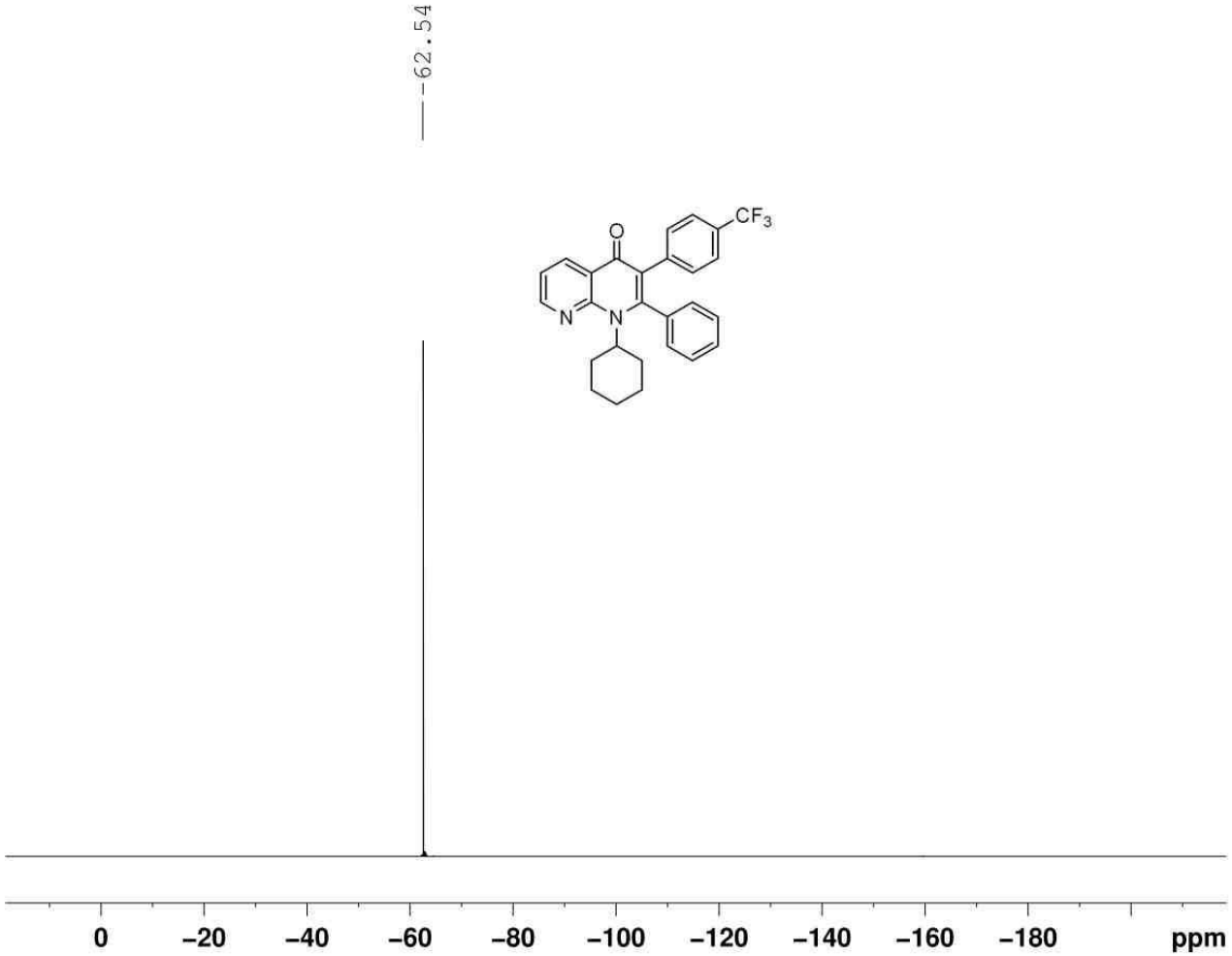
^{19}F



NAME	110215.u301	
EXPNO	10	
PROCNO	1	
Date_	20110215	
Time	8.04	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgfhigqn	
TD	131072	
SOLVENT	CDCl3	
NS	64	
DS	4	
SWH	66964.289	Hz
FIDRES	0.510897	Hz
AQ	0.9787210	sec
RG	2050	
DW	7.467	usec
DE	10.00	usec
TE	298.2	K
D1	1.00000000	sec
D11	0.03000000	sec
D12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	10.00	usec
