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Supporting Information

1,3-Dipolar [3+3] Cycloaddition of α-Halohydroxamate-based Azaoxyallyl Cations with Hydrazonoyl Chloride-derived Nitrile Imines

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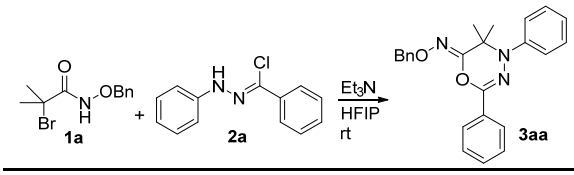
1. General Information

Proton (^{1}H) and carbon (^{13}C) NMR spectra were recorded on 400 MHz instrument (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR) and calibrated using tetramethylsilane (TMS) as internal reference. High resolution mass spectra (HRMS) were recorded under electrospray ionization (ESI) conditions. The melting point of compounds was determined by a melting point instrument. Flash column chromatography was performed on silica gel (0.035-0.070 mm) using compressed air. Thin layer chromatography (TLC) was carried out on 0.25 mm SDS silica gel coated glass plates (60F254). Eluted plates were visualized using a 254 nm UV lamp. Unless otherwise indicated, all reagents were commercially available and used without further purification. All solvents were distilled from the appropriate drying agents immediately before using. α-Halohydroxamates **1a-1f** and hydrazonoyl chlorides **2a-2n** were prepared according to literature procedures.[1-5]

2. General Procedure

To a stirred solution of α-halohydroxamate **1** (2.0 equiv, 0.2 mmol) in 0.5 mL of HFIP was added hydrazonoyl chlorides **2** (1.0 equiv, 0.1 mmol), followed by Et_3N (3.0 equiv, 0.3 mmol). The resulted reaction mixture was stirred at room temperature for 1.5-12 h. After the reaction was completed as indicated by TLC plate, the solvent was removed by evaporation and the crude product was purified by flash column chromatography on silica gel (petroleum ether / ethyl acetate = 80:1) to afford products **3** (24-96% yields).

3.Screening of ratios of 1a/2a/Et_3N.[a]

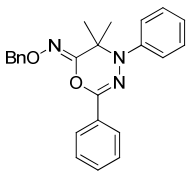


Entry	Equivalent ratio (**1a** / **2a** / Et_3N)	Time(h)	Yield[b](%)
1	1.5:1:2.5	1.5	60
2	2:1:3	1.5	67
3	2.5:1:3.5	1.5	67
4	1.8:1:2.8	1.5	64
5	2:1:3.5	1.5	67
6	2:1:2.5	1.5	65

[a]Unless otherwise noted, reactions were carried out with **1a** and **2a** in the presence of Et_3N in 0.5 mL of HFIP at the indicated equivalent ratios of **1a**/**2a**/ Et_3N at room temperature. [b]Isolated yield.

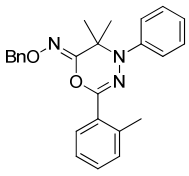
4. Characterization

(*Z*)-5,5-dimethyl-2,4-diphenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3aa):



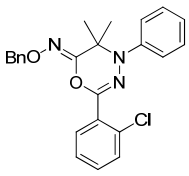
White solid, yield: 25.9 mg, 67%; M.P.=103.7-105.2 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.02-7.99 (m, 2H), 7.51 (d, *J*=7.2 Hz, 2H), 7.46-7.42 (m, 6H), 7.40-7.36 (m, 4H), 7.32-7.28 (m, 1H), 5.19 (s, 2H), 1.38 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.6, 144.9, 141.3, 137.8, 130.1, 129.7, 128.4, 128.4, 128.3, 127.9, 127.8, 126.4, 125.6, 76.7, 55.6, 20.8 ppm; HRMS (ESI) calculated for $C_{24}H_{24}N_3O_2$ $[M + H]^+$: 386.1866, found 386.1863.

(*Z*)-5,5-dimethyl-4-phenyl-2-(o-tolyl)-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ab):



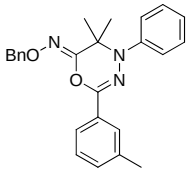
Light yellow solid, yield: 15.5 mg, 39%; M.P.=102.8-103.9 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.90 (d, *J*=8.4 Hz, 2H), 7.51 (d, *J*=7.2 Hz, 2H), 7.46-7.42 (m, 3H), 7.40-7.36 (m, 4H), 7.32-7.28 (m, 1H), 7.24 (d, *J*=8.0 Hz, 2H), 5.19 (s, 2H), 2.43 (s, 3H), 1.37 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.8, 145.0, 141.5, 139.9, 137.8, 129.1, 128.4, 128.3, 128.2, 127.9, 127.8, 127.3, 126.3, 125.6, 76.6, 55.6, 21.5, 20.7 ppm; HRMS (ESI) calculated for $C_{25}H_{26}N_3O_2$ $[M + H]^+$: 400.2020, found 400.2016.

(*Z*)-2-(2-chlorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ac):



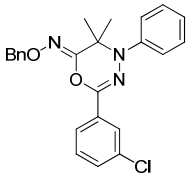
Yellow oil, yield: 10.2 mg, 24%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.71-7.68 (m, 1H), 7.48-7.44 (m, 3H), 7.41-7.38 (m, 3H), 7.36-7.33 (m, 4H), 7.32-7.31 (m, 2H), 7.29-7.25 (m, 1H), 5.13 (s, 2H), 1.40 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 144.5, 140.6, 137.7, 133.2, 133.0, 131.0, 130.7, 130.5, 129.9, 129.8, 128.4, 128.3, 128.2, 128.1, 127.8, 126.7, 126.4, 123.7, 119.7, 76.6,55.4, 20.6 ppm; HRMS (ESI) calculated for $C_{24}H_{23}ClN_3O_2$ $[M + H]^+$: 420.1473, found 420.1473.

(*Z*)-5,5-dimethyl-4-phenyl-2-(m-tolyl)-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ad):



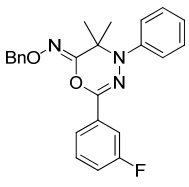
Yellow oil, yield: 20.2 mg, 51%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.81 (d, *J*=8.4 Hz, 2H), 7.53-7.51 (m, 2H), 7.46-7.41 (m, 5H), 7.38 (d, *J*=7.2 Hz, 2H), 7.35-7.29 (m, 2H), 7.28-7.25 (m, 1H), 5.20 (s, 2H), 2.43 (s, 3H), 1.37 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 144.9, 141.5, 138.0, 137.8, 130.6, 130.0, 128.4, 128.3, 128.2, 127.9, 127.8, 126.4, 126.1, 122.8, 76.6, 55.6, 21.5, 20.7 ppm; HRMS (ESI) calculated for $C_{25}H_{26}N_3O_2$ $[M + H]^+$: 400.2020, found 400.2012.

(*Z*)-2-(3-chlorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ae):



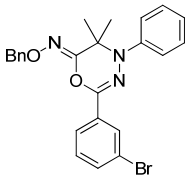
White solid, yield: 36.9 mg, 88%; M.P.=111.3-113.0 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.98 (s, 1H), 7.86 (d, *J*=7.2 Hz, 1H), 7.51 (d, *J*=6.8 Hz, 2H), 7.46-7.39 (m, 6H), 7.36-7.30 (m, 4H), 5.19 (s, 2H), 1.37 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.2, 144.6, 140.0, 137.7, 134.5, 131.9, 129.7, 129.6, 128.5, 128.4, 128.3, 127.9, 127.8, 126.6, 125.5, 123.6, 76.7, 55.7, 20.8 ppm; HRMS (ESI) calculated for $C_{24}H_{23}ClN_3O_2$ $[M + H]^+$: 420.1477, found 420.1473.

(*Z*)-2-(3-fluorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3af):



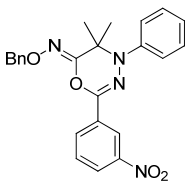
White solid, yield: 35.9 mg, 89%; M.P.=74.1-75.3 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.76 (d, *J*=8.0 Hz, 1H), 7.67 (d, *J*=9.6 Hz, 1H), 7.49 (d, *J*=7.2 Hz, 2H), 7.45-7.39 (m, 5H), 7.37-7.28 (m, 4H), 7.14-7.09 (m, 1H), 5.17 (s, 2H), 1.36 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0, 161.6, 150.2, 144.6, 140.2, 140.1, 137.7, 132.4, 132.3, 129.9, 129.8, 128.4, 128.3, 128.2, 127.9, 127.8, 126.5, 121.2, 121.1, 116.7, 116.5, 112.6, 112.4, 76.7, 55.7, 20.8 ppm; HRMS (ESI) calculated for $C_{24}H_{23}FN_3O_2$ [M + H]$^+$: 404.1769, found 404.1766.

(*Z*)-2-(3-bromophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ag):



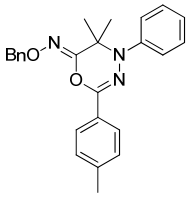
White oil, yield: 42.2 mg, 91%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.08 (s, 1H), 7.84 (d, *J*=8.0 Hz, 1H), 7.49-7.44 (m, 3H), 7.39-7.32 (m, 5H), 7.29-7.22 (m, 4H), 5.12 (s, 2H), 1.30 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 144.5, 139.8, 137.7, 132.6, 132.1, 129.9, 128.5, 128.4, 128.3, 128.0, 127.8, 126.6, 124.1, 122.6, 76.7, 55.7, 20.8 ppm; HRMS (ESI) calculated for $C_{24}H_{23}BrN_3O_2$ [M + H]$^+$: 464.0968, found 464.0960.

(*Z*)-5,5-dimethyl-2-(3-nitrophenyl)-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ah):



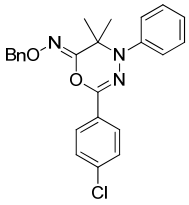
Yellow solid, yield: 41.3 mg, 96%; M.P.=121.9-123.6 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.74 (s, 1H), 8.22-8.20 (m, 2H), 7.54 (d, *J*=8.0 Hz, 1H), 7.46 (d, *J*=7.2 Hz, 2H), 7.41-7.37 (m, 4H), 7.33-7.29 (m, 4H), 5.14 (s, 2H), 1.34 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.7, 148,5, 144.2, 139.1, 137.5, 131.9, 131.0, 129.5, 128.6, 128.4, 128.0, 127.8, 126.8, 124.1, 120.5, 76.8, 55.8, 20.9 ppm; HRMS (ESI) calculated for $C_{24}H_{23}N_4O_4$ [M + H]$^+$: 431.1714, found 431.1717.

(*Z*)-5,5-dimethyl-4-phenyl-2-(p-tolyl)-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ai):



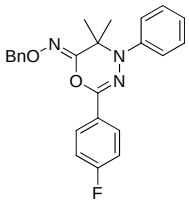
Yellow solid, yield: 18.0 mg, 45%; M.P.=118.2-120.0 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.88 (d, *J*=8.4 Hz, 2H), 7.51 (d, *J*=7.2 Hz, 2H), 7.44 (d, *J*=7.2 Hz, 2H), 7.40 (d, *J*=8.0 Hz, 2H), 7.36 (d, *J*=7.6 Hz, 3H), 7.31-7.28 (m, 1H), 7.23 (d, *J*=8.0 Hz, 2H), 5.18 (s, 2H), 2.42 (s, 3H), 1.36 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 145.0, 141.5, 139.9, 137.8, 129.1, 128.4, 128.3, 128.2, 127.9, 127.8, 127.3, 126.3, 125.6, 76.6, 55.6, 21.5, 20.7 ppm; HRMS (ESI) calculated for $C_{25}H_{26}N_3O_2$ [M + H]$^+$: 400.2020, found 400.2008.

(*Z*)-2-(4-chlorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3aj):



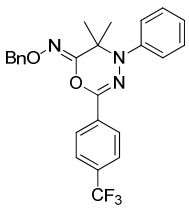
White solid, yield: 28.3 mg, 68%; M.P.=112.5-114.2 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.90 (d, *J*=8.4 Hz, 2H), 7.49 (d, *J*=6.8 Hz, 2H), 7.44-7.37 (m, 7H), 7.35-7.28 (m, 3H), 5.17 (s, 2H), 1.36 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.3, 144.7, 140.4, 137.6, 135.7, 128.6, 128.4, 128.3, 127.9, 127.8, 126.8, 126.5, 76.7, 55.6, 20.8 ppm; HRMS (ESI) calculated for $C_{24}H_{23}ClN_3O_2$ $[M + H]^+$: 420.1478, found 420.1473.

(*Z*)-2-(4-fluorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ak):



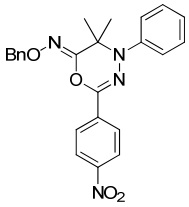
Yellow solid, yield: 27.5 mg, 67%; M.P.=97.9-99.3 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.93-7.90 (m, 2H), 7.45 (d, *J*=7.2 Hz, 2H), 7.40-7.33 (m, 5H), 7.30-7.24 (m, 3H), 7.06 (t, *J*=8.8 Hz, 2H), 5.12 (s, 2H), 1.31 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 162.6, 150.4, 144.8, 140.6, 137.7, 128.4, 128.0, 127.8, 127.7, 127.6, 126.4, 126.3, 126.2, 115.6, 115.3, 76.7, 55.6, 20.8 ppm; HRMS (ESI) calculated for $C_{24}H_{23}FN_3O_2$ $[M + H]^+$: 404.1769, found 404.1761.

(*Z*)-5,5-dimethyl-4-phenyl-2-(4-(trifluoromethyl)phenyl)-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3al):



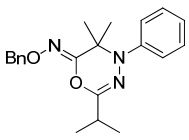
White solid, yield: 39.2 mg, 87%; M.P.=130.1-131.3 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.07 (d, *J*=8.4 Hz, 2H), 7.66 (d, *J*=8.4 Hz, 2H), 7.49 (d, *J*=7.2 Hz, 2H), 7.45-7.38 (m, 5H), 7.40-7.30 (m, 3H), 5.18 (s, 2H), 1.38 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.0, 144.4, 139.9, 137.6, 133.4, 131.4, 131.1, 128.5, 128.4, 128.0, 127.8, 126.6, 125.7, 125.4, 125.3, 125.2, 122.7, 76.7, 55.7, 20.8 ppm; HRMS (ESI) calculated for $C_{25}H_{23}F_3N_3O_2$ $[M + H]^+$: 454.1737, found 454.1733.

(*Z*)-5,5-dimethyl-2-(4-nitrophenyl)-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3am):



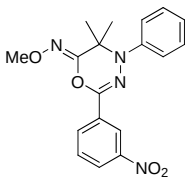
Yellow solid, yield: 41.0 mg, 95%; M.P.=130.5-132.1 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.22 (d, *J*=9.2 Hz, 2H), 8.06 (d, *J*=8.8 Hz, 2H), 7.47-7.45 (m, 2H), 7.42 (t, *J*=1.6 Hz, 1H), 7.39 (d, *J*=1.6 Hz, 2H), 7.38-7.35 (m, 2H), 7.32-7.30 (m, 2H), 7.28 (s, 1H), 5.14 (s, 2H), 1.35 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.5, 148.2, 144.1, 139.1, 137.4, 135.9, 128.6, 128.5, 128.4, 128.1, 127.8, 126.9, 126.0, 123.7, 76.8, 55.9, 53.5, 21.0 ppm; HRMS (ESI) calculated for $C_{24}H_{23}N_4O_4$ $[M + H]^+$: 431.1714, found 431.1708.

(*Z*)-2-isopropyl-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3an):



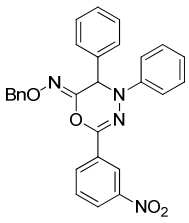
White solid, yield: 11.8 mg, 34%; M.P.=93.2-94.8 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.49-7.36 (m, 4H), 7.36-7.33 (m, 3H), 7.28-7.23 (m, 3H), 5.10 (s, 2H), 2.80-2.69 (m, 1H), 1.30 (s, 3H), 1.28 (s, 3H), 1.24 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 148.8, 145.1, 137.8, 128.3, 128.2, 128.1, 127.8, 127.5, 126.1, 76.5,55.0, 31.5, 20.2, 19.7 ppm; HRMS (ESI) calculated for $C_{21}H_{26}N_3O_2$ $[M + H]^+$: 352.2020, found 352.2017.

(*Z*)-5,5-dimethyl-2-(3-nitrophenyl)-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-methyl oxime (3bh):



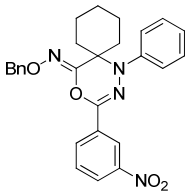
Yellow solid, yield: 33.3 mg, 94%; M.P.=116.6-117.3 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.74 (s, 1H), 8.25-8.23 (m, 2H), 7.57 (t, *J*=8.0 Hz, 1H), 7.42-7.38 (m, 2H), 7.31 (d, *J*=7.2 Hz, 3H), 3.94 (s, 3H), 1.36 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.3, 148.5, 144.2, 139.0, 131.9, 131.0, 129.4, 128.5, 127.8, 126.8, 124.1, 120.4, 62.8, 55.7, 20.8 ppm; HRMS (ESI) calculated for $C_{18}H_{19}N_4O_4$ $[M + H]^+$: 355.1401, found 355.1398.

(*Z*)-2-(3-nitrophenyl)-4,5-diphenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ch):



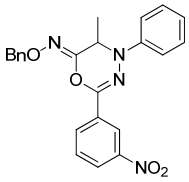
Yellow oil, yield: 25.8 mg, 54%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.76 (s, 1H), 8.22-8.17 (m, 2H), 7.54-7.45 (m, 3H), 7.40-7.39 (m, 2H), 7.37-7.31 (m, 4H), 7.24-7.21 (m, 6H), 6.99-6.96 (m, 1H), 5.92 (s, 1H), 5.19 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 148.5, 144.5, 144.4, 143.9, 138.5, 138.2, 137.5, 136.6, 133.6, 133.1, 131.6, 131.5, 131.0, 130.8, 129.5, 129.4, 129.3, 129.1, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 128.2, 126.8, 126.4, 124.1, 121.7, 121.6, 120.5, 120.3, 114.1, 113.9, 76.9, 76.8, 54.6, 50.9 ppm; HRMS (ESI) calculated for $C_{28}H_{23}N_4O_4$ $[M + H]^+$: 479.1714, found 479.1711.

(*Z*)-3-(3-nitrophenyl)-1-phenyl-4-oxa-1,2-diazaspiro[5.5]undec-2-en-5-one O-benzyl oxime (3dh):



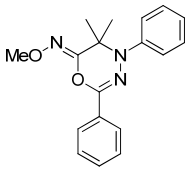
Yellow solid, yield: 42.1 mg, 90%; M.P.=141.9-143.5 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.72 (s, 1H), 8.21-8.19 (m, 2H), 7.53 (t, *J*=8.0 Hz, 1H), 7.48-7.46 (m, 2H), 7.41-7.36 (m, 4H), 7.34-7.26 (m, 4H), 5.18 (s, 2H), 2.09 (d, *J*=12.4 Hz, 2H), 1.62-1.52 (m, 5H), 1.33-1.25 (m, 2H), 0.89-0.86 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 147.3, 143.7, 138.8, 137.8, 131.9, 131.0, 129.4, 128.6, 128.5, 128.4, 128.0, 126.7, 123.9, 120.4, 76.7, 59.3, 28.8, 25.3, 22.7 ppm; HRMS (ESI) calculated for $C_{27}H_{27}N_4O_4$ $[M + H]^+$: 471.2027, found 471.2025.

(*Z*)-5-methyl-2-(3-nitrophenyl)-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3eh):



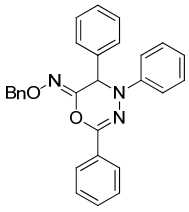
Yellow oil, yield: 10.9 mg, 25%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.85 (s, 1H), 8.33-8.26 (m, 2H), 7.65-7.61 (m, 1H), 7.47 (d, *J*=6.8 Hz, 2H), 7.44-7.36 (m, 5H), 7.32 (d, *J*=8.0 Hz, 2H), 7.05 (t, *J*=7.2 Hz, 1H), 5.19-5.12 (m, 2H), 4.95-4.90 (m, 1H), 1.34 (d, *J*=6.4 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 145.5, 144.0, 138.1, 137.3, 131.7, 131.0, 130.9, 129.6, 129.5, 128.6, 128.5, 128.2, 128.1, 124.2, 121.9, 120.5, 114.6, 76.7, 47.4, 13.1 ppm; HRMS (ESI) calculated for $C_{23}H_{21}N_4O_4$ $[M + H]^+$: 417.1557, found 417.1554.

(*Z*)-5,5-dimethyl-2,4-diphenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-methyl oxime (3ba):



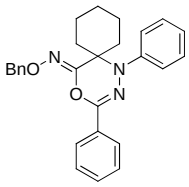
White oil, yield: 18.9 mg, 62%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.01-7.99 (m, 2H), 7.44-7.42 (m, 4H), 7.40-7.36 (m, 3H), 7.32-7.28 (m, 1H), 3.98 (s, 3H), 1.39 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.2, 144.9, 141.2, 130.1, 129.8, 128.4, 128.3, 127.8, 126.4, 125.6, 62.7, 55.5, 20.7 ppm; HRMS (ESI) calculated for $C_{18}H_{20}N_3O_2$ $[M + H]^+$: 310.1550, found 310.1546.

