**Water-Triggered and Gold(I)-Catalyzed Cascade Addition /
Cyclization of Terminal Alkynes with *ortho*-Alkynylaryl
Aldehyde**

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Supporting information

All experiments were carried out under an inert atmosphere of nitrogen, unless otherwise stated. Flash column chromatography was performed over SORBENT silica gel 30-60 μ m. ^1H NMR and ^{13}C NMR spectra were acquired by Varian 400 MHz and 100 MHz, or 300 MHz and 75 MHz, respectively, and referenced to the internal solvent signals. IR spectra were recorded by ABB Bomem MB100 interferometer. MS data were obtained by KRATOS MS25RFA Mass Spectrometer. HRMS were performed at McGill University.

Cy_3PAgCl ¹ and *ortho*-alkynylaryl aldehydes² were prepared by the reported methods. Me_3AuCl , Ph_3PAuCl and Et_3AuCl were purchased from Stream Company.

Typical procedure (entry 1, Table 2):

Me_3PAuCl (0.0019g, 0.00625 mmol, 5 mol%) was mixed with 0.5 mL distilled water, 0.5 mL toluene, 0.028 mL of phenylacetylene (**2a**) (0.25mmol, 2 equivalent) and 5 μL of *i*- Pr_2NEt (0.025 mmol, 20 mol%). The mixture was stirred at room temperature until all solid disappeared. 2-(Phenylethynyl)benzaldehyde (**1a**) (0.0258g, 0.125 mmol), was added and stirred at room temperature for 10 min, and then stirred at 70 $^\circ\text{C}$ for one day. The reaction was stopped and extracted with ether (3 $\times$ 5 mL). The extraction was dried with Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash

¹ Bowmaker, G. A.; Effendy; Harvey, P. J.; Healy, P. C.; Skelton, B. W.; White, A. H. *J. Chem. Soc., Dalton Trans.* **1996**, 2459

² Roesch, K. R.; Larock, R. C. *J. Org. Chem.* **2002**, 67, 86. The compounds were purified by column and redistillation.

column (30-40:1 hexanes and EtOAc). Compound **3a** was obtained in 81% of yield (0.0311g).

3-phenyl-1-(phenylethynyl)-1H-isochromene (3a): IR (liquid film): $\nu_{\max}$ 3063, 3034, 2232, 1625, 1602, 1490, 1457, 1333, 1268, 1051, 1027, 756, 689 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.82-7.79 (m, 2H), 7.51-7.49 (m, 2H), 7.44-7.26 (m, 9H), 7.16(dd, J = 7.6, 1.2Hz, 1H), 6.55 (s, 1H), 6.18 (s, 1H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 152.9, 134.4, 132.3, 131.4, 129.2, 129.03, 128.99, 128.6, 128.5, 128.4, 127.2, 125.6, 124.5, 124.1, 122.5, 101.9, 87.5, 85.7, 69.5; MS (EI) m/z (%) 308 (M^+), 279, 231 (100), 202, 105, 77; HRMS calcd for $\text{C}_{23}\text{H}_{16}\text{O}$: 308.1201; found: 308.1192.

3-phenyl-1-(p-tolyethynyl)-1H-isochromene (3b): IR (liquid film): $\nu_{\max}$ 3060, 3028, 2920, 2231, 1728, 1690, 1626, 1603, 1509, 1493, 1454, 1333, 1267, 1051, 816, 764, 690 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.82-7.80 (m, 2H), 7.45-7.26 (m, 8H), 7.17-7.11 (m, 3H), 6.55 (s, 1H), 6.18 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (CDCl_3 , 100MHz,

ppm) δ 152.9, 139.1, 134.3, 132.1, 131.4, 129.22, 129.18, 128.9, 128.6, 128.5, 127.1, 125.6, 124.5, 124.0, 119.4, 101.9, 87.8, 85.0, 69.7, 21.9; MS (EI) m/z (%) 322 (M^+), 307, 245 (100), 215, 202, 153, 105, 77; HRMS calcd for $C_{24}H_{18}O$: 322.1358; found: 322.1352.