PL1	-3.00	dB
PL1W	15.53680420	W
SFO1	282.3761148	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	72.00	usec
PL2	0.00	dB
PL12	17.00	dB
PL2W	11.25325108	W
PL12W	0.22453187	W
SFO2	300.1312005	MHz
SI	65536	
SF	282.4043550	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

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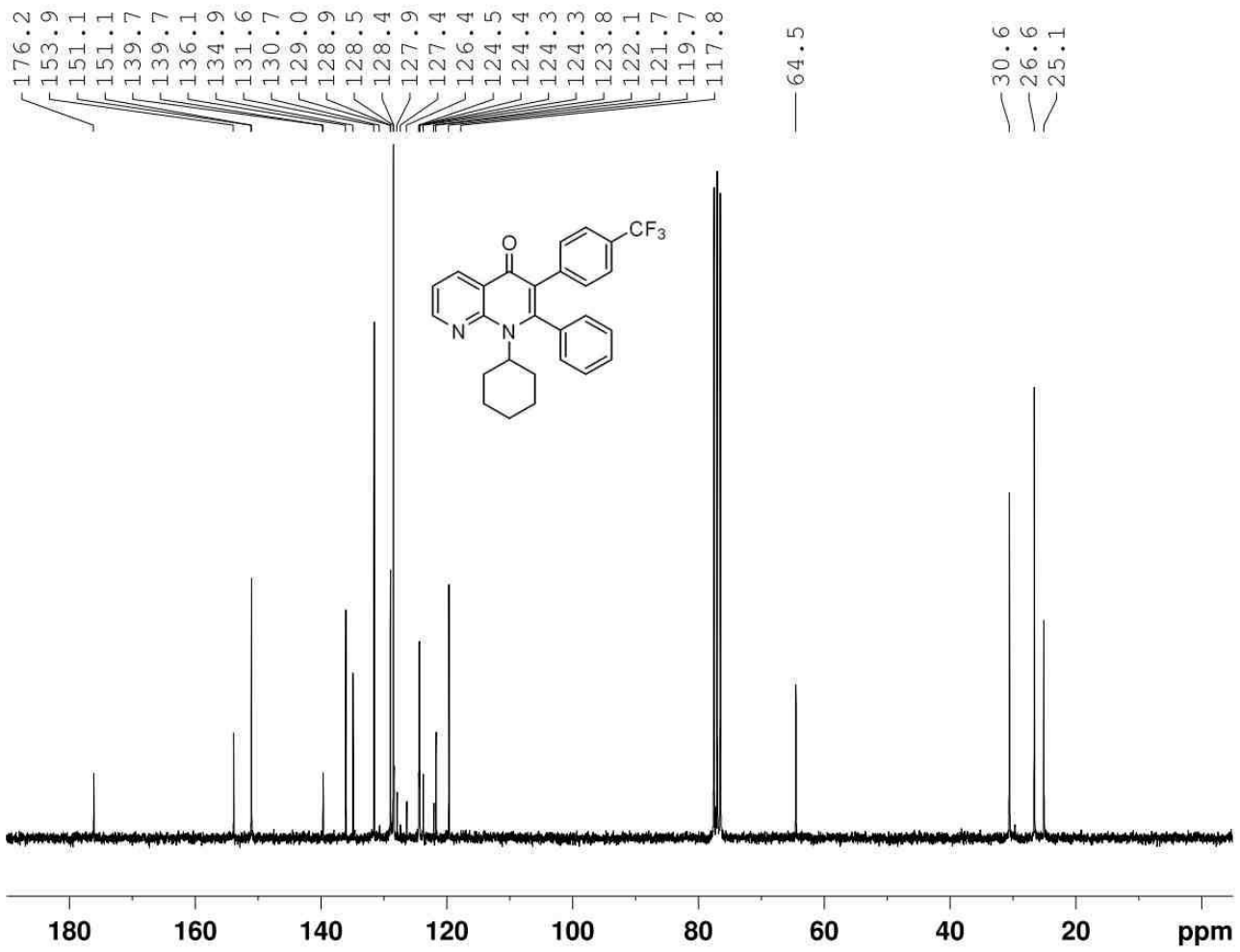

