SUPPORTING INFORMATION

Carbopalladation of Nitriles: Synthesis of 3,4-Disubstituted 2-Aminonaphthalenes and
1,3-Benzoxazine Derivatives by the Pd-Catalyzed Annulation of Alkynes by (2-
Iodophenyl)acetonitrile

*Qingping Tian, Alexandre A. Pletnev, and Richard C. Larock**

Department of Chemistry, Iowa State University, Ames, Iowa 50011

larock@iastate.edu

Table of Contents

Reagent Sources	S2
Preparation and Characterization of Starting Materials	S2
Preparation and Characterization of Annulation Products	S3
¹ H and ¹³ C NMR Spectra of All New Compounds	S7

Reagents. Diphenylacetylene, triethylamine, tri-*n*-butylamine, 4-octyne, 2,2,7,7-tetramethyl-3,5-octadiyne, phenylacetylene, 1-phenyl-2-(trimethylsilyl)acetylene and 1-triisopropylsilyl-1-propyne were obtained from Aldrich Chemical Co., Inc. Tetra-*n*-butylammonium chloride, (2-iodophenyl)acetonitrile and 4,4-dimethyl-2-pentyne were obtained from Lancaster Synthesis, Inc. 1-Phenyl-1-propyne, 1-phenyl-1-butyne, 3-phenyl-2-propyn-1-ol, 2-methyl-3-pentyn-2-ol and 2-methyl-4-phenyl-3-butyn-2-ol were obtained from Farchan Laboratories, Inc. 3,3-Dimethyl-1-phenyl-1-butyne was prepared according to a previous literature procedure.¹

(2-Iodo-4,5-dimethoxyphenyl)acetonitrile (16) was prepared from 2-iodo-4,5-dimethoxybenzyl bromide (prepared in two steps from 4,5-dimethoxybenzyl alcohol)² according to a published procedure.³ A solution of 2-iodo-4,5-dimethoxybenzyl bromide (0.853 g, 2.39 mmol) and 18-crown-6 (0.053 g, 0.2 mmol) in 5 mL of MeCN was placed over solid KCN (0.338 g, 5.2 mmol). The reaction mixture was stirred vigorously for 24 h, after which it was filtered and the amount of solvent was reduced on a rotary evaporator. The mixture was diluted with water, extracted with CH₂Cl₂, dried (Na₂SO₄), evaporated and the residue was purified by column chromatography using 1:1 hexanes/ethyl acetate to produce 0.605 g (84%) of **16**: white solid, mp 110-111 °C (hexanes/ethyl acetate); ¹H NMR (CDCl₃) δ 3.76 (s, 2H), 3.87 (s, 3H), 3.90 (s, 3H), 6.98 (s, 1H), 7.24 (s, 1H); ¹³C NMR (CDCl₃) δ 29.2, 55.9, 56.1, 86.8, 111.5, 117.4, 121.5, 125.1, 149.1, 149.5; IR (neat) 3086, 2967, 2916, 2845, 2257 cm⁻¹; HRMS *m/z* 302.97609 (calcd for C₁₀H₁₀INO₂, 302.97563).

2-Acetoxy-2-(2-iodophenyl)acetonitrile (19c). To a cold (0 °C) solution of 2-iodobenzaldehyde (1.469 g, 6.33 mmol) in aq 2M NaHSO₃ (15 mL) was added a solution of KCN (1.645 g, 25.3 mmol) in 3.25 mL of water. The reaction mixture was stirred for 1.5 h at room temperature, then extracted with ether. The organic extracts were washed with water, dried (Na₂SO₄) and evaporated to afford 1.245 g (76%) of 2-hydroxy-2-(2-iodophenyl)acetonitrile,⁴ 0.39 g (1.5 mmol) of which was dissolved in a mixture of 7 mL of Ac₂O and 7 mL of pyridine and stirred overnight at room temperature.⁵ The reaction mixture was then poured into water and extracted with ether. The organic extracts were washed with aq HCl, aq NaHCO₃, and water, dried (Na₂SO₄), evaporated and the residue was purified by column chromatography using 4:1 hexanes/ethyl acetate to afford 0.42 g (93%) of **19c**: white solid, mp 57-59 °C

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(3) Cook, F. L.; Bowers, C. W.; Liotta, C. L. *J. Org. Chem.* **1974**, 39, 3416.