1-((4-bromophenyl)ethynyl)-3-phenyl-1H-isochromene (3c): IR (liquid film): $\nu_{\max}$ 3067, 3030, 2231, 1229, 1689, 1627, 1486, 1454, 1393, 1332, 1267, 1052, 1010, 823, 764, 689 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.80-7.77 (m, 2H), 7.46-7.24 (m, 10H), 7.17 (dd, $J = 7.6, 1.2\text{Hz}$, 1H), 6.55 (s, 1H), 6.17 (s, 1H); ^{13}C NMR (CDCl_3 , 100MHz, ppm) δ 152.7, 134.2, 133.6, 131.7, 131.2, 129.2, 129.1, 128.6, 128.1, 127.2, 125.6, 124.4, 124.2, 123.3, 121.4, 101.9, 87.1, 86.4, 69.4; MS (EI) m/z (%) 386 (M^+), 309, 276, 230 (100), 202, 153, 138, 106, 77; HRMS calcd for $C_{23}H_{15}\text{BrO}$: 386.0306; found: 386.0299.

1-(cyclohexenylethynyl)-3-phenyl-1H-isochromene (3d): IR (liquid film): $\nu_{\max}$ 3061, 3024, 2927, 2857, 2215, 1602, 1493, 1454, 1330, 1267, 1051, 1027, 764 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.78-7.76 (m, 2H), 7.41-7.34 (m, 4H), 7.30-7.21 (m, 2H), 7.14

(dd, $J = 7.6, 1.2\text{Hz}$, 1H), 6.51 (s, 1H), 6.21 (dddd, $J = 4, 4, 2, 2\text{Hz}$, 1H), 6.05 (s, 1H), 2.17(m, 2H), 2.12 (m, 2H), 1.68-1.55 (m, 4H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 152.9, 136.6, 134.3, 131.4, 129.1, 128.8, 128.7, 128.5, 127.0, 125.6, 124.5, 123.9, 120.1, 101.8, 89.6, 82.9, 69.7, 29.4, 26.0, 22.6, 21.8; MS (EI) m/z (%) 312 (M^+ , 100), 293, 258, 239, 178, 165, 106, 77; HRMS calcd for $\text{C}_{23}\text{H}_{20}\text{O}$: 312.1514 ; found: 312.1504.

1-(oct-1-ynyl)-3-phenyl-1H-isochromene (3e): IR (liquid film): ν_{max} 3064, 2954, 2930, 2857, 2236, 1740, 1627, 1603, 1493, 1454, 1332, 1268, 1049, 1026, 764, 689cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.78-7.75 (m, 2H), 7.41-7.34 (m, 4H), 7.28-7.21 (m, 2H), 7.12 (dd, $J = 1.2, 7.2\text{Hz}$, 1H), 6.50 (s, 1H), 5.92 (s, 1H), 2.31 (td, $J = 7.2, 2.0\text{Hz}$, 2H), 1.57 (tt, $J = 7.2, 7.2\text{Hz}$, 2H), 1.41 (m, 2H), 1.30-1.27 (m, 4H), 0.89 (t, $J = 6.8\text{Hz}$, 3H); ^{13}C NMR (CD_2Cl_2 , 75MHz, ppm) δ 152.7, 134.4, 131.2, 129.2, 129.1, 128.8, 128.6, 127.0, 125.4, 124.3, 124.0, 101.6, 88.9, 76.7, 69.2, 31.5, 28.7³, 22.7, 18.9, 14.0; MS (EI) m/z (%) 316 (M^+), 245, 231, 202, 139, 105 (100), 77 ; HRMS calcd for $\text{C}_{23}\text{H}_{24}\text{O}$: 316.1827; found: 316.1823.