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NAME	110204.228
EXPNO	10
PROCNO	1
Date_	20110206
Time	15.12
INSTRUM	spect
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PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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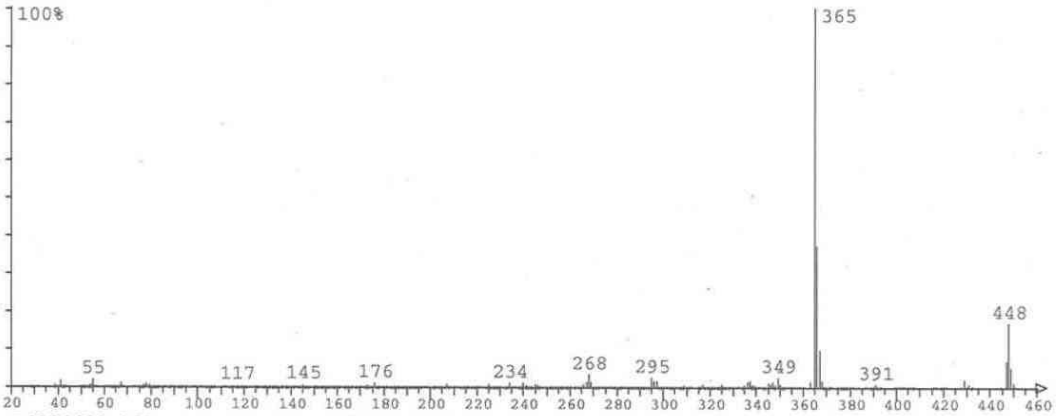
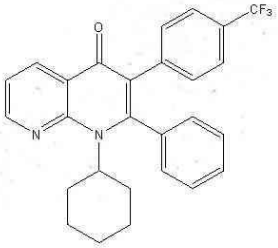
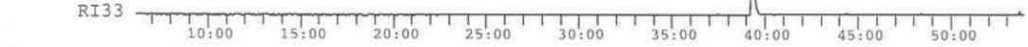


