Supplementary Material (ESI) for Chemical Communications

Supporting Information

Gold-catalyzed Cycloisomerization of 1,6-Diyne-4-en-3-ols to form Naphthyl Ketone Derivatives.

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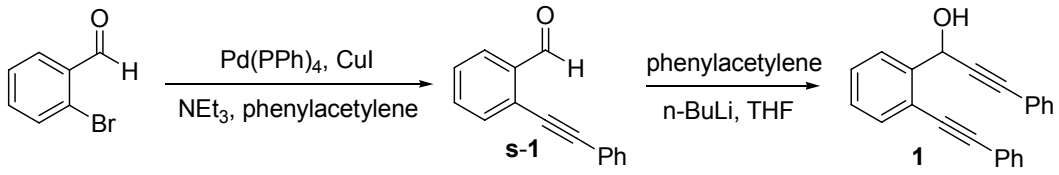
Contents:

(I) Experimental procedures for synthesis of the substrates

(1) Synthesis of 3-phenyl-1-(2-(phenylethynyl)phenyl)prop-2-yn-1-ol (1).



(a) Synthesis of 2-(phenylethynyl)benzaldehyde (s-1).

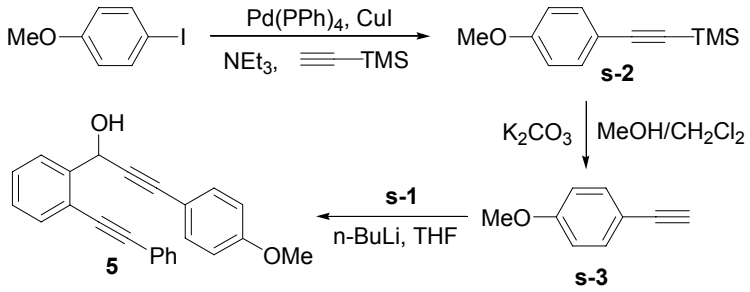
To a triethylamine solution (10 ml) of 2-bromobenzaldehyde (1.0 g, 5.44 mmol) was added $Pd(PPh_3)_4$ (313.9 mg, 0.3 mmol) and CuI (51.8 mg, 0.3 mmol) at 28 ℃, and the mixture was stirred for 5 min before addition of phenylacetylene (582.5 mg, 5.71 mmol). The resulting mixture was stirred for 12 h, and the solvent was removed in vacuo, and added with a saturated $NaHCO_3$ solution. The organic layer was extracted with ethyl acetate, washed with a saturated NaCl solution and dried over anhydrous $MgSO_4$. The residues were chromatographed through a silica gel column (hexane: ethyl acetate/9:1, $R_f = 0.8$) to afford compound **s-1** (1.03 g, 5.0 mmol, 92%) as yellow oil.

(b) Synthesis of 3-phenyl-1-(2-(phenylethynyl)phenyl)prop-2-yn-1-ol (1).

To a THF solution (10.0 mL) of phenylacetylene (544.7 mg, 5.34 mmol) was added n-BuLi (5.34 mmol) at –78 ℃, and the mixture was stirred for 20 min before addition of compound **s-1** (1.0 g, 4.85 mmol).The resulting solution was warmed to 28 ℃ and kept on stirring for 2 h before addition a saturated ammonium chloride solution. The organic layer was extracted with ethyl acetate, washed with water, dried over $MgSO_4$, and concentrated in vacuo. The residues were chromatographed on a silica columnl (hexane: ethyl acetate/1:1, $R_f = 0.5$) to afford compound **1** (1.29 g, 4.17 mmol, 86%) as colorless oil.

(2) Synthesis of 3-(4-methoxyphenyl)-1-(2-(phenylethynyl)phenyl) prop-2-

yn-1-ol (5).



(a) Synthesis of 1-ethynyl-4-methoxybenzene (s-3).

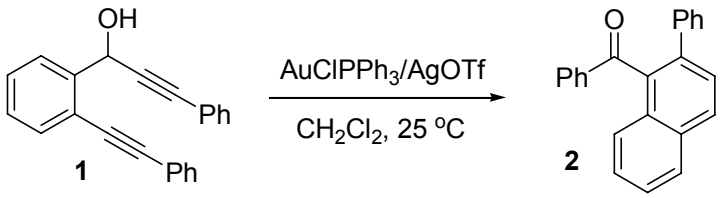
To a triethylamine solution (10 ml) of 1-iodo-4-methoxybenzene (3.0 g, 12.8 mmol) was added $Pd(PPh_3)_4$ (740.5 mg, 06 mmol) and CuI (122.1 mg, 0.6 mmol) at 28 ℃, and the mixture was stirred for 5 min before addition of ethynyltrimethylsilane (1.38 g, 14.1 mmol). The resulting mixture was stirred for 12 h, and the solvent was removed in vacuo, and added with a saturated $NaHCO_3$ solution. The organic layer was extracted with ethyl acetate, washed with a saturated NaCl solution and dried over anhydrous $MgSO_4$. The residues were chromatographed through a silica gel column (hexane: ethyl acetate/9:1, R_f = 0.6) to afford compound **s-2** (2.12 g, 10.4 mmol, 81%) as yellow oil. To a $MeOH/CH_2Cl_2$ mixture solution (20.0 mL) of compound **s-2** (2.12 g, 10.4 mmol) was added moderate K_2CO_3 at 25 ℃. The resulting mixture was stirred for 30 min, and the solvent was removed in vacuo, and added with a saturated NH_4Cl solution. The organic layer was extracted with ethyl acetate, washed with water, dried over $MgSO_4$, and concentrated in vacuo. The residues were chromatographed on a silica columnl (hexane: ethyl acetate/1:9, R_f = 0.5) to afford compound **s-3** (1.30 g, 9.87 mmol, 95%) as colorless oil.

(b) Synthesis of 3-(4-methoxyphenyl)-1-(2-(phenylethynyl)phenyl)prop-2-yn-1-ol (5).

To a THF solution (10.0 mL) of compound **s-3** (704.9 mg, 5.34 mmol) was added n-BuLi (5.34 mmol) at –78 ℃, and the mixture was stirred for 20 min before addition

of compound **s-1** (1.0 g, 4.85 mmol).The resulting solution was warmed to 28 ℃ and kept on stirring for 2 h before addition a saturated ammonium chloride solution. The organic layer was extracted with ethyl acetate, washed with water, dried over $MgSO_4$, and concentrated in vacuo. The residues were chromatographed on a silica columnl (hexane: ethyl acetate/1:1, R_f = 0.4) to afford compound **5** (1.25 g, 3.69 mmol, 76%) as colorless oil.