³ In CDCl_3 , the two carbons can be distinguished: 28.9 and 28.8

3-butyl-1-(phenylethynyl)-1H-isochromene (3f): IR (liquid film): $\nu_{\max}$ 3063, 2956, 2929, 2871, 2236, 1730, 1649, 1603, 1489, 1455, 1336, 1153, 1104, 1033, 1020, 755, 691 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.51-7.49 (m, 2H), 7.37-7.17 (m, 6H), 6.99 (dd, $J = 7.6, 1.2\text{Hz}$, 1H), 6.01 (s, 1H), 5.77 (s, 1H), 2.29 (t, $J = 7.2\text{Hz}$, 2H), 1.65 (tt, $J = 7.2, 7.2\text{Hz}$, 2H), 1.44 (m, 2H), 0.96 (t, $J = 7.2\text{Hz}$, 3H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 157.6, 132.2, 131.4, 128.92, 128.90, 128.5, 127.5, 126.3, 124.4, 123.0, 122.6, 101.8, 87.2, 86.1, 69.1, 33.6, 29.2, 22.5, 14.1; MS (EI) m/z (%) 288 (M^+), 259, 245, 231, 215, 202 (100), 105; HRMS calcd for $\text{C}_{21}\text{H}_{20}\text{O}$: 288.1514; found: 288.1511.

3-butyl-1-(p-tolylethynyl)-1H-isochromene (3g): IR (liquid film): $\nu_{\max}$ 3027, 2956, 2929, 2871, 2236, 1733, 1647, 1603, 1509, 1455, 1377, 1336, 1153, 1104, 973, 815, 751 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.38 (d, $J = 8.0\text{Hz}$, 2H), 7.35 (d, $J = 7.6\text{Hz}$, 2H), 7.26-7.17 (m, 2H), 7.12 (d, $J = 8\text{Hz}$, 2H), 6.97 (d, $J = 7.2\text{Hz}$, 1H), 5.98 (s, 1H), 5.75 (s, 1H), 2.36 (s, 3H), 2.27 (t, $J = 7.6\text{Hz}$, 2H), 1.63 (tt, $J = 7.6\text{Hz}$, 2H), 1.45-1.40 (m, 2H), 0.94 (t, $J = 7.2\text{Hz}$, 3H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 157.6, 139.0, 132.1, 131.4,

129.2, 128.8, 127.6, 126.3, 124.4, 122.9, 119.4, 101.8, 87.5, 85.3, 69.3, 33.8, 29.4, 22.7, 21.9, 14.3; MS (EI) m/z (%) 302 (M^+), 273, 259, 245 (100), 231, 215, 202, 189, 119; HRMS calcd for $C_{22}H_{22}O$: 302.1671; found: 302.1677.

1-((4-bromophenyl)ethynyl)-3-butyl-1H-isochromene (3h): IR (liquid film): $\nu_{\max}$ 3066, 2956, 2929, 2870, 2238, 2200, 1732, 1679, 1651, 1586, 1486, 1455, 1327, 1153, 1070, 1011, 824, 757cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.46-7.43 (m, 2H), 7.35-7.29 (m, 3H), 7.27-7.23 (m, 1H), 7.20-7.16 (m, 1H), 6.98 (dd, $J = 7.2, 0.8\text{Hz}$, 1H), 5.98 (s, 1H), 5.76 (s, 1H), 2.27 (t, $J = 7.6\text{Hz}$, 2H), 1.62 (tt, $J = 7.6, 7.6\text{Hz}$, 2H), 1.42 (m, 2H), 0.94 (t, $J = 7.6\text{Hz}$, 3H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 157.4, 133.6, 131.7, 131.3, 128.9, 127.2, 126.4, 124.3, 123.2, 123.1, 121.5, 101.8, 87.3, 86.0, 69.0, 33.7, 29.4, 22.7, 14.3; MS (EI) m/z (%) 366 (M^+), 323, 311, 231, 215, 202 (100), 183, 155, 101; HRMS calcd for $C_{21}H_{19}\text{BrO}$: 366.0619; found: 366.0608.