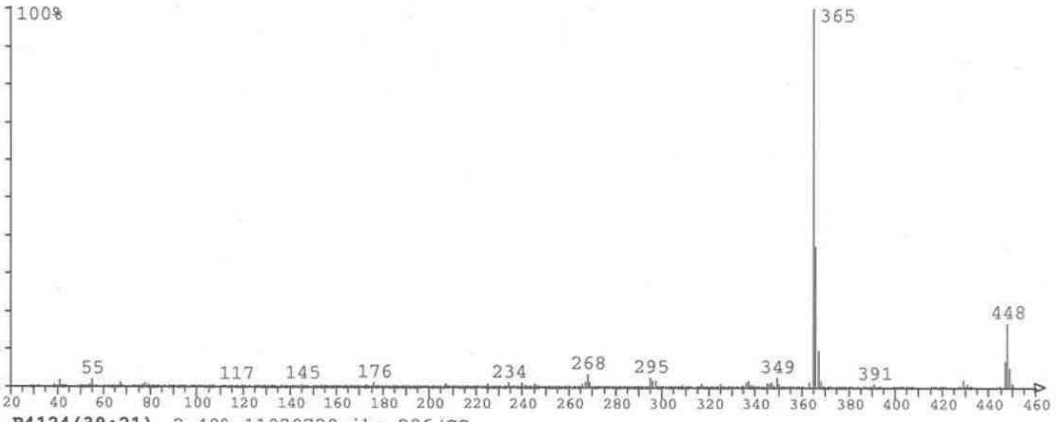
B4124(39:21) 2 40% 11020720 ikp 286/GC

11020720

39:21







B4124(39:21) 2 40% 11020720 ikp 286/GC

29	0.25	145	0.41	190	0.22	242	0.33	294	0.22	346	0.61	420	0.15
39	0.48	146	0.24	191	0.15	243	0.21	295	2.23	347	1.20	429	1.77
41	1.47	148	0.33	193	0.24	244	0.20	296	1.37	348	0.46	430	0.36
51	0.19	151	0.25	194	0.29	245	0.63	297	1.38	349	2.36	431	0.57
52	0.14	152	0.18	196	0.24	246	0.52	298	0.32	350	0.59	447	6.63
53	0.34	159	0.14	206	0.16	251	0.16	308	0.28	351	0.28	448	16.73
54	0.42	161	0.16	207	0.56	258	0.14	309	0.40	363	1.24	449	4.91
55	1.69	163	0.23	213	0.27	262	0.18	310	0.21	365	100.00	450	0.68
65	0.18	164	0.35	214	0.31	265	0.18	315	0.34	366	36.97		
67	0.75	165	0.29	215	0.15	266	0.61	317	0.58	367	9.57		
76	0.19	172	0.17	218	0.16	267	1.12	318	0.15	368	1.37		
77	0.44	173	0.37	225	0.56	268	3.08	321	0.17	369	0.19		
78	0.53	174	0.15	226	0.22	269	0.96	322	0.25	376	0.15		
79	0.51	175	0.23	227	0.37	270	0.24	325	0.63	377	0.33		
81	0.16	176	0.71	232	0.24	271	0.15	326	0.16	378	0.28		
83	0.18	177	0.23	233	0.32	279	0.16	335	0.38	379	0.37		
104	0.15	178	0.14	234	0.85	285	0.16	336	1.14	380	0.23		
117	0.19	183	0.26	235	0.20	286	0.22	337	1.30	389	0.21		
120	0.16	184	0.29	238	0.24	287	0.29	338	0.46	391	0.55		
134	0.19	188	0.19	240	0.82	288	0.15	339	0.42	405	0.18		
139	0.17	189	0.24	241	0.50	289	0.20	345	0.85	419	0.17		