(II) A typical procedure for catalytic cyclization of 1,6-Diyne-4-en-3-ol.



(a) Synthesis of phenyl(2-phenylnaphthalen-1-yl)methanone (2).

A solution of PPh_3AuOTf (2 mol%) was prepared by mixing PPh_3AuCl (3.2 mg, 0.006 mmol) and AgOTf (1.7 mg, 0.006 mmol) in dichloromethane (1.0 mL). To this solution was added compound **1** (100 mg, 0.32 mmol) at 25 ℃, the mixture was stirred for 3 h. The resulting solution was filtered through a celite bed, and eluted through a silica gel column (ethyl acetate/hexane = 1/15) to give compound **2** (85.0 mg, 0.28 mmol, 85%) as yellow solid.

(III) Spectral Data for Compounds 1-32

Spectra data for 3-phenyl-1-(2-(phenylethynyl)phenyl)prop-2-yn-1-ol (1).

Yellow oil; IR (neat, cm^{-1}): 3550(s), 2920(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.80 (d, J = 8.0 Hz, 1H), 7.59~7.57 (m, 3H), 7.46 (d, J = 8.0 Hz, 2H), 7.40 (t, J = 8.0 Hz, 1H), 7.36~7.32 (m, 4H), 7.31~7.26 (m, 3H), 6.18 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.2, 132.4, 131.7 (2×CH), 131.5 (2×CH), 128.9, 128.6, 128.4, 128.3, 128.2

(2×CH), 128.1 (2×CH), 126.7, 122.7, 122.4, 121.4, 95.0, 88.3, 86.6, 86.4, 63.7; HRMS calcd for $C_{23}H_{16}O$: 308.1201, found: 308.1200.

Spectra data for phenyl(2-phenylnaphthalen-1-yl)methanone (2).

Yellow solid, m.p. 121.0~121.6 ℃; IR (neat, cm^{-1}): 3085(s), 1660(s); ^1H NMR (500 MHz, $CDCl_3$): δ 8.01 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.62 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.51 (t, J = 8.0 Hz, 1H), 7.45 (t, J = 8.0 Hz, 1H), 7.39~7.34 (m, 3H), 7.24~7.20 (m, 4H), 7.16 (t, J = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.7, 140.1, 137.8, 137.4, 135.6, 133.2, 132.4, 130.6, 129.5 (2×CH), 129.4 (3×CH), 128.2 (2×CH), 128.1 (3×CH), 127.5, 127.4, 127.2, 126.3, 125.5; HRMS calcd for $C_{23}H_{16}O$: 308.1201, found: 308.1200.

Spectra data for 1-(2-(phenylethynyl)phenyl)-3-*p*-tolylprop-2-yn-1-ol (3).

Yellow oil; IR (neat, cm^{-1}): 3552(s), 2930(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.77 (d, J = 8.0 Hz, 1H), 7.59~7.53 (m, 3H), 7.39 (t, J = 8.0 Hz, 1H), 7.35~7.31 (m, 6H), 7.08 (d, J = 8.0 Hz, 2H), 6.13 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.3, 138.6, 132.4, 131.6 (2×CH), 131.5 (2×CH), 129.0 (2×CH), 128.9, 128.6, 128.4 (2×CH), 128.2, 126.8, 122.8, 121.4, 119.4, 95.0, 87.6, 88.6 (2×C), 63.7, 21.4; HRMS calcd for $C_{24}H_{18}O$: 322.1358, found: 322.1355.

Spectra data for 3-(4-fluorophenyl)-1-(2-(phenylethynyl)phenyl)prop-2-yn-1-ol (4).

Yellow oil; IR (neat, cm^{-1}): 3553(s), 2923(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.50 (d, J = 7.5 Hz, 1H), 7.58~7.53 (m, 3H), 7.42~7.38 (m, 3H), 7.35~7.32 (m, 4H), 6.96 (t, J = 9.0 Hz, 2H), 6.12 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.4 (d, J_{CF} = 249.1 Hz), 142.1, 133.5 (d, J_{CF} = 7.8 Hz, 2×CH), 132.4, 131.4 (2×CH), 128.8, 128.5, 128.3 (2×CH), 128.2, 126.5, 122.7, 121.2, 118.5, 115.3 (d, J_{CF} = 22.1 Hz, 2×CH), 95.0, 88.1, 86.6, 85.2, 63.5; HRMS calcd for $C_{23}H_{15}FO$: 326.1107, found: 326.1107.

Spectra data for 3-(4-methoxyphenyl)-1-(2-(phenylethynyl)phenyl)prop-2-yn-1-ol

(5).

Yellow oil; IR (neat, cm^{-1}): 3552(s), 2922(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, J = 8.0 Hz, 1H), 7.57~7.55 (m, 3H), 7.40~7.37 (m, 3H), 7.35~7.30 (m, 4H), 6.79 (d, J = 8.0 Hz, 2H), 6.14 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.7, 142.5, 133.2 (2×CH), 132.4, 131.5 (2×CH), 128.9, 128.6, 128.4 (2×CH), 128.2, 126.7, 122.8, 121.4, 114.6, 113.8 (2×CH), 94.9, 86.9, 88.6, 86.4, 63.7, 55.2; HRMS calcd for $C_{24}H_{18}O_2$: 338.1307, found: 338.1306.

Spectra data for 1-(2-(phenylethynyl)phenyl)but-2-yn-1-ol (6).

Yellow oil; IR (neat, cm^{-1}): 3555(s), 2925(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.72 (d, J = 7.5 Hz, 1H), 7.55~7.53 (m, 3H), 7.38~7.34 (m, 4H), 7.29 (t, J = 7.5 Hz, 1H), 5.93 (s, 1H), 1.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.8, 132.3, 131.5 (2×CH), 128.8, 128.5, 128.3 (2×CH), 128.0, 126.5, 122.8, 121.2, 94.7, 86.6, 82.9, 78.6, 63.2, 3.7; HRMS calcd for $C_{18}H_{14}O$: 246.1405, found: 246.1406.

Spectra data for 1-(2-(phenylethynyl)phenyl)hept-2-yn-1-ol (7).