(*Z*)-2,4,5-triphenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-benzyl oxime (3ca):



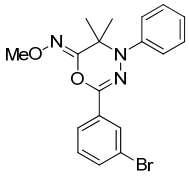
White solid, yield: 14.3 mg, 33%; M.P.=149.3-151.2 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.03-8.01 (m, 2H), 7.50 (d, *J*=6.8 Hz, 2H), 7.44-7.42 (m, 5H), 7.38-7.33 (m, 3H), 7.28 (d, *J*=7.2 Hz, 7H), 6.99 (t, *J*=7.2 Hz, 1H), 5.95 (s, 1H), 5.24 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.9, 144.8, 140.3, 137.7, 133.5, 129.8, 129.7, 129.3, 129.1, 129.0, 128.7, 128.6, 128.5, 128.4, 128.3, 128.1, 128.0, 126.9, 126.6, 125.6, 125.5, 121.0, 113.9, 113.7, 76.7, 54.4 ppm; HRMS (ESI) calculated for $C_{28}H_{24}N_3O_2$ $[M + H]^+$: 434.1863, found 434.1860.

(*Z*)-1,3-diphenyl-4-oxa-1,2-diazaspiro[5.5]undec-2-en-5-one O-benzyl oxime (3da):



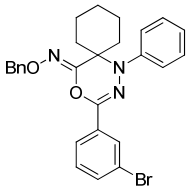
White solid, yield: 11.4 mg, 27%; M.P.=118.0-119.0 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.99-7.96 (m, 2H), 7.51 (d, *J*=7.2 Hz, 2H), 7.44-7.40 (m, 6H), 7.38-7.36 (m, 1H), 7.34-7.29 (m, 4H), 5.22 (s, 2H), 7.16 (d, *J*=12.4 Hz, 2H), 1.66-1.51 (m, 5H), 1.36-1.28 (m, 2H), 0.96-0.92 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.2, 144.4, 141.1, 138.2, 130.0, 129.6, 128.6, 128.4, 128.3, 128.2, 128.1, 127.8, 126.3, 125.6, 76.6, 59.0, 28.7, 25.4, 22.8 ppm; HRMS (ESI) calculated for $C_{27}H_{28}N_3O_2$ $[M + H]^+$: 426.2176, found 426.2179.

(*Z*)-2-(3-bromophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-methyl oxime (3bg):



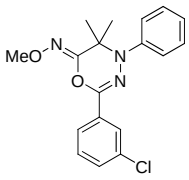
White oil, yield: 34.1 mg, 88%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.07 (s, 1H), 7.86 (d, *J*=8.0 Hz, 1H), 7.50 (d, *J*=8.0 Hz, 1H), 7.40-7.36 (m, 2H), 7.31-7.25 (m, 4H), 3.93 (s, 3H), 1.33 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.8, 144.5, 139.7, 132.6, 132.0, 129.9, 128.5, 128.3, 127.8, 126.6, 124.1, 122.5, 62.7, 55.5, 20.7 ppm; HRMS (ESI) calculated for $C_{18}H_{19}BrN_3O_2$ $[M + H]^+$: 388.0655, found 388.0655.

(*Z*)-3-(3-bromophenyl)-1-phenyl-4-oxa-1,2-diazaspiro[5.5]undec-2-en-5-one O-benzyl oxime (3dg):



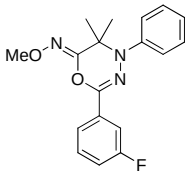
White oil, yield: 29.4 mg, 58%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.05 (s, 1H), 7.84-7.82 (m, 1H), 7.49-7.45 (m, 3H), 7.39-7.34 (m, 5H), 7.27-7.22 (m, 4H), 5.16 (s, 2H), 2.08 (d, *J*=12.4 Hz, 2H), 1.56-1.49 (m, 5H), 1.30-1.22 (m, 2H), 0.88-0.84 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.7, 144.0, 139.6, 138.0, 132.5, 132.0, 129.9, 128.6, 128.5,128.4, 128.3, 128.2, 127.9, 126.5, 124.0, 122.5, 76.6, 59.1, 28.7, 25.4, 22.8 ppm; HRMS (ESI) calculated for $C_{27}H_{27}BrN_3O_2$ $[M + H]^+$: 504.1281, found 504.1279.

(*Z*)-2-(3-chlorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-methyl oxime (3be):



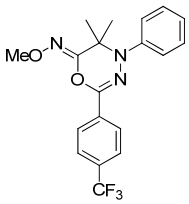
White oil, yield: 25.6 mg, 75%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.92 (s, 1H), 7.83-7.80 (m, 1H), 7.40-7.34 (m, 3H), 7.33-7.31 (m, 2H), 7.29-7.24 (m, 2H), 3.93 (s, 3H), 1.33 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.8, 144.5, 139.9, 134.5, 131.8, 129.7, 129.6, 128.5, 127.8, 126.6, 125.5, 123.6, 62.7, 55.5, 20.7 ppm; HRMS (ESI) calculated for $C_{18}H_{19}ClN_3O_2$ $[M + H]^+$: 344.1160, found 344.1158.

(*Z*)-2-(3-fluorophenyl)-5,5-dimethyl-4-phenyl-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-methyl oxime (3bf):



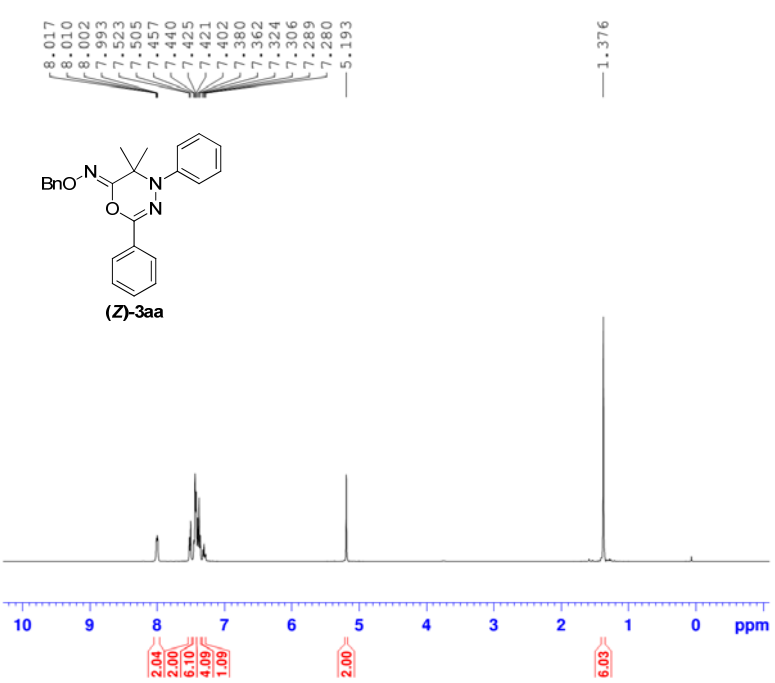
White oil, yield: 26.7 mg, 82%; ^{1}H NMR (400 MHz,$CDCl_3$): δ 7.71 (d, J=7.6 Hz, 1H), 7.65-7.62 (m, 1H), 7.39-7.33 (m, 3H), 7.31-7.24 (m, 3H), 7.09-7.05 (m, 1H), 3.92 (s, 3H), 1.33 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0, 161.6, 149.8, 144.6, 140.1, 140.0, 132.3, 132.2, 130.0, 129.9, 128.4, 127.8, 126.5, 121.2, 121.1, 116.7, 116.5, 112.6, 112.4, 62.7, 55.5, 20.7 ppm; HRMS (ESI) calculated for $C_{18}H_{19}FN_3O_2$ $[M + H]^+$: 328.1456, found 328.1451.

(*Z*)-5,5-dimethyl-4-phenyl-2-(4-(trifluoromethyl)phenyl)-*4H*-1,3,4-oxadiazin-6(*5H*)-one O-methyl oxime (3bl):



White oil, yield: 34.1 mg, 90%; M.P.=84.5-84.9 ℃; ^{1}H NMR (400 MHz,$CDCl_3$): δ 8.04 (d, J=8.4 Hz, 2H), 7.63 (d, J=8.4 Hz, 2H), 7.41-7.37 (m, 2H), 7.31-7.27 (m, 3H), 3.93 (s, 3H), 1.35 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.6, 144.4, 139.8, 133.4, 131.4, 131.1, 128.5, 127.8, 126.7, 125.7, 125.5, 125.4, 125.3, 125.2, 125.1, 122.7, 76.7, 62.7, 55.6, 20.8 ppm; HRMS (ESI) calculated for $C_{19}H_{19}F_3N_3O_2$ $[M + H]^+$: 378.1424, found 378.1424.

5. ^{1}H and ^{13}C NMR spectra

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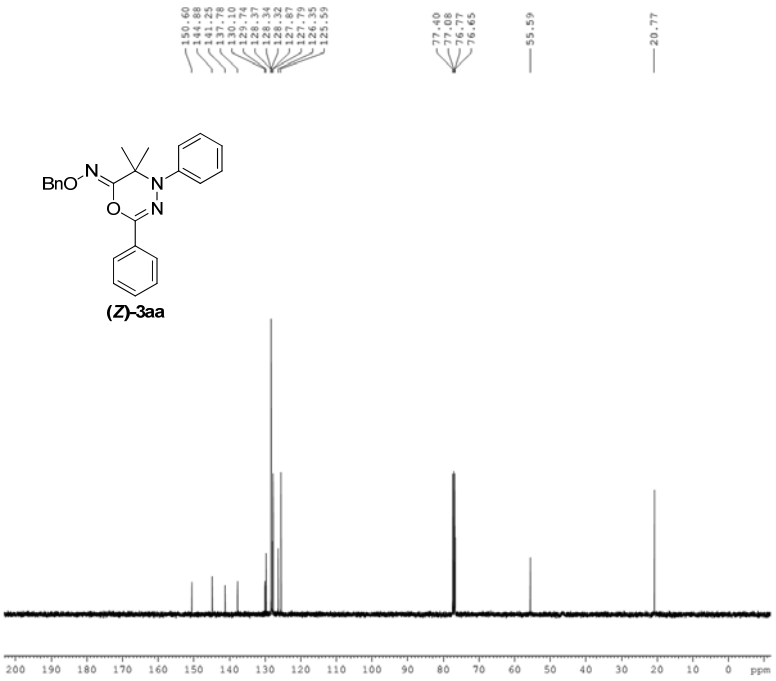
NAME                  NMR
EXPNO                4680
PROCNO                  1
Date_            20161205
Time                14.44
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    144
DW                60.800 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.50 usec
PL1                -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI                  32768
SF            400.1700000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```




```
NAME                  NMR
EXPNO                4681
PROCNO                  1
Date_            20161205
Time                14.49
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     35
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   1290
DW                20.800 usec
DE                 6.50 usec
TE                296.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.70 usec
PL1                -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.83 dB
PL12               12.00 dB
PL13               14.00 dB
PL2W          16.91636658 W
PL12W          0.55629748 W
PL13W          0.35100001 W
SFO2          400.1716007 MHz
SI                  32768
SF            100.6228270 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
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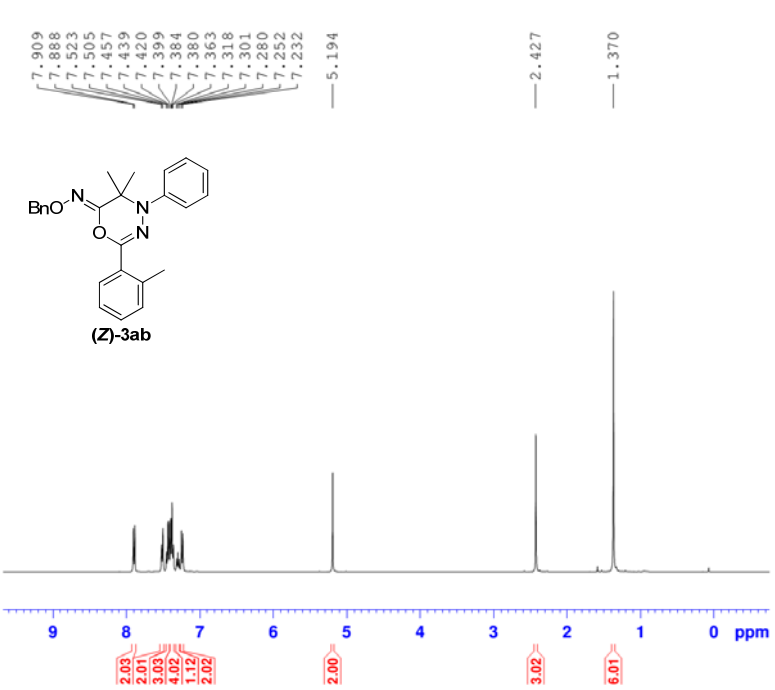


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NAME                NMR
EXPNO              4710
PROCNO                1
Date_          20161226
Time              10.30
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  114
DW               60.800 usec
DE                6.50 usec
TE               673.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1               14.50 usec
PL1              -2.83 dB
PL1W       16.91636658 W
SFO1       400.1724712 MHz
SI                32768
SF         400.1700000 MHz
WDW                EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
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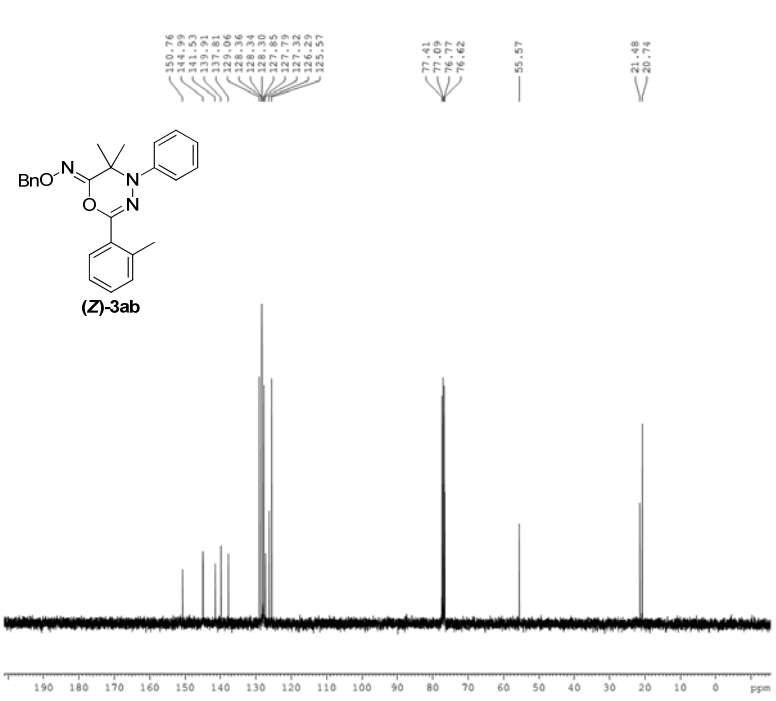


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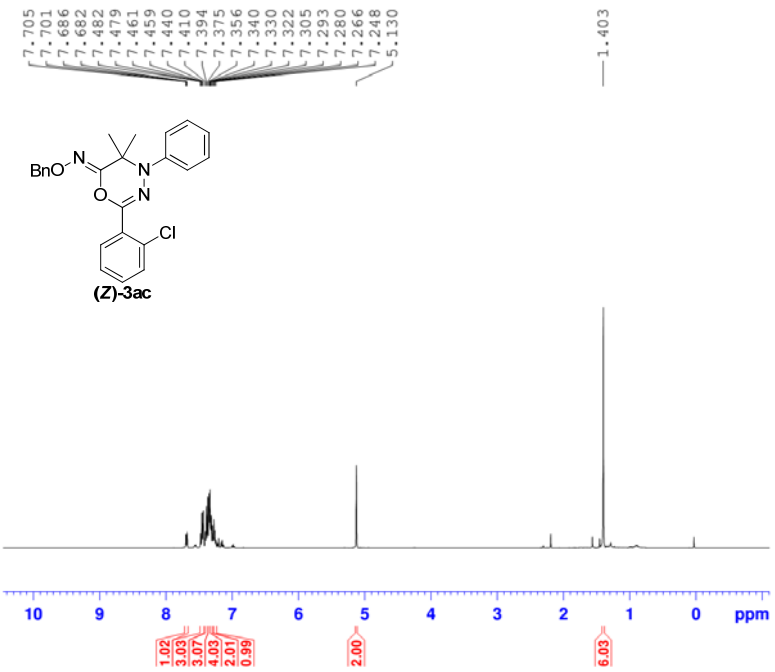
NAME                NMR
EXPNO              4709
PROCNO                1
Date_          20161226
Time              10.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   18
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  812
DW               20.800 usec
DE                6.50 usec
TE               673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1               13C
P1               11.70 usec
PL1              -2.00 dB
PL1W       48.76812744 W
SFO1       100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -2.83 dB
PL12             12.00 dB
PL13             14.00 dB
PL2W       16.91636658 W
PL12W       0.55629748 W
PL13W       0.35100001 W
SFO2       400.1716007 MHz
SI                32768
SF         100.6228270 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

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NAME                 NMR
EXPNO                4717
PROCNO                  1
Date_            20161228
Time                14.18
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      9
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    114
DW                60.800 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.50 usec
PL1                -2.83 dB
PL1W         16.91636658 W
SFO1         400.1724712 MHz
SI                  32768
SF           400.1700000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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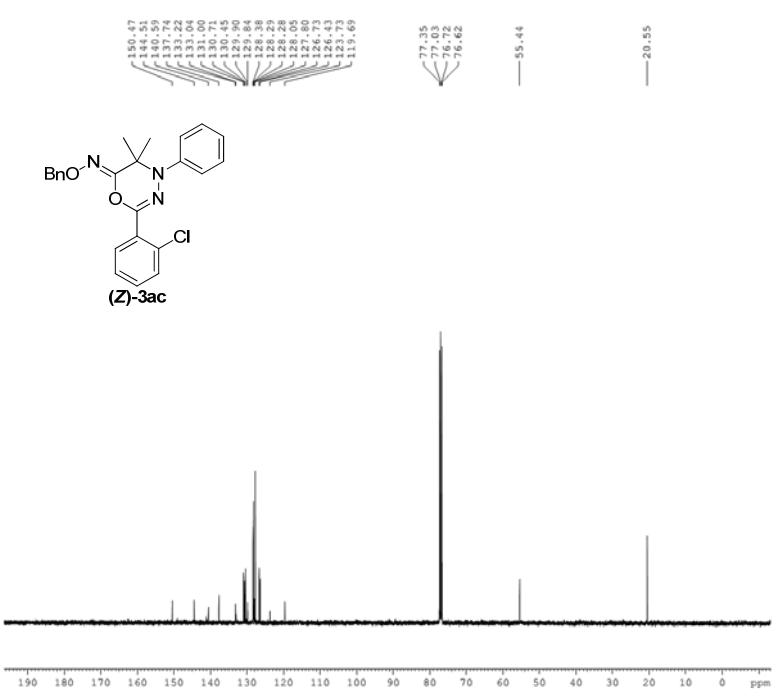
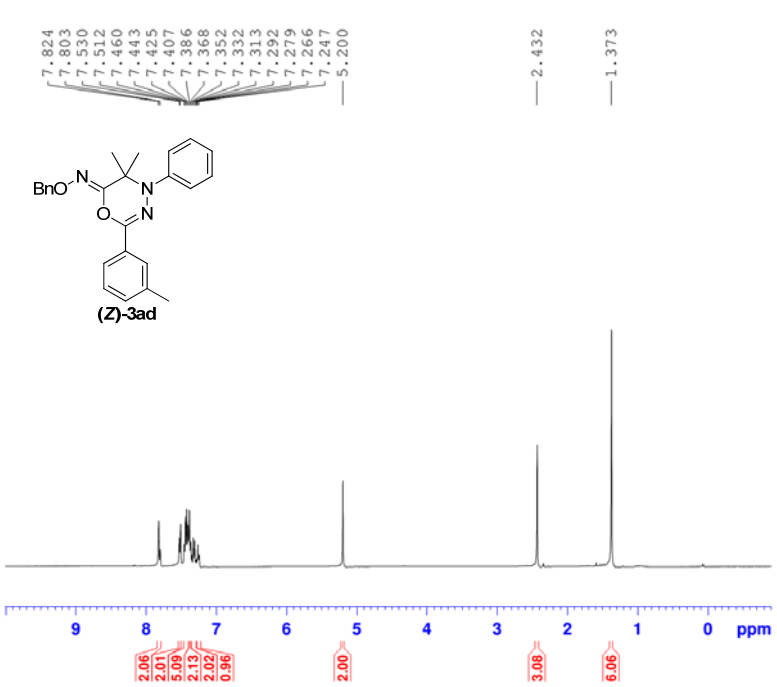



```
NAME                 NMR
EXPNO                4718
PROCNO                  1
Date_            20161228
Time                14.34
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    195
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    812
DW                20.800 usec
DE                 6.50 usec
TE                673.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