B4124(39:21) 2 40% 11020720 ikp 286/GC lim: 0.14%

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Admin,HOK, Rostock

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(E) X-Ray structures

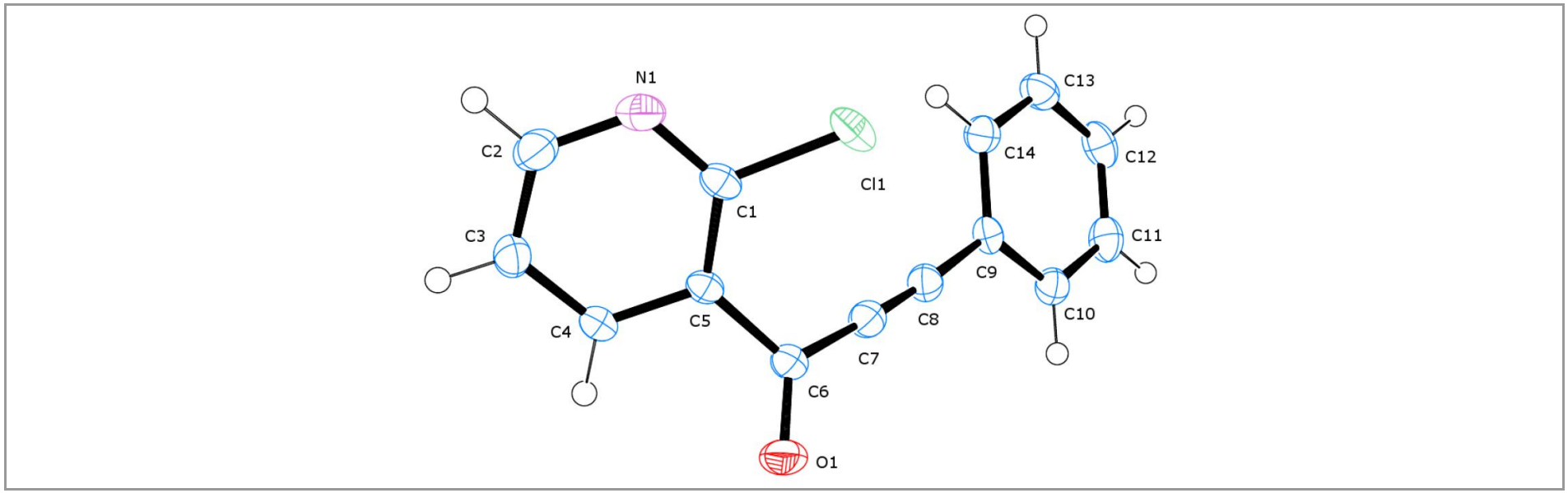

Figure 1. Structure of compound **3a.**

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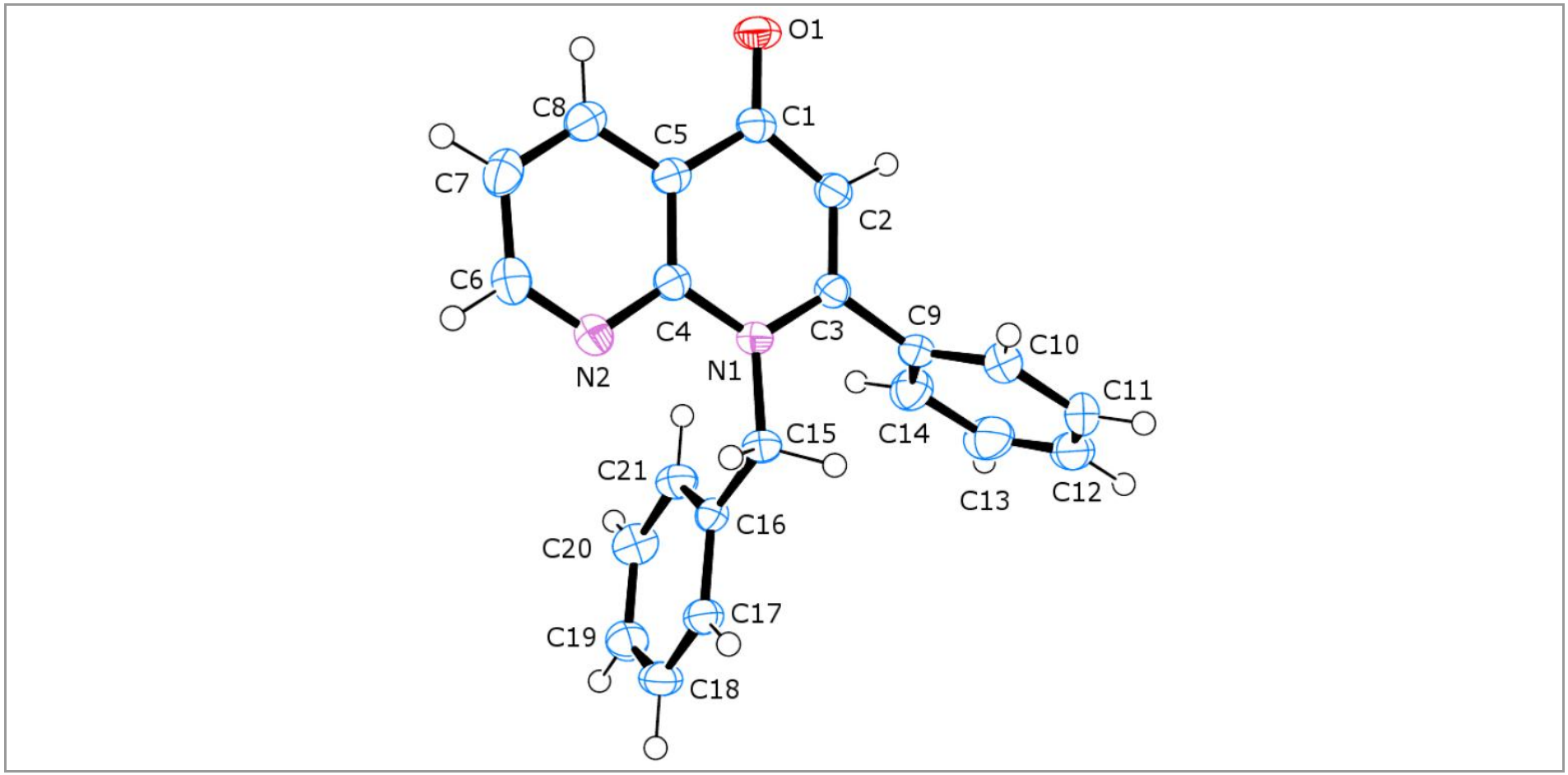