Yellow oil; IR (neat, cm^{-1}): 3560(s), 2929(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.72 (d, J = 7.5 Hz, 1H), 7.56~7.52 (m, 3H), 7.37~7.34 (m, 4H), 7.28 (t, J = 7.5 Hz, 1H), 5.94 (s, 1H), 2.25 (t, J = 7.0 Hz, 2H), 1.52~1.46 (m, 2H), 1.42~1.35 (m, 2H), 0.86 (t, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.9, 132.2, 131.5 (2×CH), 128.7, 128.4, 128.3 (2×CH), 127.9, 126.5, 122.8, 121.2, 94.6, 87.3, 86.6, 79.4, 63.2, 30.5, 21.8, 18.4, 13.5; HRMS calcd for $C_{21}H_{20}O$: 288.1514, found: 288.1512.

Spectra data for 1-(2-((4-methoxyphenyl)ethynyl)phenyl)-3-phenylprop-2-yn-1-ol (8).

Yellow oil; IR (neat, cm^{-1}): 3561(s), 2930(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.77 (d, J = 7.5 Hz, 1H), 7.55 (d, J = 7.5 Hz, 1H), 7.49 (d, J = 7.5 Hz, 2H), 7.45 (d, J = 7.5 Hz, 2H), 7.37 (t, J = 7.5 Hz, 1H), 7.33~7.26 (m, 4H), 6.86 (d, J = 7.5 Hz, 2H), 6.15 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.8, 142.0, 133.0 (2×CH),

132.2, 131.7 (2×CH), 128.5, 128.4, 128.2 (3×CH), 126.7, 122.5, 122.7, 114.8, 114.0 (2×CH), 95.1, 88.4, 86.3, 85.3, 63.7, 55.2; HRMS calcd for $C_{24}H_{18}O_2$: 338.1307, found: 338.1306.

Spectra data for 3-(4-fluorophenyl)-1-(2-((4-methoxyphenyl)ethynyl)phenyl)-prop-2-yn-1-ol (9).

Yellow oil; IR (neat, cm^{-1}): 3552(s), 2922(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.73 (d, J = 8.0 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.47 (d, J = 9.0 Hz, 2H), 7.42~7.39 (m, 2H), 7.36 (t, J = 8.0 Hz, 1H), 7.31 (t, J = 8.0 Hz, 1H), 6.96 (t, J = 8.0 Hz, 2H), 6.86 (t, J = 9.0 Hz, 2H), 6.11 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.6 (d, J_{CF} = 248.4 Hz), 159.9, 141.9, 133.7 (d, J_{CF} = 7.8 Hz, 2×CH), 133.2 (2×CH), 132.3, 128.6, 128.3, 126.7, 121.7, 118.6, 115.5 (d, J_{CF} = 22.1 Hz, 2×CH), 114.8, 114.1 (2×CH), 95.2, 88.1, 85.3 (2×C), 63.8, 55.3; HRMS calcd for $C_{24}H_{17}FO_2$: 356.1213, found: 356.1211.

Spectra data for 1-(2-((4-methoxyphenyl)ethynyl)phenyl)but-2-yn-1-ol (10).

Yellow oil; IR (neat, cm^{-1}): 3556(s), 2926(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.69 (d, J = 8.0 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.47 (d, J = 8.5 Hz, 2H), 7.34 (t, J = 8.0 Hz, 1H), 7.27 (t, J = 8.0 Hz, 1H), 6.87 (d, J = 8.5 Hz, 2H), 5.90 (s, 1H), 3.80 (s, 3H), 1.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.0, 142.5, 133.0 (2×CH), 132.1, 128.5, 128.0, 126.6, 121.5, 114.9, 114.0 (2×CH), 94.8, 85.3, 82.9, 78.5, 63.3, 55.3, 3.8; HRMS calcd for $C_{19}H_{16}O_2$: 276.1150, found: 276.1151.

Spectra data for 3-phenyl-1-(2-(*p*-tolylethynyl)phenyl)prop-2-yn-1-ol (11).

Yellow oil; IR (neat, cm^{-1}): 3563(s), 2933(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, J = 7.5 Hz, 1H), 7.56 (d, J = 7.5 Hz, 1H), 7.47~7.45 (m, 4H), 7.38 (t, J = 7.5 Hz, 1H), 7.34~7.26 (m, 4H), 7.15 (d, J = 7.5 Hz, 2H), 6.16 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.1, 138.8, 132.4, 131.7 (2×CH), 131.4 (2×CH), 129.1 (2×CH), 128.7, 128.4, 128.2, 128.1 (2×CH), 126.7, 122.5, 121.6, 119.7, 95.3, 88.3, 86.4, 86.0, 63.8, 21.5; HRMS calcd for $C_{24}H_{18}O$: 322.1358, found: 322.1359.

Spectra data for 3-*p*-tolyl-1-(2-(*p*-tolylethynyl)phenyl)prop-2-yn-1-ol (12).

Yellow oil; IR (neat, cm^{-1}): 3558(s), 2927(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.77 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.45 (d, J = 8.0 Hz, 2H), 7.38 (t, J = 8.0 Hz, 1H), 7.36~7.30 (m, 3H), 7.15 (d, J = 8.0 Hz, 2H), 7.08 (d, J = 8.0 Hz, 2H), 6.14 (s, 1H), 2.36 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.2, 138.8, 138.6, 132.4, 131.6 (2×CH), 131.5 (2×CH), 129.2 (2×CH), 129.0 (2×CH), 128.7, 128.2, 126.8, 121.7, 119.7, 119.4, 95.2, 87.6, 86.7, 86.0, 63.8, 21.5, 21.4; HRMS calcd for $C_{25}H_{20}O$: 336.1514, found: 336.1514.

Spectra data for 3-(4-fluorophenyl)-1-(2-(*p*-tolylethynyl)phenyl)prop-2-yn-1-ol (13).