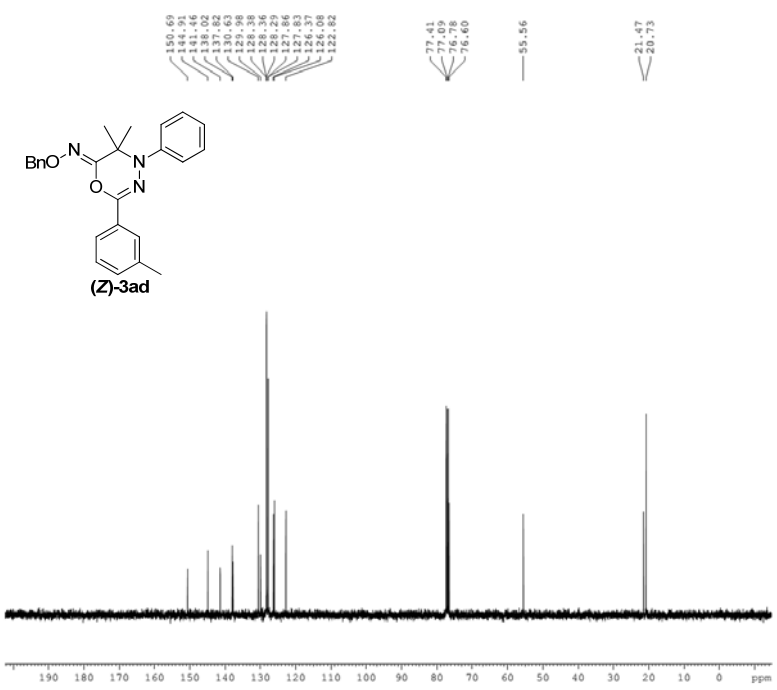
======== CHANNEL f1 ========
NUC1                 13C
P1                 11.70 usec
PL1                -2.00 dB
PL1W         48.76812744 W
SFO1         100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.83 dB
PL12               12.00 dB
PL13               14.00 dB
PL2W         16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2         400.1716007 MHz
SI                  32768
SF           100.6228270 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
NAME                NMR
EXPNO              4725
PROCNO                1
Date_          20161230
Time              16.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                 90.5
DW               60.800 usec
DE                6.50 usec
TE               294.3 K
D1            1.00000000 sec
TD0                   1

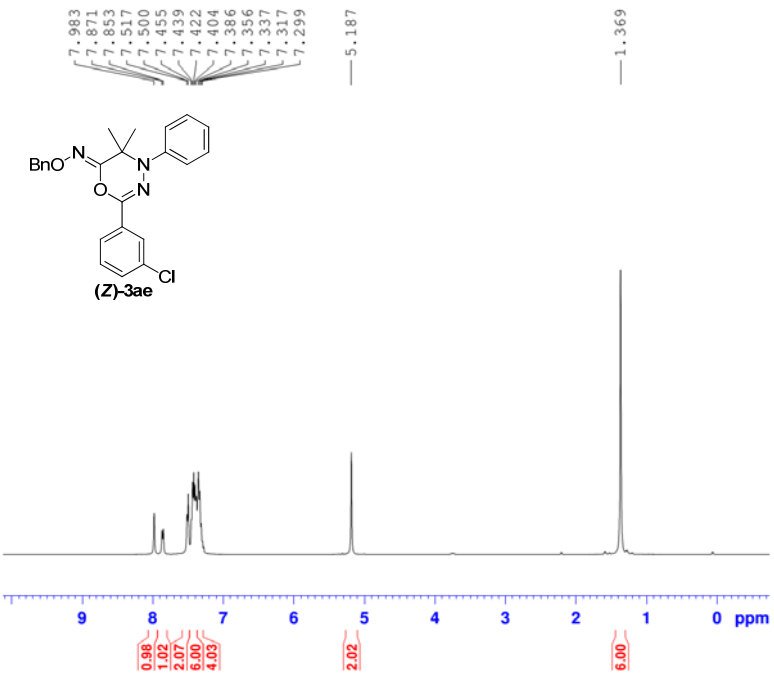
======== CHANNEL f1 ========
NUC1                 1H
P1                14.50 usec
PL1               -2.83 dB
PL1W        16.91636658 W
SFO1        400.1724712 MHz
SI                32768
SF          400.1700000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
NAME                NMR
EXPNO              4726
PROCNO                1
Date_          20161230
Time              16.09
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  406
DW               20.800 usec
DE                6.50 usec
TE               294.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

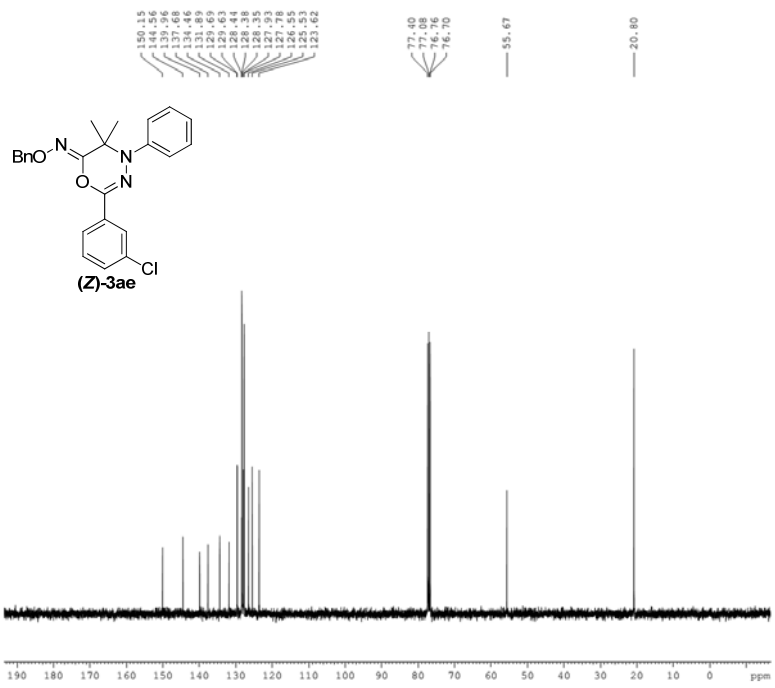
======== CHANNEL f1 ========
NUC1                13C
P1                11.70 usec
PL1               -2.00 dB
PL1W        48.76812744 W
SFO1        100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -2.83 dB
PL12              12.00 dB
PL13              14.00 dB
PL2W        16.91636658 W
PL12W        0.55629748 W
PL13W        0.35100001 W
SFO2        400.1716007 MHz
SI                32768
SF          100.6228270 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
NAME                NMR
EXPNO              4676
PROCNO                1
Date_          20161202
Time              10.13
INSTRUM           spect
PROBHD  5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  128
DW               60.800 usec
DE                6.50 usec
TE               297.1 K
D1            1.00000000 sec
TD0                   1

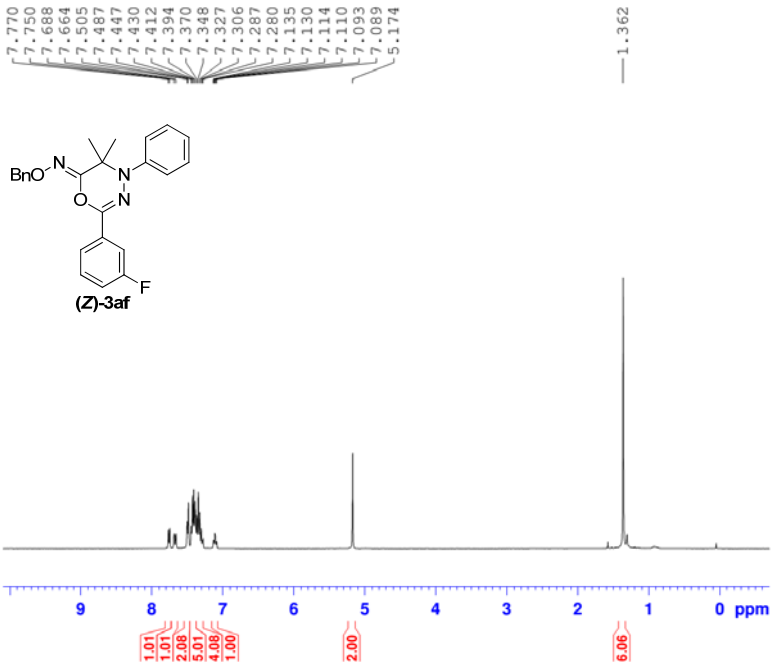
======== CHANNEL f1 ========
NUC1                1H
P1               14.50 usec
PL1              -2.83 dB
PL1W        16.91636658 W
SFO1        400.1724712 MHz
SI                32768
SF          400.1700000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```




```
NAME                NMR
EXPNO              4677
PROCNO                1
Date_          20161202
Time              10.19
INSTRUM           spect
PROBHD  5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   64
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  724
DW               20.800 usec
DE                6.50 usec
TE               297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

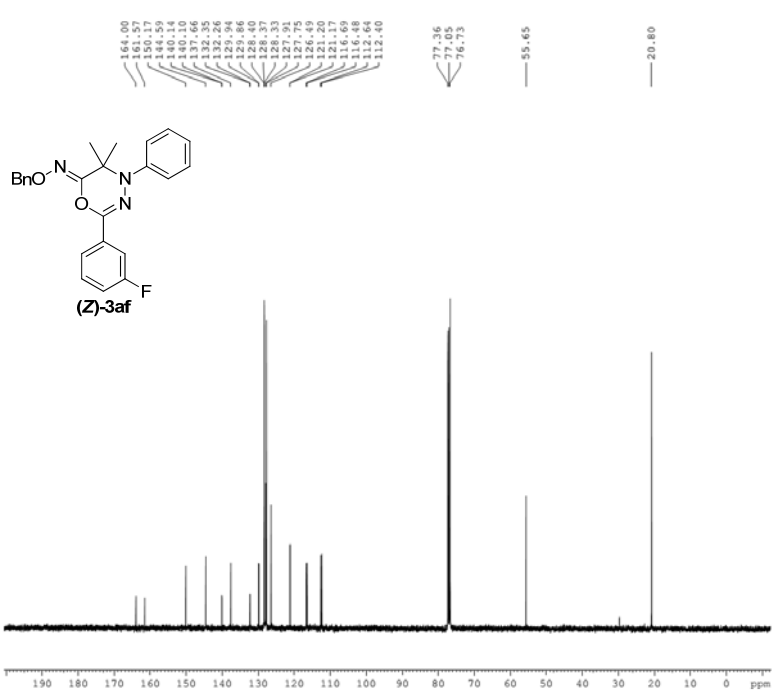
======== CHANNEL f1 ========
NUC1                13C
P1               11.70 usec
PL1              -2.00 dB
PL1W        48.76812744 W
SFO1        100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -2.83 dB
PL12             12.00 dB
PL13             14.00 dB
PL2W        16.91636658 W
PL12W        0.55629748 W
PL13W        0.35100001 W
SFO2        400.1716007 MHz
SI                32768
SF          100.6228270 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```




```
NAME                 NMR
EXPNO                4749
PROCNO                  1
Date_            20170112
Time                16.07
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     12
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    144
DW                60.800 usec
DE                 6.50 usec
TE                296.4 K
D1            1.00000000 sec
TD0                     1

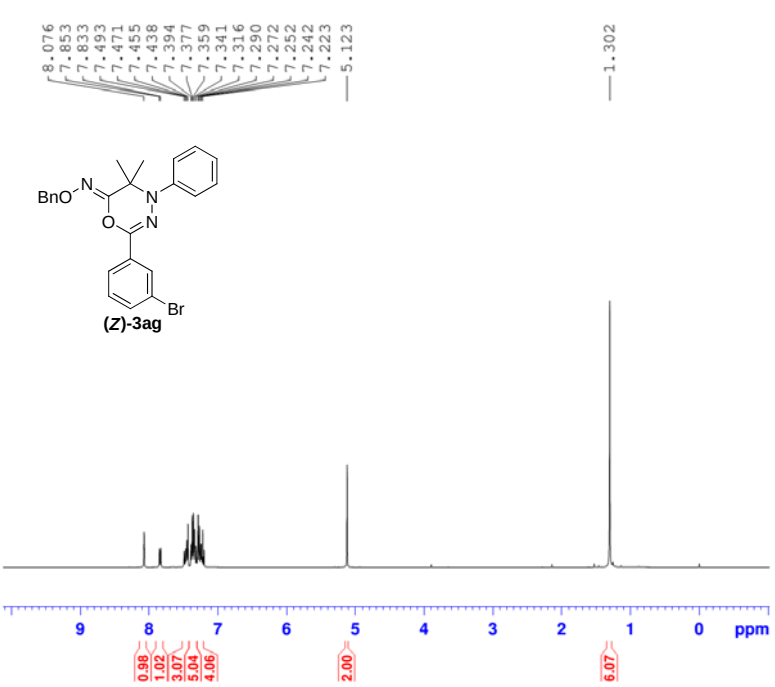
======== CHANNEL f1 ========
NUC1                  1H
P1                 14.50 usec
PL1                -2.83 dB
PL1W         16.91636658 W
SFO1         400.1724712 MHz
SI                  32768
SF           400.1700000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```



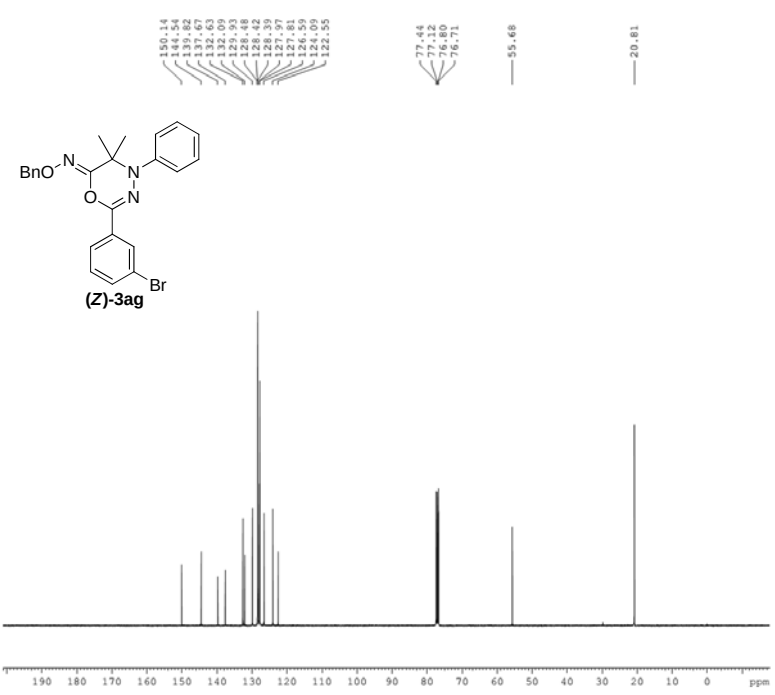

```
NAME                 NMR
EXPNO                4748
PROCNO                  1
Date_            20170112
Time                14.58
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    812
DW                20.800 usec
DE                 6.50 usec
TE                296.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.70 usec
PL1                -2.00 dB
PL1W         48.76812744 W
SFO1         100.6328888 MHz

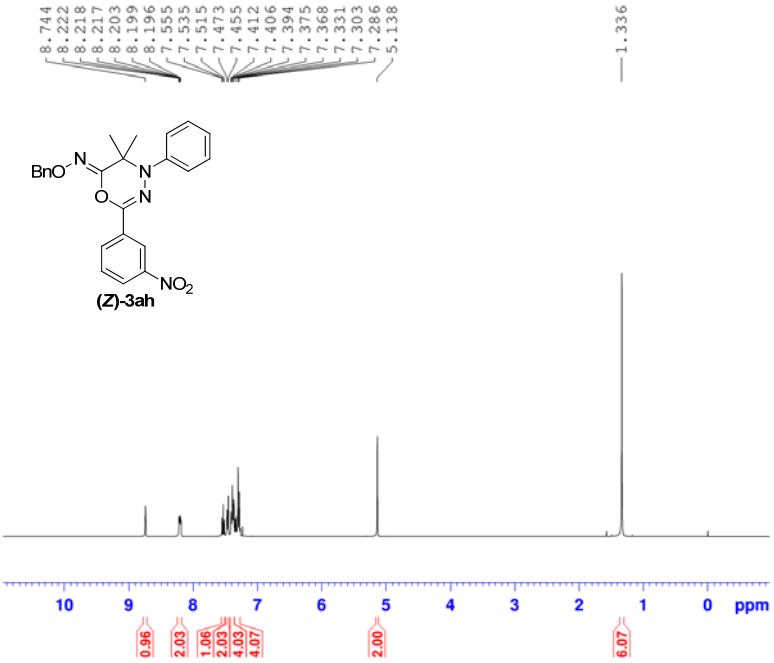
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.83 dB
PL12               12.00 dB
PL13               14.00 dB
PL2W         16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2         400.1716007 MHz
SI                  32768
SF           100.6228270 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```



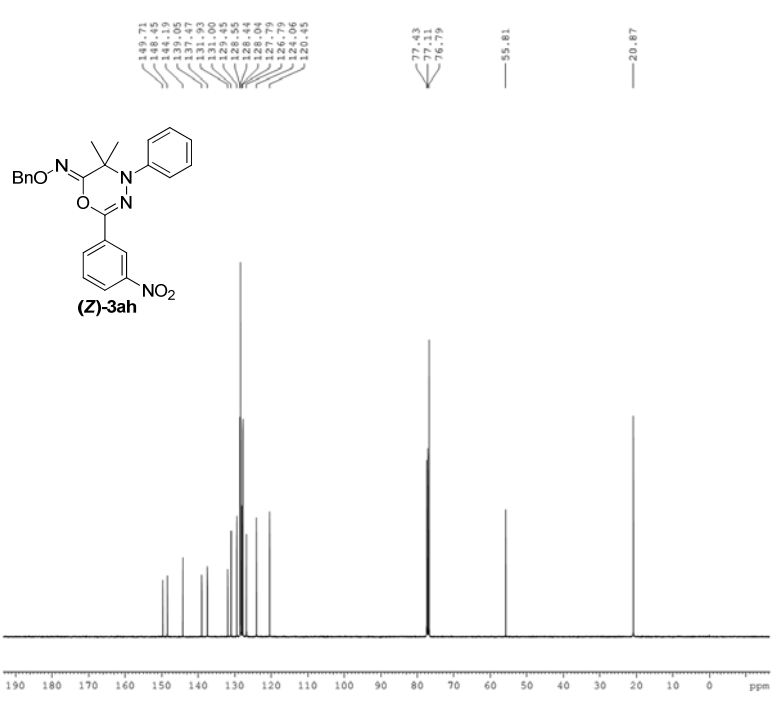

```
NAME                 NMR
EXPNO                201739
PROCNO               1
Date_                20170307
Time                 23.58 h
INSTRUM              spect
PROBHD     Z116098_0406 (
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                   16
DS                   2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894966 sec
RG                   30.91
DW                   62.400 usec
DE                   6.50 usec
TE                   293.5 K
D1                   1.00000000 sec
TD0                  1
SFO1                 400.1324708 MHz
NUC1                 1H
P1                   10.00 usec
SI                   65536
SF                   400.1300296 MHz
WDW                  EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```



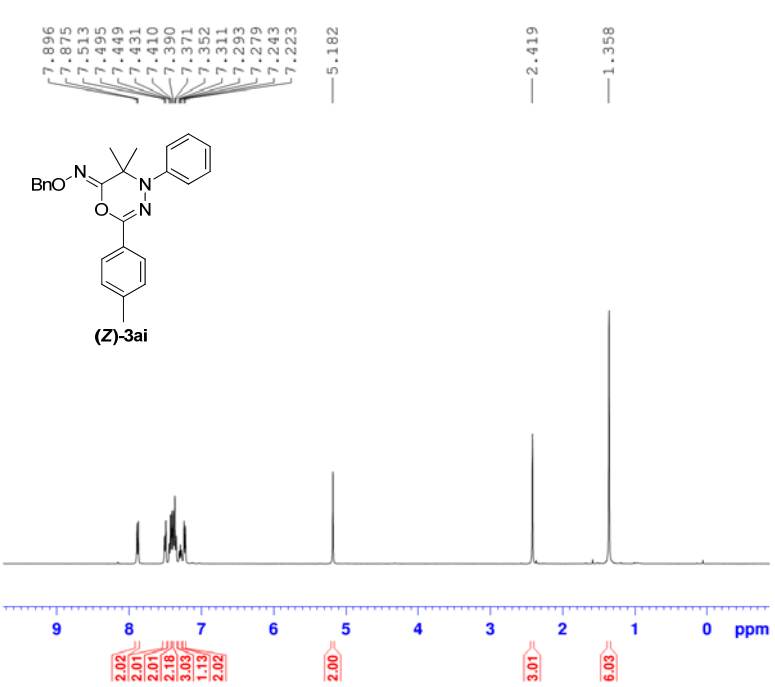

```
NAME                 NMR
EXPNO                201740
PROCNO               1
Date_                20170308
Time                 0.59 h
INSTRUM              spect
PROBHD     Z116098_0406 (
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   1024
DS                   4
SWH                  24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                   196.12
DW                   20.800 usec
DE                   6.50 usec
TE                   294.2 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                  1
SFO1                 100.6228298 MHz
NUC1                 13C
P1                   10.00 usec
SI                   32768
SF                   100.6127685 MHz
WDW                  EM
SSB                  0
LB                   1.00 Hz
GB                   0
PC                   1.40
```




```
NAME                NMR
EXPNO               201741
PROCNO                   1
Date_             20170307
Time                20.31 h
INSTRUM               spect
PROBHD    Z116098_0406 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894966 sec
RG                    30.91
DW                    62.400 usec
DE                     6.50 usec
TE                    293.1 K
D1                 1.00000000 sec
TD0                       1
SFO1               400.1324708 MHz
NUC1                      1H
P1                    10.00 usec
SI                    65536
SF                 400.1300196 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

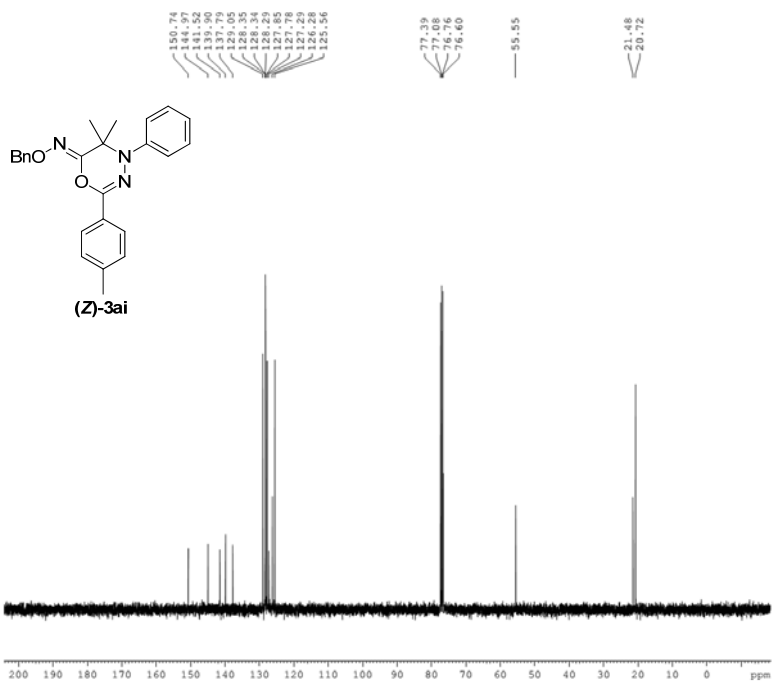