3-butyl-1-(cyclohexenylethynyl)-1H-isochromene (3i): IR (liquid film): $\nu_{\max}$ 3062, 3024, 2954, 2930, 2859, 2223, 1734, 1603, 1484, 1455, 1286, 1152, 1018, 918, 751cm^{-1} ;

^1H NMR (CDCl_3 , 500MHz, ppm) δ 7.28 (d, $J = 7.5\text{Hz}$, 1H), 7.22 (dd, $J = 7, 7.5\text{Hz}$, 1H), 7.15 (dd, $J = 7, 7.5\text{Hz}$, 1H), 6.94 (d, $J = 7.5\text{Hz}$, 1H), 6.20 (m, 1H), 5.86 (s, 1H), 5.72 (s, 1H), 2.23 (t, $J = 7.5\text{Hz}$, 2H), 2.17 (m, 2H), 2.10 (m, 2H), 1.65-1.56 (m, 7H), 1.44-1.37 (m, 3H), 0.93 (t, $J = 7.5\text{Hz}$, 3H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 157.7, 136.4, 131.4, 128.7, 127.8, 126.2, 124.4, 122.8, 120.2, 101.7, 89.3, 83.3, 69.3, 33.7, 29.41, 29.38, 26.0, 26.7, 26.6, 21.8, 14.3; MS (EI) m/z (%) 292 (M^+), 263, 249 (100), 235, 221, 207, 191, 178, 165, 152, 109, 81; HRMS calcd for $\text{C}_{21}\text{H}_{24}\text{O}$: 292.1827; found: 292.1830.

3-butyl-1-((4-methoxyphenyl)ethynyl)-1H-isochromene (3j): IR (liquid film): ν_{max} 3063, 2956, 2931, 2870, 2836, 2233, 1730, 1647, 1605, 1510, 1455, 1290, 1249, 1172, 1034, 832, 752cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.46-7.43 (m, 2H), 7.36 (d, $J = 7.6\text{Hz}$, 1H), 7.27-7.16 (m, 2H), 6.98 (d, $J = 7.2\text{Hz}$, 1H), 6.84 (d, $J = 8.4\text{Hz}$, 2H), 5.98 (s, 1H), 5.76 (s, 1H), 3.81 (s, 3H), 2.26 (t, $J = 7.6\text{Hz}$, 2H), 1.62 (tt, $J = 7.6, 7.6\text{Hz}$, 2H), 1.42 (m, 2H), 0.93 (t, $J = 7.6\text{Hz}$, 3H); ^{13}C NMR (CDCl_3 , 100MHz, ppm) δ 160.1, 157.7, 133.7, 131.5, 128.8, 127.7, 126.3, 124.5, 123.0, 114.6, 114.1, 101.7, 87.3, 84.6, 69.3, 55.5, 33.6, 29.2, 22.5, 14.2; MS (EI) m/z (%) 318 (M^+), 289, 275, 261 (100), 202, 189, 163, 135, 94; HRMS calcd for $\text{C}_{22}\text{H}_{22}\text{O}$: 318.1620; found: 318.1623.

3-tert-butyl-1-(phenylethynyl)-1H-isochromene (3k): IR (liquid film): $\nu_{\max}$ 3062, 3023, 2964, 2934, 2868, 2233, 1737, 1640, 1602, 1489, 1453, 1327, 1215, 1082, 914, 809, 754, 690cm^{-1} ; ^1H NMR (CDCl_3 , 500MHz, ppm) δ 7.46-7.44 (m, 2H), 7.31-7.30 (m, 4H), 7.26-7.23 (m, 1H), 7.18 (m, 1H), 7.02 (d, $J = 6.4\text{Hz}$, 1H), 5.99 (s, 1H), 5.84 (s, 1H), 1.23 (s, 9H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 164.2, 132.0, 131.4, 128.8, 128.7, 128.4, 127.9, 126.4, 124.3, 123.7, 122.7, 98.7, 86.6, 86.5, 69.0, 35.6, 28.1; MS (EI) m/z (%) 288 (M^+), 273, 245, 231 (100), 202, 105; HRMS calcd for $\text{C}_{21}\text{H}_{20}\text{O}$: 288.1514; found: 288.1512.