(4) Anhoury, M.-L.; Crooy, P.; De Neys, R.; Eliaers, J. *J. Chem. Soc., Perkin Trans. I* **1974**, 1015.

(5) Aufderhaar, E.; Baldwin, J. E.; Barton, D. H. R.; Faulkner, D. J.; Slaytor, M. *J. Chem. Soc. C* **1971**, 2175.

(hexanes/ethyl acetate); ^1H NMR (CDCl_3) δ 2.21 (s, 3H), 6.52 (s, 1H), 7.19 (td, $J = 7.8, 1.5$ Hz, 1H), 7.48 (td, $J = 7.8, 1.2$ Hz, 1H), 7.73 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.92 (dd, $J = 7.8, 1.2$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 20.2, 67.0, 97.9, 115.4, 129.0, 129.3, 131.9, 134.1, 140.2, 168.6; IR (neat) 3064, 2935, 2845, 2246, 1756 cm^{-1} ; HRMS m/z 300.96058 (calcd for $\text{C}_{10}\text{H}_8\text{INO}_2$, 300.95998).

2-Amino-3-(2-methylphenyl)-4-phenylnaphthalene (3). Obtained as a brown solid in a 44% yield from the reaction of (2-iodophenyl)acetonitrile and 2-(phenylethynyl)toluene after purification by column chromatography using 4:1 hexanes/ethyl acetate ($R_f = 0.44$): mp 172-174 °C (hexanes/ethyl acetate); ^1H NMR (CDCl_3) δ 1.93 (s, 3H), 3.75 (br s, 2H), 7.01-7.25 (m, 12H), 7.36 (t, $J = 8.0$ Hz, 1H), 7.66 (d, $J = 8.0$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 20.0, 108.2, 122.5, 124.8, 125.6, 126.1, 126.5, 126.9, 127.0, 128.1, 128.3, 128.9, 129.3, 129.6, 130.7, 131.1, 134.3, 136.5, 138.5, 142.4 (1 sp^2 carbon missing due to overlap); IR (neat) 3469, 3368, 3043, 3024, 2928, 1617, 1435 cm^{-1} ; HRMS m/z 309.15227 (calcd for $\text{C}_{23}\text{H}_{19}\text{N}$, 309.15175). NOE was detected between the NH_2 (3.75 ppm) and CH_3 (1.93 ppm) groups in the 2D NOESY spectrum of **3**.

2-Amino-4-(2-methylphenyl)-3-phenylnaphthalene (4). Obtained as an amber oil in a 45% yield from the reaction of (2-iodophenyl)acetonitrile and 2-(phenylethynyl)toluene after purification by column chromatography using 4:1 hexanes/ethyl acetate ($R_f = 0.48$): ^1H NMR (CDCl_3) δ 2.08 (s, 3H), 3.66 (br s, 2H), 7.00-7.26 (m, 11H), 7.33-7.38 (m, 2H), 7.67 (d, $J = 7.6$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 19.8, 107.9, 122.3, 125.6, 125.7, 126.0, 126.5, 126.8, 127.2, 127.3, 127.4, 127.5, 129.3, 129.9, 131.0, 131.1, 134.5, 136.8, 139.1, 139.4, 142.3; IR (neat) 3476, 3380, 3058, 3019, 2923, 1616 cm^{-1} ; HRMS m/z 309.15227 (calcd for $\text{C}_{23}\text{H}_{19}\text{N}$, 309.15175). No NOE was detected between the NH_2 (3.66 ppm) and CH_3 (2.08 ppm) groups.

2-Amino-4-ethyl-3-phenylnaphthalene (6). Obtained as a light brown solid in a 37% yield from the reaction of (2-iodophenyl)acetonitrile and 1-phenyl-1-propyne after purification by column chromatography using 15:1 hexanes/ethyl acetate: mp 131-132 °C (hexanes/EtOAc); ^1H NMR (CDCl_3) δ 1.14 (t, $J = 7.5$ Hz, 3H), 2.78 (q, $J = 7.5$ Hz, 2H), 3.55 (br s, 2H), 6.98 (s, 1H), 7.25-7.54 (m, 7H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.95 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 15.5, 23.0, 107.0, 122.4, 124.5, 125.9, 126.1, 126.4, 127.6, 129.1, 129.9, 134.9, 137.4, 139.1, 142.6 (1 sp^2 carbon missing due to overlap); IR (CDCl_3) 3427, 3304, 3065, 2980, 1621 cm^{-1} ; HRMS m/z 247.1315 (calcd for $\text{C}_{18}\text{H}_{17}\text{N}$, 247.1361).

2-Amino-3-ethenyl-4-phenylnaphthalene (7). Obtained as an orange solid in a 17% yield from the reaction of (2-iodophenyl)acetonitrile and 1-phenyl-1-propyne after purification by column chromatography using 15:1 hexanes/ethyl acetate: mp 128-130 °C (hexanes/EtOAc); ^1H NMR (CDCl_3) δ 4.14 (br s, 2H), 5.40 (dd, $J = 11.7, 1.8$ Hz, 1H), 5.47 (dd, $J = 18.3, 1.8$ Hz, 1H), 6.42 (dd, $J = 18.0, 11.7$

Hz, 1H), 7.05-7.10 (m, 2H), 7.24-7.50 (m, 7H), 7.59 (d, $J = 8.1$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 108.9, 120.9, 122.5, 125.5, 125.6, 126.2, 126.7, 127.0, 127.4, 128.1, 130.7, 134.0, 134.1, 139.4, 139.6, 142.0; IR (CDCl_3) 3444, 3375, 3051, 2961, 1624 cm^{-1} ; HRMS m/z 245.1202 (calcd for $\text{C}_{18}\text{H}_{15}\text{N}$, 245.1204).

2-Amino-4-hydroxymethyl-3-phenylnaphthalene (8). Obtained as a yellow oil in a 29% yield from the reaction of (2-iodophenyl)acetonitrile and 3-phenyl-2-propyn-1-ol after purification by column chromatography using 2:1 hexanes/ethyl acetate: ^1H NMR (CDCl_3) δ 1.60 (br s, 1H), 3.80 (br s, 2H), 4.79 (s, 2H), 7.09 (s, 1H), 7.31-7.36 (m, 3H), 7.40-7.47 (m, 2H), 7.50-7.54 (m, 2H), 7.65 (d, $J = 8.0$ Hz, 1H), 8.12 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 59.8, 109.2, 123.2, 124.4, 126.2, 126.3, 128.0, 128.9, 129.1, 129.8, 131.2, 134.4, 134.8, 137.0, 142.2; IR (neat) 3450, 3390, 3063, 3025, 2929, 2851, 1621 cm^{-1} ; HRMS m/z 249.11577 (calcd for $\text{C}_{17}\text{H}_{15}\text{NO}$, 249.11536).

2-Amino-3-tert-butyl-4-phenylnaphthalene (10). Obtained as a light orange solid in a 27% yield from the reaction of (2-iodophenyl)acetonitrile and 3,3-dimethyl-1-phenyl-1-butyne after purification by column chromatography using 15:1 hexanes/ethyl acetate: mp 164-165 $^{\circ}\text{C}$ (hexanes/EtOAc); ^1H NMR (CDCl_3) δ 1.31 (s, 9H), 4.14 (br s, 2H), 6.92 (d, $J = 8.4$ Hz, 1H), 6.97 (dt, $J = 6.6, 1.2$ Hz, 1H), 7.24-7.40 (m, 7H), 7.53 (d, $J = 8.1$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 32.9, 37.4, 112.4, 122.2, 124.6, 125.6, 126.7, 127.2, 127.3, 129.4, 131.4, 132.6, 134.1, 138.7, 142.8, 144.1; IR (CDCl_3) 3478, 3367, 3061, 2956, 1618 cm^{-1} ; HRMS m/z 275.1680 (calcd for $\text{C}_{20}\text{H}_{21}\text{N}$, 275.1674).

2-Amino-1-tert-butylfluoranthene (11). Obtained as a light yellow solid in a 15% yield from the reaction of (2-iodophenyl)acetonitrile and 3,3-dimethyl-1-phenyl-1-butyne after purification by column chromatography using 15:1 hexanes/ethyl acetate: mp 95-96 $^{\circ}\text{C}$ (hexanes/EtOAc); ^1H NMR (CDCl_3) δ 1.55 (s, 9H), 4.08 (br s, 2H), 6.80 (s, 1H), 7.32-7.39 (m, 4H), 7.73-7.78 (m, 2H), 8.04 (m, 1H); ^{13}C NMR (CDCl_3) δ 30.6, 33.3, 117.1, 119.7, 124.6, 126.8, 127.6, 127.8, 127.9, 129.4, 135.4, 137.1, 137.5, 140.2, 140.8, 147.1, (2 sp^2 carbons missing due to overlap); IR (CDCl_3) 3467, 3374, 3063, 2930, 1622 cm^{-1} ; HRMS m/z 273.1512 (calcd for $\text{C}_{20}\text{H}_{19}\text{N}$, 273.1518).

{2-(Phenylethynyl)phenyl}acetonitrile (12). Obtained as a red oil in a 58% yield from the reaction of (2-iodophenyl)acetonitrile and 1-phenyl-2-(trimethylsilyl)acetylene after purification by column chromatography using 30:1 hexanes/ethyl acetate: ^1H NMR (CDCl_3) δ 3.98 (s, 2H), 7.32-7.42 (m, 5H), 7.50-7.62 (m, 4H); ^{13}C NMR (CDCl_3) δ 22.9, 86.1, 95.8, 117.5, 122.6, 122.9, 128.3, 128.5, 128.6, 129.0, 129.1, 131.7, 131.8, 132.5; IR (CDCl_3) 3059, 2925, 2248, 2214, 1599 cm^{-1} ; HRMS m/z 217.0891 (calcd for $\text{C}_{16}\text{H}_{11}\text{N}$, 217.0892). Compound **12** was also obtained in a 51% from the reaction of (2-iodophenyl)acetonitrile and phenylacetylene.

2-Amino-4-methyl-3-(triisopropylsilyl)naphthalene (13). Obtained as a green oil in a 54% yield from the reaction of (2-iodophenyl)acetonitrile and 1-triisopropylsilyl-1-propyne after purification by

column chromatography using 10:1 hexanes/ethyl acetate: ^1H NMR (CDCl_3) δ 1.16 (d, $J = 7.5$ Hz, 18H), 1.65 (heptet, $J = 7.5$ Hz, 3H), 2.79 (s, 3H), 3.97 (br s, 2H), 6.84 (d, $J = 1.2$ Hz, 1H), 7.24 (td, $J = 8.4$, 1.5 Hz, 1H), 7.35 (td, $J = 8.1$ Hz, 1H), 7.52 (dd, $J = 8.1$, 0.6 Hz, 1H), 7.91 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.1, 19.4, 21.8, 108.2, 122.0, 124.2, 125.7, 126.4, 127.7, 135.1, 144.1, 149.6 (1 sp^2 carbon missing due to overlap); IR (neat) 3490, 3381, 3062, 2948, 2871, 1615 cm^{-1} ; HRMS m/z 313.22300 (calcd for $\text{C}_{20}\text{H}_{31}\text{NSi}$, 313.22258).

2-Amino-3-*tert*-butyl-4-(3,3-dimethyl-1-butynyl)naphthalene (15). Obtained as an inseparable mixture with the other regioisomer (about 6%) as a brown oil in a 91% yield from the reaction of (2-iodophenyl)acetonitrile and 2,2,7,7-tetramethyl-3,5-octadiyne after column chromatography using 4:1 hexanes/ethyl acetate: ^1H NMR (CDCl_3) δ 1.43 (s, 9H), 1.78 (s, 9H), 4.05 (br s, 2H), 6.92 (s, 1H), 7.24-7.34 (m, 2H), 7.46-7.49 (m, 1H), 8.34-8.37 (m, 1H); ^{13}C NMR (CDCl_3) δ 29.3, 30.6, 32.3, 38.0, 79.2, 110.6, 113.3, 120.6, 123.2, 125.0, 125.9, 126.4, 130.1, 132.5, 138.0, 143.7; IR (neat) 3510, 3392, 3067, 2969, 2923, 2866, 2207, 1619 cm^{-1} ; HRMS m/z 279.19915 (calcd for $\text{C}_{20}\text{H}_{25}\text{N}$, 279.19870).

2-Amino-6,7-dimethoxy-3,4-diphenylnaphthalene (17). Obtained as an off-white solid in an 81% yield from the reaction of **16** and diphenylacetylene after purification by column chromatography using 2:1 hexanes/ethyl acetate: mp 177-179 $^\circ\text{C}$ (EtOH); ^1H NMR (CDCl_3) δ 3.64 (br s, 2H), 3.66 (s, 3H), 4.00 (s, 3H), 6.70 (s, 1H), 6.98 (s, 1H), 7.04 (s, 1H), 7.09-7.26 (m, 10H); ^{13}C NMR (CDCl_3) δ 55.6, 55.8, 104.4, 106.2, 107.9, 122.3, 126.3, 126.7, 127.5, 128.2, 130.2, 130.7, 130.8, 137.9, 138.4, 139.4, 141.1, 146.9, 149.8 (1 sp^2 carbon missing due to overlap); IR (neat) 3460, 3366, 3059, 3000, 2962, 2934, 2834, 1614, 1495 cm^{-1} ; HRMS m/z 355.15787 (calcd for $\text{C}_{24}\text{H}_{21}\text{NO}_2$, 355.15723).

2-Methyl-4,5-diphenylnaphtho[2,1-*d*]oxazole (20). Obtained as a white solid in a 53% yield from the reaction of **19c** and diphenylacetylene after purification by column chromatography using 2:1 hexanes/ethyl acetate: mp 222-224 $^\circ\text{C}$ (hexanes/ethyl acetate); ^1H NMR (CDCl_3) δ 2.03 (s, 3H), 7.01-7.02 (m, 1H), 7.06-7.10 (m, 3H), 7.16-7.28 (m, 5H), 7.35-7.40 (m, 1H), 7.44-7.46 (m, 1H), 7.49-7.54 (m, 1H), 8.50 (d, $J = 8.8$ Hz, 1H), 9.56 (s, 1H); ^{13}C NMR (CDCl_3) δ 23.5, 117.9, 123.1, 125.6, 126.3, 126.4, 126.5, 126.9, 127.5, 127.6, 128.5, 130.6, 131.3, 131.6, 131.9, 132.7, 136.8, 138.6, 144.2, 170.3; IR (neat) 3060, 1646, 1513, 1494, 1277 cm^{-1} ; HRMS m/z 335.13157 (calcd for $\text{C}_{24}\text{H}_{17}\text{NO}$, 335.13101).

2,4,4,5-Tetramethyl-1,4-dihydro-2*H*-naphtho[2,3-*d*][1,3]oxazine (21a). Obtained as a light brown solid in a 25% yield from the reaction of (2-iodophenyl)acetonitrile and 2-methyl-3-pentyn-2-ol after purification by column chromatography using 4:1 hexanes/ethyl acetate ($R_f = 0.44$): mp 95-97 $^\circ\text{C}$; ^1H NMR (CDCl_3) δ 1.44 (d, $J = 5.6$ Hz, 3H), 1.75 (s, 3H), 1.83 (s, 3H), 2.73 (s, 3H), 4.30 (br s, 1H), 4.92 (q, $J = 5.6$ Hz, 1H), 6.89 (s, 1H), 7.24-7.28 (m, 1H), 7.32-7.36 (m, 1H), 7.55 (d, $J = 8.4$ Hz, 1H), 7.92 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 17.7, 21.8, 28.4, 30.2, 73.3, 76.2, 109.9, 122.7, 123.9, 125.7, 126.1,

128.6, 130.5, 133.0, 140.7 (1 sp^2 carbon missing due to overlap); IR (neat) 3375, 3056, 2983, 2934, 2875, 1618 cm^{-1} ; HRMS m/z 241.14703 (calcd for $\text{C}_{16}\text{H}_{19}\text{NO}$, 241.14666).

3-*E*-{1-[2-Cyanomethylphenyl]ethylidene}-5-{1-hydroxy-1-methylethyl}-2,2,4-trimethyl-2,3-dihydrofuran (22). Obtained as a yellow oil in a 26% yield from the reaction of (2-iodophenyl)acetonitrile and 2-methyl-3-pentyn-2-ol after purification by column chromatography using 4:1 hexanes/ethyl acetate (R_f = 0.26): ^1H NMR (CDCl_3) δ 1.03 (s, 3H), 1.40 (s, 6H), 1.57 (s, 3H), 1.62 (s, 3H), 2.04 (s, 3H), 2.10 (s, 1H), 3.55-3.70 (m, 2H), 7.16-7.19 (m, 1H), 7.23-7.28 (m, 2H), 7.36-7.38 (m, 1H); ^{13}C NMR (CDCl_3) δ 10.6, 21.3, 22.4, 26.1, 26.2, 28.7, 29.0, 70.9, 85.7, 104.3, 116.5, 118.2, 127.3, 127.8, 128.0, 128.2, 130.1, 144.1, 161.9; IR (neat) 3334, 2978, 2930, 2875, 2253 cm^{-1} ; HRMS m/z 311.18908 (calcd for $\text{C}_{20}\text{H}_{25}\text{NO}_2$, 311.18853).

4,4-Dimethyl-5-phenyl-2-*n*-propyl-1,4-dihydro-2*H*-naphtho[2,3-*d*][1,3]oxazine (21c). Obtained as a light yellow solid in a 38% yield from the reaction of (2-iodophenyl)acetonitrile, 2-methyl-4-phenyl-3-butyne-2-ol and $n\text{-Bu}_3\text{N}$ after purification by column chromatography using 4:1 hexanes/ethyl acetate: mp 142-144 $^\circ\text{C}$ (EtOH); ^1H NMR (CDCl_3) δ 1.00 (t, J = 7.4 Hz, 3H), 1.21 (s, 3H), 1.52 (s, 3H), 1.46-1.73 (m, 4H), 4.41 (br s, 1H), 4.87 (m, 1H), 6.85 (d, J = 8.4 Hz, 1H), 6.97-7.02 (m, 2H), 7.24-7.32 (m, 3H), 7.42-7.46 (m, 3H), 7.55 (d, J = 8.0 Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.0, 17.7, 29.5, 30.4, 37.9, 76.2, 110.4, 122.3, 125.1, 125.8, 126.9, 127.3, 127.4, 127.5, 128.9, 130.1, 130.9, 132.4, 132.9, 137.1, 140.2, 140.5; IR (neat) 3381, 3057, 3021, 2969, 2933, 2871, 1619 cm^{-1} ; HRMS m/z 331.19399 (calcd for $\text{C}_{23}\text{H}_{25}\text{NO}$, 331.19361).

1.068
0.043

77.482
77.058
76.635

108.873

141.960
139.590
139.394
134.094
134.031
130.695
128.098
127.356
127.054
126.730
126.179
125.607
125.490
122.491
119.954

2-Amino-3-ethenyl-4-phenylnaphthalene (7)

180 160 140 120 100 80 60 40 20 0 ppm

/drx1/data/qtian/nmr/ctian.299.fid/1/pdata/1 unknown Sun Nov 2 11:32:33 1997

1.311
1.292
1.223
0.994

4.143

5.299

7.549
7.522
7.400
7.390
7.379
7.293
7.290
7.277
7.269
7.258
7.246
7.080
6.991
6.987
6.969
6.965
6.931
6.903

2-Amino-3-tert-butyl-4-phenylnaphthalene (10)

1.75

2-Amino-3-tert-butyl-4-phenylnaphthalene (10)

2-Amino-1-tert-butylfluoranthene (11)

33.303
30.560147.144
140.778
140.209
137.513
137.081
135.376
129.447
127.889
127.806
127.588
126.851
124.651
119.694
117.061

2-Amino-1-tert-butylfluoranthene (11)

0.089

22.881

76.704
77.128
77.552

86.075

95.770

132.470
131.788
131.697
129.131
128.965
128.595
128.472
128.267
122.911
122.589
117.529

{2-(Phenylethynyl)phenyl}acetonitrile (12)

180 160 140 120 100 80 60 40 20 0 ppm

/drx1/data/qtian/nmr/ctian.303.fid/1/pdata/1 unknown Sat Nov 1 18:31:21 1997

VI-28-B-2