```
NAME                NMR
EXPNO               201710
PROCNO                   1
Date_             20170224
Time                23.12 h
INSTRUM               spect
PROBHD    Z116098_0406 (
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH                24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631988 sec
RG                   196.12
DW                    20.800 usec
DE                     6.50 usec
TE                    292.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1
SFO1               100.6228298 MHz
NUC1                      13C
P1                    10.00 usec
SI                    32768
SF                 100.6127685 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```




```
NAME                 NMR
EXPNO                4728
PROCNO                  1
Date_            20161230
Time                16.20
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    144
DW                60.800 usec
DE                 6.50 usec
TE                294.7 K
D1             1.00000000 sec
TD0                     1

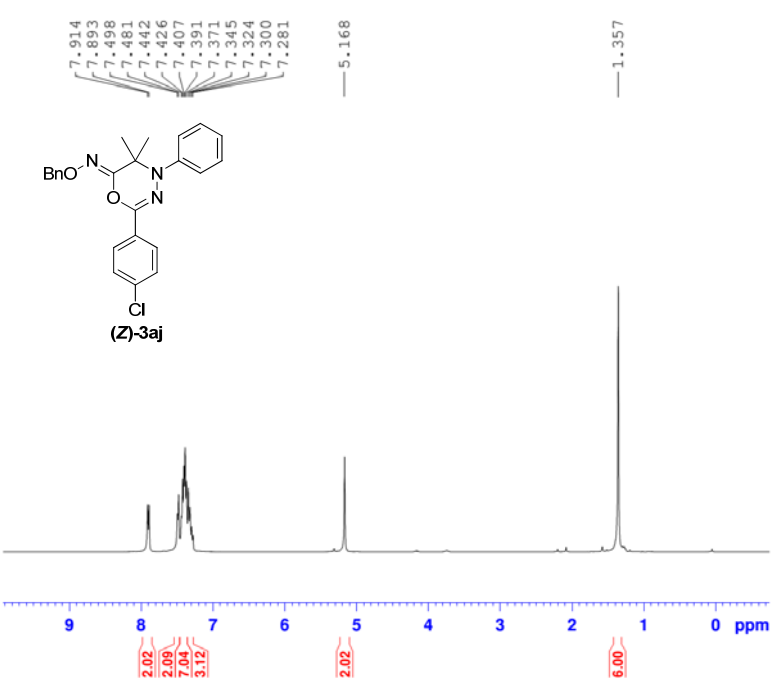
======== CHANNEL f1 ========
NUC1                  1H
P1                 14.50 usec
PL1                -2.83 dB
PL1W          16.91636658 W
SFO1         400.1724712 MHz
SI                  32768
SF           400.1700000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```




```
NAME                 NMR
EXPNO                4727
PROCNO                  1
Date_            20161230
Time                16.15
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   1030
DW                20.800 usec
DE                 6.50 usec
TE                294.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

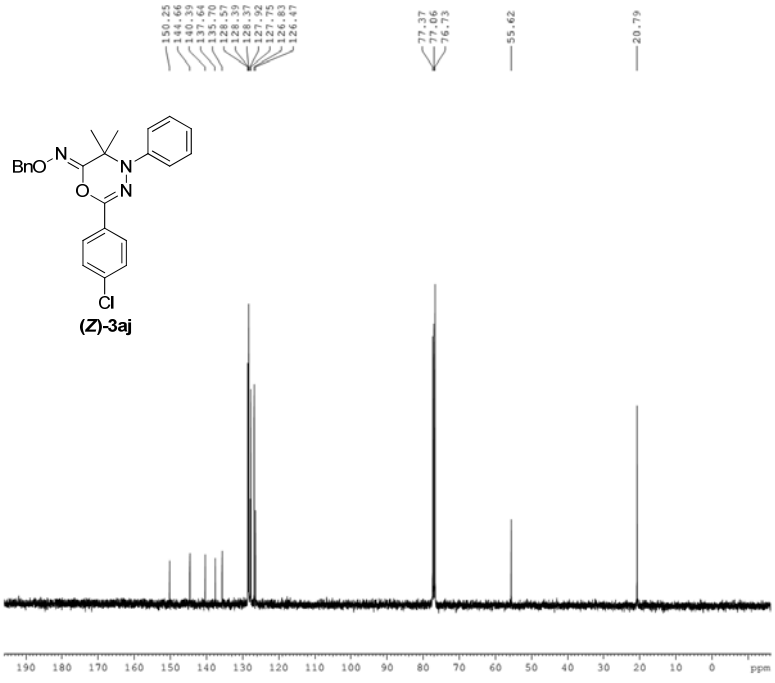
======== CHANNEL f1 ========
NUC1                 13C
P1                 11.70 usec
PL1                -2.00 dB
PL1W          48.76812744 W
SFO1         100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.83 dB
PL12               12.00 dB
PL13               14.00 dB
PL2W          16.91636658 W
PL12W          0.55629748 W
PL13W          0.35100001 W
SFO2         400.1716007 MHz
SI                  32768
SF           100.6228270 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```




```
NAME                 NMR
EXPNO                4679
PROCNO                  1
Date_            20161202
Time                10.35
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    144
DW                 60.800 usec
DE                  6.50 usec
TE                 297.7 K
D1              1.00000000 sec
TD0                     1

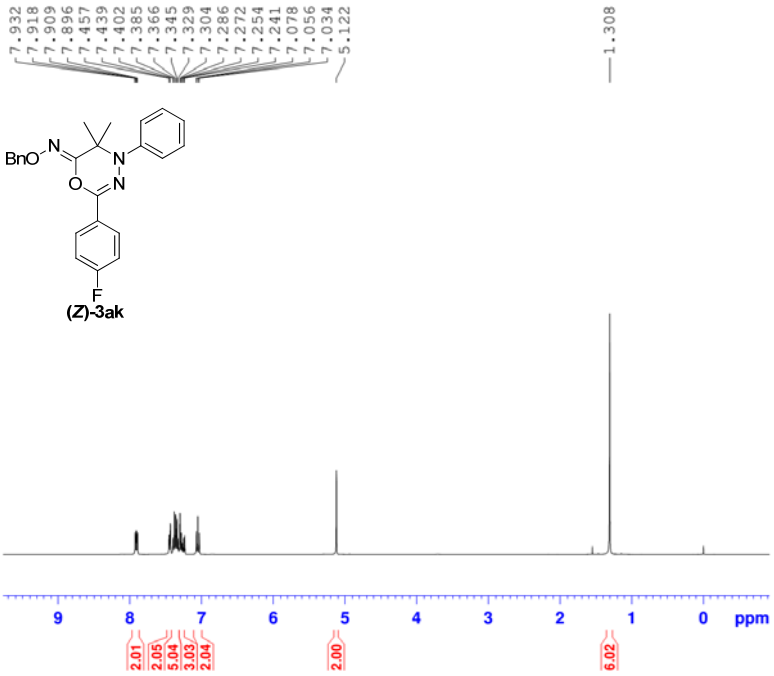
======== CHANNEL f1 ========
NUC1                   1H
P1                  14.50 usec
PL1                 -2.83 dB
PL1W           16.91636658 W
SFO1          400.1724712 MHz
SI                   32768
SF            400.1700000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



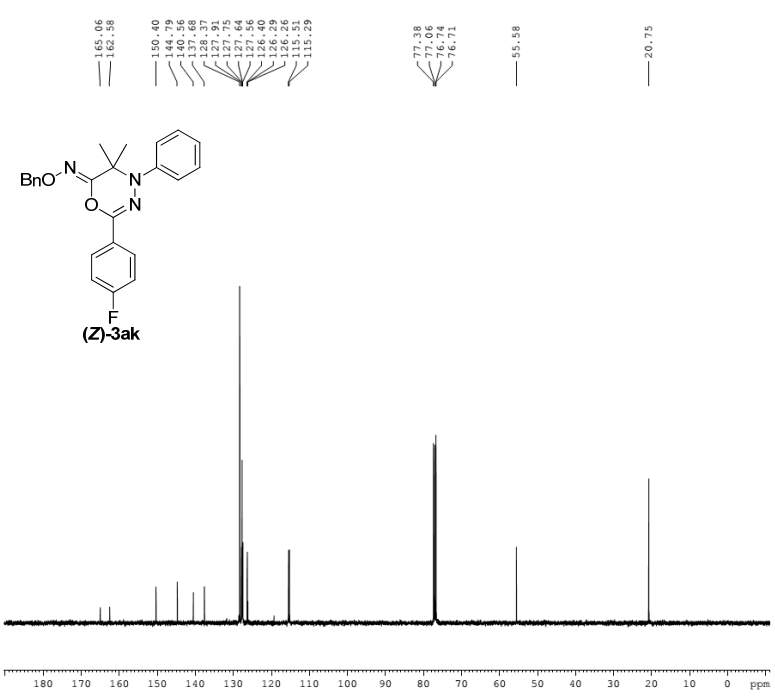

```
NAME                 NMR
EXPNO                4678
PROCNO                  1
Date_            20161202
Time                10.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    103
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    724
DW                 20.800 usec
DE                  6.50 usec
TE                 297.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  11.70 usec
PL1                 -2.00 dB
PL1W           48.76812744 W
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -2.83 dB
PL12                12.00 dB
PL13                14.00 dB
PL2W           16.91636658 W
PL12W           0.55629748 W
PL13W           0.35100001 W
SFO2          400.1716007 MHz
SI                   32768
SF            100.6228270 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



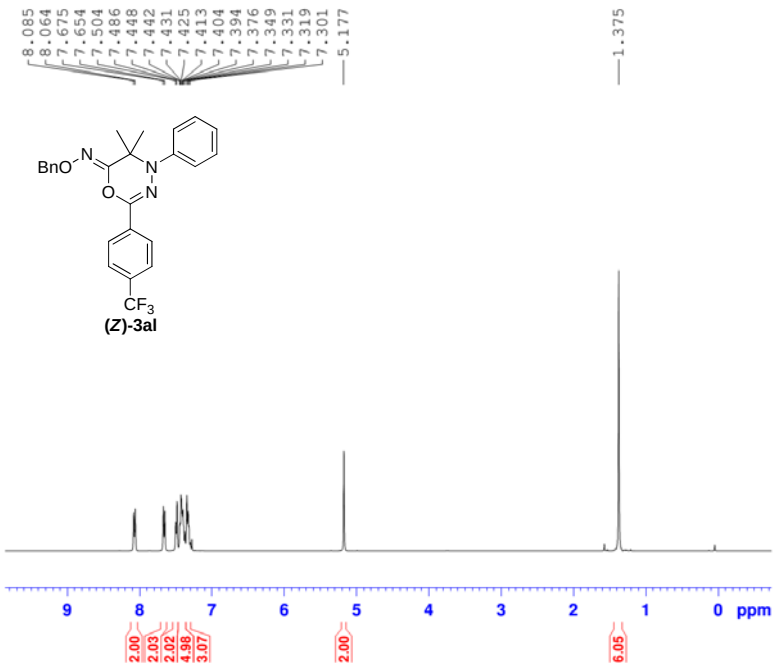

```
NAME                NMR
EXPNO               201703
PROCNO              1
Date_               20170221
Time                22.19 h
INSTRUM             spect
PROBHD     Z116098_0406 (
PULPROG             zg30
TD                  65536
SOLVENT             CDCl3
NS                  16
DS                  2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894966 sec
RG                  56.71
DW                  62.400 usec
DE                  6.50 usec
TE                  291.2 K
D1                  1.00000000 sec
TD0                 1
SFO1                400.1324708 MHz
NUC1                1H
P1                  10.00 usec
SI                  65536
SF                  400.1300173 MHz
WDW                 EM
SSB                 0
LB                  0.30 Hz
GB                  0
PC                  1.00
```




```
NAME                NMR
EXPNO               5262
PROCNO              1
Date_               20171121
Time                10.14
INSTRUM             spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  153
DS                  4
SWH                 24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                  2050
DW                  20.800 usec
DE                  6.50 usec
TE                  297.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                 1

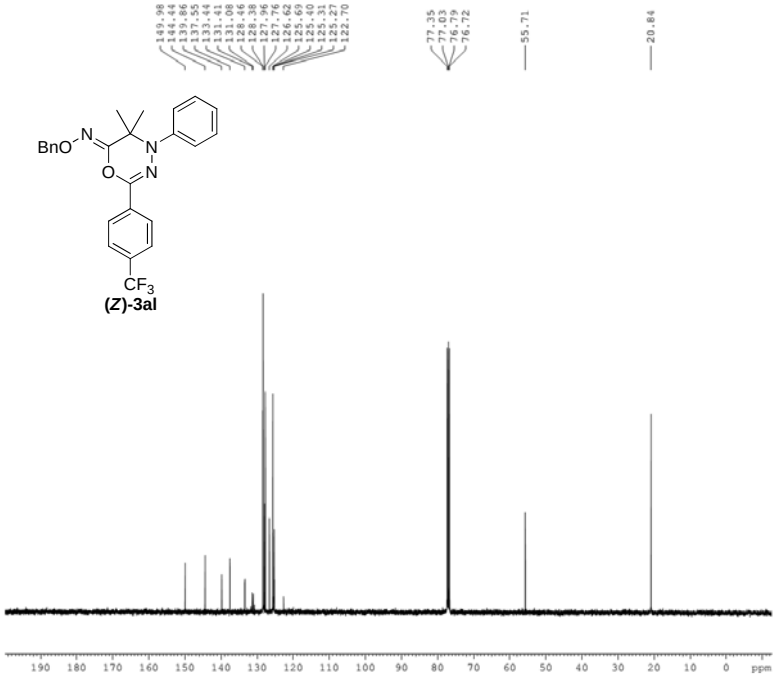
======== CHANNEL f1 ========
NUC1                13C
P1                  11.70 usec
PL1                 -2.00 dB
PL1W                48.76812744 W
SFO1                100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                1H
PCPD2               80.00 usec
PL2                 -2.83 dB
PL12                12.00 dB
PL13                14.00 dB
PL2W                16.91636658 W
PL12W               0.55629748 W
PL13W               0.35100001 W
SFO2                400.1716007 MHz
SI                  32768
SF                  100.6228270 MHz
WDW                 EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
```




```
NAME                  NMR
EXPNO                4746
PROCNO                  1
Date_             20170112
Time                 14.34
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    114
DW                 60.800 usec
DE                  6.50 usec
TE                 295.9 K
D1                1.00000000 sec
TD0                     1

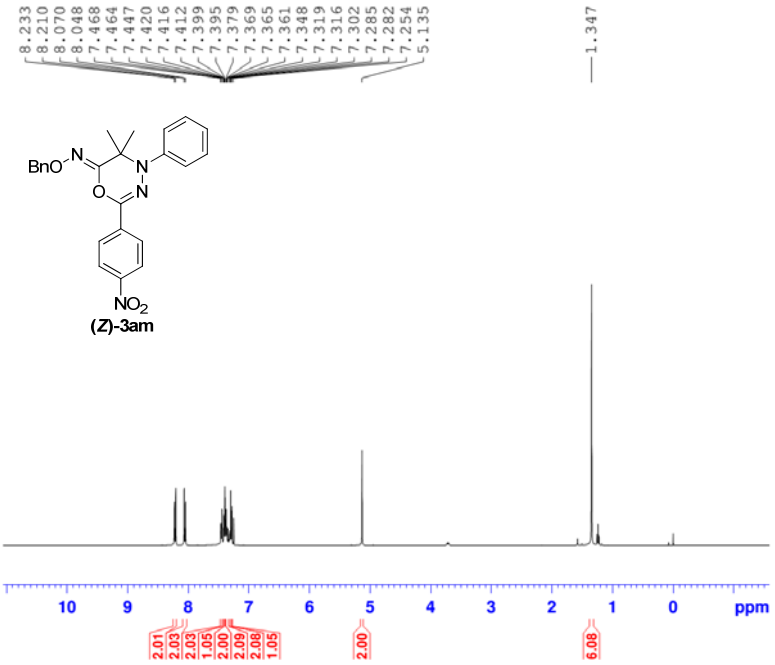
======== CHANNEL f1 ========
NUC1                   1H
P1                  14.50 usec
PL1                 -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI                  32768
SF            400.1700000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```



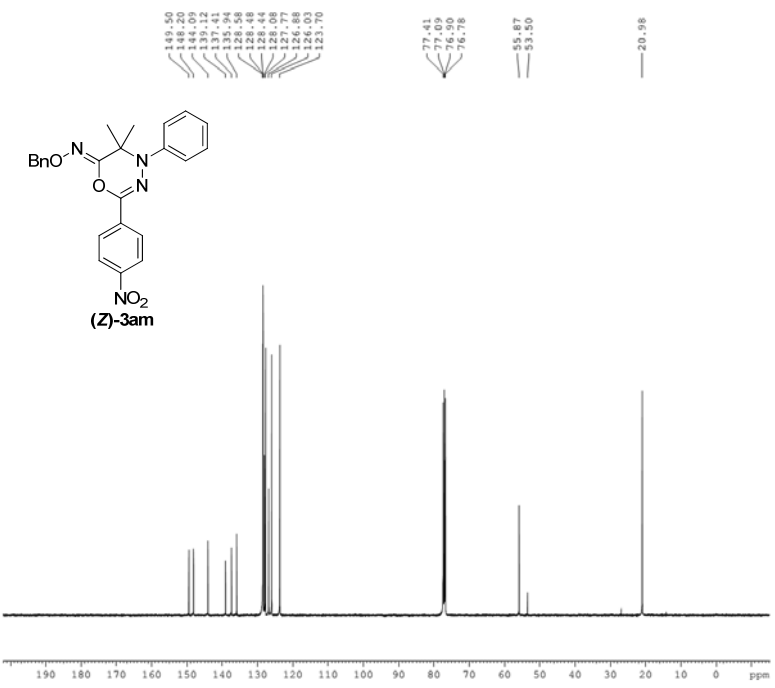

```
NAME                  NMR
EXPNO                4747
PROCNO                  1
Date_             20170112
Time                 14.38
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    212
DS                      4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    812
DW                 20.800 usec
DE                  6.50 usec
TE                 296.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                  11.70 usec
PL1                 -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