Figure 2. Structure of compound **5b.**

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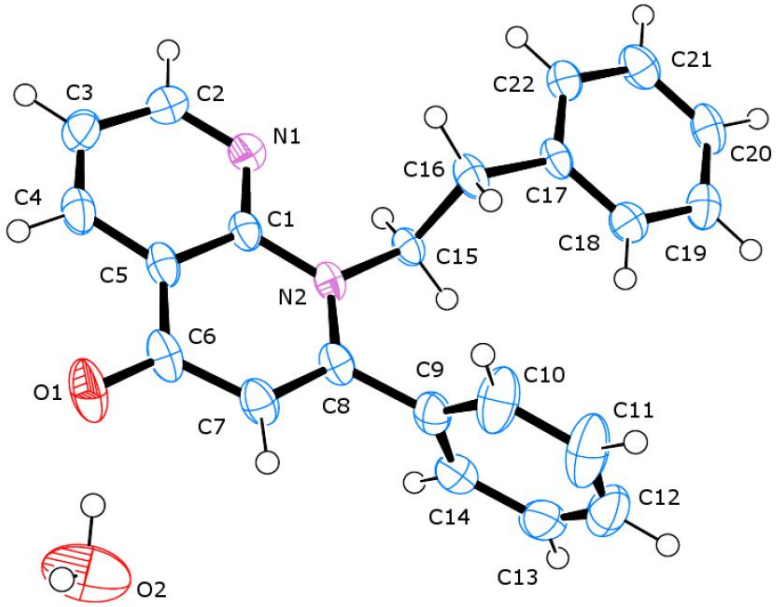