Yellow oil; IR (neat, cm^{-1}): 3555(s), 2927(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.77 (d, J = 7.5 Hz, 1H), 7.57 (d, J = 7.5 Hz, 1H), 7.47 (d, J = 7.5 Hz, 2H), 7.43~7.36 (m, 3H), 7.32 (t, J = 7.5 Hz, 1H), 7.15 (d, J = 7.5 Hz, 2H), 6.96 (t, J = 7.5 Hz, 2H), 6.16 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.4 (d, J_{CF} = 248.4 Hz), 142.0, 138.8, 133.6 (d, J_{CF} = 8.9 Hz, 2×CH), 132.3, 131.4 (2×CH), 129.1 (2×CH), 128.6, 128.2, 126.5, 121.5, 119.6, 118.5, 115.4 (d, J_{CF} = 22.1 Hz, 2×CH), 95.3, 88.1, 86.0, 85.2, 63.5, 21.4; HRMS calcd for $C_{24}H_{17}FO$: 340.1263, found: 340.1260.

Spectra data for 3-(4-methoxyphenyl)-1-(2-(*p*-tolylethynyl)phenyl)prop-2-yn-1-ol (14).

Yellow oil; IR (neat, cm^{-1}): 3551(s), 2920(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.77 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 2H), 7.39~7.36 (m, 3H), 7.31 (t, J = 8.0 Hz, 1H), 7.15 (d, J = 8.0 Hz, 2H), 6.80 (d, J = 8.0 Hz, 2H), 6.13 (s, 1H), 3.77 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.7, 142.3, 138.8, 133.2 (2×CH), 132.4, 131.5 (2×CH), 129.2 (2×CH), 128.7, 128.2, 126.8, 121.6, 119.7, 114.6, 113.8 (2×CH), 95.2, 86.9, 86.4, 86.0, 63.8, 55.2, 21.5; HRMS calcd for $C_{25}H_{20}O_2$: 352.1643, found: 352.1643.

Spectra data for 1-(2-(*p*-tolylethynyl)phenyl)but-2-yn-1-ol (15).

Yellow oil; IR (neat, cm^{-1}): 3545(s), 2910(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.71 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 2H), 7.36 (t, J = 8.0 Hz, 1H), 7.29 (t, J = 8.0 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 5.91 (s, 1H), 2.36 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.6, 138.7, 132.2, 131.4 (2×CH), 129.1 (2×CH), 128.6, 128.0, 126.6, 121.4, 119.7, 95.0, 85.9, 83.0, 78.5, 63.3, 21.5, 3.7; HRMS calcd for $C_{19}H_{16}O$: 260.1201, found: 260.1200.

Spectra data for 1-(2-(prop-1-ynyl)phenyl)but-2-yn-1-ol (16).

Yellow oil; IR (neat, cm^{-1}): 3541(s), 2912(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.64 (d, J = 7.5 Hz, 1H), 7.36 (d, J = 7.5 Hz, 1H), 7.27 (t, J = 7.5 Hz, 1H), 7.20 (t, J = 7.5 Hz, 1H), 5.80 (s, 1H), 2.05 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.6, 132.2, 128.0, 127.9, 126.5, 122.0, 91.3, 82.7, 78.6, 77.0, 63.0, 4.4, 3.6; HRMS calcd for $C_{13}H_{12}O$: 184.0888, found: 184.0886.

Spectra data for 1-(2-(prop-1-ynyl)phenyl)hept-2-yn-1-ol (17).

Yellow oil; IR (neat, cm^{-1}): 3540(s), 2900(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.65 (d, J = 7.5 Hz, 1H), 7.37 (d, J = 7.5 Hz, 1H), 7.29 (t, J = 7.5 Hz, 1H), 7.21 (t, J = 7.5 Hz, 1H), 5.82 (s, 1H), 2.25 (t, J = 7.5 Hz, 2H), 2.07 (s, 3H), 1.53~1.46 (m, 2H), 1.44~1.38 (m, 2H), 0.89 (t, J = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.6, 132.4, 128.0, 127.9, 126.5, 122.1, 91.3, 87.3, 79.2, 77.1, 63.3, 30.6, 21.7, 18.5, 13.5, 4.44; HRMS calcd for $C_{16}H_{18}O$: 226.1358, found: 226.1358.

Spectra data for phenyl(2-*p*-tolylnaphthalen-1-yl)methanone (18).

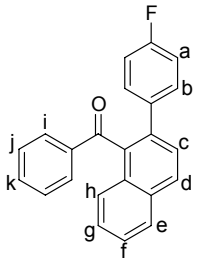
Yellow solid, m.p. 117.6~118.0 ℃; IR (neat, cm^{-1}): 3081(s), 1665(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, J = 8.5 Hz, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.69 (d, J = 8.5 Hz, 1H), 7.63 (d, J = 8.5 Hz, 2H), 7.55 (d, J = 8.5 Hz, 1H), 7.49 (t, J = 8.5 Hz, 1H), 7.43 (t, J = 8.5 Hz, 1H), 7.39 (t, J = 8.5 Hz, 1H), 7.24~7.22 (m, 4H), 7.02 (d, J = 8.0 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.8, 137.9, 137.4, 137.3,

137.1, 135.5, 133.2, 132.3, 130.6, 129.6 (2×CH), 129.4, 129.3 (2×CH), 128.9 (2×CH), 128.3 (2×CH), 128.1, 127.7, 127.1, 126.1, 125.5, 21.0; HRMS calcd for $C_{24}H_{18}O$: 322.1358, found: 322.1357.

Spectra data for (2-(4-fluorophenyl)naphthalen-1-yl)(phenyl)methanone (19).

Yellow solid, m.p. 113.9~114.5 ℃; IR (neat, cm^{-1}): 3079(s), 1662(s); ^1H NMR (500 MHz, $CDCl_3$): δ 8.00 (d, J = 8.0 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.53~7.50 (m, 2H), 7.45 (t, J = 8.0 Hz, 1H), 7.40 (t, J = 8.0 Hz, 1H), 7.33~7.30 (m, 2H), 7.24 (t, J = 8.0 Hz, 2H), 6.91 (t, J = 8.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.6, 162.2 (d, J_{CF} = 246.1 Hz), 137.7, 136.2, 136.2, 135.8, 133.4, 132.4, 131.1 (d, J_{CF} = 7.8 Hz, 2×CH), 130.6, 129.5 (3×CH), 128.4 (2×CH), 128.1, 127.4, 127.3, 126.4, 125.5, 115.1 (d, J_{CF} = 22.2 Hz, 2×CH); HRMS calcd for $C_{23}H_{15}FO$: 326.1107, found: 326.1106.