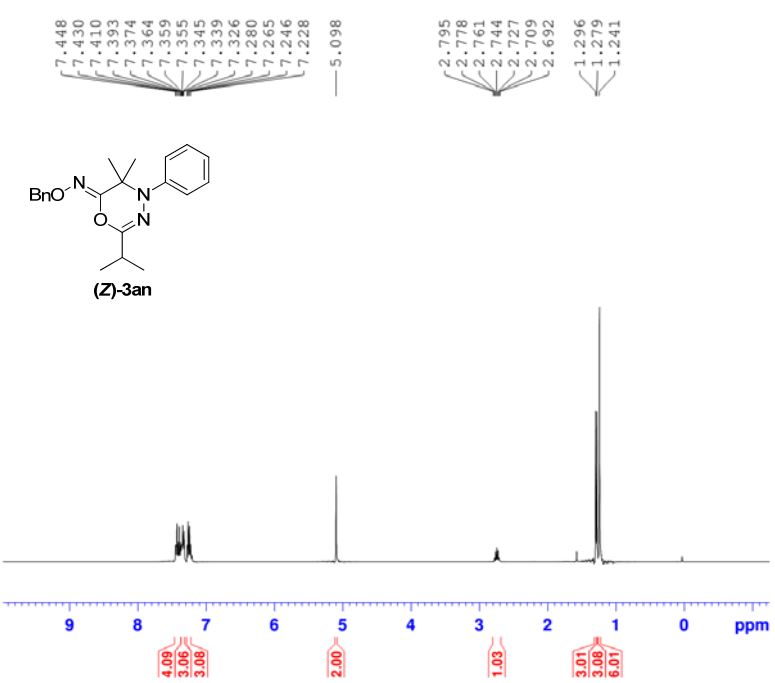
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -2.83 dB
PL12                12.00 dB
PL13                14.00 dB
PL2W          16.91636658 W
PL12W          0.55629748 W
PL13W          0.35100001 W
SFO2          400.1716007 MHz
SI                  32768
SF            100.6228270 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```




```
NAME              NMR
EXPNO          201701
PROCNO              1
Date_        20170221
Time            20.53 h
INSTRUM          spect
PROBHD   Z116098_0406 (
PULPROG          zg30
TD              65536
SOLVENT         CDCl3
NS                 16
DS                  2
SWH          8012.820 Hz
FIDRES          0.122266 Hz
AQ           4.0894966 sec
RG                 71.01
DW              62.400 usec
DE               6.50 usec
TE              290.7 K
D1           1.00000000 sec
TD0                 1
SFO1         400.1324708 MHz
NUC1               1H
P1              10.00 usec
SI              65536
SF           400.1300122 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

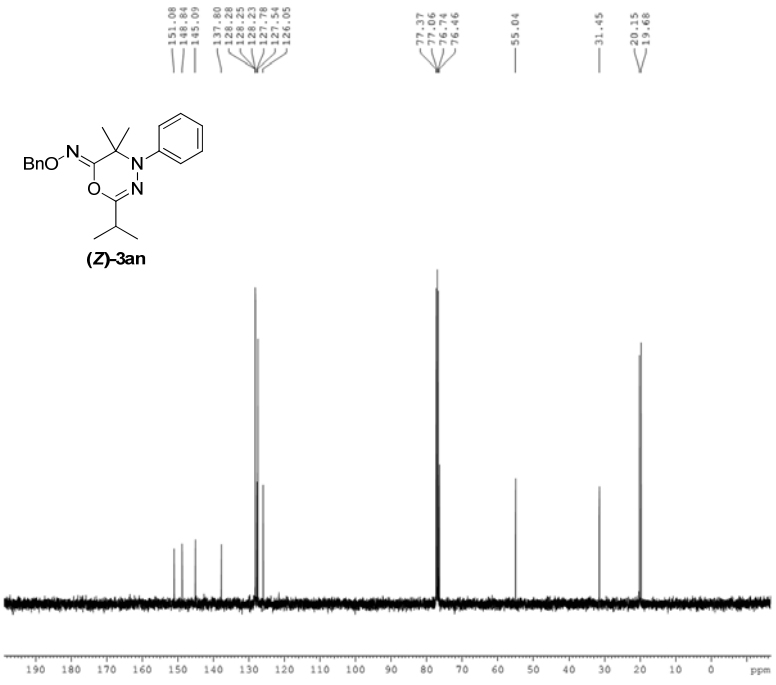



```
NAME              NMR
EXPNO          201713
PROCNO              1
Date_        20170301
Time            13.35 h
INSTRUM          spect
PROBHD   Z116098_0406 (
PULPROG        zgpg30
TD              65536
SOLVENT         CDCl3
NS               1024
DS                  4
SWH         24038.461 Hz
FIDRES          0.366798 Hz
AQ           1.3631988 sec
RG                196.12
DW              20.800 usec
DE               6.50 usec
TE              294.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                 1
SFO1         100.6228298 MHz
NUC1               13C
P1              10.00 usec
SI              32768
SF           100.6127685 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```




```
NAME                 NMR
EXPNO                4716
PROCNO                  1
Date_            20161228
Time                14.13
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      5
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    114
DW                60.800 usec
DE                 6.50 usec
TE                673.2 K
D1            1.00000000 sec
TD0                     1

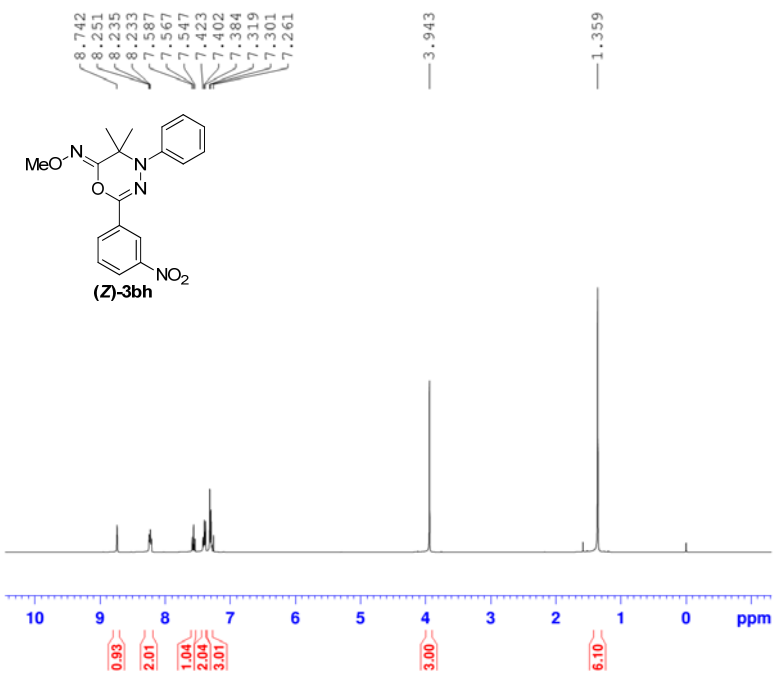
======== CHANNEL f1 ========
NUC1                  1H
P1                 14.50 usec
PL1                -2.83 dB
PL1W         16.91636658 W
SFO1         400.1724712 MHz
SI                  32768
SF           400.1700000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



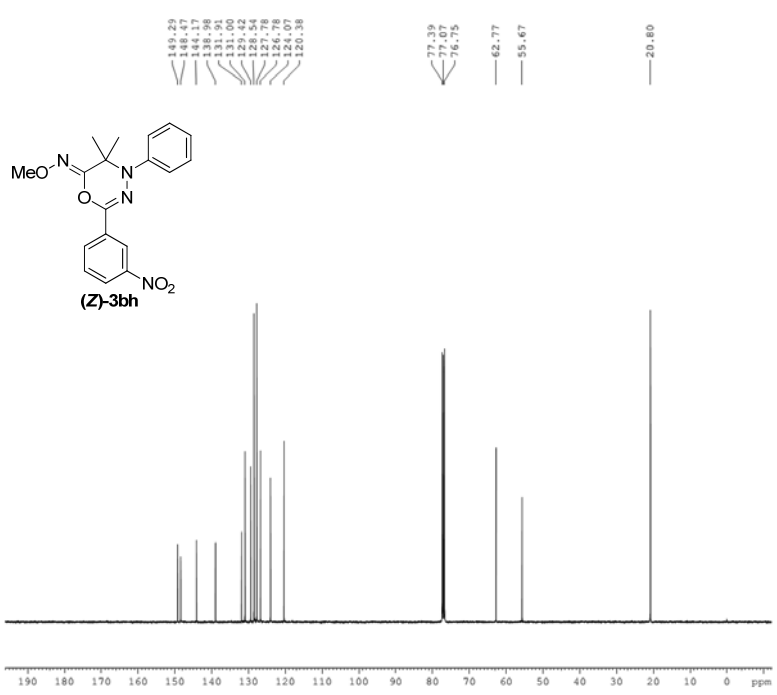

```
NAME                 NMR
EXPNO                4722
PROCNO                  1
Date_            20161229
Time                17.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     52
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    812
DW                20.800 usec
DE                 6.50 usec
TE                673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.70 usec
PL1                -2.00 dB
PL1W         48.76812744 W
SFO1         100.6328888 MHz

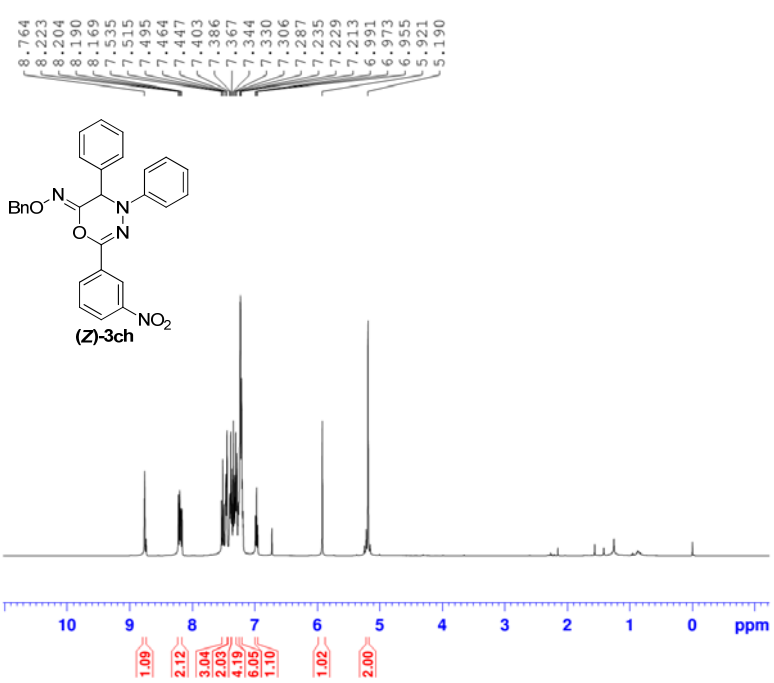
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.83 dB
PL12               12.00 dB
PL13               14.00 dB
PL2W         16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2         400.1716007 MHz
SI                  32768
SF           100.6228270 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



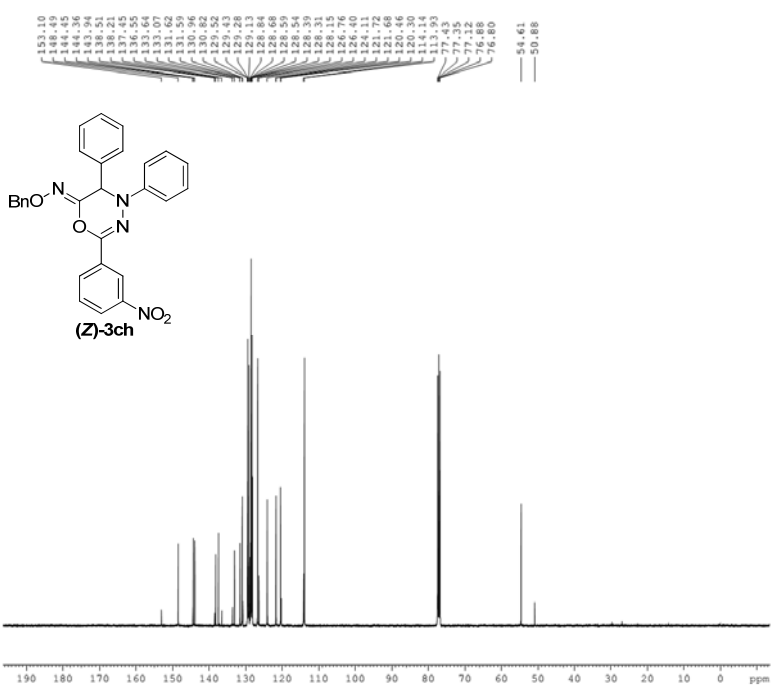

```
NAME                NMR
EXPNO             201715
PROCNO                 1
Date_           20170301
Time               12.31 h
INSTRUM             spect
PROBHD   Z116098_0406 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 78.23
DW                 62.400 usec
DE                  6.50 usec
TE                293.5 K
D1              1.00000000 sec
TD0                    1
SFO1            400.1324708 MHz
NUC1                  1H
P1                 10.00 usec
SI                 65536
SF              400.1300097 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



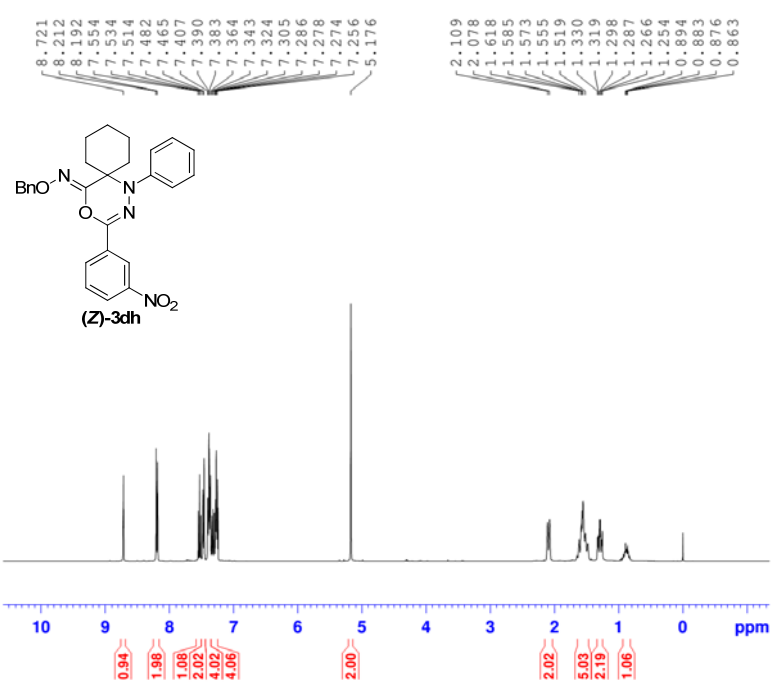

```
NAME                NMR
EXPNO             201746
PROCNO                 1
Date_           20170307
Time               21.42 h
INSTRUM             spect
PROBHD   Z116098_0406 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                196.12
DW                 20.800 usec
DE                  6.50 usec
TE                293.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1            100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
SI                 32768
SF              100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



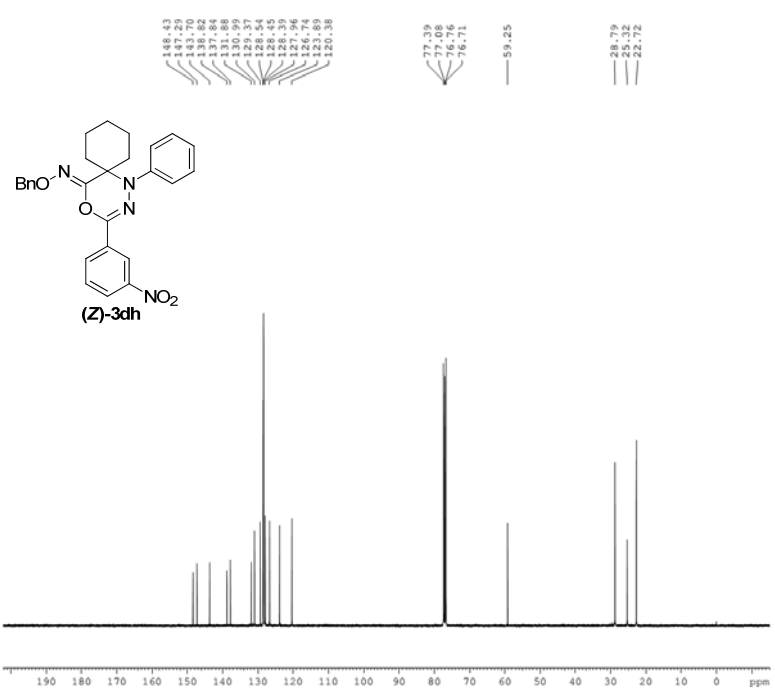

```
NAME                NMR
EXPNO             201742
PROCNO                 1
Date_           20170307
Time               21.47 h
INSTRUM             spect
PROBHD   Z116098_0406 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 30.91
DW                 62.400 usec
DE                  6.50 usec
TE                293.4 K
D1              1.00000000 sec
TD0                    1
SFO1           400.1324708 MHz
NUC1                  1H
P1                 10.00 usec
SI                 65536
SF             400.1300270 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



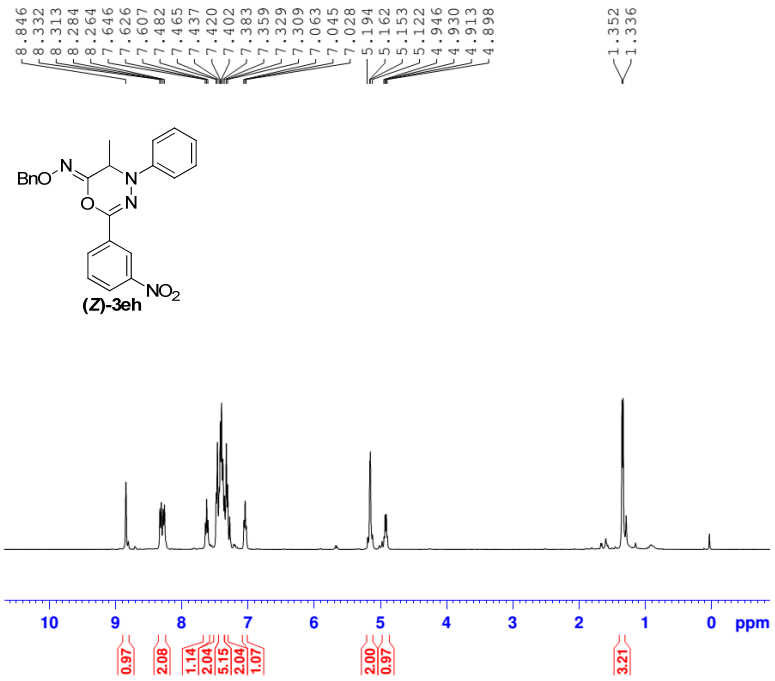

```
NAME                NMR
EXPNO             201743
PROCNO                 1
Date_           20170307
Time               22.47 h
INSTRUM             spect
PROBHD   Z116098_0406 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                196.12
DW                 20.800 usec
DE                  6.50 usec
TE                294.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
SI                 32768
SF             100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
NAME                 NMR
EXPNO              201744
PROCNO                  1
Date_            20170307
Time                18.07 h
INSTRUM              spect
PROBHD    Z116098_0406 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES              0.122266 Hz
AQ               4.0894966 sec
RG                  30.91
DW                  62.400 usec
DE                   6.50 usec
TE                 292.0 K
D1               1.00000000 sec
TD0                     1
SFO1           400.1324708 MHz
NUC1                   1H
P1                  10.00 usec
SI                  65536
SF             400.1300152 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

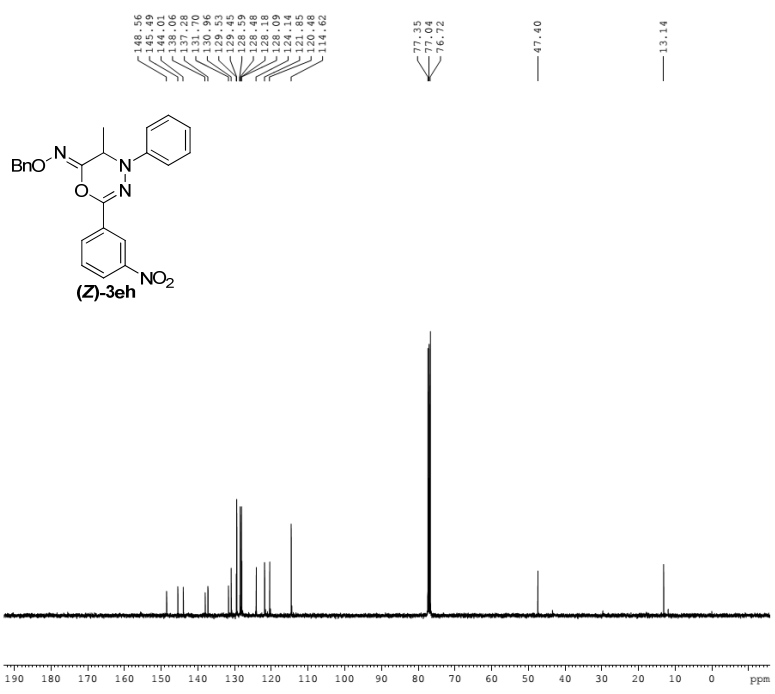



```
NAME                 NMR
EXPNO              201745
PROCNO                  1
Date_            20170307
Time                19.08 h
INSTRUM              spect
PROBHD    Z116098_0406 (
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES              0.366798 Hz
AQ               1.3631988 sec
RG                 196.12
DW                  20.800 usec
DE                   6.50 usec
TE                 293.4 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                     1
SFO1           100.6228298 MHz
NUC1                   13C
P1                  10.00 usec
SI                  32768
SF             100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
NAME                 NMR
EXPNO                5645
PROCNO               1
Date_                20171127
Time                 9.25
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                   16
DS                   2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                   128
DW                   60.800 usec
DE                   6.50 usec
TE                   296.4 K
D1                   1.00000000 sec
TD0                  1

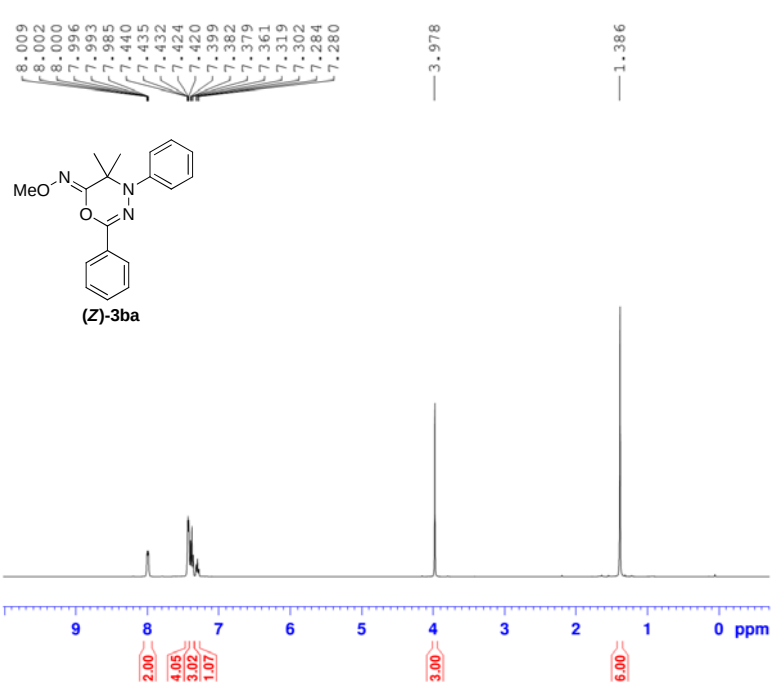
======== CHANNEL f1 ========
NUC1                 1H
P1                   14.50 usec
PL1                  -2.83 dB
PL1W                 16.91636658 W
SFO1                 400.1724712 MHz
SI                   32768
SF                   400.1700000 MHz
WDW                  EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```