1-((4-bromophenyl)ethynyl)-3-tert-butyl-1H-isochromene (3l): IR (liquid film): $\nu_{\max}$ 3064, 3020, 2964, 2868, 2232, 1638, 1485, 1453, 1326, 1288, 1080, 1069, 1010, 914, 820, 754cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.44-7.41 (m, 2H), 7.31-7.16 (m, 5H), 7.02 (dd, $J = 7.2, 1.6\text{Hz}$, 1H), 5.97 (s, 1H), 5.83 (s, 1H), 1.23 (s, 9H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 164.1, 133.5, 137.1, 131.2, 128.9, 127.6, 126.4, 124.2, 123.8, 123.0,

121.6, 98.7, 87.8, 85.4, 68.8, 35.6, 28.1; MS (EI) m/z (%) 366 (M^+), 351, 323, 309 (100), 230, 202, 183, 57; HRMS calcd for $C_{21}H_{19}BrO$: 366.0619; found: 366.0616.

3-tert-butyl-1-((4-methoxyphenyl)ethynyl)-1H-isochromene (3m): IR (liquid film):

$\nu_{\max}$ 3069, 2963, 2231, 1638, 1605, 1509, 1453, 1289, 1249, 1081, 1034, 914, 831, 751 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.41-7.37 (m, 2H), 7.32-7.16 (m, 3H), 7.04-6.99 (m, 1H), 6.85-6.80 (m, 2H), 5.96 (s, 1H), 5.83 (s, 1H), 3.80 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (CDCl_3 , 100MHz, ppm) δ 164.4, 160.0, 133.6, 131.4, 128.7, 128.1, 126.4, 124.3, 123.7, 114.8, 114.1, 98.7, 86.6, 85.0, 69.0, 55.5, 35.5, 28.0; MS (EI) m/z (%) 318 (M^+), 303, 275, 261 (100), 218, 202, 189, 135; HRMS calcd for $C_{22}H_{22}O_2$: 318.1620; found: 318.1616.

3-cyclohexenyl-1-(phenylethynyl)-1H-isochromene (3n): IR (liquid film): $\nu_{\max}$ 3066,

2929, 2858, 2233, 1729, 1635, 1599, 1489, 1452, 1325, 1238, 1062, 1039, 922, 908, 798, 754, 690 cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.52-7.46 (m, 2H), 7.40-7.38 (m, 1H),

7.34-7.30 (m, 3H), 7.27-7.17 (m, 2H), 7.06 (m, dd, $J = 7.2, 1.2$ Hz, 1H), 6.57 (t, $J = 4$ Hz, 1H), 6.00 (s, 1H), 5.97 (s, 1H), 2.28 (m, 2H), 2.23 (m, 2H), 1.73 (m, 2H), 1.67-1.62(m, 2H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 153.9, 132.3, 131.8, 130.4, 128.9, 128.8, 128.7, 128.5, 128.1, 126.6, 124.4, 124.0, 122.6, 100.5, 87.3, 85.9, 69.1, 25.9, 24.6, 22.8, 22.3; MS (EI) m/z (%) 312 (M^+ , 100), 284, 231, 202, 79; HRMS calcd for $\text{C}_{23}\text{H}_{20}\text{O}$: 312.1514 ; found: 312.1504.

3-cyclohexenyl-1-(p-tolylethynyl)-1H-isochromene (3o): IR (liquid film): ν_{max} 3066, 3026, 2929, 2859, 2232, 1728, 1635, 1609, 1509, 1482, 1452, 1325, 1238, 1062, 1037, 816, 798, 751cm^{-1} ; ^1H NMR (CDCl_3 , 400MHz, ppm) δ 7.42-7.39 (m, 3H), 7.28-7.18 (m, 2H), 7.13 (d, $J = 8$ Hz, 2H), 7.06 (d, $J = 7.2$ Hz, 1H), 6.58 (t, $J = 4$ Hz, 1H), 6.00 (s, 1H), 5.97 (s, 1H), 2.37 (s, 3H), 2.29 (m, 2H), 2.23 (m, 2H), 1.75 (m, 2H), 1.66-1.64 (m, 2H); ^{13}C NMR (CDCl_3 , 75MHz, ppm) δ 154.0, 139.1, 132.2, 131.8, 130.4, 129.2, 128.82, 128.97, 128.07, 126.6, 124.4, 123.9, 119.5, 100.5, 87.6, 85.1, 69.2, 25.9, 24.6, 22.80, 22.83, 22.3, 21.8; MS (EI) m/z (%) 326 (M^+ , 100), 297, 255, 245, 215, 202, 189, 79; HRMS calcd for $\text{C}_{24}\text{H}_{22}\text{O}$: 326.1671; found: 326.1667.