NOE-map of compound **19**

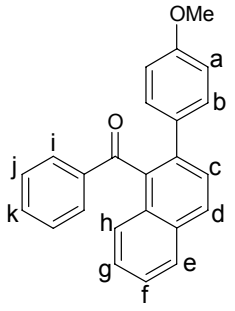


irradiation	enhancement (%)
H^a (δ 6.91)	H^b (δ 7.31, 0.14 %)
H^b (δ 7.31)	H^c (δ 7.52, 0.93 %); H^a (δ 6.91, 1.56 %)
H^d (δ 7.94)	H^e (δ 8.00, 1.49 %); H^c (δ 7.51, 1.39 %)
H^e (δ 8.00)	H^d (δ 7.94, 0.75 %); H^f (δ 7.45, 1.87 %)
H^h (δ7.72)	H^g (δ 7.40, 1.08 %)

Spectra data for (2-(4-methoxyphenyl)naphthalen-1-yl)(phenyl)methanone (20).

Yellow solid, m.p. 123.0~123.5 ℃; IR (neat, cm^{-1}): 3081(s), 1663(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 8.0 Hz, 1H), 7.48 (t, J = 8.0 Hz, 1H), 7.42 (t, J = 8.0 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 7.27 (d, J = 9.0 Hz, 2H), 7.23 (t, J = 8.0 Hz, 2H), 6.74 (d, J = 9.0 Hz, 2H), 3.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.9, 158.9, 137.9, 137.0, 135.4, 133.2, 132.6, 132.2, 130.6, 130.6 (2×CH), 129.5 (2×CH), 129.4, 128.3 (2×CH), 128.1, 127.7, 127.1, 126.1, 125.4, 113.7 (2×CH), 55.1; HRMS calcd for $C_{24}H_{18}O_2$: 338.1307, found: 338.1306.

NOE map of compound **20**



irradiation	enhancement (%)
Me (δ 3.71)	H^a (δ 6.74, 1.54 %)
H^a (δ 6.74)	H^b (δ 7.27, 1.59 %); Me (δ 3.71, 2.24 %)
H^b (δ 7.27)	H^i (7.61, 0.54 %); H^c (δ 7.53, 0.82 %); H^a (δ 6.74, 2.73 %)
H^i (δ 7.61)	H^b (δ 7.27, 0.54 %); H^j (δ 7.23, 1.71 %)
H^d (δ 7.91)	H^e (δ 7.98, 1.21 %); H^c (δ 7.53, 1.52 %)
H^e (δ 7.98)	H^d (δ 7.91, 1.28 %); H^f (δ 7.48, 2.59 %)

Spectra data for (2-methylnaphthalen-1-yl)(phenyl)methanone (21).

Yellow oil; IR (neat, cm^{-1}): 3075(s), 1654(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.86~7.82 (m, 4H), 7.57 (t, J = 8.5 Hz, 1H), 7.48 (d, J = 8.5 Hz, 1H), 7.42 (t, J = 8.5 Hz, 3H), 7.38~7.33 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.3, 137.5, 135.9, 133.8, 132.2, 131.6, 130.6, 129.7 (2×CH), 128.9, 128.8 (2×CH), 128.5, 128.0, 126.7, 125.4, 124.9, 19.7; HRMS calcd for $C_{18}H_{14}O$: 246.1045, found: 246.1044.

Spectra data for (2-butylnaphthalen-1-yl)(phenyl)methanone (22).

Yellow oil; IR (neat, cm^{-1}): 3088(s), 1666(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.87~7.80 (m, 4H), 7.56 (t, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.42~7.39 (m, 4H), 7.33 (t, J = 8.0 Hz, 1H), 2.55 (t, J = 7.5 Hz, 2H), 1.56~1.52 (m, 2H), 1.27~1.20 (m, 2H), 0.79 (t, J = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.3, 137.9, 137.3, 135.6, 133.7, 131.7, 130.6, 129.8 (2×CH), 129.0, 128.7 (2×CH),128.0, 127.4, 126.6, 125.4, 125.1, 33.4, 33.3, 22.5, 13.8; HRMS calcd for $C_{21}H_{20}O$: 288.1514, found: 288.1513.

Spectra data for (4-methoxyphenyl)(2-phenylnaphthalen-1-yl)methanone (23A).

Yellow solid, m.p. 122.2~122.8 ℃; IR (neat, cm^{-1}): 3084(s), 1664(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, J = 8.5 Hz, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.73 (d, J = 8.5 Hz, 1H), 7.63 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 8.5 Hz, 1H), 7.50 (t, J = 8.5 Hz, 1H), 7.44 (d, J = 8.5 Hz, 1H), 7.40 (d, J = 8.5 Hz, 2H), 7.24 (t, J = 8.5 Hz, 2H), 7.18 (t, J =

8.5 Hz, 1H), 6.70 (d, J = 8.5 Hz, 2H), 3.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.0, 163.5, 140.2, 136.9, 135.8, 132.3, 131.9 (2×CH), 131.0, 130.6, 129.3 (2×CH), 129.1, 128.1 (2×CH), 128.0, 127.6, 127.3, 127.0, 126.2, 125.5, 113.5 (2×CH), 55.2; HRMS calcd for $C_{24}H_{18}O_2$: 338.1307, found: 338.1306.

Spectra data for 2-phenylnaphthalene (23B).

Yellow solid, m.p. 101.0~101.5 ℃; IR (neat, cm^{-1}): 3071(s); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 (s, 1H), 7.94 (t, J = 8.0 Hz, 2H), 7.89 (d, J = 8.0 Hz, 1H), 7.80~7.76 (m, 3H), 7.56~7.51 (m, 4H), 7.42 (t, J = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 141.1, 138.5, 133.6, 132.6, 128.8 (2×CH), 128.4, 128.2, 127.6, 127.4 (2×CH), 127.3, 126.3, 125.9, 125.8, 125.6; HRMS calcd for $C_{16}H_{12}$: 204.0939, found: 204.0938.

Spectra data for (2-(4-fluorophenyl)naphthalen-1-yl)(4-methoxyphenyl)-methanone (24A).