```
NAME                 NMR
EXPNO                5646
PROCNO               1
Date_                20171127
Time                 9.30
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   385
DS                   4
SWH                  24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                   2050
DW                   20.800 usec
DE                   6.50 usec
TE                   296.5 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 13C
P1                   11.70 usec
PL1                  -2.00 dB
PL1W                 48.76812744 W
SFO1                 100.6328888 MHz

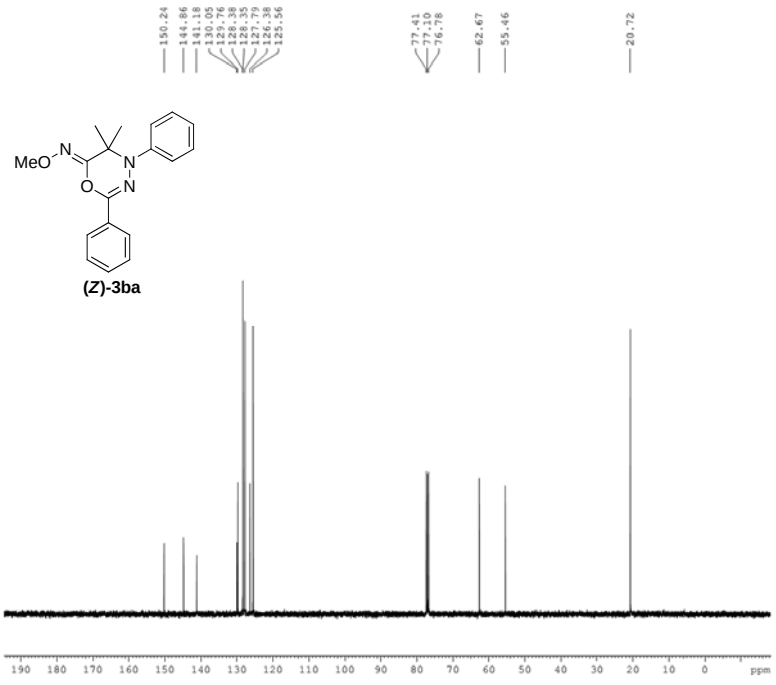
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                 1H
PCPD2                80.00 usec
PL2                  -2.83 dB
PL12                 12.00 dB
PL13                 14.00 dB
PL2W                 16.91636658 W
PL12W                0.55629748 W
PL13W                0.35100001 W
SFO2                 400.1716007 MHz
SI                   32768
SF                   100.6228270 MHz
WDW                  EM
SSB                  0
LB                   1.00 Hz
GB                   0
PC                   1.40
```



(*Z*)-3ba

```
NAME                 NMR
EXPNO                4696
PROCNO                  1
Date_            20161216
Time                 9.51
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   90.5
DW                60.800 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.50 usec
PL1                 -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI                   32768
SF            400.1700000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

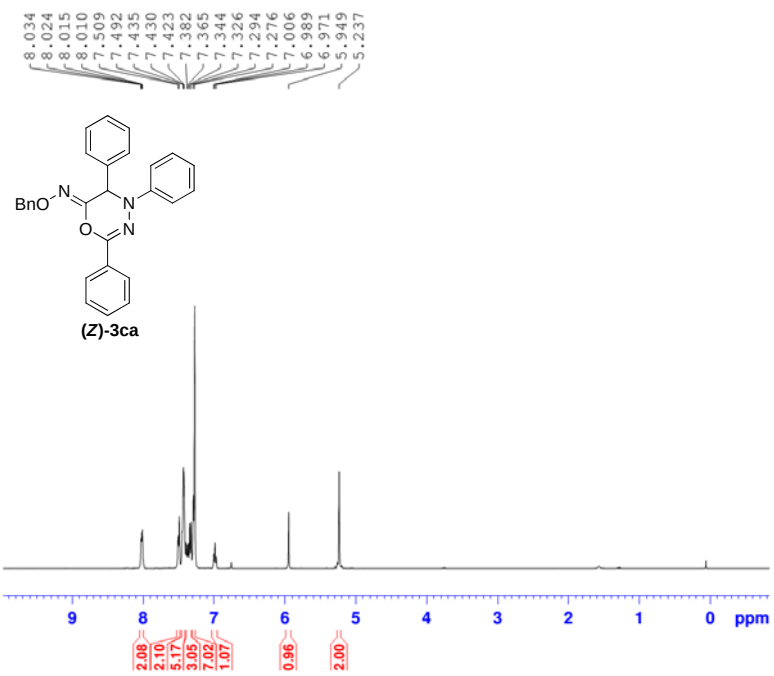


(*Z*)-3ba

```
NAME                 NMR
EXPNO                4699
PROCNO                  1
Date_            20161219
Time                13.58
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     38
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   1440
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

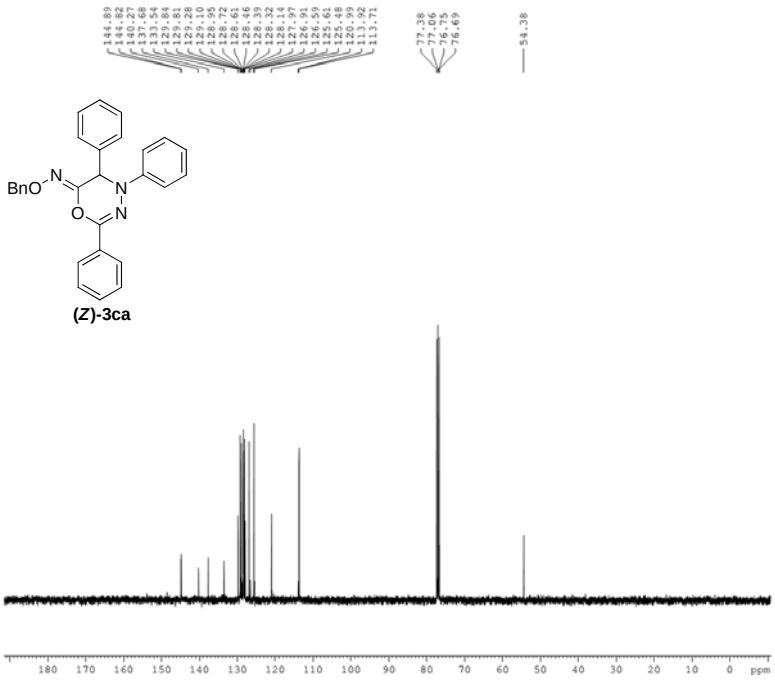
======== CHANNEL f1 ========
NUC1                  13C
P1                  11.70 usec
PL1                 -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 -2.83 dB
PL12                12.00 dB
PL13                14.00 dB
PL2W          16.91636658 W
PL12W          0.55629748 W
PL13W          0.35100001 W
SFO2          400.1716007 MHz
SI                   32768
SF            100.6228270 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
NAME                 NMR
EXPNO                4697
PROCNO                  1
Date_            20161219
Time                13.46
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      6
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                   90.5
DW                60.800 usec
DE                 6.50 usec
TE                295.4 K
D1             1.00000000 sec
TD0                     1

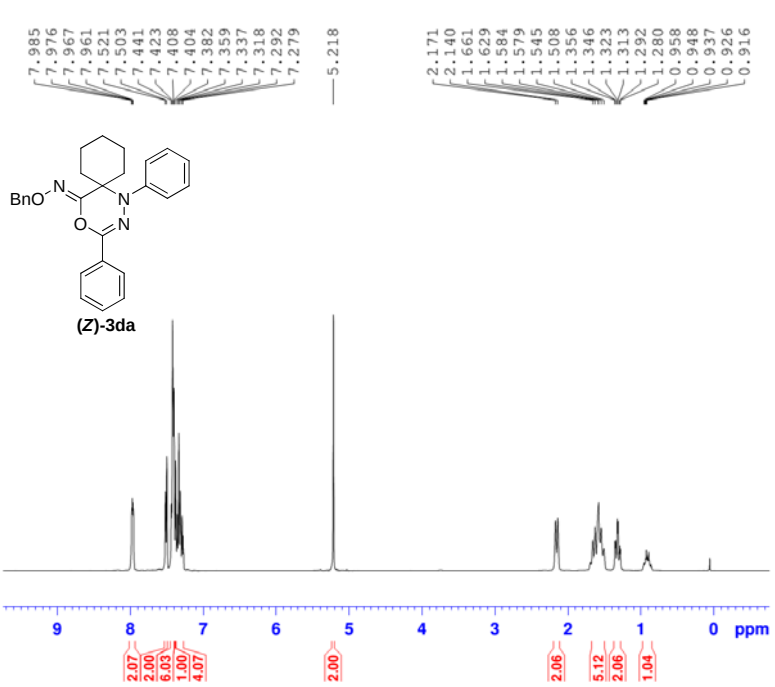
======== CHANNEL f1 ========
NUC1                   1H
P1                 14.50 usec
PL1                -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI                  32768
SF            400.1700000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```




```
NAME                 NMR
EXPNO                4698
PROCNO                  1
Date_            20161219
Time                13.49
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     65
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   1030
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

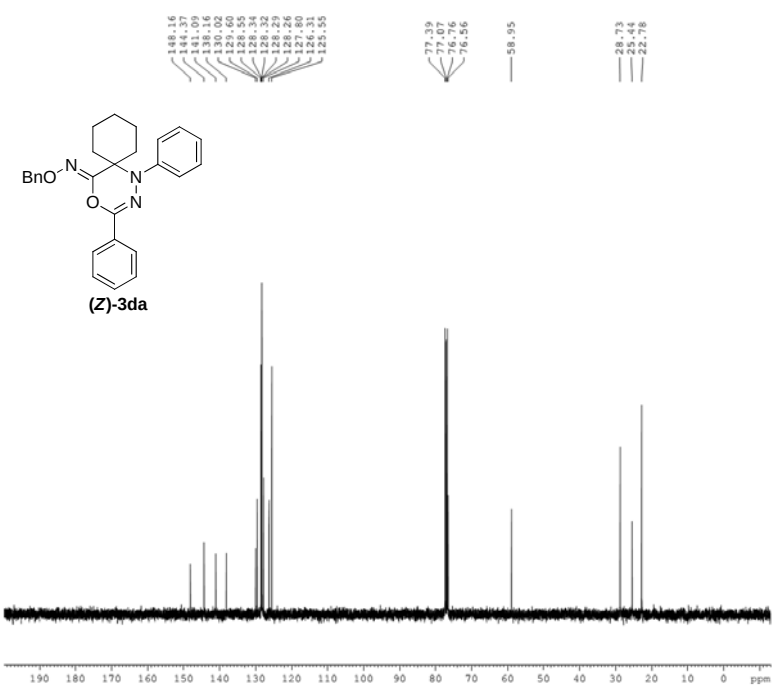
======== CHANNEL f1 ========
NUC1                  13C
P1                 11.70 usec
PL1                -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -2.83 dB
PL12               12.00 dB
PL13               14.00 dB
PL2W          16.91636658 W
PL12W          0.55629748 W
PL13W          0.35100001 W
SFO2          400.1716007 MHz
SI                  32768
SF            100.6228270 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```




```
NAME                NMR
EXPNO              4724
PROCNO                1
Date_          20161229
Time              17.41
INSTRUM           spect
PROBHD  5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  161
DW               60.800 usec
DE                6.50 usec
TE               673.2 K
D1            1.00000000 sec
TD0                   1

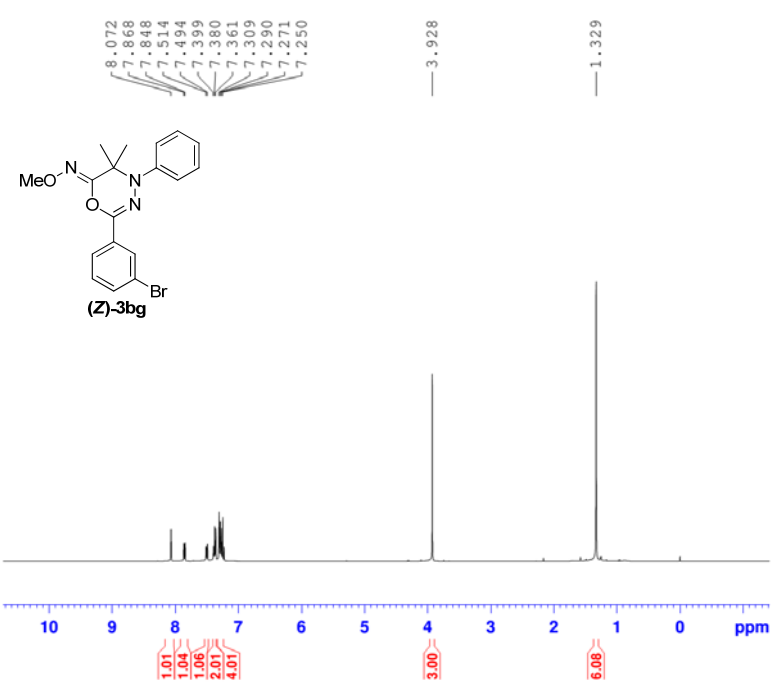
======== CHANNEL f1 ========
NUC1                1H
P1               14.50 usec
PL1              -2.83 dB
PL1W        16.91636658 W
SFO1       400.1724712 MHz
SI                32768
SF         400.1700000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



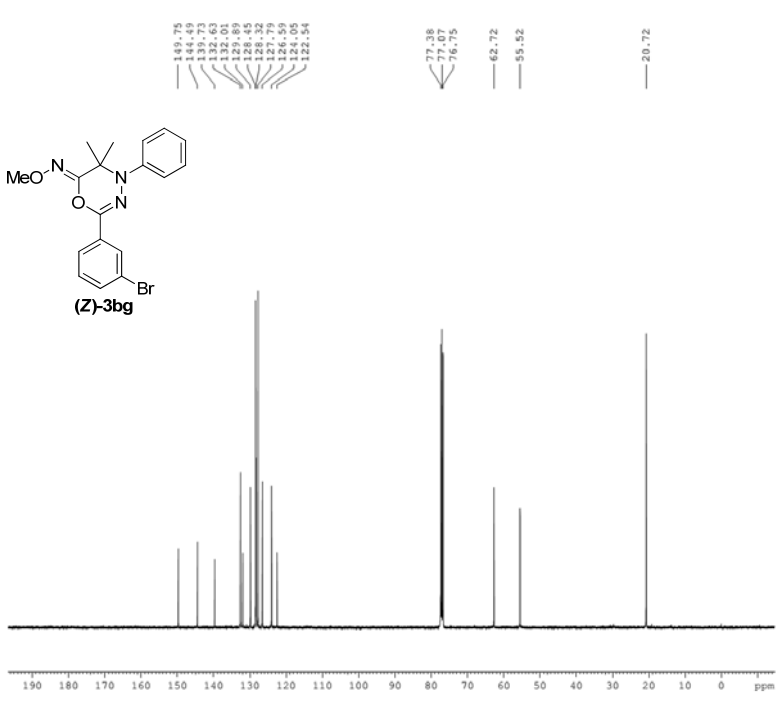

```
NAME                NMR
EXPNO              4723
PROCNO                1
Date_          20161229
Time              17.37
INSTRUM           spect
PROBHD  5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  812
DW               20.800 usec
DE                6.50 usec
TE               673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1               11.70 usec
PL1              -2.00 dB
PL1W        48.76812744 W
SFO1       100.6328888 MHz

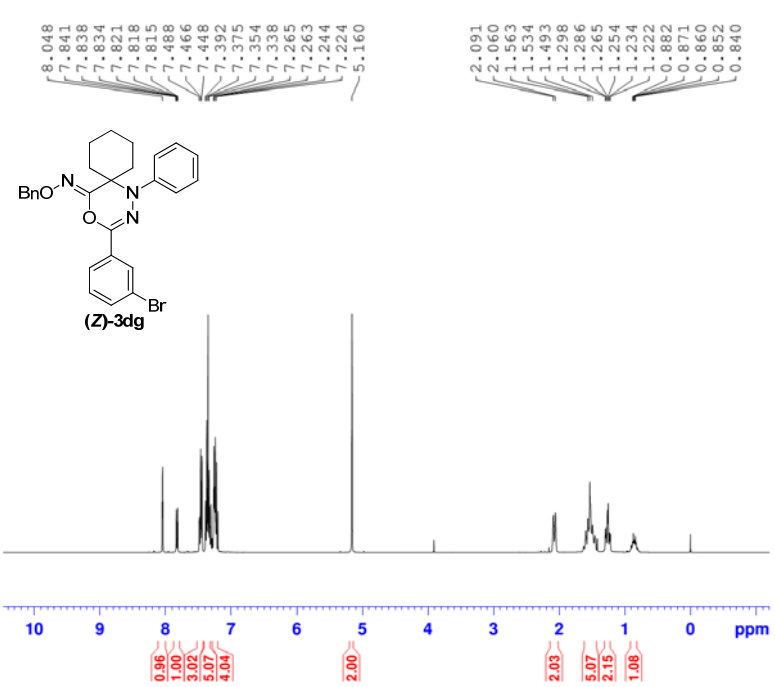
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -2.83 dB
PL12             12.00 dB
PL13             14.00 dB
PL2W        16.91636658 W
PL12W        0.55629748 W
PL13W        0.35100001 W
SFO2       400.1716007 MHz
SI                32768
SF         100.6228270 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



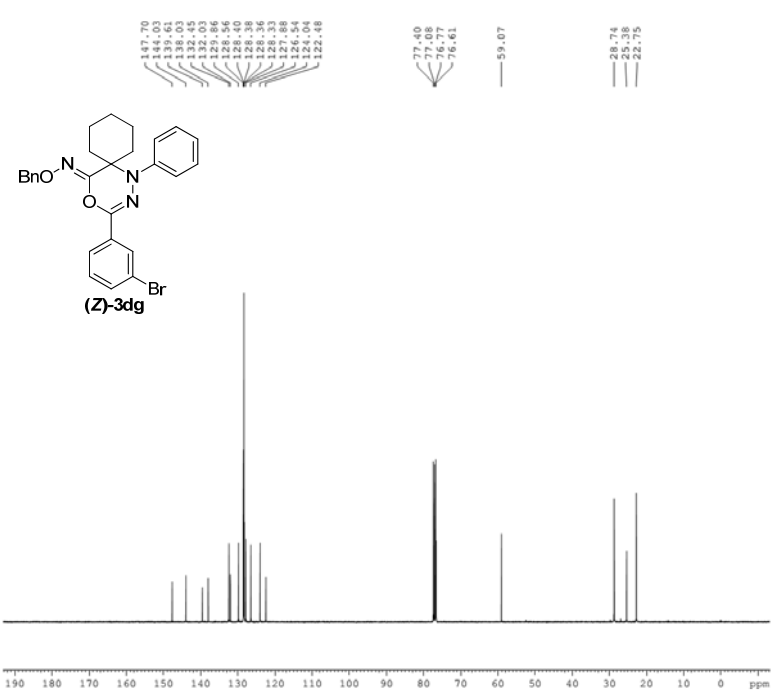

```
NAME                 NMR
EXPNO              201737
PROCNO                  1
Date_            20170307
Time                19.19 h
INSTRUM             spect
PROBHD    Z116098_0406 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                 50.56
DW                 62.400 usec
DE                  6.50 usec
TE                292.8 K
D1                1.00000000 sec
TD0                    1
SFO1           400.1324708 MHz
NUC1                   1H
P1                 10.00 usec
SI                 65536
SF             400.1300140 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



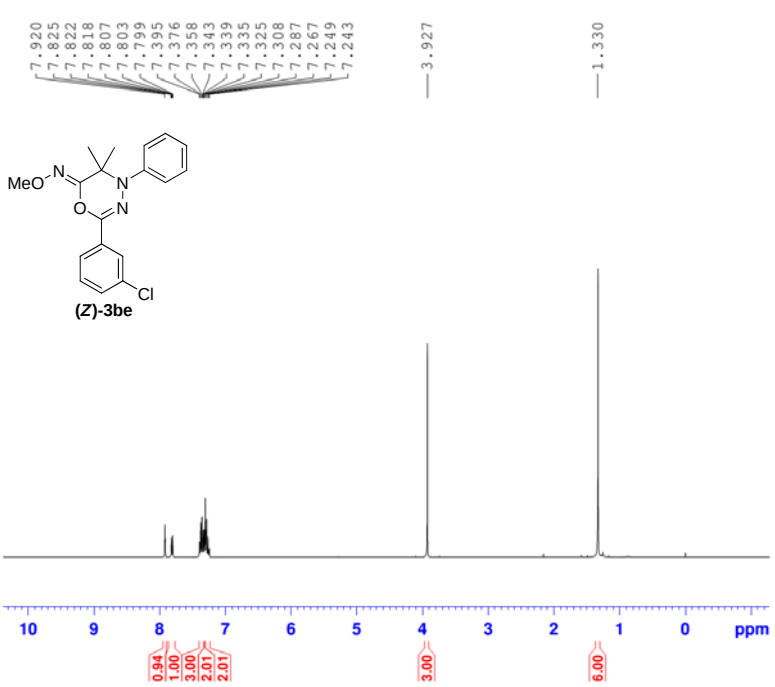