Figure 3. Molecular structure of compound **5f.**

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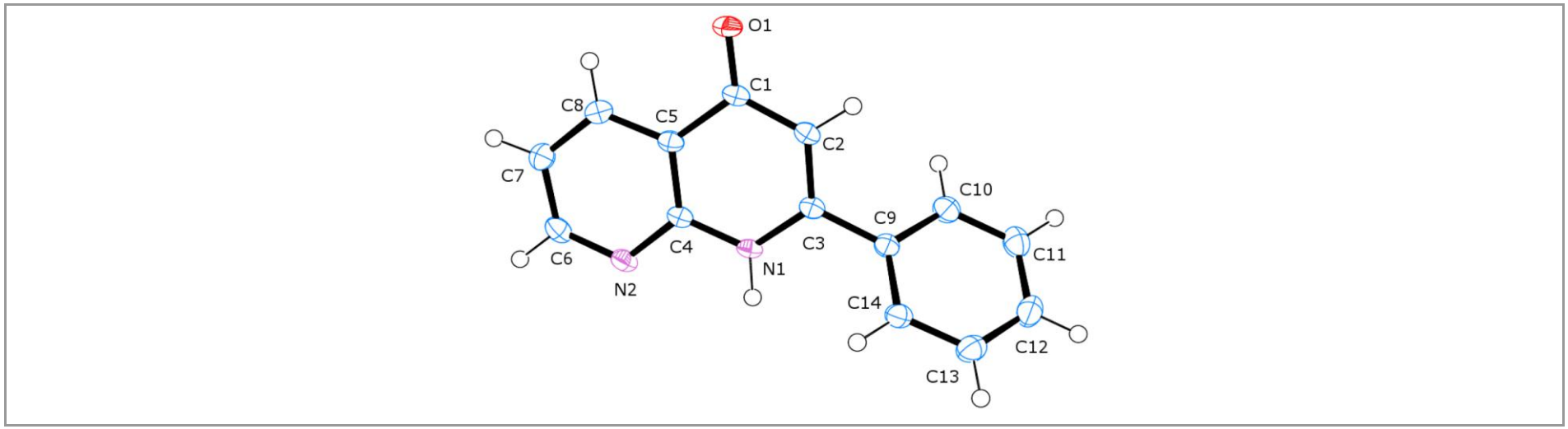