Yellow solid, m.p. 117.1~117.8 ℃; IR (neat, cm^{-1}): 3081(s), 1661(s); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.97 (d, J = 9.0 Hz, 1H), 7.91 (d, J = 9.0 Hz, 1H), 7.70 (d, J = 9.0 Hz, 1H), 7.60 (d, J = 9.0 Hz, 2H), 7.51~7.48 (m, 2H), 7.43 (t, J = 8.0 Hz, 1H), 7.35~7.32 (m, 2H), 6.92 (t, J = 9.0 Hz, 2H), 6.71 (d, J = 9.0 Hz, 2H), 3.74 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 197.9, 163.7, 162.1 (d, J_{CF} = 246.3 Hz), 136.3, 136.0, 135.9, 132.3, 132.0 (2×CH), 131.0 (d, J_{CF} = 7.8 Hz, 2×CH), 130.9, 130.6, 129.2, 128.1, 127.4, 127.1, 126.3, 125.6, 115.1 (d, J_{CF} = 22.1 Hz, 2×CH), 113.6 (2×CH), 55.3; HRMS calcd for $C_{24}H_{17}FO_2$: 356.1213, found: 356.1211.

Spectra data for 2-(4-fluorophenyl)naphthalene (24B).

Yellow solid, m.p. 99.1~99.5 ℃; IR (neat, cm^{-1}): 3071(s); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.98 (s, 1H), 7.91~7.85 (m, 3H), 7.69~7.65 (m, 3H), 7.50~7.46 (m, 2H), 7.16 (t, J = 8.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.4 (d, J_{CF} = 246.1 Hz), 137.5, 137.2, 133.6, 132.5, 128.9 (d, J_{CF} = 7.8 Hz, 2×CH), 128.5, 128.1, 127.6, 126.4,

126.0, 125.6, 125.4, 115.7 (d, J_{CF} = 21.0 Hz, 2×CH); HRMS calcd for $C_{16}H_{11}F$: 222.0845, found: 222.0844.

Spectra data for (4-methoxyphenyl)(2-methylnaphthalen-1-yl)methanone (25).

Yellow oil; IR (neat, cm^{-1}): 3079(s), 1655(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.84~7.78 (m, 4H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.36~7.32 (m, 2H), 6.87 (d, *J* = 7.5 Hz, 2H), 3.80 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.6, 164.0, 136.2, 132.0 (2×CH), 131.9, 131.5, 130.6, 130.5, 128.6, 128.4, 127.9, 126.5, 125.2, 124.9, 119.4 (2×CH), 55.4, 19.6; HRMS calcd for $C_{19}H_{16}O_2$: 276.1150, found: 276.1151.

Spectra data for (2-phenylnaphthalen-1-yl)(*p*-tolyl)methanone (26).

Yellow solid, m.p. 122.0~122.6 ℃; IR (neat, cm^{-1}): 3085(s), 1660(s); ^1H NMR (500 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.59~7.56 (m, 3H), 7.50 (t, *J* = 8.5 Hz, 1H), 7.43 (t, *J* = 8.5 Hz, 1H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.24 (t, *J* = 8.5 Hz, 2H), 7.18 (t, *J* = 8.5 Hz, 1H), 7.03 (d, *J* = 8.5 Hz, 2H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.2, 144.1, 140.2, 137.1, 135.8, 135.4, 132.3, 130.6, 129.7 (2×CH), 129.4 (2×CH), 129.2, 129.0 (2×CH), 128.1 (2×CH), 128.0, 127.6, 127.3, 127.0, 126.2, 125.5, 21.6; HRMS calcd for $C_{24}H_{18}O$: 322.1358, found: 322.1358.

Spectra data for *p*-tolyl(2-*p*-tolylnaphthalen-1-yl)methanone (27).

Yellow solid, m.p. 123.1~123.8 ℃; IR (neat, cm^{-1}): 3083(s), 1662(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.58~7.55 (m, 3H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.28(d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 4H), 2.29 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.3, 144.1, 137.3, 137.1, 137.0, 135.7, 135.5, 132.2, 130.6, 129.8 (2×CH), 129.2 (2×CH), 129.1, 129.0 (2×CH), 128.9 (2×CH), 128.0, 127.8, 127.0, 126.1, 125.5, 21.6, 21.0; HRMS calcd for $C_{25}H_{20}O$: 336.1514, found: 336.1513.

Spectra data for (2-(4-fluorophenyl)naphthalen-1-yl)(*p*-tolyl)methanone (28).

Yellow solid, m.p. 116.0~116.6 ℃; IR (neat, cm^{-1}): 3082(s), 1662(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, J = 8.5 Hz, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 8.5 Hz, 1H), 7.54~7.48 (m, 4H), 7.43 (t, J = 8.5 Hz, 1H), 7.35~7.32 (m, 2H), 7.04 (d, J = 8.5 Hz, 2H), 6.92 (t, J = 8.5 Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.1, 162.1 (d, J_{CF} = 246.1 Hz), 144.4, 136.2, 136.0, 135.3, 132.3, 131.0 (d, J_{CF} = 7.8 Hz, 2×CH), 130.6 (2×C), 129.7 (2×CH), 129.3, 129.1 (2×CH), 128.1, 127.4, 127.2, 126.3, 125.5, 115.1 (d, J_{CF} = 21.0 Hz, 2×CH), 21.6; HRMS calcd for $C_{24}H_{17}FO$: 340.1263, found: 340.1263.

Spectra data for (2-(4-methoxyphenyl)naphthalen-1-yl)(*p*-tolyl)methanone (29).

Yellow solid, m.p. 124.5~124.6 ℃; IR (neat, cm^{-1}): 3089(s), 1669(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.97 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.56~7.53 (m, 3H), 7.47 (t, J = 8.0 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 7.31 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.0 Hz, 2H), 6.77 (d, J = 8.0 Hz, 2H), 3.71 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.4, 158.8, 144.1, 136.7, 135.6, 135.4, 132.6, 132.1, 130.6, 130.5 (2×CH), 129.7 (2×CH), 129.2, 129.1 (2×CH), 128.0, 127.7, 127.0, 126.0, 125.4, 113.6 (2×CH), 55.1, 21.6; HRMS calcd for $C_{25}H_{20}O_2$: 352.1463, found: 352.1463.

Spectra data for (2-methylnaphthalen-1-yl)(*p*-tolyl)methanone (30).

Yellow oil; IR (neat, cm^{-1}): 3089(s), 1667(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, J = 8.5 Hz, 2H), 7.73 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.5 Hz, 1H), 7.41 (t, J = 8.5 Hz, 1H), 7.37~7.33 (m, 2H), 7.21 (d, J = 8.5 Hz, 2H), 2.39 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.8, 144.8, 136.1, 135.1, 132.0, 131.6, 130.6, 129.8 (2×CH), 129.8 (2×CH), 128.7, 128.4, 128.0, 126.6, 125.3, 124.9, 21.7, 19.7; HRMS calcd for $C_{19}H_{16}O$: 260.1201, found: 260.1200.