```
NAME                 NMR
EXPNO              201738
PROCNO                  1
Date_            20170307
Time                20.19 h
INSTRUM             spect
PROBHD    Z116098_0406 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                196.12
DW                 20.800 usec
DE                  6.50 usec
TE                293.7 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                    1
SFO1           100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
SI                 32768
SF             100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



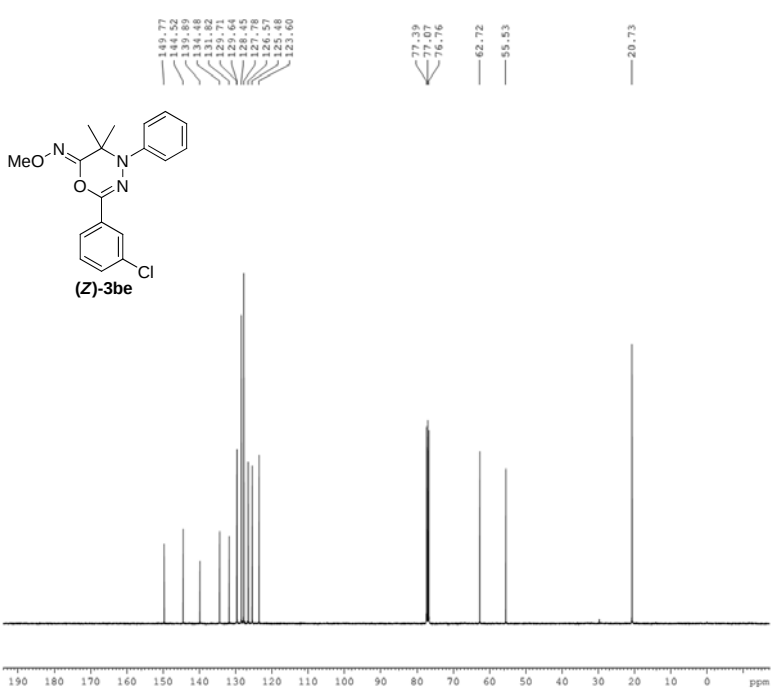

```
NAME                 NMR
EXPNO              201735
PROCNO                  1
Date_            20170307
Time                22.53 h
INSTRUM              spect
PROBHD    Z116098_0406 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  30.91
DW                 62.400 usec
DE                  6.50 usec
TE                 293.5 K
D1              1.00000000 sec
TD0                     1
SFO1           400.1324708 MHz
NUC1                   1H
P1                 10.00 usec
SI                  65536
SF             400.1300218 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



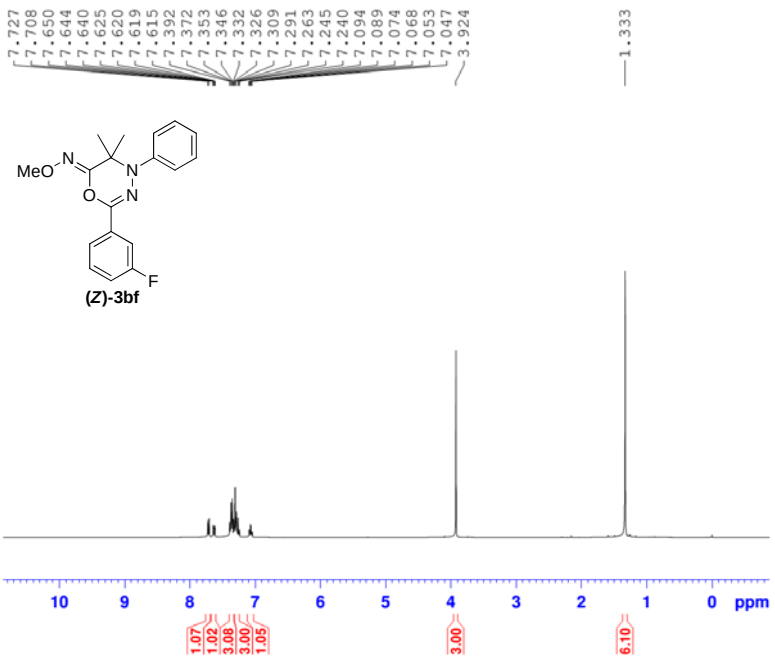

```
NAME                 NMR
EXPNO              201736
PROCNO                  1
Date_            20170307
Time                23.53 h
INSTRUM              spect
PROBHD    Z116098_0406 (
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                 196.12
DW                 20.800 usec
DE                  6.50 usec
TE                 294.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1           100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
SI                  32768
SF             100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



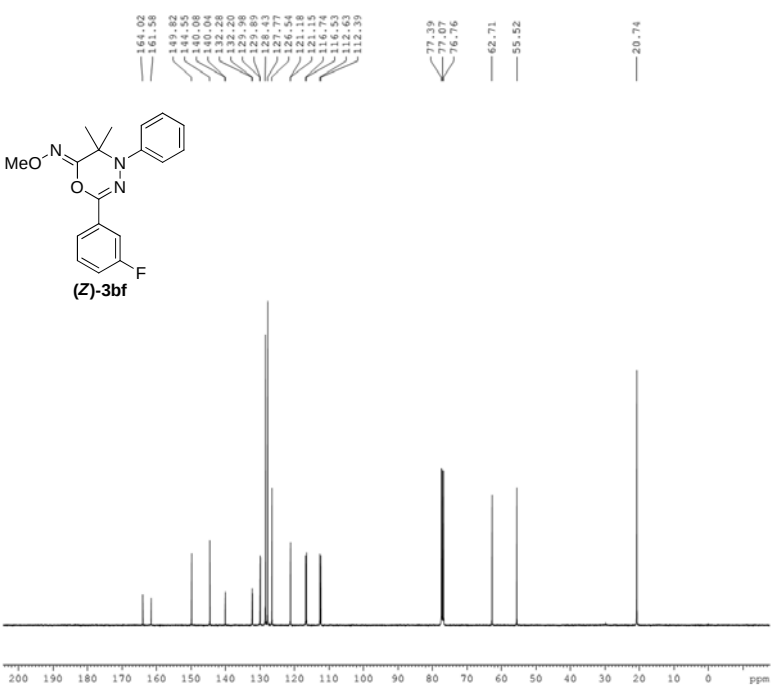

```
NAME                 NMR
EXPNO              201729
PROCNO                  1
Date_           20170308
Time                2.10 h
INSTRUM             spect
PROBHD     Z116098_0406 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES              0.122266 Hz
AQ                4.0894966 sec
RG                    30.91
DW                   62.400 usec
DE                    6.50 usec
TE                  293.7 K
D1                1.00000000 sec
TD0                     1
SFO1             400.1324708 MHz
NUC1                    1H
P1                   10.00 usec
SI                   65536
SF               400.1300166 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



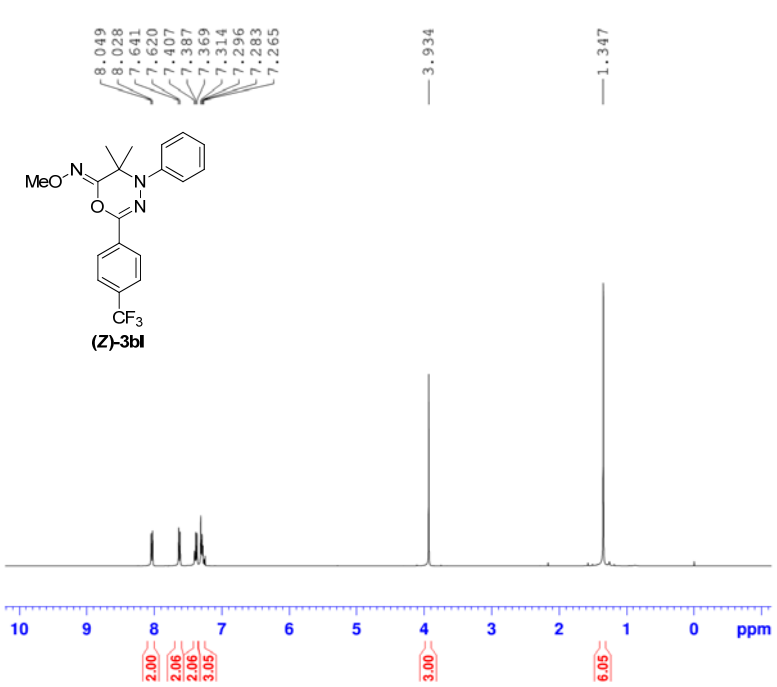

```
NAME                 NMR
EXPNO              201730
PROCNO                  1
Date_           20170308
Time                3.11 h
INSTRUM             spect
PROBHD     Z116098_0406 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                   196.12
DW                   20.800 usec
DE                    6.50 usec
TE                  294.4 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                     1
SFO1             100.6228298 MHz
NUC1                    13C
P1                   10.00 usec
SI                   32768
SF               100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



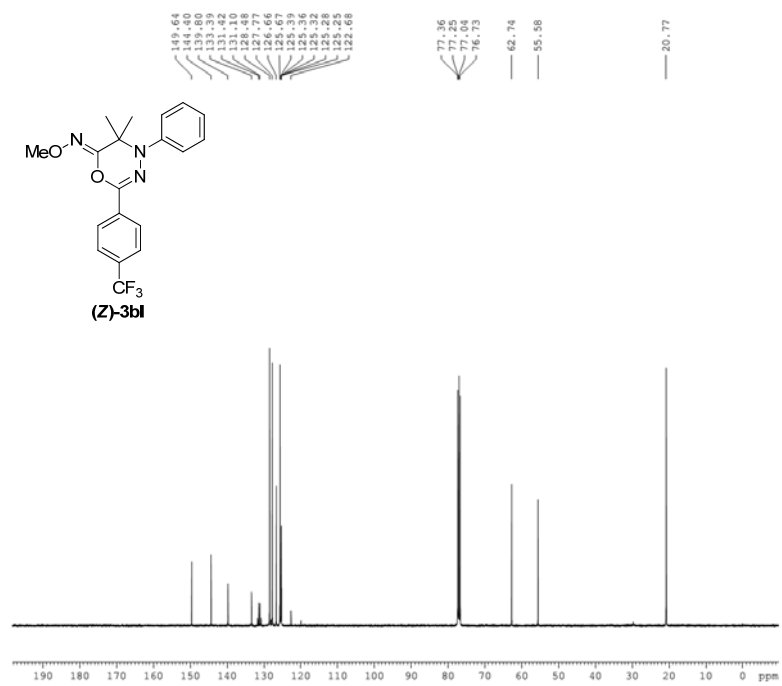

```
NAME                NMR
EXPNO             201731
PROCNO                 1
Date_           20170308
Time                1.05 h
INSTRUM            spect
PROBHD    Z116098_0406 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                 30.91
DW                 62.400 usec
DE                  6.50 usec
TE                293.6 K
D1                1.00000000 sec
TD0                    1
SFO1           400.1324708 MHz
NUC1                  1H
P1                 10.00 usec
SI                 65536
SF             400.1300179 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME                NMR
EXPNO             201732
PROCNO                 1
Date_           20170308
Time                2.05 h
INSTRUM            spect
PROBHD    Z116098_0406 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                196.12
DW                 20.800 usec
DE                  6.50 usec
TE                294.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                    1
SFO1           100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
SI                 32768
SF             100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
NAME                NMR
EXPNO               201733
PROCNO              1
Date_               20170308
Time                3.16 h
INSTRUM             spect
PROBHD     Z116098_0406 (
PULPROG             zg30
TD                  65536
SOLVENT             CDCl3
NS                  16
DS                  2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894966 sec
RG                  50.56
DW                  62.400 usec
DE                  6.50 usec
TE                  293.8 K
D1                  1.00000000 sec
TD0                 1
SFO1                400.1324708 MHz
NUC1                1H
P1                  10.00 usec
SI                  65536
SF                  400.1300141 MHz
WDW                 EM
SSB                 0
LB                  0.30 Hz
GB                  0
PC                  1.00
```




```
NAME                NMR
EXPNO               201734
PROCNO              1
Date_               20170308
Time                4.17 h
INSTRUM             spect
PROBHD     Z116098_0406 (
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  1024
DS                  4
SWH                 24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                  196.12
DW                  20.800 usec
DE                  6.50 usec
TE                  294.4 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                 1
SFO1                100.6228298 MHz
NUC1                13C
P1                  10.00 usec
SI                  32768
SF                  100.6127685 MHz
WDW                 EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
```

6. X-Ray crystal data of compound (*Z*)-3ae

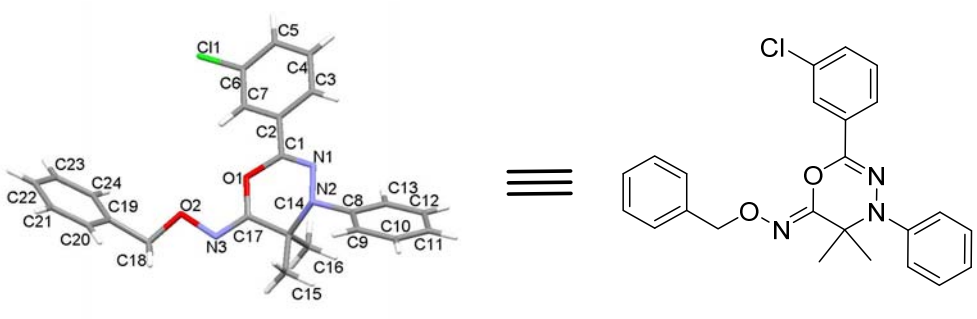


Figure 1.X-ray single crystal structure of (*Z*)-3ae (with thermal ellipsoils shown at the 50% probability level)

Identification code	**(Z)-3ae**	
Empirical formula	$C_{24}H_{22}ClN_3O_2$	
Formula weight	419.89	
Temperature	113 K	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 7.9332(14) A b = 10.9116(18) A c = 12.9665(19) A	alpha = 96.881(4) deg. beta = 92.036(2) deg. gamma = 109.013(5) deg.
Volume	1050.2(3) A^3	
Z, Calculated density	2, 1.328 g/cm^3	
Absorption coefficient	0.208 mm^-1	
F(000)	440.0	
Crystal size	0.2 × 0.18 × 0.14 mm^3	
Radiation	MoKα (λ = 0.71073)	
Theta range for data collection	6.084 to 55.034 deg.	
Index ranges	-10 ⩽ h ⩽ 10, -13 ⩽ k ⩽ 14, -16 ⩽ l ⩽ 16	

Reflections collected / uniqueIndependent reflections	13555 / 4737 [Rint = 0.0248, Rsigma = 0.0237]
Data / restraints / parameters	4737/84/313
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0867
R indices (all data)	R1 = 0.0399, wR2 = 0.0905
Largest diff. peak and hole	0.30/-0.29 e.A^-3

7. Computational methods

(1) The geometric structures of all reactants, transition states (TS), intermediates (Int) and products were optimized by the density functional theory (DFT) method with the hybrid functional B3LYP[6-8] at the 6-31+G(d) theoretical level. The analytical computations of vibrational frequencies were performed for all stationary points to verify either that they were energy minima with all positive frequencies or that they were transition states with only one imaginary frequency. The intrinsic reaction coordinate (IRC) calculations were performed to confirm that every transition state connects the corresponding reactant and product through the minimized-energy pathway. Cartesian coordinates, the number of imaginary frequencies and computed thermochemical values of the optimized geometries are provided in the Supporting Information. All computations presented in this work were performed with GAUSSIAN 09 program package.

Cartesian coordinates, the number of imaginary frequencies and computed thermochemical values of the optimized structures

Structure Number: **4**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -632.11403938 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.836762	0.989761	0.514411
2	8	0	-0.117040	-0.513872	-0.944107
3	7	0	-1.515820	-0.882075	-0.877111
4	6	0	-3.756535	-0.241215	-0.207362
5	6	0	-4.255154	-0.644247	1.181481
6	1	0	-5.345361	-0.753897	1.210539
7	1	0	-3.961780	0.155736	1.866003
8	1	0	-3.793493	-1.572326	1.530007
9	6	0	-4.462615	1.033856	-0.687192
10	1	0	-4.163839	1.307369	-1.705607
11	1	0	-4.166739	1.855233	-0.031323
12	1	0	-5.551745	0.912677	-0.657161
13	6	0	-2.203461	0.008374	-0.166645
14	6	0	0.591731	-0.944849	0.222863
15	1	0	0.613318	-2.045346	0.262646
16	1	0	0.071424	-0.569627	1.112517
17	6	0	1.989542	-0.381370	0.154479
18	6	0	3.109462	-1.212922	0.037308
19	1	0	2.972051	-2.291616	-0.011997
20	6	0	4.399975	-0.673231	-0.012672
21	1	0	5.260638	-1.332805	-0.098178
22	6	0	4.579611	0.710631	0.045037
23	1	0	5.580817	1.133682	0.006800
24	6	0	3.464397	1.550671	0.154585
25	1	0	3.599101	2.628921	0.201886
26	6	0	2.179553	1.008778	0.210595

27	1	0	1.307747	1.652560	0.296351

Zero-point correction=	0.219653 (Hartree/Particle)
Thermal correction to Energy=	0.233526
Thermal correction to Enthalpy=	0.234470
Thermal correction to Gibbs Free Energy=	0.175691
Sum of electronic and zero-point Energies=	-631.894386
Sum of electronic and thermal Energies=	-631.880513
Sum of electronic and thermal Enthalpies=	-631.879569
Sum of electronic and thermal Free Energies=	-631.938349

Structure Number: **5**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1070.43974016 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	4.269372	2.125701	0.000034
2	7	0	-0.973275	-1.194222	-0.001371
3	7	0	-2.190125	-1.525746	-0.000717
4	6	0	0.188955	-1.028347	-0.002725
5	6	0	1.598594	-0.892921	-0.001326
6	6	0	2.434564	-2.031472	0.000368
7	1	0	1.994677	-3.023504	0.000550
8	6	0	3.816988	-1.871260	0.001787
9	1	0	4.456868	-2.749266	0.002991
10	6	0	4.396883	-0.598730	0.001709
11	1	0	5.474406	-0.474436	0.002856
12	6	0	3.559353	0.519355	0.000145
13	6	0	2.173978	0.397951	-0.001346
14	1	0	1.544362	1.280690	-0.002581
15	6	0	-3.142013	-0.491021	-0.000154
16	6	0	-4.490698	-0.893180	0.000732
17	1	0	-4.715450	-1.955843	0.000948
18	6	0	-5.506793	0.058597	0.001297
19	1	0	-6.543885	-0.267875	0.001971
20	6	0	-5.202711	1.425914	0.000993
21	1	0	-5.997841	2.166351	0.001454
22	6	0	-3.863792	1.827321	0.000129
23	1	0	-3.613426	2.885656	-0.000100
24	6	0	-2.835823	0.882680	-0.000440
25	1	0	-1.800138	1.211758	-0.001069

Zero-point correction=	0.185600 (Hartree/Particle)
Thermal correction to Energy=	0.199025
Thermal correction to Enthalpy=	0.199969
Thermal correction to Gibbs Free Energy=	0.142175
Sum of electronic and zero-point Energies=	-1070.254140
Sum of electronic and thermal Energies=	-1070.240715
Sum of electronic and thermal Enthalpies=	-1070.239771
Sum of electronic and thermal Free Energies=	-1070.297565

Structure Number: **TS1**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1702.54919172 (Hartrees)
Number of imaginary frequencies: -140.23*i* cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.979819	5.507204	0.515449
2	8	0	0.216075	-1.047569	-2.325813
3	8	0	-1.124317	-1.913205	-0.206994
4	7	0	1.859549	0.772485	-0.573038
5	7	0	2.937597	0.080408	-0.743481
6	7	0	0.256730	-2.119576	-0.222807
7	6	0	0.835057	1.330337	-0.639793
8	6	0	-0.416040	2.011580	-0.721314
9	6	0	-1.490799	1.391595	-1.392776
10	1	0	-1.338418	0.404925	-1.827846
11	6	0	-2.705888	2.071864	-1.466065
12	1	0	-3.543737	1.608303	-1.976749
13	6	0	-2.866984	3.332718	-0.883121
14	1	0	-3.816760	3.854838	-0.938368
15	6	0	-1.786395	3.922469	-0.219892
16	6	0	-0.555708	3.283872	-0.130947
17	1	0	0.275181	3.755727	0.379050
18	6	0	3.853737	0.131214	0.339129
19	6	0	3.485535	0.431478	1.661265
20	1	0	2.448070	0.642392	1.901368
21	6	0	4.453753	0.445316	2.667548
22	1	0	4.158878	0.681674	3.686989
23	6	0	5.788381	0.149158	2.375515
24	1	0	6.536050	0.160744	3.162890
25	6	0	6.152649	-0.157842	1.059386
26	1	0	7.188678	-0.381081	0.818205
27	6	0	5.195567	-0.163794	0.044807
28	1	0	5.475645	-0.370998	-0.983239
29	6	0	2.239618	-1.915125	-1.407380
30	6	0	2.915502	-2.791599	-0.401386
31	1	0	3.983004	-2.561709	-0.328616
32	1	0	2.835389	-3.829319	-0.762258
33	1	0	2.444923	-2.742853	0.579074
34	6	0	2.870597	-1.826822	-2.759108
35	1	0	2.439987	-1.010606	-3.340430
36	1	0	2.631083	-2.761956	-3.289695
37	1	0	3.959332	-1.742093	-2.700179
38	6	0	0.776398	-1.652473	-1.367399
39	6	0	-1.659541	-2.512120	0.976723
40	1	0	-1.245648	-2.013899	1.864689
41	1	0	-1.342910	-3.565457	1.005923
42	6	0	-3.165204	-2.403080	0.949752
43	6	0	-3.872707	-2.043162	2.105162