ysc-4-72-1

Data Collected on: m400-mercury400
Archive directory: /export/home/ysc/vnmr/sys/data
Sample directory: /usr/local/lib
File: PROTON

Pulse Sequence: zgpg30

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.898 sec

Width 6410.3 Hz

8 repetitions

OBSERVE H1, 400.1245662 MHz

DATA PROCESSING

FT size 32768

Total time 0 min

ysc-4-72-1

Data Collected on: m400-mercury400
Archive directory: /export/home/ysc/vnmr/sys/data
Sample directory: /usr/local/lib
File: PROTON

Pulse Sequence: zgpg30

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.898 sec

Width 6410.3 Hz

8 repetitions

OBSERVE H1, 400.1245662 MHz

DATA PROCESSING

FT size 32768

Total time 0 min

yxq-4-72-1

Pulse Sequence: zgpg30

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

UNITY-500 "dante"

Pulse 38.3 degrees
Acq. time 1.300 sec
Width 27481.4 Hz
5568 repetitions
OBSERVE C13, 125.8885203 MHz
DECOUPLE H1, 499.8008858 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 18 hr, 12 min, 49 sec

STANDARD IN OBSERVE

Pulse Sequence: gHMQC

Solvent: CDCl₃
Ambient temperature
Mercury-400BB "m400"

Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 5571.4 Hz
AQ Width 27034.0 Hz
4 repetitions
2 x 128 increments
OBSERVE H1, 400.1213604 MHz
DECOUPLE C13, 100.6182683 MHz
Power 52 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.066 sec
F1 DATA PROCESSING
Gauss apodization 0.014 sec
FT size 1024 x 512
Total time 22 min, 54 sec

STANDARD IN

Pulse Sequence

SC
SC

yxq-4-71-1

Date Collected On: m400-mercury400
Archive directory: /export/home/xyao/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.958 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 400.1245662 MHz
DATA PROCESSING
FT size 32768
Total time 0 min

yxq-4-71-1

Data Collected on: m300-mercury300
Archive directory: /export/home/xyao/vnmrSYS/data
Sample directory:
File: CARBON

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 21.3 C / 294.4 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18807.9 Hz
1472 repetitions
OBSERVE C13, 75.4500158 MHz
DECOUPLE H1, 800.0510289 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 32 hr, 21 min

yxq-4-78-8

Data Collected on: n400-mercury400
Archive directory: /export/home/xyad/vmr/sys/data
Sample directory:
File: CARBON

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp. 25.0 C / 298.1 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.189 sec
Width 25125.6 Hz
9920 repetitions
OBSERVE C13, 100.6113782 MHz
DECOUPLE H1, 400.1266027 MHz
Power 24 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 62 hr, 35 min

yxq-4-71-2

Data Collected on: m400-mercury400
 Archive directory: /export/home/xyao/vnmrsys/data
 Sample directory:
 File: PROTON

Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.990 sec
 Width 6410.3 Hz
 8 repetitions
 OBSERVE H1, 400.1245662 MHz
 DATA PROCESSING
 FT size 32768
 Total time 9 min

yxq-4-71-2

Data Collected on: m300-mercury300
Archive directory: /export/home/xyao/vnmrsys/data
Sample directory:
File: CARBON

Pulse Sequence: zgpg30
Solvent: CDCl3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18867.9 Hz
25792 repetitions
OBSERVE C13, 75.4500158 MHz
DECOUPLE H1, 300.0610239 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 121072
Total time 40 hr, 27 min

yxq-4-S8-2-1

Data Collected on: m400-mercury400

Archive directory: /export/home/xyao/vnarsys/data

Sample directory:

File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.938 sec

Width 6410.3 Hz

8 repetitions

OBSERVE H1, 400.1245662 MHz

DATA PROCESSING

FT size 32768

Total time 0 min

yxq-4-58-2-1 in CD2C12

Pulse Sequence: s2pd1

Solvent: CD2C12

Ambient temperature

File: entry5-C13_CD2C12

Mercury-300 "m300"

Relax. delay 1.500 sec

Pulse 58.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

3632 repetitions

OBSERVE C13, 75.4490141 MHz

DECOUPLE H1, 300.6570086 MHz

Power 34 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 0 min, 0 sec

yxq-4-58-2-1

Data Collected on: m300-mercury300
Archive directory: /export/home/xyao/vnmrsys/data
Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 22.2 C / 295.4 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.815 sec

Width 18367.3 Hz

8336 repetitions

OBSERVE C13, 75.4500158 MHz

DECOUPLE H1, 300.0610299 MHz

Power 35 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 16 hr, 10 min

YXQ-4-64-ph

Data Collected on: m400-mercury400
Archive Directory: /export/home/xyao/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.895 sec
Width 6410.3 Hz
4 repetitions
OBSERVE H1, 400.1245682 MHz
DATA PROCESSING
FT size 32768
Total time 0 min

YXQ-4-64-toluene

Data Collected on: n400-mercury400
Archive directory: /export/home/xyao/vnarsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl3
Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.255 sec
Width 6410.5 Hz
4 repetitions
OBSERVE H1, 400.1245662 MHz
DATA PROCESSING
FT size 32768
Total time 0 min

YXQ-4-64-toluene

Data Collected on: n400-mercury400
Archive directory: /export/home/xyao/vnarsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl3
Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.255 sec
Width 6410.5 Hz
4 repetitions

OBSERVE H1, 400.1245662 MHz
DATA PROCESSING
FT size 32768
Total time 0 min

yxq-4-54-Yo1

Data Collected on: m300-mercury300
Archive directory: /export/home/yxq/vnmrsys/data
Sample directory:
File: CARBON

Pulse Sequence: zgpg30

Solvent: CDCl3

Temp. 21.0 C / 294.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.815 sec

Width 18867.3 Hz

2112 repetitions

OBSERVE C13, 75.4500158 MHz

DECOUPLE H1, 300.0810299 MHz

Power 35 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 16 hr, 10 min

VXQ-4-54-Br

YNA-4-54-Br

Data Collected on: m400-mercury400

File: 4-54-Br

Archive directory: /export/home/xyeo/vnhrsyz/data/archive

Sample directory: /export/home/xyeo/vnhrsyz/data/sample

File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.999 sec

Width 6410.3 Hz

8 repetitions

DBSERVE M1, 400.1245662 MHz

DATA PROCESSING

FT size 32768

Total time 0 min

yxq-4-4-Br

Data Collected on: m300-mercury300
Archive directory: /export/home/xyao/vnarsys/data
Sample directory:
File: CARBON

Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 21.4 C / 294.6 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18857.9 Hz
4032 repetitions
OBSERVE C13, 75.4500158 MHz
DECOUPLE H1, 300.0610293 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
FT size 131072
Total time 4 hr, 51 min

yxq-4-70-2

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

UNITY-500 "dante"

Pulse 70.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

4 repetitions

OBSERVE M1, 499.8989908 MHz

DATA PROCESSING

FI size 32768

Total time 0 min, 7 sec

YKQ-4-70-2

Data Collected on: m300-mercury300
Archive directory: /export/home/xyao/vnmrsws/data
Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18867.9 Hz
25104 repetitions
OBSERVE C13, 75.4500150 MHz
DECOUPLE H1, 300.0610239 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
FT size 131072
Total time 80 hr, 54 min

yxq-4-79-1

Pulse Sequence: zgpg30

Solvent: CDCl3

Ambient temperature

Mercury-400BB "m400"

Relax. delay 1.000 sec

Pulse 92.0 degrees

Acq. time 1.993 sec

Width 6006.0 Hz

4 repetitions

OBSERVE H1, 400.1219604 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 13 sec

yxq-4-79-1

Pulse Sequence: zgpg30

Solvent: CDCl3

Ambient temperature

Mercury-400BB "m400"

yxq-4-79-1

Pulse Sequence: zgpg30

Solvent: CDCl3

Ambient temperature

Mercury-400BB "m400"

yxq-4-29-1

Pulse Sequence: zgpg30

Solvent: CDCl₃

Ambient temperature

Mercury-400BB "m400"

Relax. delay 2.500 sec

Pulse 42.5 degrees

Acq. time 1.188 sec

Width 25000.0 Hz

9532 repetitions

OBSERVE C13, 100.6107230 MHz

DECOUPLE H1, 400.1238934 MHz

Power 35 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

FT size 65536

Total time 110 hr, 10 min, 45 sec

yxq-4-29-1

Pulse Sequence: zgpg30

Solvent: CDCl₃

Ambient temperature

Mercury-400BB "m400"

yxq-68-1-1

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

UNITY-500 "dante"

Pulse 70.4 degrees

Acq. time 1.832 sec

Width 8000.0 Hz

8 repetitions

OBSERVE H1, 499.8922908 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 15 sec

yxb-4-63-1-1

Data Collected on: m300-mercury300
Archive directory: /export/home/xyao/vnmr\$ys/data
Sample directory:
File: CARBON

Pulse Sequence: s2pul

Solvent: CDCl3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18867.3 Hz
3988 repetitions
OBSERVE C13, 75.4500153 MHz
DECOUPLE H1, 300.0610293 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 18 hr, 10 min

3k

yxq-4-69A

Sample Data

Data Collected on: 8400-mercury400

Data Date:

Archive directory: /export/home/xyao/vnmr/sys/data

Sample Name:

Sample directory:

Sample:

File: PRDTON

Exp:

Pulse Sequence: s2pul

Proc:

Solvent: CDCl₃

Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.998 sec

Width 6410.3 Hz

3 repetitions

OBSERVE H1, 400.1245662 MHz

DATA PROCESSING

FT size 32768

Total time 0 min

yxq-4-68A-CB

Data Collected on: m300-mercury800
Archive directory: /export/home/xyao/vnarsys/data
Sample directory:
File: CARBON

Pulse Sequence: szpul
Solvent: CDCl₃
Temp. 21.4 C / 294.6 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18867.9 Hz
18176 repetitions
OBSERVE C13, 75.4509158 MHz
DECOUPLE H1, 300.0619283 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
FT size 131072
Total time 80 hr, 54 min

3l

yxq-4-81-2

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
Mercury-200 "a200"

Relax. delay 1.000 sec
Pulse 55.3 degrees
Acq. time 1.952 sec
Width 3003.0 Hz
15 repetitions
OBSERVE H1, 200.0616317 MHz
DATA PROCESSING
FT size 16384
Total time 0 min, 0 sec

Yg-4-81-2
100 MHz

yxq-4-76Ph-C13

Pulse Sequence: s2p1

Solvent: CDCl3

Ambient temperature

File: yxq-4-76-PhC13

Mercury-300 "m300"

Relax. delay 1.500 sec

Pulse 58.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

2986 repetitions

OBSERVE C13, 75.4486632 MHz

DECOUPLE H1, 300.0564325 MHz

Power 34 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 100 hr, 20 min, 12 sec

yxq-4-76-CH3

yxq-4-76-CH3

Data Collected on: m400-mercury400
Archive directory: /export/home/xyao/vnmrsys/data
Sample directory: /export/home/xyao/vnmrsys/data
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 25.0 C / 298.1 K

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.988 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 400.1245662 MHz
DATA PROCESSING
FT size 32768
Total time 0 min

yxq-4-76CH3-C13

Pulse Sequence: s2pH1

Solvent: CDCl3

Ambient temperature

File: yxq-4-76-CH3-C13

Mercury-300 "mS90"

Relax. delay 1.500 sec

Pulse 58.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

2272 repetitions

OBSERVE C13, 75.4483692 MHz

DECOUPLE H1, 300.0564925 MHz

Power 34 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

FT size 131072

Total time 100 hr, 20 min, 12 sec