Spectra data for 1-(2-methylnaphthalen-1-yl)ethanone (31A).

Yellow oil; IR (neat, cm^{-1}): 3091(s), 1670(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 8.0 Hz, 1H), 7.43 (t, J = 8.0 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H), 2.62 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 208.3, 138.7, 131.7, 129.9, 128.8, 128.7, 128.6, 128.2, 126.9, 125.4, 123.9, 32.9, 19.3; HRMS calcd for $C_{13}H_{12}O$: 184.0888, found: 184.0887.

Spectra data for 2-methylnaphthalene (31B).

Brown solid, m.p. 34~36 ℃; IR (neat, cm^{-1}): 3051(s), 292(w); ^1H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, J = 8.5 Hz, 1H), 7.52~7.73 (m, 2H), 7.61 (s, 1H), 7.45~7.38 (m, 2H), 7.30 (d, J = 8.5 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.3, 133.6, 131.7, 128.0, 127.6, 127.5, 127.2, 126.8, 125.8, 124.9, 21.6; HRMS calcd for $C_{11}H_{10}$: 142.0783, found: 142.0782.

Spectra data for 1-(2-butylnaphthalen-1-yl)ethanone (32).

Yellow oil; IR (neat, cm^{-1}): 3086(s), 1662(s); ^1H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, J = 8.5 Hz, 1H), 7.77 (d, J = 8.5 Hz, 1H), 7.57 (d, J = 8.5 Hz, 1H), 7.47 (t, J = 8.5 Hz, 1H), 7.43 (t, J = 8.5 Hz, 1H), 7.33 (d, J = 8.5 Hz, 1H), 2.66 (t, J = 7.5 Hz, 2H), 2.62 (s, 3H),1.66~1.60 (m, 2H), 1.41~1.34 (m, 2H), 0.92 (t, J =7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 208.3, 138.4, 135.0, 131.8, 128.9, 128.8, 128.3, 127.5, 126.8, 125.5, 124.0, 33.8, 33.5, 33.3, 22.7, 13.9; HRMS calcd for $C_{16}H_{18}O$: 226.1358, found: 226.1357.

(V) x-Ray data of compound 2.

(1) ORTEP-Drawing of compound 2. (The ellipsoids of atoms are drawn to compass 50% probability.)

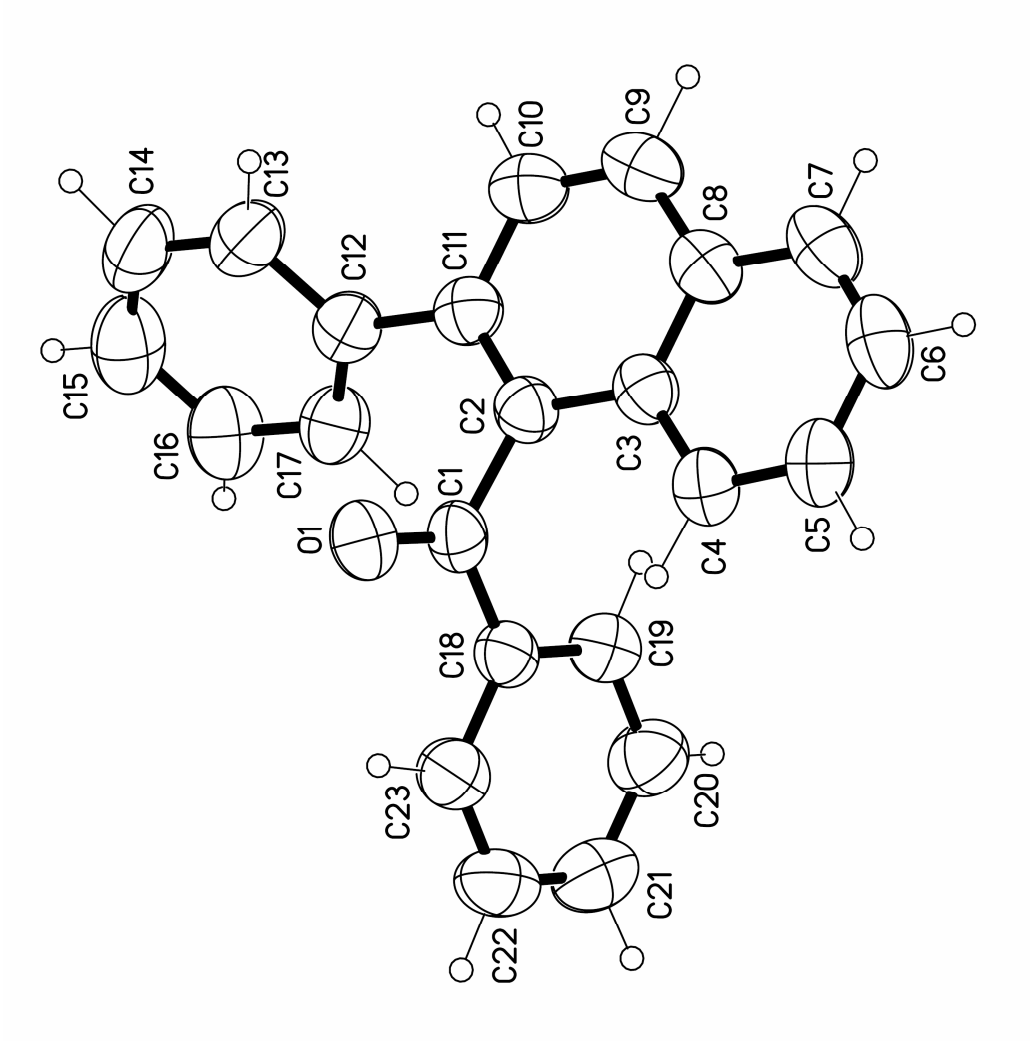


Table 1. Crystal data and structure refinement for compound 2.