44	1	0	-3.325737	-1.797130	3.013949
45	6	0	-5.270742	-1.994336	2.103149
46	1	0	-5.803367	-1.715204	3.009397
47	6	0	-5.978127	-2.293636	0.936677
48	1	0	-7.064256	-2.252653	0.930904
49	6	0	-5.278619	-2.643935	-0.224376
50	1	0	-5.822000	-2.875115	-1.138044
51	6	0	-3.884297	-2.702187	-0.217414
52	1	0	-3.342122	-2.966976	-1.120776

Zero-point correction=	0.406264 (Hartree/Particle)
Thermal correction to Energy=	0.434077
Thermal correction to Enthalpy=	0.435021
Thermal correction to Gibbs Free Energy=	0.343060
Sum of electronic and zero-point Energies=	-1702.142927
Sum of electronic and thermal Energies=	-1702.115115
Sum of electronic and thermal Enthalpies=	-1702.114171
Sum of electronic and thermal Free Energies=	-1702.206132

Structure Number: **Int1**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1702.56622518 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-8.018838	-0.005580	-1.091279
2	8	0	1.794873	-1.319244	0.748909
3	8	0	3.698952	-0.448448	-1.131961
4	7	0	-1.994081	-0.038131	0.090360
5	7	0	-0.667201	0.026698	0.072782
6	7	0	2.408424	-0.306137	-1.321811
7	6	0	-3.118768	-0.242737	0.329658
8	6	0	-4.475907	-0.477892	0.641217
9	6	0	-4.813749	-1.026720	1.889459
10	1	0	-4.027580	-1.278044	2.619563
11	6	0	-6.155002	-1.250784	2.192898
12	1	0	-6.428670	-1.681815	3.169468
13	6	0	-7.153048	-0.935197	1.271549
14	1	0	-8.211957	-1.116131	1.520408
15	6	0	-6.807230	-0.388716	0.028462
16	6	0	-5.468868	-0.156018	-0.298123
17	1	0	-5.197003	0.272253	-1.276393
18	6	0	-0.135293	1.385939	0.105929
19	6	0	0.868375	1.642460	1.060357
20	1	0	1.265822	0.819821	1.686427
21	6	0	1.399606	2.927908	1.155761
22	1	0	2.194283	3.125460	1.891792
23	6	0	0.945761	3.949637	0.323857
24	1	0	1.374236	4.959662	0.407253
25	6	0	-0.041042	3.688029	-0.626911
26	1	0	-0.386615	4.489094	-1.297078
27	6	0	-0.582635	2.410786	-0.746265
28	1	0	-1.341734	2.215365	-1.518065
29	6	0	0.050977	-0.910387	-0.875827
30	6	0	-0.160668	-0.539486	-2.337800
31	1	0	-1.224408	-0.704239	-2.638934
32	1	0	0.492241	-1.190441	-2.970541
33	1	0	0.117363	0.524030	-2.537083
34	6	0	-0.391337	-2.357970	-0.661816
35	1	0	-0.273827	-2.652446	0.410085
36	1	0	0.287341	-3.006867	-1.269758
37	1	0	-1.441605	-2.530027	-0.995400
38	6	0	1.582475	-0.867032	-0.414109
39	6	0	4.299527	0.239039	0.001082
40	1	0	3.721282	0.006085	0.936912
41	1	0	4.274973	1.343643	-0.193142
42	6	0	5.700898	-0.247593	0.142393
43	6	0	6.706647	0.636773	0.549771
44	1	0	6.466822	1.695909	0.722256

45	6	0	8.010273	0.179598	0.734879
46	1	0	8.795052	0.878102	1.058355
47	6	0	8.320778	-1.160877	0.508234
48	1	0	9.348753	-1.520096	0.655863
49	6	0	7.323886	-2.043637	0.092102
50	1	0	7.567442	-3.099895	-0.091215
51	6	0	6.018436	-1.590828	-0.090129
52	1	0	5.222869	-2.275817	-0.423706

Zero-point correction=	0.409236	(Hartree/Particle)
Thermal correction to Energy=	0.436912	
Thermal correction to Enthalpy=	0.437856	
Thermal correction to Gibbs Free Energy=	0.346186	
Sum of electronic and zero-point Energies=	-1702.156990	
Sum of electronic and thermal Energies=	-1702.129313	
Sum of electronic and thermal Enthalpies=	-1702.128369	
Sum of electronic and thermal Free Energies=	-1702.220039	

Structure Number: **3ae**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1702.65437723 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-3.088620	5.280017	-0.413587
2	8	0	0.410284	-0.018227	0.332827
3	8	0	2.606169	-1.257351	0.158849
4	7	0	-1.891888	0.027814	-0.148282
5	7	0	-1.897044	-1.349792	-0.207054
6	7	0	1.480657	-2.057861	0.379077
7	6	0	-0.791364	0.628654	0.109986
8	6	0	-0.680156	2.096472	0.143034
9	6	0	0.554728	2.705187	0.429251
10	1	0	1.417889	2.080891	0.632514
11	6	0	0.657321	4.092914	0.453591
12	1	0	1.613197	4.559188	0.677067
13	6	0	-0.456414	4.899778	0.193595
14	1	0	-0.380596	5.982061	0.209873
15	6	0	-1.674684	4.283628	-0.086613
16	6	0	-1.805791	2.896039	-0.114142
17	1	0	-2.765825	2.441209	-0.326532
18	6	0	-3.231941	-1.872543	-0.340036
19	6	0	-3.472751	-2.909273	-1.249696
20	1	0	-2.652988	-3.292108	-1.848908
21	6	0	-4.761284	-3.427228	-1.400494
22	1	0	-4.935653	-4.231265	-2.110936
23	6	0	-5.824324	-2.899130	-0.662882
24	1	0	-6.828313	-3.295748	-0.788884
25	6	0	-5.589774	-1.846059	0.226419
26	1	0	-6.411757	-1.420583	0.796808
27	6	0	-4.300724	-1.335423	0.391180
28	1	0	-4.118044	-0.508417	1.069825
29	6	0	-0.938738	-2.037866	0.725293
30	6	0	-0.870593	-3.541925	0.446072
31	1	0	-1.829262	-4.014900	0.673365
32	1	0	-0.101380	-3.990567	1.078694
33	1	0	-0.608200	-3.741770	-0.595929
34	6	0	-1.324592	-1.791221	2.205496
35	1	0	-1.375288	-0.724074	2.443133
36	1	0	-0.583104	-2.253693	2.865021
37	1	0	-2.302424	-2.237983	2.413818
38	6	0	0.400663	-1.378562	0.438621
39	6	0	3.769510	-2.109704	0.083337
40	1	0	3.625391	-2.828887	-0.731771
41	1	0	3.863837	-2.661853	1.026032
42	6	0	4.965718	-1.228979	-0.162441
43	6	0	5.346976	-0.895338	-1.469324
44	1	0	4.778004	-1.288475	-2.309040

45	6	0	6.444562	-0.063107	-1.699901
46	1	0	6.730306	0.187132	-2.718460
47	6	0	7.174831	0.445423	-0.621480
48	1	0	8.030856	1.091536	-0.799215
49	6	0	6.802495	0.119213	0.685883
50	1	0	7.367200	0.511427	1.527907
51	6	0	5.703840	-0.713414	0.911513
52	1	0	5.413903	-0.965112	1.929434

Zero-point correction=	0.412874 (Hartree/Particle)
Thermal correction to Energy=	0.439153
Thermal correction to Enthalpy=	0.440097
Thermal correction to Gibbs Free Energy=	0.352236
Sum of electronic and zero-point Energies=	-1702.241503
Sum of electronic and thermal Energies=	-1702.215224
Sum of electronic and thermal Enthalpies=	-1702.214280
Sum of electronic and thermal Free Energies=	-1702.302142

Structure Number: **TS2**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1702.53557663 (Hartrees)
Number of imaginary frequencies: -227.25*i* cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-4.484057	5.157505	0.199745
2	8	0	2.185975	-1.550673	2.295221
3	8	0	2.153553	0.040162	0.101178
4	7	0	-2.059439	-0.688687	0.470726
5	7	0	-1.773098	-1.940518	0.624826
6	7	0	1.033524	-0.837249	0.370126
7	6	0	-2.380408	0.433149	0.451786
8	6	0	-2.239573	1.820404	0.143419
9	6	0	-0.982659	2.276160	-0.308386
10	1	0	-0.156021	1.577187	-0.416358
11	6	0	-0.834578	3.633908	-0.586926
12	1	0	0.127081	4.006118	-0.927365
13	6	0	-1.906114	4.518899	-0.436784
14	1	0	-1.786409	5.574207	-0.661349
15	6	0	-3.143975	4.043326	0.010328
16	6	0	-3.325591	2.699530	0.315121
17	1	0	-4.281636	2.334551	0.674089
18	6	0	-2.134815	-2.774255	-0.513982
19	6	0	-1.516878	-2.583642	-1.752572
20	1	0	-0.737932	-1.830249	-1.833104
21	6	0	-1.897273	-3.392647	-2.825928
22	1	0	-1.421387	-3.257084	-3.793518
23	6	0	-2.875148	-4.378377	-2.657130
24	1	0	-3.163488	-5.006683	-3.495775
25	6	0	-3.482561	-4.558228	-1.410542
26	1	0	-4.243693	-5.322195	-1.277565
27	6	0	-3.117071	-3.749251	-0.331615
28	1	0	-3.584487	-3.868673	0.641454
29	6	0	-0.052459	-2.320687	1.951303
30	6	0	0.268115	-3.815544	1.900557
31	1	0	-0.564100	-4.426707	2.268409
32	1	0	1.135627	-3.973859	2.546291
33	1	0	0.534103	-4.144307	0.892045
34	6	0	-0.472211	-1.904718	3.367413
35	1	0	-0.764055	-0.849269	3.413256
36	1	0	0.386871	-2.032165	4.029306
37	1	0	-1.306583	-2.519630	3.724481
38	6	0	1.210030	-1.487714	1.517406
39	6	0	3.238389	-0.670594	-0.505348
40	1	0	2.940591	-1.027023	-1.504055
41	1	0	3.487588	-1.537293	0.118935
42	6	0	4.416737	0.266950	-0.597891
43	6	0	4.930814	0.677360	-1.833495

44	1	0	4.468317	0.318475	-2.751205
45	6	0	6.032418	1.538276	-1.900433
46	1	0	6.423868	1.843767	-2.868179
47	6	0	6.625002	2.004860	-0.724926
48	1	0	7.481299	2.673667	-0.772899
49	6	0	6.112563	1.605568	0.515776
50	1	0	6.571720	1.964556	1.434095
51	6	0	5.018073	0.742009	0.578747
52	1	0	4.613592	0.425838	1.537020

Zero-point correction=	0.405318 (Hartree/Particle)
Thermal correction to Energy=	0.434041
Thermal correction to Enthalpy=	0.434985
Thermal correction to Gibbs Free Energy=	0.339175
Sum of electronic and zero-point Energies=	-1702.130259
Sum of electronic and thermal Energies=	-1702.101536
Sum of electronic and thermal Enthalpies=	-1702.100592
Sum of electronic and thermal Free Energies=	-1702.196402

Structure Number: **Int2**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1702.56121065 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	5.677474	-3.420209	-0.355289
2	8	0	-1.853164	1.401355	2.535885
3	8	0	-1.746715	-0.658071	0.660299
4	7	0	1.632512	1.158460	0.221771
5	7	0	1.181778	2.370902	0.550051
6	7	0	-0.917571	0.361709	0.627810
7	6	0	1.932125	0.033482	0.162821
8	6	0	2.333791	-1.314397	0.034307
9	6	0	1.334592	-2.303504	0.050302
10	1	0	0.266651	-2.018738	0.154894
11	6	0	1.716897	-3.641795	-0.054274
12	1	0	0.944038	-4.427296	-0.034566
13	6	0	3.059007	-3.991552	-0.180478
14	1	0	3.349330	-5.051905	-0.263902
15	6	0	4.043663	-2.992444	-0.199852
16	6	0	3.692251	-1.647277	-0.089621
17	1	0	4.464764	-0.862366	-0.099461
18	6	0	0.813749	3.166420	-0.619465
19	6	0	-0.229462	2.821710	-1.497256
20	1	0	-0.832163	1.911222	-1.330957
21	6	0	-0.516470	3.647869	-2.582763
22	1	0	-1.337684	3.377136	-3.264418
23	6	0	0.222155	4.808998	-2.803374
24	1	0	-0.013772	5.458622	-3.659872
25	6	0	1.261088	5.147704	-1.936335
26	1	0	1.844290	6.064955	-2.107976
27	6	0	1.571110	4.331954	-0.851008
28	1	0	2.393067	4.612065	-0.173806
29	6	0	0.145200	2.373883	1.672029
30	6	0	-0.554653	3.733399	1.703401
31	1	0	0.176471	4.566474	1.827392
32	1	0	-1.256010	3.719210	2.577164
33	1	0	-1.156412	3.899601	0.778363
34	6	0	0.887362	2.168248	2.997949
35	1	0	1.410281	1.183719	3.028919
36	1	0	0.118321	2.178267	3.812119
37	1	0	1.626951	2.982915	3.180407
38	6	0	-0.982155	1.272988	1.628122
39	6	0	-3.171236	-0.368443	0.645805
40	1	0	-3.381176	0.573869	0.073780
41	1	0	-3.491509	-0.222858	1.713450
42	6	0	-3.903111	-1.507402	0.022273
43	6	0	-5.298051	-1.418355	-0.090602

44	1	0	-5.816261	-0.523234	0.284379
45	6	0	-6.025067	-2.454673	-0.670782
46	1	0	-7.118511	-2.376694	-0.756060
47	6	0	-5.368549	-3.591667	-1.143523
48	1	0	-5.943297	-4.408300	-1.602261
49	6	0	-3.982594	-3.687198	-1.030729
50	1	0	-3.463051	-4.582702	-1.400152
51	6	0	-3.251991	-2.650157	-0.450850
52	1	0	-2.157284	-2.720935	-0.361000

Zero-point correction=	0.409287 (Hartree/Particle)
Thermal correction to Energy=	0.436970
Thermal correction to Enthalpy=	0.437915
Thermal correction to Gibbs Free Energy=	0.346486
Sum of electronic and zero-point Energies=	-1702.151923
Sum of electronic and thermal Energies=	-1702.124240
Sum of electronic and thermal Enthalpies=	-1702.123296
Sum of electronic and thermal Free Energies=	-1702.214724

Structure Number: **3ae'**
SCF Energy at B3LYP/6-31+G(d) theoretical level: -1702.66345200 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.730207	5.234874	-1.146196
2	8	0	0.045052	-3.177817	0.070616
3	8	0	1.554386	-0.941667	-0.113003
4	7	0	-1.667033	0.431002	0.055553
5	7	0	-2.378433	-0.724991	-0.176681
6	7	0	0.242440	-0.918809	0.388486
7	6	0	-0.407800	0.337774	0.309463
8	6	0	0.370709	1.580737	0.519530
9	6	0	1.348516	1.618106	1.525327
10	1	0	1.491111	0.746427	2.155158
11	6	0	2.122032	2.763254	1.709767
12	1	0	2.872045	2.787529	2.495701
13	6	0	1.939050	3.888125	0.900421
14	1	0	2.533343	4.784904	1.041942
15	6	0	0.970264	3.836481	-0.101325
16	6	0	0.188576	2.701848	-0.303066
17	1	0	-0.536482	2.685116	-1.108288
18	6	0	-3.782253	-0.458144	-0.367040
19	6	0	-4.457743	-1.077237	-1.424866
20	1	0	-3.910737	-1.734622	-2.093124
21	6	0	-5.818338	-0.833265	-1.627741
22	1	0	-6.332829	-1.319397	-2.452679
23	6	0	-6.508509	0.047780	-0.790896
24	1	0	-7.564564	0.244693	-0.955842
25	6	0	-5.827696	0.686705	0.250003
26	1	0	-6.352891	1.383543	0.898484
27	6	0	-4.471090	0.435505	0.464607
28	1	0	-3.934362	0.943943	1.259184
29	6	0	-1.975449	-1.919528	0.636411
30	6	0	-2.720922	-3.181395	0.197293
31	1	0	-3.788435	-3.091637	0.413664
32	1	0	-2.321714	-4.037729	0.746132
33	1	0	-2.584974	-3.376978	-0.869333
34	6	0	-2.181320	-1.686279	2.151520
35	1	0	-1.686811	-0.773991	2.498623
36	1	0	-1.775376	-2.533938	2.714900
37	1	0	-3.250318	-1.606100	2.375639
38	6	0	-0.478353	-2.102956	0.314314
39	6	0	2.494221	-1.569777	0.811930
40	1	0	2.122619	-2.567447	1.054259
41	1	0	2.559274	-0.965552	1.722965
42	6	0	3.816289	-1.631432	0.098701
43	6	0	4.061875	-2.650539	-0.833334
44	1	0	3.289757	-3.391016	-1.027833

45	6	0	5.282169	-2.711512	-1.508059
46	1	0	5.463666	-3.505797	-2.227694
47	6	0	6.271171	-1.754921	-1.254861
48	1	0	7.223410	-1.804963	-1.777082
49	6	0	6.033849	-0.736253	-0.328111
50	1	0	6.799032	0.009373	-0.127787
51	6	0	4.809504	-0.674101	0.342645
52	1	0	4.624885	0.122395	1.060152

Zero-point correction=	0.412945 (Hartree/Particle)
Thermal correction to Energy=	0.439168
Thermal correction to Enthalpy=	0.440112
Thermal correction to Gibbs Free Energy=	0.353241
Sum of electronic and zero-point Energies=	-1702.250507
Sum of electronic and thermal Energies=	-1702.224284
Sum of electronic and thermal Enthalpies=	-1702.223340
Sum of electronic and thermal Free Energies=	-1702.310211

(2) The relative Gibbs free energy in solvent was calculated in a hexafluoroisopropanol solution. The energy data of all structures in solvent were obtained from the single point energy calculation at the CPCM-B3LYP/6-311+G(d,p) theoretical level and the thermal correction to Gibbs free energy calculated at the B3LYP/6-31+G(d) theoretical level. The Gibbs free energy of [4 + 5] was set to 0 kcal/mol as a reference.

Table S1 Relative Gibbs free energy of all stationary points for the two plausible reaction pathways obtained at the B3LYP/6-31+G(d) and the CPCM-B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d) theoretical levels (kcal/mol)

Structures		Computational methods	
		B3LYP/6-31+G(d)	CPCM-B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d) *
Pathway 1	4 + 5	0	0
	TS1	18.7	18.2
	Int1	10.0	7.9
	3ae	-41.6	-34.0
Pathway 2	4 + 5	0	0
	TS2	24.8	24.9
	Int2	13.3	10.4
	3ae2	-46.6	-41.6

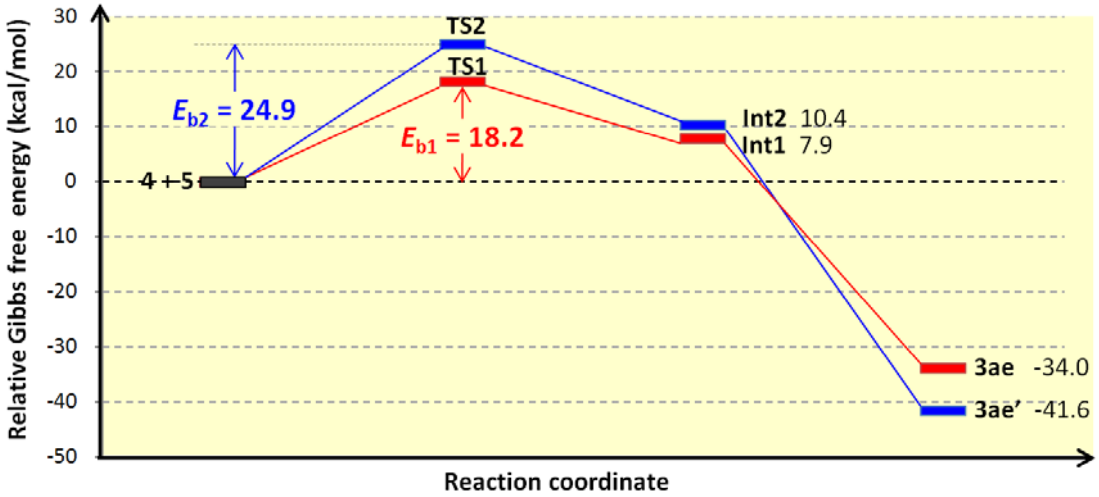


Figure S1 Energy profile for the two plausible reaction pathways obtained at the CPCM-B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d) theoretical level.

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