Figure 4. Molecular structure of compound **5k.**

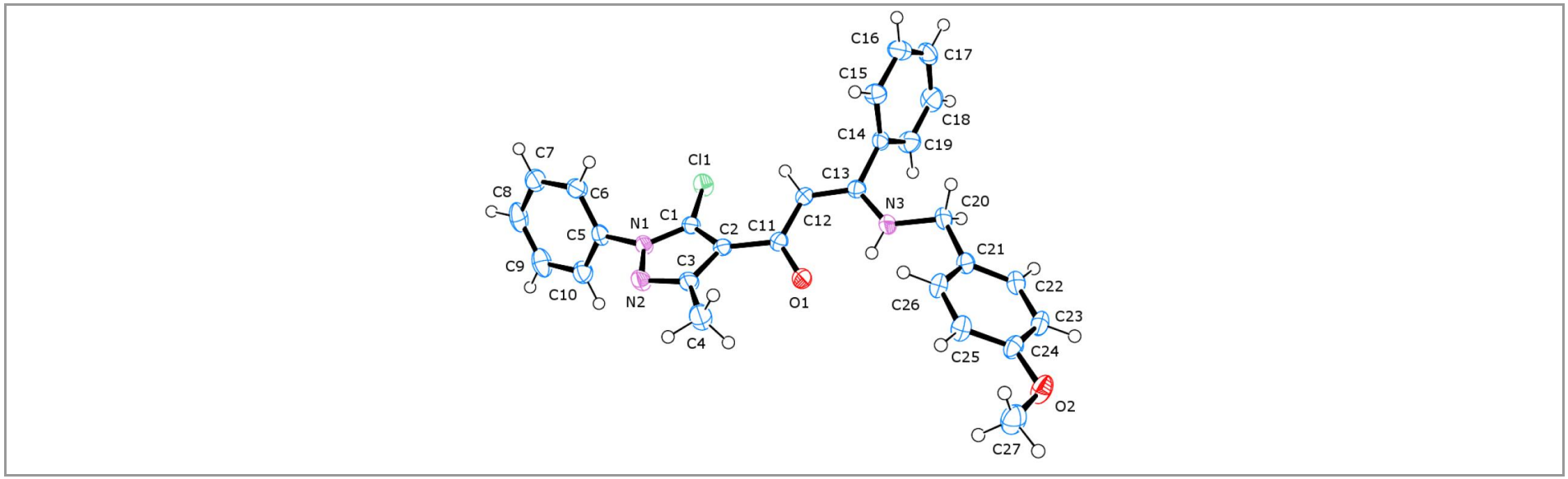

Figure 5. Molecular structure of compound **10.**

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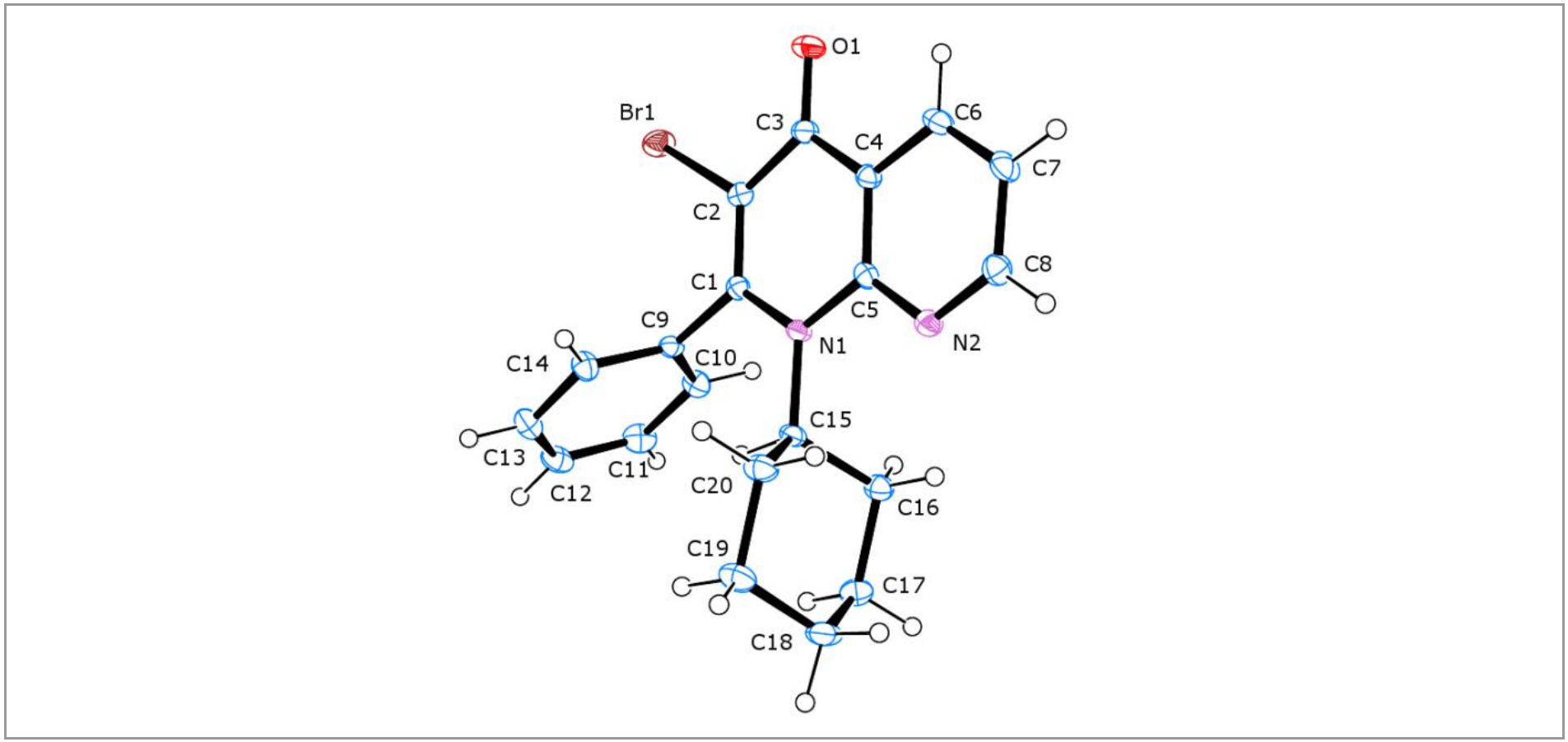

Figure 6. Structure **20.**