Identification code	06mr53m	
Empirical formula	C23 H16 O	
Formula weight	308.36	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 9.3540(17) Å	α= 92.763(3)°.
	b = 9.4771(18) Å	β= 116.301(3)°.
	c = 10.2788(19) Å	γ = 91.150(3)°.
Volume	815.1(3) $Å^3$	
Z	2	
Density (calculated)	1.256 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	324	
Crystal size	0.98 x 0.8 x 0.09 mm^3	
Theta range for data collection	2.15 to 28.34°	
Index ranges	$-12 \le h \le 12$, $-12 \le k \le 12$, $-13 \le l \le 13$	
Reflections collected	9686	
Independent reflections	4060 [R(int) = 0.0395]	
Completeness to theta = 28.34°	99.4 %	
Absorption correction	Empirical	
Max. and min. transmission	0.94704 and 0.83150	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4060 / 0 / 217	
Goodness-of-fit on F^2	0.914	
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1121	
R indices (all data)	R1 = 0.0930, wR2 = 0.1294	
Largest diff. peak and hole	0.149 and -0.134 e. $Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for compound 2.

O(1)-C(1)	1.2187(16)
C(1)-C(18)	1.482(2)
C(1)-C(2)	1.509(2)
C(2)-C(11)	1.3803(19)
C(2)-C(3)	1.4281(19)
C(3)-C(4)	1.4174(19)
C(3)-C(8)	1.418(2)
C(4)-C(5)	1.371(2)
C(4)-H(4A)	1.0753
C(5)-C(6)	1.406(2)
C(5)-H(5A)	1.0456
C(6)-C(7)	1.356(2)
C(6)-H(6A)	1.0062
C(7)-C(8)	1.410(2)
C(7)-H(7A)	0.9910
C(8)-C(9)	1.421(2)
C(9)-C(10)	1.350(2)
C(9)-H(9A)	1.0461
C(10)-C(11)	1.418(2)
C(10)-H(10A)	1.0138
C(11)-C(12)	1.488(2)
C(12)-C(17)	1.388(2)
C(12)-C(13)	1.397(2)
C(13)-C(14)	1.387(2)
C(13)-H(13A)	1.0990
C(14)-C(15)	1.371(3)
C(14)-H(14A)	0.9963
C(15)-C(16)	1.371(2)
C(15)-H(15A)	1.0501
C(16)-C(17)	1.380(2)
C(16)-H(16A)	1.0329
C(17)-H(17A)	1.0316
C(18)-C(19)	1.387(2)
C(18)-C(23)	1.393(2)
C(19)-C(20)	1.374(2)
C(19)-H(19A)	0.9785

C(20)-C(21)	1.370(2)
C(20)-H(20A)	1.0145
C(21)-C(22)	1.376(2)
C(21)-H(21A)	1.0336
C(22)-C(23)	1.375(2)
C(22)-H(22A)	0.9878
C(23)-H(23A)	1.0548

O(1)-C(1)-C(18)	121.40(14)
O(1)-C(1)-C(2)	118.74(14)
C(18)-C(1)-C(2)	119.84(13)
C(11)-C(2)-C(3)	120.74(14)
C(11)-C(2)-C(1)	120.47(13)
C(3)-C(2)-C(1)	118.46(13)
C(4)-C(3)-C(8)	118.08(13)
C(4)-C(3)-C(2)	122.51(14)
C(8)-C(3)-C(2)	119.40(13)
C(5)-C(4)-C(3)	120.85(15)
C(5)-C(4)-H(4A)	120.7
C(3)-C(4)-H(4A)	118.3
C(4)-C(5)-C(6)	120.38(15)
C(4)-C(5)-H(5A)	117.9
C(6)-C(5)-H(5A)	121.6
C(7)-C(6)-C(5)	120.10(14)
C(7)-C(6)-H(6A)	119.6
C(5)-C(6)-H(6A)	120.3
C(6)-C(7)-C(8)	121.09(16)
C(6)-C(7)-H(7A)	120.7
C(8)-C(7)-H(7A)	118.2
C(7)-C(8)-C(3)	119.47(15)
C(7)-C(8)-C(9)	122.16(15)
C(3)-C(8)-C(9)	118.35(14)
C(10)-C(9)-C(8)	120.91(15)
C(10)-C(9)-H(9A)	121.6
C(8)-C(9)-H(9A)	117.5
C(9)-C(10)-C(11)	121.95(14)
C(9)-C(10)-H(10A)	117.7
C(11)-C(10)-H(10A)	120.3

C(2)-C(11)-C(10)	118.61(14)
C(2)-C(11)-C(12)	123.48(14)
C(10)-C(11)-C(12)	117.88(13)
C(17)-C(12)-C(13)	118.91(14)
C(17)-C(12)-C(11)	121.17(13)
C(13)-C(12)-C(11)	119.78(15)
C(14)-C(13)-C(12)	119.44(17)
C(14)-C(13)-H(13A)	118.2
C(12)-C(13)-H(13A)	122.3
C(15)-C(14)-C(13)	120.91(16)
C(15)-C(14)-H(14A)	121.7
C(13)-C(14)-H(14A)	117.3
C(14)-C(15)-C(16)	119.84(16)
C(14)-C(15)-H(15A)	123.7
C(16)-C(15)-H(15A)	116.3
C(15)-C(16)-C(17)	120.28(17)
C(15)-C(16)-H(16A)	120.2
C(17)-C(16)-H(16A)	119.0
C(16)-C(17)-C(12)	120.61(15)
C(16)-C(17)-H(17A)	120.9
C(12)-C(17)-H(17A)	118.4
C(19)-C(18)-C(23)	119.02(15)
C(19)-C(18)-C(1)	121.26(14)
C(23)-C(18)-C(1)	119.72(14)
C(20)-C(19)-C(18)	120.35(16)
C(20)-C(19)-H(19A)	122.5
C(18)-C(19)-H(19A)	117.1
C(21)-C(20)-C(19)	120.40(16)
C(21)-C(20)-H(20A)	118.0
C(19)-C(20)-H(20A)	121.2
C(20)-C(21)-C(22)	119.79(17)
C(20)-C(21)-H(21A)	119.8
C(22)-C(21)-H(21A)	120.3
C(23)-C(22)-C(21)	120.63(16)
C(23)-C(22)-H(22A)	123.1
C(21)-C(22)-H(22A)	116.3
C(22)-C(23)-C(18)	119.81(16)
C(22)-C(23)-H(23A)	128.6

C(18)-C(23)-H(23A)	111.6

Symmetry transformations used to generate equivalent atoms: