Supporting Information

Synthesis of Dibenzo[g,p]chrysenes From Bis(biaryl)acetylenes via Sequential ICl-induced Cyclization and Mizoroki-Heck coupling..

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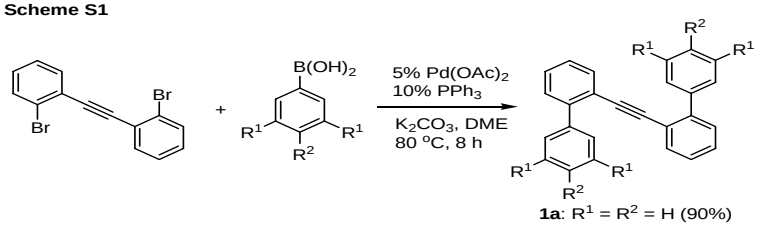
Contents:

(1) **Representative synthetic procedures for compound 1a**

Scheme S1



1a: $R^1 = R^2 = H$ (90%)

To a solution of $Pd(OAc)_2$ (67 mg, 0.30 mmol), PPh_3 (156 mg, 0.59 mmol) and K_2CO_3 (3.29 g, 23.81 mmol) in DME (30 mL) and H_2O (10 mL) at room temperature was added phenylboricacid (2.18 g, 17.85 mmol), and resulting mixture was stirred for 10 min. To this solution was added 1,2-bis(2-bromophenyl)ethyne[s1] (2.00 g, 5.95 mmol), and the mixture was heated to 80 ^oC for 8 h. The solution was cooled to room temperature before adding saturated ammonium chloride solution. The solution was extracted with ethyl acetate (2 x 30 mL), washed with brine solution, and dried over $MgSO_4$. The organic layer was filtered, concentrated, and eluted through a silica column to give the bromo biarlyl **1a** (1.57 g, 4.76 mmol) in 80%.

(s1). For preparation of 1,2-bis(2-bromophenyl)ethyne see: (a) Chang, H.-K.; Datta, S.; Das, A.; Odedra, A.; Liu, R.-S. *Angew. Chem. Ent. Ed*. **2007**, *46*, 4744. (b) Mio, M. J.; Kopel, L. C.; Braun, J. B.; Gadzikwa, T. L.; Hull, K. L.; Brisbois, R. G.; Markworth, C. J.; Grieco, P. A. *Org. Lett*. **2002**, *4*, 3199.

(2) Procedure for calculation of the relative energies of states VI and **VI'**

The geometries of carbocations **VI** and **VI'** had been fully optimized had been calculated using the B3LYP method[s2,s3] with the 6-31+G* basis set[s4] (B3LYP/6-31+G*). 3-21G* was used for iodine atom since 6-31+G* is not available. Density Functional Theory (DFT) has been recognized as a valuable tool in the study of structural isomers. The vibrational frequencies, at the same level of theory, were computed for both species to characterize them as true minima on the

potential energy hypersurfaces. All of the calculations were performed with the GAUSSIAN 03 package.[s5] The unscaled zero-point vibrational energies (ZPE) are included in the reported energies.

(s2) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

(s3) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev.* **1988**, *B37*, 785.

(s4) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650.

(s5) Frisch, M. J. et al. *Gaussian 03*, revision A1; Gaussian, Inc.: Pittsburgh, PA, 2003.

(3) Spectral data for key compounds

Spectral data for 1,2-di(biphenyl-2-yl)ethyne (**1a**).

IR (neat, cm^{-1}): 3059, 3010, 1605; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.71 (d, 4H, J = 8 Hz), 7.55 (d, 2H, J = 8 Hz) 7.470-7.53 (m, 8H), 7.43 (t, 2H, J = 8 Hz), 7.36 (t, 2H, J = 8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 143.4, 140.4, 132.9, 129.3, 129.2, 128.3, 127.8, 127.4, 127.0, 121.7, 91.9; HRMS calcd. for $C_{26}H_{18}$: 330.1409, found 330.1406.

Spectral data for 1,2-bis(4'-fluorobiphenyl-2-yl)ethyne (**1b**).

IR (neat, cm^{-1}): 3050, 2999, 1602, 1210; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.45-7.49 (m, 4H), 7.40 (d, 2H, J = 7.6 Hz), 7.26-7.36 (m, 8H), 7.01 (t, 2H, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.3 (d, J_{CF} = 244.3 Hz), 142.4, 136.3, 133.0, 130.8 (d, J_{CF} = 9.2 Hz), 129.3, 128.5, 127.1, 121.5, 114.7 (d, J_{CF} = 22.4 Hz), 91.8; HRMS calcd. for $C_{26}H_{16}F_2$: 366.1220, found 366.1217.

Spectral data for 1,2-bis(3',5'-dimethoxybiphenyl-2-yl)ethyne (**1c**).

IR (neat, cm^{-1}): 3058, 3010, 1603, 1245; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.41-7.45 (m, 4H), 7.35 (t, 2H, J = 4.8 Hz), 7.3 (t, 2H, J = 4.8 Hz), 6.79 (d, 4H, J = 2.4 Hz), 6.49 (t, 2H, J = 2.4 Hz), 3.80 (s, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.2, 143.3, 142.2, 133.0, 129.2, 128.3, 127.1, 121.6, 107.2, 100.1, 92.3, 55.2; HRMS calcd. for

$C_{30}H_{26}O_4$: 450.1831, found 450.1834.

Spectral data for bis[2-(3,4,5- trimethoxyphenyl)phenyl]ethyne (**1d**).

IR (neat, cm^{-1}): 3060, 3015, 1600, 1247; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.25-7.40 (m, 8H), 6.84 (s, 4H), 3.90 (s, 6H), 3.83 (s, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.7, 143.4, 137.6, 136.0, 132.9, 129.2, 128.5, 127.1, 121.5, 106.6, 92.5, 60.9, 56.1; HRMS calcd. for $C_{32}H_{30}O_6$: 510.2042, found 510.2045.

Spectral data for 9-(biphenyl-2-yl)-10-iodophenanthrene (**2a**).

IR (neat, cm^{-1}): 3066, 3024, 2834, 1610; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.58-8.65 (m, 2H); 8.35-8.37 (m, 1H), 7.51-7.66 (m, 7H), 7.41 (t, 1H, J = 6.8 Hz,), 7.29 (d, 1H, J = 6.8 Hz,), 7.18-7.22 (m, 2H), 6.94-6.99 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 144.5, 143.0, 141.4, 140.6, 134.4, 132.6, 132.3, 131.2, 130.5, 130.3, 130.0, 128.8, 128.7, 128.5, 127.8, 127.5, 127.4, 127.4, 127.0, 126.9, 122.6, 108.0 (two peaks meared); HRMS calcd. for $C_{26}H_{17}I$: 456.0375, found 456.0371.

Spectral data for 2-fluoro-10-(4'-fluorobiphenyl-2-yl)-9-iodophenanthrene (**2b**).

IR (neat, cm^{-1}): 3059, 3010, 2835, 1605, 1205; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.56-8.60 (m, 1H), 8.47-8.49 (m, 1H), 8.38-8.40 (m, 1H), 7.60-7.66 (m, 3H), 7.52-7.57 (m, 2H), 7.28-7.36 (m, 2H), 7.12-7.20 (m, 3H), 6.66-6.72 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.7 (d, J_{CF} = 244.3 Hz), 161.3 (d, J_{CF} = 245.8 Hz), 143.6, 140.3, 136.5 (d, J_{CF} = 3 Hz), 134.5, 133.6 (d, J_{CF} = 9.2 Hz), 133.8, 131.1, 130.5, 130.3, 130.3, 129.8, 128.8, 127.9, 127.8, 126.6, 125.0, 122.4, 115.9, 114.5 (d, J_{CF} = 21.4 Hz), 112.9 (d, J_{CF} = 21.4 Hz), 109.6 (one peak meaged); HRMS calcd. for $C_{26}H_{15}F_2I$: 492.0186, found 492.0189.

Spectral data for 9-iodo-10-(4'-iodo-3',5'-dimethoxybiphenyl-2-yl)-1,3-dimethoxy phenanthrene (**2c**).

IR (neat, cm^{-1}): 3065, 3025, 2832, 1607, 1240; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.47 (d, 1H, *J* = 9.6 Hz), 8.30 (d, 1H, *J* = 9.6 Hz), 7.64 (d, 1H, *J* = 2.4 Hz), 7.57-7.59 (m, 2H), 7.42-7.45 (m, 3H), 7.16 (d, 1H, *J* = 8.8 Hz), 6.53 (d, 1H, *J* = 1.2 Hz), 6.38 (s, 2H), 3.89 (s, 3H), 3.41 (s, 3H), 3.31 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.2, 158.3, 157.2, 148.6, 143.5, 141.6, 139.1, 134.7, 133.3, 133.0, 129.7, 129.3, 128.7, 128.4, 127.0, 126.9, 126.8, 123.2, 119.4, 107.4, 107.0, 105.4, 99.2, 96.3, 75.3, 56.1, 55.7, 55.4; HRMS calcd. for $C_{30}H_{24}I_2O_4$: 701.9764, found 701.9763.

Spectral data for 9-iodo-1,2,3-trimethoxy-10-(3',4',5'-trimethoxybiphenyl-2-yl)-phenanthrene (**2d**).

IR (neat, cm^{-1}): 3060, 3023, 2846, 1605, 1245; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.43 (d, 1H, *J* = 8 Hz), 8.36 (d, 1H, *J* = 8 Hz), 7.83 (s, 1H), 7.56-7.60 (m, 2H), 7.27-7.48 (m, 3H), 7.27-7.29 (m, 1H), 6.47 (s, 2H), 4.06 (s, 3H), 3.81 (s, 3H), 3.65 (s, 3H), 3.35 (s, 6H), 3.32 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 153.2, 151.9, 149.8, 147.9, 142.4, 141.4, 139.9, 136.8, 136.3, 134.8, 132.4, 129.6, 129.3, 129.1, 127.9, 127.7, 127.1, 127.0, 126.3, 123.1, 122.6, 109.3, 106.6, 99.4, 60.7, 60.6, 60.5, 55.8, 55.5; HRMS calcd for $C_{32}H_{29}IO_6$: 636.1009, found 636.1015.

Spectral data for 1,2-bis(4'-methoxybiphenyl-2-yl)ethyne (**3a**).

IR (neat, cm^{-1}): 3063, 3015, 1605, 1245; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, 4H, *J* = 8.0 Hz), 7.47 (d, 2H, *J* = 6.8 Hz), 7.35-7.38 (m, 4H), 7.22-7.26 (m, 2H), 6.92 (d, 4H, *J* = 5.2 Hz), 3.85 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.0, 143.0, 133.1, 132.9, 130.4, 129.2, 128.3, 126.4, 121.6, 113.3, 92.0, 55.2; HRMS calcd. for $C_{28}H_{22}O_2$: 390.1620, found 390.1626.

Spectral data for 1,2-bis(4,4'-dimethoxybiphenyl-2-yl)ethyne (**3b**).

IR (neat, cm^{-1}): 3065, 3010, 1607, 1243; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.47 (d, 4H, *J* = 6.8 Hz), 7.26 (d, 2H, *J* = 8.8 Hz), 6.87-6.97 (m, 8H), 3.83 (s, 6H), 3.80 (s, 6H); ^{13}C

NMR ($CDCl_3$, 100 MHz) δ 158.8, 158.0, 136.1, 132.6, 130.3 (x 2), 122.3, 117.2, 115.3, 113.2, 91.8, 55.3, 55.2; HRMS calcd. for $C_{30}H_{26}O_4$: 450.1831, found 450.1833.

Spectral data for spiro hexadienone (**4a**).

IR (neat, cm^{-1}): 3060, 3010, 1675, 1610, 1525; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.20-7.45 (m, 8H), 7.03 (d, 1H, *J* = 6.8 Hz), 6.92 (d, 1H, *J* = 6.8 Hz), 6.80 (d, 2H, *J* = 8.4 Hz), 6.22-6.23 (m, 2H), 5.91 (d, 1H, *J* = 10.0 Hz), 5.11 (dd, 1H, *J* = 10.0, 2.4 Hz), 3.75 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.4, 159.0, 153.1, 147.1, 146.1, 145.1, 141.0, 140.6, 133.6, 131.1, 131.0, 130.5, 129.9, 129.1, 129.0, 127.6, 126.7, 123.3, 123.2, 113.3, 104.6, 63.0, 55.1; HRMS calcd. for $C_{27}H_{19}IO_2$: 502.0430, found 502.0425.

Spectral data for spiro compound (**4b**).

IR (neat, cm^{-1}): 3059, 3017, 1670, 1605, 1500; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.22 (d, 1H, *J* = 8.4 Hz), 7.17 (d, 2H, *J* = 8.8 Hz), 6.96 (d, 1H, *J* = 2.4 Hz), 6.92 (dd, 1H, *J* = 8.8, 2.4 Hz), 6.73-6.81 (m, 4H), 6.55 (d, 1H, *J* = 2.4 Hz), 6.20-6.22 (m, 2H), 5.86 (dd, 1H, *J* = 10.0, 1.6 Hz), 5.09 (dd, 1H, *J* = 10.0, 2.4 Hz), 3.86 (s, 3H), 3.80 (s, 3H), 3.74 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.0, 160.8, 158.7, 158.0, 154.0, 147.4, 146.5, 134.8, 133.6, 133.4, 132.1, 131.6, 131.0, 130.1, 129.5, 123.9, 116.8, 113.9, 113.6, 113.2, 108.9, 104.4, 62.3, 55.6, 55.3, 55.1 (one peak mearged); HRMS calcd. for $C_{29}H_{23}IO_4$: 562.0641, found 562.0642.

Spectral data for 4′-methoxy-2-*p*-tolylethynyl biphenyl (**5b**).

IR (neat, cm^{-1}): 3057, 3015, 1597, 1492, 1245: ^1H NMR (400MHz, $CDCl_3$) δ 7.60 (d, 2H, *J* = 8.8 Hz), 7.38-7.31 (m, 2H), 7.28-7.23 (m, 4H), 7.08 (d, 2H, *J* = 8.0 Hz), 6.97 (d, 2H, *J* = 8.8 Hz), 3.84 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz) δ 159.1, 143.3, 138.1, 133.1, 132.8, 131.0, 130.4, 129.2, 129.0, 128.2, 126.5, 121.6, 120.4, 113.2, 92.2, 88.8, 55.2, 21.4; HRMS calcd for $C_{22}H_{18}O$: 298.1358, found 298.1355.

Spectral data for 4'-methoxy-2-((4-methoxyphenyl)ethynyl)biphenyl (**5c**).

IR (neat, cm^{-1}): 3060, 3017, 1600, 1492, 1247: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.61-7.58 (m, 3H), 7.39-7.23 (m, 5H), 6.95 (d, 2H, *J* = 8.4 Hz), 6.77 (d, 2H, *J* = 8.4 Hz), 3.79 (s, 3H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.4, 159.0, 143.0, 133.0, 132.7, 132.6, 130.4, 129.2, 128.1, 126.5, 121.6, 115.6, 113.8, 113.2, 92.1, 88.2, 55.2, 55.1; HRMS calcd. for $C_{22}H_{18}O_2$: 314.1307, found 314.1305.

Spectral data for 2-((4'-methoxybiphenyl-2-yl)ethynyl)furan (**5d**).

IR (neat, cm^{-1}): 3057, 1597, 1492, 1239: ^{1}H NMR (400MHz, $CDCl_3$) δ 7.66-7.60 (m, 3H), 7.43-7.37 (m, 3H), 7.30 (td, 1H, *J* = 8.0, 2.0 Hz), 7.00 (d, 2H, *J* = 8.0 Hz), 6.53 (d, 1H, *J* = 3.6 Hz), 6.38 (dd, 1H, *J* = 3.6, 1.6 Hz), 3.85 (s, 3H); ^{13}C NMR (100 MHz) δ 159.1, 143.4, 143.2, 137.2, 132.8, 132.5, 130.3, 129.3, 128.9, 126.5, 120.3, 115.0, 113.4, 110.9, 93.3, 82.1, 55.1; HRMS calcd. for $C_{19}H_{14}O_2$: 274.0994, found 274.0991.

Spectral data for 2-((4'-methoxybiphenyl-2-yl)ethynyl)thiophene (**5e**).

IR (neat, cm^{-1}): 3060, 1602, 1500, 1478, 1240: ^{1}H NMR (400MHz, $CDCl_3$) δ 7.64-7.60 (m, 3H), 7.44-7.36 (m, 2H), 7.30 (td, 1H, *J* = 8.0, 2.0), 7.24 (dd, 1H, *J* = 5.2, 1.2 Hz), 7.16 (dd, 1H, *J* = 3.6, 0.8 Hz), 7.01 (d, 2H, *J* = 8.0 Hz), 6.97 (dd, 1H, J = 5.2, 3.6 Hz), 3.87 (s, 3H); ^{13}C NMR (100 MHz) δ 159.1, 143.2, 132.8, 132.5, 131.4, 130.4, 129.3, 128.6, 127.1, 127.0, 126.6, 123.5, 121.0, 113.4, 93.3, 85.4, 55.2; HRMS calcd. for $C_{19}H_{14}OS$: 290.0765, found 290.0767.

Spectral data for 2-((4'-methoxybiphenyl-2-yl)ethynyl)benzofuran (**5f**).

IR (neat, cm^{-1}): 3060, 1597, 1482, 1441, 1247; ^{1}H NMR (400MHz, $CDCl_3$) δ 7.70 (dd, 1H, *J* = 8.0, 0.8 Hz), 7.64 (d, 2H, *J* = 8.8 Hz), 7.54 (dd, 1H, *J* = 8.0, 0.8 Hz), 7.48-7.43 (m, 3H), 7.35-7.31 (m, 2H), 7.26 (t, 1H, *J* = 7.6 Hz), 7.03 (d, 2H, *J* = 8.8 Hz), 6.87 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz) δ 159.2, 154.7, 143.6, 138.8, 133.1, 132.4, 130.3, 129.4, 129.3, 127.7, 126.6, 125.4, 123.1, 121.0, 119.9, 113.5,

111.4, 111.1 95.2, 82.3, 55.2; HRMS calcd for $C_{23}H_{16}O_2$: 324.1150, found 324.1153.

Spectral data for 2-((4'-methoxybiphenyl-2-yl)ethynyl)benzo[b]thiophene (**5g**).

IR (neat, cm^{-1}): 3065, 1597, 1482, 1245; ^1H NMR (400MHz, $CDCl_3$) δ 7.78-7.72 (m, 2H), 7.70-7.65 (m, 3H), 7.47-7.31 (m, 6H), 7.06 (d, 2H, *J* = 8.8 Hz), 3.89 (s, 3H); ^{13}C NMR (100 MHz) δ 159.2, 143.4, 140.2, 139.0, 132.7, 132.6, 130.3, 129.3, 128.9, 128.1, 126.6, 125.2, 124.6, 123.6, 123.4, 121.8, 120.6, 113.4, 95.2, 85.7, 55.2; HRMS calcd. for $C_{23}H_{16}OS$: 340.0922, found 340.0917.

Spectral data for 4'-methoxy-2-(oct-1-ynyl)biphenyl (**5h**).

IR (neat, cm^{-1}): 3065, 2895, 1597, 1482, 1240; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, 2H, *J* = 8.8 Hz), 7.40-7.47 (m, 1H), 7.24-7.29 (m, 2H), 7.18-7.24 (m, 1H), 6.92 (d, 2H, *J* = 8.8 Hz), 3.83 (s, 3H), 2.28 (t, 2H, *J* = 6.8 Hz), 1.41-1.45 (m, 2H), 1.23-1.33 (m, 6H), 0.86 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.8, 143.1, 133.2, 133.0, 130.3, 129.2, 127.6, 126.4, 122.2, 113.1, 93.2, 80.3, 55.0, 31.3, 28.4, 28.4, 22.5, 19.4, 14.0; HRMS calcd. for $C_{21}H_{24}O$: 292.1827, found 292.1827.

Spectral data for 4,4'-dimethoxy-2-(phenylethynyl)biphenyl (**5i**).

IR (neat, cm^{-1}): 3065, 3012, 1605, 1502, 1240; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.58 (d, 2H, *J* = 8.8 Hz), 7.35-7.37 (m, 2H), 7.29-7.32 (m, 4H), 7.15 (d, 1H, *J* = 1.6 Hz), 6.96-6.98 (m, 3H), 3.86 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.8, 158.1, 136.4, 132.8, 131.4, 130.4, 128.2, 128.1, 123.4, 122.1, 117.1, 115.4, 113.3, 91.8, 89.6, 55.4, 55.3 (one peak mearged); HRMS calcd. for $C_{22}H_{18}O_2$: 314.1307, found 314.1307.

Spectral data for 4,4'-dimethoxy-2-((4-methoxyphenyl)ethynyl)biphenyl (**5j**).

IR (neat, cm^{-1}): 3063, 3010, 1600, 1503, 1245; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.61 (d, 2H, *J* = 8.8 Hz), 7.30-7.35 (m, 3H), 7.17 (d, 1H, *J* = 2.4 Hz), 6.99 (d, 2H, *J* = 8.8 Hz),

6.94 (dd, 1H, *J* = 8.4, 2.4 Hz), 6.84 (d, 2H, *J* = 8.8 Hz), 3.86 (s, 3H), 3.85 (s, 3H), 3.79 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.5, 158.7, 158.1, 136.0, 132.8, 130.4, 122.4, 116.8, 115.5, 115.0, 113.9, 113.5, 113.2, 91.9, 88.3, 55.3, 55.2 (two peaks mearged); HRMS calcd. for $C_{23}H_{20}O_3$: 344.1412, found 344.1412.

Spectral data for 2-((4,4'-dimethoxybiphenyl-2-yl)ethynyl)furan (**5k**).

IR (neat, cm^{-1}): 3060, 1597, 1498, 1483, 1243: ^{1}H NMR (400MHz, $CDCl_3$) δ 7.54 (d, 2H, *J* = 8.0 Hz), 7.38 (dd, 1H, *J* = 2.0, 0.8 Hz), 7.31 (d, 1H, *J* = 8.4 Hz), 7.15 (d, 1H, *J* = 2.8 Hz), 6.99-6.94 (m, 3H), 6.53 (dd, 1H, *J* = 3.2, 0.4 Hz), 6.38 (dd, 1H, J = 3.2, 1.6 Hz), 3.84 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (100 MHz) δ 158.8, 158.0, 143.5, 137.1, 136.1, 132.3, 130.5, 130.2, 121.1, 116.8, 115.9, 115.2, 113.3, 111.0, 93.4, 81.8, 55.3, 55.2; HRMS calcd. for $C_{20}H_{16}O_3$: 304.1099, found 304.1094.

Spectral data for 2-((4,4'-dimethoxybiphenyl-2-yl)ethynyl)thiophene (**5l**).

IR (neat, cm^{-1}): 3059, 1597, 1492, 1485, 1242: ^{1}H NMR (400MHz, $CDCl_3$) δ 7.53 (d, 2H, *J* = 8.8 Hz), 7.29 (d, 1H, *J* = 8.4), 7.23 (dd, 1H, *J* = 5.2, 1.2 Hz), 7.12 (dd, 1H, *J* = 3.2, 0.8 Hz), 7.10 (d, 1H, *J* = 3.2 Hz), 6.96-6.91 (m, 4H), 3.86 (s, 6H); ^{13}C NMR (100 MHz) δ 158.7, 158.0, 136.0, 132.4, 131.5, 130.3, 130.2, 127.2, 126.9, 123.3, 121.7, 116.5, 115.5, 113.3, 93.4, 85.2, 55.3, 55.1; HRMS calcd. for $C_{20}H_{16}O_2S$: 320.0871, found 320.0864.

Spectral data for 4,4'-dimethoxy-2-(oct-1-ynyl)biphenyl (**5m**).

IR (neat, cm^{-1}): 3063, 3012, 2893, 1605, 1502, 1243; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.49 (dd, 2H, *J* = 8.8, 0.8 Hz), 7.23 (d, 1H, *J* = 8.4 Hz), 7.01 (d, 1H, *J* = 2.4 Hz), 6.92 (d, 2H, *J* = 8.8 Hz), 6.87 (dd, 1H, *J* = 8.4, 2.4 Hz), 3.83 (s, 3H), 3.81 (s, 3H), 2.29 (t, 2H, *J* = 6.8 Hz), 1.46-1.48 (m, 2H), 1.23-1.33 (m, 6H), 0.87 (t, 3H, *J* = 6.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.6, 158.0, 136.1, 133.0, 130.3, 123.0, 117.3, 114.5, 113.1, 93.2, 80.3, 55.3, 55.2, 31.4, 28.5, 28.4, 22.5, 19.5, 14.0 (one peak mearged);

HRMS calcd. for $C_{22}H_{26}O_2$: 322.1933, found 322.1933.

Spectral data for 4',5-dimethoxy-2-((4-methoxyphenyl)ethynyl)biphenyl (**5n**).

IR (neat, cm^{-1}): 3065, 3010, 1605, 1498, 1243; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.65 (d, 2H, *J* = 8.8 Hz), 7.55 (d, 1H, *J* = 8.4 Hz), 7.30 (d, 2H, *J* = 8.4 Hz), 6.99 (d, 2H, *J* = 8.8 Hz), 6.94 (d, 1H, *J* = 2.4 Hz), 6.86-6.81 (m, 3H), 3.86 (s, 3H), 3.84 (s, 3H), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.3, 159.2, 159.1, 144.6, 134.0, 133.0, 132.5, 130.4, 115.9, 114.7, 114.0, 113.8, 113.2, 112.4, 90.5, 88.1, 55.3, 55.2, 55.1; HRMS calcd. for $C_{23}H_{20}O_3$: 344.1412, found 344.1415.

Spectral data for spiro compound (**6b**).

IR (neat, cm^{-1}): 3054, 2835, 1675, 1600, 1495; ^1H NMR (400MHz, $CDCl_3$): δ 7.44 (d, 2H, *J* = 4.0 Hz), 7.30-7.24 (m, 3H), 7.13 (d, 2H, *J* = 7.6 Hz), 7.07 (d, 1H, *J* = 7.6 Hz), 6.51-6.43 (m, 4H), 2.33 (s, 3H); ^{13}C NMR (100 MHz): 185.8, 150.2, 147.3, 145.9, 140.0, 138.8, 131.8, 131.0, 129.1, 129.0, 128.2, 127.7, 123.7, 123.3, 99.4, 62.4, 21.3; HRMS calcd. for $C_{21}H_{15}IO$, 410.0168, found 410.0164.

Spectral data for spiro compound (**6c**).

IR (neat, cm^{-1}): 3052, 2836, 1673, 1605, 1500, 1145; ^1H NMR (400MHz, $CDCl_3$): δ 7.45-7.41 (m, 2H), 7.36 (d, 2H, *J* = 8.8 Hz), 7.30-7.25 (m, 1H), 7.07 (d, 1H, *J* = 7.2 Hz), 6.85 (d, 2H, *J* = 8.8 Hz), 6.51-6.43 (m, 4H), 3.80 (s, 3H); ^{13}C NMR (100 MHz): 185.8, 159.8, 149.7, 147.6, 146.0, 139.9, 131.0, 129.8, 129.2, 127.7, 127.0, 123.7, 123.3, 113.7, 99.0, 62.4, 55.2; HRMS calcd. for $C_{21}H_{15}IO_2$, 426.0117, found 426.0113.

Spectral data for spiro compound (**6d**).

IR (neat, cm^{-1}): 3062, 2812, 1670, 1615, 1412; ^1H NMR (400MHz, $CDCl_3$): δ 7.45-7.42 (m, 3H), 7.27-7.23 (m, 1H), 7.05-7.01 (m, 2H), 6.54-6.44 (m, 5H); ^{13}C

NMR ($CDCl_3$, 100 MHz): 186.1, 148.7, 148.2, 146.3, 143.0, 138.5, 138.3, 130.3, 129.2, 127.8, 123.6, 123.0, 111.6, 111.3, 92.9, 60.8; HRMS calcd. for $C_{18}H_{11}IO_2$: 385.9804, found 385.9800.

Spectral data for spiro compound (**6e**).

IR (neat, cm^{-1}): 3075, 2842, 1675, 1423; ^1H NMR (400MHz, $CDCl_3$): δ 7.45-7.42 (m, 3H), 7.36 (d, 1H, *J* = 5.2 Hz), 7.28-7.23 (m, 1H), 7.05-7.02 (m, 2H), 6.54-6.44 (m, 4H); ^{13}C NMR (100 MHz): 185.5, 148.7 (x 2), 146.4, 138.6, 136.1, 131.0 (x 2), 129.3, 128.0, 127.9, 126.8, 123.9, 123.0, 96.8, 62.6; HRMS calcd for $C_{18}H_{11}IOS$: 401.9575, found 401.9571.

Spectral data for spiro compound (**6f**).

IR (neat, cm^{-1}): 3062, 2834, 1676, 1432; ^1H NMR (400MHz, $CDCl_3$): δ 7.55 (d, 1H, *J* = 7.6 Hz), 7.50-7.41 (m, 3H), 7.32-7.28 (m, 3H), 7.20 (t, 1H, *J* = 8.0 Hz), 7.09 (d, 1H, *J* = 7.6 Hz), 6.59-6.50 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): 185.9, 154.4, 150.1, 148.0, 146.2, 139.0, 138.1, 130.5, 129.3, 128.3, 127.7, 125.6, 124.1, 123.2, 123.0, 121.4, 111.1, 107.1, 96.5, 60.9; HRMS calcd for $C_{22}H_{13}IO_2$: 435.9960, found 435.9956.

Spectral data for spiro compound (**6g**).

IR (neat, cm^{-1}): 3060, 2840, 1665, 1413; ^1H NMR (400MHz, $CDCl_3$): δ 7.87-7.85 (m, 1H), 7.58- 7.56 (m, 1H), 7.53-7.47 (m, 2H), 7.37-7.32 (m, 3H), 7.29 (s, 1H), 7.16 (d, 1H, *J* = 7.2 Hz), 6.52 (d, 2H, *J* = 7.2 Hz), 6.39 (d, 2H, *J* = 9.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 185.48, 145.7 (x 2), 145.5, 140.7, 139.6, 136.7, 131.6 (x 2), 129.7, 129.3, 128.1, 125.9, 124.6, 124.1, 123.6, 123.5, 122.8, 102.7, 63.4; HRMS calcd for $C_{22}H_{13}IOS$: 451.9732, found 451.9728.

Spectral data for spiro compound (**6h**).

IR (neat, cm^{-1}): 3060, 2945, 2840, 1665, 1413; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 (t, 1H, *J* = 7.6 Hz), 7.31 (d, 1H, *J* = 7.6 Hz), 7.21 (t, 1H, *J* = 7.6 Hz), 7.03 (d, 1H, *J* = 7.6 Hz), 6.52 (d, 2H, *J* = 10.0 Hz), 6.32 (d, 2H, *J* = 10.0 Hz), 2.20-2.24 (m, 2H), 1.40-1.47 (m, 2H), 1.23-1.32 (m, 6H), 0.86 (t, 3H, *J* = 6.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.1, 151.5, 147.4, 145.8, 140.1, 131.2, 129.0, 127.1, 123.2, 122.5, 98.8, 61.8, 31.3, 30.3, 29.4, 29.1, 22.5, 14.0; HRMS calcd. for $C_{20}H_{21}IO$: 404.0637, found 404.0635.

Spectral data for spiro compound (**6i**).

IR (neat, cm^{-1}): 3060, 2840, 1665, 1600, 1495; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 (b, 5H), 6.97-6.99 (m, 2H), 6.82 (dd, 1H, *J* = 8.4, 2.0 Hz), 6.48 (d, 2H, *J* = 10.4 Hz), 6.40 (d, 2H, *J* = 10.4 Hz), 3.87 (s 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.7, 161.0, 151.2, 147.4, 147.3, 134.8, 131.5, 130.7, 128.8, 128.4, 128.3, 124.1, 113.9, 109.4, 99.7, 61.7, 55.7; HRMS calcd. for $C_{21}H_{15}IO_2$: 426.0117, found 426.0119.

Spectral data for spiro compound (**6j**).

IR (neat, cm^{-1}): 3050, 2998, 2847, 1665, 1605; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 (d, 2H, *J* = 8.8 Hz), 6.97 (s, 1H), 6.96 (d, 1H, *J* = 6Hz), 6.85 (d, 2H, *J* = 8.8 Hz), 6.80 (dd, 1H, *J* = 6.0, 2.4 Hz), 6.48 (d, 2H, *J* = 10.0 Hz), 6.43 (d, 2H, *J* = 10.0 Hz), 3.87 (s, 3H), 3.79 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.8, 161.0, 159.9, 150.8, 147.8, 147.5, 131.4, 130.7, 129.7, 127.1, 124.1, 113.7, 113.7, 109.4, 98.8, 61.7, 55.7, 55.2; HRMS: calcd for $C_{22}H_{17}IO_3$: 456.0222, found 456.0217.

Spectral data for spiro compound (**6k**).

IR (neat, cm^{-1}): 3042, 2856, 1675, 1615, 1433, 1245; ^{1}H NMR (400MHz, $CDCl_3$): δ 7.44 (s, 1H), 7.01- 6.93 (m, 3H), 6.78 (d, 1H, *J* = 8.4 Hz), 6.51- 6.44 (m, 5H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 186.0, 160.9, 148.6, 148.5, 147.7, 142.9, 139.1,

129.8, 123.7, 114.1, 113.8, 111.4, 111.2, 109.0, 92.6, 59.9, 55.5; HRMS calcd for $C_{19}H_{13}IO_3$: 415.9909, found 415.9903.

Spectral data for spiro compound (**6l**).

IR (neat, cm^{-1}): 3055, 2852, 1665, 1453; ^1H NMR (400MHz, $CDCl_3$): δ 7.45 (d, 1H, *J* = 4.0 Hz), 7.36 (d, 1H, *J* = 4.8 Hz), 7.02 (t, 1H, *J* = 4.8 Hz), 6.96-6.92 (m, 2H), 6.80-6.73 (m, 1H), 6.52 (s, 4H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 185.7, 160.9, 149.0, 147.7, 143.3, 136.1, 130.5, 129.8, 127.8, 126.9, 126.8, 123.8, 113.9, 109.3, 96.5, 61.3, 55.6; HRMS calcd. for $C_{19}H_{13}IO_2S$: 431.9681, found 431.9679.

Spectral data for spiro compound (**6m**).

IR (neat, cm^{-1}): 3060, 2960, 2840, 1667, 1600, 1495; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.91 (d, 1H, *J* = 8.8 Hz), 6.84 (d, 1H, *J* = 2.8 Hz), 6.73 (dd, 1H, *J* = 8.8, 2.8 Hz), 6.47 (d, 2H, *J* = 10.4 Hz), 6.28 (d, 2H, *J* = 10.4 Hz), 3.84 (s, 3H), 2.18-2.22 (m, 2H), 1.27-1.29 (m, 2H), 1.23-1.26 (m, 6H), 0.85 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.1, 160.9, 152.7, 147.8, 147.3, 131.6, 130.8, 124.0, 112.9, 108.2, 98.6, 61.1, 55.6, 31.3, 30.4, 29.3, 29.0, 22.4, 14.0; HRMS calcd. for $C_{21}H_{23}IO_2$: 434.0743, found 434.0743.

Spectral data for compound (**6n**).

IR (neat, cm^{-1}): 3085, 2882, 1685, 1243; ^1H NMR (400MHz, $CDCl_3$): δ 7.32-7.28 (m, 4H), 6.94 (d, 1H, *J* = 8.4 Hz), 6.82 (d, 1H, *J* = 8.8 Hz), 6.62 (s, 1H), 6.49 (d, 2H, *J* = 10.4 Hz), 6.42 (d, 2H, *J* = 10.4 Hz), 3.76 (s, 6H); ^{13}C NMR (100 MHz): 185.7, 159.9, 159.5, 147.6, 146.9, 141.3, 138.9, 130.7, 129.7, 127.0, 124.2, 114.7, 113.5, 108.9, 98.1, 62.3, 55.6, 55.0; HRMS calcd for $C_{22}H_{17}IO_3$, 456.0222, found 456.0219.

Spectral data for 2',4-dimethoxy-2-((4-methoxyphenyl)ethynyl)biphenyl (**7**).

IR (neat, cm^{-1}): 3065, 3015, 1603, 1243; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.37 (m,

2H), 7.30 (d, 1H, *J* = 4.4 Hz), 7.13-7.16 (m, 2H), 7.03 (t, 1H, *J* = 7.6 Hz), 6.99 (d, 1H, *J* = 8 Hz), 6.93 (dd, 2H, *J* = 8.0, 1.2 Hz), 6.79 (dd, 2H, *J* = 8.0, 1.2 Hz), 3.85 (s, 3H), 3.77 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.4, 158.3, 157.1, 133.6, 132.8, 131.7, 131.2, 129.6, 128.6, 124.2, 120.0, 116.1, 115.6, 114.4, 113.8, 110.8, 91.5, 88.1, 55.6, 55.3, 55.2; HRMS calcd. for $C_{23}H_{20}O_3$: 344.1412, found 344.1406.

Spectral data for 10-iodo-2,5-dimethoxy-9-(4-methoxyphenyl)phenanthrene (**8**).

IR (neat, cm^{-1}): 3075, 3025, 2832, 1607, 1243; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.64 (d, 1H, *J* = 9.6 Hz), 7.96 (d, 1H, *J* = 2.8 Hz), 7.24-7.29 (m, 2H), 7.12-7.17 (m, 3H), 7.04-7.05 (m, 3H), 4.11 (s, 3H), 4.00 (s, 3H), 3.91 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.1, 158.6, 157.7, 145.5, 139.2, 134.5, 133.9, 131.0, 130.5, 125.6, 124.8, 121.9, 121.2, 116.8, 115.8, 113.8, 109.1, 108.8, 56.0, 55.4, 55.3; HRMS calcd. for $C_{23}H_{19}IO_3$: 470.0379, found 470.0375.

Spectral data for 9-iodo-2-methoxy-10-*p*-tolyl phenanthrene (**9b**).

IR (neat, cm^{-1}): 3069, 3020, 1597, 1402, 1249; ^{1}H NMR (400MHz, $CDCl_3$): δ 8.59 (d, 1H, *J* = 8.8 Hz), 8.53 (d, 1H, *J* = 8.0 Hz), 8.43 (d, 1H, *J* = 8.8 Hz), 7.67-7.58 (m, 2H), 7.35 (d, 2H, *J* = 8.0 Hz), 7.26 (d, 1H, *J* = 8.8 Hz), 7.17 (d, 2H, *J* = 8.8 Hz), 6.80 (s, 1H), 3.69 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.2, 144.7, 142.5, 137.4, 134.6, 133.8, 131.4, 130.5, 129.6, 129.2, 127.4, 126.9, 124.6, 124.1, 122.0, 116.7, 109.9, 107.4, 55.1, 21.4; HRMS calcd. for $C_{22}H_{17}IO$: 424.0324, found 424.0320.

Spectral data for 9-iodo-2-methoxy-10-(4-methoxyphenyl)phenanthrene (**9c**).

IR (neat, cm^{-1}): 3075, 3025, 1600, 1403, 1248; ^{1}H NMR (400MHz, $CDCl_3$): δ 8.60 (d, 1H, *J* = 8.8 Hz), 8.54 (d, 1H, *J* = 8.0 Hz), 8.43 (dd, 1H, *J* = 8.8, 0.8 Hz), 7.67-7.57 (m, 2H), 7.25 (dd, 1H, *J* = 8.0, 2.8 Hz), 7.19 (d, 2H, *J* = 8.8 Hz), 7.06 (d, 2H, *J* = 8.8 Hz),

6.80 (d, 1H, *J* = 2.8 Hz), 3.89 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.0, 158.3, 144.4, 138.0, 134.7, 134.0, 131.5, 131.0, 130.5, 127.5, 127.0, 124.6, 124.1, 122.1, 116.8, 113.9, 109.7, 108.0, 55.3, 55.2; HRMS calcd. for $C_{22}H_{17}IO_2$: 440.0273, found 440.0279.

Spectral data for 2-(10-iodo-7-methoxy phenathren-9-yl)-furan (**9d**).

IR (neat, cm^{-1}): 3072, 3020, 2929, 1597, 1440, 1250; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.55 (d, 1H, *J* = 6.0 Hz), 8.50 (d, 1H, *J* = 5.6 Hz), 8.38 (d, 1H, *J* = 5.6 Hz), 7.65 (t, 2H, *J* = 5.6 Hz), 7.58 (t, 1H, *J* = 5.6 Hz), 7.27 (d, 1H, *J* = 5.6 Hz), 6.89 (d, 1H, *J* = 5.6 Hz), 6.64 (t, 1H, *J* = 6.0 Hz), 6.55 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.4, 155.1, 141.9, 135.0, 134.8, 134.0, 131.0, 130.9, 128.2, 126.9, 124.4, 124.0, 122.0, 117.2, 110.6, 110.6, 109.9, 108.0, 55.1; HRMS calcd. for $C_{19}H_{13}IO_2$: 399.9960, found: 399.9957.

Spectral data for 2-(10-iodo-7-methoxy phenathren-9-yl)-thiophene (**9e**).

IR (neat, cm^{-1}): 3070, 3012, 2895, 1602, 1245; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, 1H, *J* = 9.2 Hz), 8.49 (d, 1H, *J* = 8.0 Hz), 8.41 (d, 1H, *J* = 8.0 Hz), 7.64 (t, 1H, *J* = 7.2 Hz), 7.58 (t, 1H, *J* = 7.2 Hz), 7.53 (d, 1H, *J* = 4.0 Hz), 7.28-7.22 (m, 2H), 7.06 (d, 1H, *J* = 4.0 Hz), 6.98 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.5, 146.3, 137.4, 134.9, 134.3, 131.3, 130.8, 128.4, 128.0, 127.0, 126.9, 126.2, 124.4, 124.0, 122.1, 117.2, 110.8, 109.4, 55.1; HRMS calcd. for $C_{19}H_{13}IOS$: 415.9732, found 415.9729.

Spectral data for 2-(10-iodo-7-methoxy phenathren-9-yl)-benofuran (**9f**).

IR (neat, cm^{-1}): 3085, 3015, 2975, 1604, 1501, 1249; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, 1H, *J* = 7.6 Hz), 8.52 (d, 1H, *J* = 8.0 Hz), 8.41 (d, 1H, *J* = 8.8 Hz), 7.74 (d, 1H, *J* = 7.2 Hz), 7.68 (t, 1H, *J* = 6.8 Hz), 7.64-7.58 (m, 2H), 7.41-7.33 (m, 2H), 7.25

(d, 1H, *J* = 8.8 Hz), 6.98 (s, 1H), 6.94 (s, 1H), 3.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.6, 157.2, 154.7, 135.0, 134.7, 133.5, 133.1, 131.0, 128.5, 128.3, 127.1, 124.5, 124.2, 123.0, 122.1, 121.3, 117.3, 111.5, 109.8, 109.7, 108.2, 107.8, 55.2; HRMS calcd for $C_{23}H_{15}IO_2$: 450.0117, found 450.0113.

Spectral data for 2-(10-iodo-7-methoxy phenathren-9-yl)-benzothiophene (**9g**).

IR (neat, cm^{-1}): 3059, 2971, 1556, 1244; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64 (d, 1H, *J* = 9.2 Hz), 8.59 (d, 1H, *J* = 8.0 Hz), 8.43 (d, 1H, *J* = 8.4 Hz), 7.99 (d, 1H, *J* = 7.2 Hz), 7.70 (t, 1H, *J* = 7.2 Hz), 7.63 (t, 1H, *J* = 7.2 Hz), 7.43 (s, 1H), 7.39 (t, 1H, *J* = 8.0 Hz), 7.32-7.22 (m, 3H), 6.79 (s, 1H), 3.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.5, 140.5, 139.8, 138.6, 138.3, 134.7, 133.8, 131.5, 130.8, 127.8 (x 2), 127.0, 125.9, 124.6, 124.3, 124.2, 123.1, 122.7, 122.2, 117.0, 109.2, 108.7, 55.1; HRMS calcd. for $C_{23}H_{15}IOS$: 465.9888, found 465.9885.

Spectral data for 10-hexyl-9-iodo-2-methoxyphenanthrene (**9h**).

IR (neat, cm^{-1}): 3059, 2971, 2895, 1556, 1243; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.58 (d, 1H, *J* = 9.2 Hz), 8.46 (d, 1H, *J* = 6 Hz), 8.38 (d, 1H, *J* = 6 Hz), 7.52-7.58 (m, 2H), 7.48 (d, 1H, *J* = 2.4 Hz), 7.28 (dd, 1H, *J* = 9.2, 2.4 Hz), 3.96 (s, 3H), 3.40-3.44 (m, 2H), 1.65-1.80 (m, 2H), 1.57-1.61 (m, 2H), 1.38-1.43 (m, 4H), 0.93 (t, 3H, *J* = 6.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.6, 141.4, 134.4, 132.1, 131.8, 130.2, 126.8, 126.7, 124.8, 124.7, 122.0, 116.3, 108.2, 107.2, 55.3, 40.5, 31.6, 29.7, 28.9, 22.7, 14.1; HRMS calcd. for $C_{21}H_{23}IO$: 418.0794, found 418.0791.

Spectral data for 9-iodo-2,7-dimethoxy-10-phenylphenanthrene (**9i**).

IR (neat, cm^{-1}): 3066, 3015, 1556, 1248; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.43-8.49 (m, 2H), 7.85 (d, 1H, *J* = 2.4 Hz), 7.43-7.49 (m, 3H), 7.25-7.29 (m, 4H), 6.72 (d, 1H, *J* = 2.8 Hz), 3.99 (s, 3H), 3.66 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.8, 157.5, 145.6, 145.2, 132.8, 132.5, 129.8, 128.5, 127.8, 124.9, 124.8, 123.9, 123.6, 117.9, 117.1,

115.4, 109.6, 106.6, 55.5, 55.1; HRMS calcd. for $C_{22}H_{17}IO_2$: 440.0273, found 440.0277.

Spectral data for 9-iodo-2,7-dimethoxy-10-(4-methoxyphenyl)phenanthrene (**9j**).

IR (neat, cm^{-1}): 3069, 3020, 1612, 1250; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.44-8.50 (m, 2H), 7.85 (d, 1H, *J* = 2.4 Hz), 7.22-7.26 (m, 2H), 7.18 (d, 2H, *J* = 8.4 Hz), 7.06 (d, 2H, *J* = 8.4 Hz), 6.78 (d, 1H, *J* = 2.4 Hz), 3.99 (s, 3H), 3.92 (s, 3H), 3.68 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.9, 158.6, 157.4, 144.8, 138.0, 132.8, 132.7, 130.9, 124.7, 123.8, 123.5, 117.7, 116.9, 115.4, 113.7, 109.5, 107.5, 55.3, 55.2, 55.0 (one peak mearged); HRMS calcd. for $C_{23}H_{19}IO_3$: 470.0379, found 470.0382.

Spectral data for 2-(10-iodo-2, 7-methoxy phenathren-9-yl)-furan (**9k**)

IR (neat, cm^{-1}): 3102, 3014, 2954, 1580, 1250; ^1H NMR (400 MHz,$CDCl_3$): δ 8.49-8.44 (m, 2H), 7.81 (s, 1H), 7.64 (s, 1H), 7.31-7.28 (m, 2H), 6.87 (d, 1H, *J* = 2.8 Hz), 6.63 (dd, 1H, *J* = 3.2, 1.6 Hz), 6.53 (d, 1H, *J* = 2.8 Hz), 3.99 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.7, 157.8, 155.3, 142.0, 135.6, 133.0, 132.6, 125.4, 124.7, 124.0, 123.6, 118.8, 117.6, 115.6, 110.6, 109.3, 108.0, 103.3, 55.5, 55.2; HRMS calcd. for $C_{20}H_{15}IO_3$: 430.0066, found 430.0062.

Spectral data for 2-(10-iodo-2, 7-methoxy phenathren-9-yl)-thiophene (**9l**).

IR (neat, cm^{-1}): 3096, 3016, 2975, 1574, 1435; ^1H NMR (400 MHz, $CDCl_3$): δ 8.47-8.42 (m, 2H), 7.82 (s, 1H), 7.52 (d, 1H, *J* = 5.2 Hz), 7.29-7.20 (m, 3H), 7.03 (t, 1H, *J* = 4.0 Hz), 6.94 (d, 1H, *J* = 2.8 Hz), 3.99 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.7, 157.7, 146.5, 137.9, 133.2, 132.8, 128.3, 126.9, 126.2, 125.2, 124.6, 123.9, 123.5, 118.5, 117.4, 116.0, 115.7, 109.3, 55.5, 55.1; HRMS calcd for $C_{20}H_{15}IO_2S$: 445.9837, found 445.9834.

Spectral data for 9-hexyl-10-iodo-2,7-dimethoxyphenanthrene (**9m**).

IR (neat, cm^{-1}): 3096, 3016, 2895, 1574, 1239, ^1H NMR ($CDCl_3$, 400 MHz): δ 8.45 (d, 1H, *J* = 9.2 Hz), 8.35 (d, 1H, *J* = 9.2 Hz), 7.81 (d, 1H, *J* = 2.0 Hz), 7.44 (d, 1H, *J* = 2.8 Hz), 7.26 (dd, 1H, *J* = 9.2, 2.0 Hz), 7.18 (dd, 1H, *J* = 9.0. 2.8 Hz), 3.98 (s, 3H), 3.94 (s, 3H), 3.39 (t, 2H, *J* = 8.0 Hz), 1.74-1.67 (m, 2H), 1.60-1.55 (m, 2H), 1.45-1.38 (m, 4H), 0.93 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.4, 157.7, 141.8, 133.1, 130.8, 127.2, 124.3, 124.1, 13.7, 116.9, 116.4, 115.4, 106.9, 103.8, 55.3, 55.2, 40.6, 31.6, 29.7, 28.8, 22.7, 14.1; HRMS calcd. for $C_{22}H_{25}IO_2$: 448.0899, found 448.0896.

Spectral data for 9-iodo-2,7-dimethoxy-10-(4-methoxy phenyl)-phenanthrene (**9n**).
IR (neat, cm^{-1}): 3084, 3027, 2922, 1597, 1246; ^1H NMR (400 MHz, $CDCl_3$): δ 8.51 (d, 1H, *J* = 9.2 Hz), 8.32 (d, 1H, *J* = 9.2 Hz), 7.93 (s, 1H), 7.25-7.16 (m, 4H), 7.05 (d, 2H, *J* = 8.8 Hz), 6.78 (s, 1H), 4.02 (s, 3H), 3.91 (s, 3H), 3.68 (s, 3H); ^{13}C NMR (100 MHz): 159.0 (x 2), 158.3, 138.0, 136.6, 134.2, 131.6, 131.2 (x 2), 126.2, 124.1, 116.4 (x 2), 113.8 (x 2), 109.7, 103.5, 55.5, 55.2, 55.1, 29.6; HRMS calcd for $C_{23}H_{19}IO_3$: 470.0379, found 470.0375.

Spectral data for 9-iodo-2-methoxy-10-(4'-methoxybiphenyl-2-yl)phenanthrene (**10a**).
IR (neat, cm^{-1}): 3120, 3027, 2922, 1597, 1249; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.53 (d, 1H, *J* = 9.2 Hz), 8.48 (d, 1H, *J* = 8.4 Hz), 8.32 (d, 1H, *J* = 8.4 Hz), 7.47-7.60 (m, 5H), 7.19-7.25 (m, 2H), 7.12 (d, 2H, *J* = 6.8 Hz), 6.83 (d, 1H, *J* = 2.8 Hz), 6.51 (d, 2H, *J* = 6.8 Hz), 3.69 (s, 3H), 3.56 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.3, 144.3, 143.1, 140.9, 134.4, 133.9, 133.2, 131.2, 130.4, 129.8, 128.5, 127.4, 127.2, 126.8, 124.4, 124.2, 122.1, 116.9, 113.1, 109.5, 108.7, 55.2, 54.9 (three peaks merged); HRMS calcd. for $C_{28}H_{21}IO_2$: 516.0586, found 516.0585.

Spectral data for 9-(4,4'-dimethoxybiphenyl-2-yl)-10-iodo-2,7-dimethoxy-

phenanthrene (**10b**).

IR (neat, cm^{-1}): 3115, 3030, 2945, 1605, 1250; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.37-8.42 (m, 2H), 7.76 (d, 1H, *J* = 2.8 Hz), 7.43 (d, 1H, *J* = 8.8 Hz), 7.17-7.23 (m, 2H), 7.06-7.11 (m, 3H), 6.86 (d, 1H, *J* = 2.4 Hz), 6.78 (d, 1H, *J* = 2.4 Hz), 6.50 (d, 2H, *J* = 8.8 Hz), 3.95 (s, 3H), 3.84 (s, 3H), 3.70 (s, 3H), 3.56 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.6, 158.0, 157.6, 144.7, 144.2, 133.6, 132.9, 133.8, 132.6, 131.5, 129.9, 124.6, 123.9, 123.6, 117.8, 117.2, 116.0, 114.6, 113.1, 109.5, 108.0, 55.4, 55.2, 55.2, 54.9 (three peaks merged); HRMS calcd. for $C_{30}H_{25}IO_4$: 576.0798, found 576.0795.

Spectral data for 2,10-difluorodibenzo[*g*,*p*]chrysene (**11b**).

IR (neat, cm^{-1}): 3120, 3025, 2937, 1605, 1208; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.56-8.60 (m, 2H), 8.50-8.54 (m, 4H), 8.23 (dd, 2H, *J* = 9.6, 2.4 Hz), 7.54-7.65 (m, 4H), 7.33-7.38 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.4 (d, J_{CF} = 242.8 Hz), 130.4, 130.3, 128.5, 128.2, 127.6, 127.4, 127.0, 126.5, 125.8, 125.7, 115.2 (d, J_{CF} = 22.9 Hz), 113.8 (d, J_{CF} = 22.9 Hz); HRMS calcd. for $C_{26}H_{14}F_2$: 364.1064, found 364.1068.

Spectral data for 1,3,9,11-tetramethoxydibenzo[*g*,*p*]chrysene (**11c**).

IR (neat, cm^{-1}): 3117, 3027, 2945, 1605, 1245; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.45 (d, 2H, *J* = 3.6 Hz), 7.78 (dd, 2H, *J* = 8.0, 1.2 Hz), 7.71 (d, 2H, *J* = 2.4 Hz), 7.42-7.48 (m, 4H), 6.76 (d, 2H, *J* = 2.4 Hz), 4.06 (s, 6H), 3.76 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.1, 157.4, 133.5, 131.3, 130.7, 128.7, 126.8, 125.3, 125.1, 122.8, 114.2, 98.6, 97.7, 55.6, 55.0; HRMS calcd for $C_{30}H_{24}O_4$: 448.1675, found 448.1669.

Spectral data for 1,2,3,9,10,11-hexamethoxydibenzo[*g*,*p*]chrysene (**11d**).

IR (neat, cm^{-1}): 3122, 3034, 2945, 1615, 1245; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.42 (d, 2H, *J* = 8.0 Hz), 7.96 (d, 2H, *J* = 8.0 Hz), 7.91 (s, 2H), 7.43-7.53 (m, 4H), 4.15 (s, 6H),

4.09 (s, 6H), 3.26 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.6, 150.4, 142.1, 130.8, 130.0, 128.9, 128.1, 126.8, 125.8, 125.3, 122.1, 117.3, 101.2, 61.6, 60.4, 56.1; HRMS calcd. for $C_{32}H_{28}O_6$: 508.1886, found 508.1881.

Spectral data for 2,7,10,15-tetramethoxydibenzo[*g*,*p*]chrysene (**11e**).

IR (neat, cm^{-1}): 3120, 3035, 2945, 1617, 1249;^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.44 (d, 4H, *J* = 8.8 Hz), 8.19 (d, 4H, *J* = 2.4 Hz), 7.23 (dd, 4H, *J* = 8.8, 2.4 Hz), 3.90 (s, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.4, 129.6, 128.4, 124.9, 124.6, 116.0, 110.1, 55.4; HRMS calcd. for $C_{30}H_{24}O_4$: 448.1675, found 488.1663.

Spectral data for spiro compound (**12**).

Mp. 223.1-224.9 ^{o}C; IR (neat, cm^{-1}): 3125, 3060, 3010, 1677, 1610, 1515, 1242; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.53 (d, 1H, *J* = 9.2 Hz), 8.44 (d, 1H, *J* = 8.8 Hz), 8.08 (d, 1H, *J* = 2.4 Hz), 7.84 (d, 1H, *J* = 2.0 Hz), 7.31 (dd, 1H, *J* = 9.2, 2.4 Hz), 7.20-7.16 (m, 3H), 6.90 (dd, 1H, *J* = 8.8, 2.0 Hz) 6.64 (d, 2H, *J* = 10.0 Hz), 6.55 (d, 2H, *J* = 10.0 Hz), 4.02 (s, 3H), 3.91 (s, 3H), 3.72 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.2, 160.5, 157.9, 157.8, 151.9, 144.0, 138.7, 135.6, 133.0, 129.8, 128.9, 128.4, 126.0, 125.1, 124.9, 124.6, 124.3, 117.9, 116.7, 111.6, 110.6, 105.8, 103.6, 56.8, 55.6, 55.4, 55.1; HRMS calcd. for $C_{29}H_{22}O_4$: 434.1518, found 434.1516.

(3) Crystallographic data for compounds 6j.

(a) ORTEP drawing for spiro **6j**

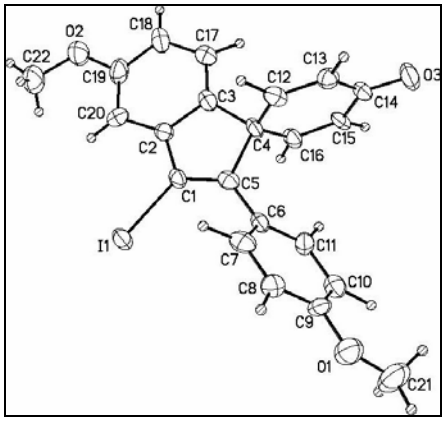


Table 1. Crystal data and structure refinement for compound **6j.**

Empirical formula	C22 H17 I O3	
Formula weight	456.26	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*P*2(1)/n	
Unit cell dimensions	a = 10.8190(7) Å	α= 90°.
	b = 9.8363(7) Å	β= 92.424(2)°.
	c = 18.3221(12) Å	γ = 90°.
Volume	1948.1(2) $Å^3$	
Z	4	
Density (calculated)	1.556 Mg/m^3	
Absorption coefficient	1.661 mm^{-1}	
F(000)	904	
Theta range for data collection	2.15 to 28.32°.	
Index ranges	-13<=h<=14, -13<=k<=11, -22<=l<=24	
Reflections collected	14200	
Independent reflections	4836 [R(int) = 0.1129]	
Completeness to theta = 28.32°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4836 / 0 / 235	
Goodness-of-fit on F^2	0.520	
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0564	
R indices (all data)	R1 = 0.1659, wR2 = 0.0685	
Largest diff. peak and hole	0.567 and -0.291 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **6j**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	8418(1)	3162(1)	854(1)	57(1)
O(1)	14427(4)	1848(5)	1228(2)	77(1)
O(2)	4811(4)	3404(5)	-1568(2)	83(1)
O(3)	12553(3)	838(4)	-2692(2)	76(1)
C(1)	8862(5)	2723(5)	-225(2)	43(2)
C(2)	7948(5)	2795(5)	-813(3)	42(1)
C(3)	8502(5)	2419(5)	-1462(3)	52(2)
C(4)	9873(5)	2061(6)	-1285(2)	45(2)
C(5)	9970(5)	2308(5)	-437(3)	43(2)
C(6)	11150(5)	2136(6)	-11(3)	41(2)
C(7)	11622(5)	3252(6)	402(3)	55(2)
C(8)	12728(5)	3124(7)	817(3)	58(2)
C(9)	13339(5)	1874(7)	808(3)	55(1)
C(10)	12903(6)	747(6)	409(3)	56(2)
C(11)	11788(5)	916(6)	-18(3)	55(2)
C(12)	10702(4)	3075(6)	-1645(2)	51(2)
C(13)	11572(5)	2649(6)	-2118(3)	49(2)
C(14)	11733(5)	1204(6)	-2280(3)	48(2)
C(15)	10921(5)	199(5)	-1949(2)	51(2)
C(16)	10079(5)	583(6)	-1475(2)	49(2)
C(17)	7844(6)	2381(6)	-2118(3)	62(2)
C(18)	6579(6)	2740(6)	-2143(3)	75(2)
C(19)	6060(5)	3097(7)	-1482(3)	65(2)
C(20)	6690(5)	3147(6)	-803(3)	51(1)
C(21)	15094(5)	607(7)	1300(3)	109(3)
C(22)	4183(5)	3863(6)	-949(3)	93(2)

Table 3. Bond lengths [Å] and angles [°] for product **6j**.

I(1)-C(1)	2.098(4)	C(18)-C(19)	1.401(6)
O(1)-C(9)	1.379(6)	C(18)-H(18)	1.1718
O(1)-C(21)	1.421(6)	C(19)-C(20)	1.393(6)
O(2)-C(19)	1.387(5)	C(20)-H(20)	0.8922
O(2)-C(22)	1.419(5)	C(21)-H(21A)	0.9600
O(3)-C(14)	1.242(5)	C(21)-H(21B)	0.9600
C(1)-C(5)	1.340(6)	C(21)-H(21C)	0.9600
C(1)-C(2)	1.432(6)	C(22)-H(22A)	0.9600
C(2)-C(20)	1.405(6)	C(22)-H(22B)	0.9600
C(2)-C(3)	1.403(6)	C(22)-H(22C)	0.9600
C(3)-C(17)	1.372(6)	C(9)-O(1)-C(21)	119.1(5)
C(3)-C(4)	1.545(6)	C(19)-O(2)-C(22)	118.4(4)
C(4)-C(12)	1.512(6)	C(5)-C(1)-C(2)	113.2(4)
C(4)-C(16)	1.514(7)	C(5)-C(1)-I(1)	125.4(4)
C(4)-C(5)	1.570(6)	C(2)-C(1)-I(1)	121.4(4)
C(5)-C(6)	1.478(6)	C(20)-C(2)-C(3)	121.5(5)
C(6)-C(11)	1.385(7)	C(20)-C(2)-C(1)	129.9(5)
C(6)-C(7)	1.417(7)	C(3)-C(2)-C(1)	108.6(5)
C(7)-C(8)	1.396(6)	C(17)-C(3)-C(2)	121.7(5)
C(7)-H(7)	1.0819	C(17)-C(3)-C(4)	129.4(5)
C(8)-C(9)	1.397(7)	C(2)-C(3)-C(4)	108.8(5)
C(8)-H(8)	1.0236	C(12)-C(4)-C(16)	115.9(4)
C(9)-C(10)	1.399(7)	C(12)-C(4)-C(3)	109.9(4)
C(10)-C(11)	1.419(6)	C(16)-C(4)-C(3)	108.7(4)
C(10)-H(10)	1.0387	C(12)-C(4)-C(5)	108.3(4)
C(11)-H(11)	1.0223	C(16)-C(4)-C(5)	111.8(4)
C(12)-C(13)	1.371(6)	C(3)-C(4)-C(5)	101.3(4)
C(12)-H(12)	1.1517	C(1)-C(5)-C(6)	130.2(5)
C(13)-C(14)	1.463(6)	C(1)-C(5)-C(4)	108.1(4)
C(13)-H(13)	0.9680	C(6)-C(5)-C(4)	121.7(4)
C(14)-C(15)	1.470(6)	C(11)-C(6)-C(7)	120.5(5)
C(15)-C(16)	1.340(6)	C(11)-C(6)-C(5)	120.9(5)
C(15)-H(15)	1.1812	C(7)-C(6)-C(5)	118.5(5)
C(16)-H(16)	0.9741	C(8)-C(7)-C(6)	120.2(6)
C(17)-C(18)	1.412(6)	C(8)-C(7)-H(7)	121.9
C(17)-H(17)	1.0450	C(6)-C(7)-H(7)	117.7

C(7)-C(8)-C(9)	117.9(6)	C(19)-C(20)-H(20)	119.5
C(7)-C(8)-H(8)	126.9	O(1)-C(21)-H(21A)	109.5
C(9)-C(8)-H(8)	114.6	O(1)-C(21)-H(21B)	109.5
O(1)-C(9)-C(10)	122.5(6)	H(21A)-C(21)-H(21B)	109.5
O(1)-C(9)-C(8)	113.8(6)	O(1)-C(21)-H(21C)	109.5
C(10)-C(9)-C(8)	123.7(5)	H(21A)-C(21)-H(21C)	109.5
C(9)-C(10)-C(11)	117.1(5)	H(21B)-C(21)-H(21C)	109.5
C(9)-C(10)-H(10)	108.0	O(2)-C(22)-H(22A)	109.5
C(11)-C(10)-H(10)	134.3	O(2)-C(22)-H(22B)	109.5
C(6)-C(11)-C(10)	120.6(5)	H(22A)-C(22)-H(22B)	109.5
C(6)-C(11)-H(11)	121.1	O(2)-C(22)-H(22C)	109.5
C(10)-C(11)-H(11)	117.9	H(22A)-C(22)-H(22C)	109.5
C(13)-C(12)-C(4)	120.7(5)	H(22B)-C(22)-H(22C)	109.5
C(13)-C(12)-H(12)	124.9		
C(4)-C(12)-H(12)	113.2	Symmetry transformations used to generate equivalent atoms:	
C(12)-C(13)-C(14)	121.1(5)		
C(12)-C(13)-H(13)	120.6		
C(14)-C(13)-H(13)	118.3		
O(3)-C(14)-C(13)	120.0(5)		
O(3)-C(14)-C(15)	120.6(6)		
C(13)-C(14)-C(15)	119.4(5)		
C(16)-C(15)-C(14)	120.8(5)		
C(16)-C(15)-H(15)	118.5		
C(14)-C(15)-H(15)	120.6		
C(15)-C(16)-C(4)	122.0(5)		
C(15)-C(16)-H(16)	121.2		
C(4)-C(16)-H(16)	116.7		
C(3)-C(17)-C(18)	119.1(5)		
C(3)-C(17)-H(17)	116.3		
C(18)-C(17)-H(17)	119.9		
C(17)-C(18)-C(19)	117.3(5)		
C(17)-C(18)-H(18)	121.7		
C(19)-C(18)-H(18)	118.9		
O(2)-C(19)-C(20)	122.1(5)		
O(2)-C(19)-C(18)	112.4(5)		
C(20)-C(19)-C(18)	125.5(5)		
C(2)-C(20)-C(19)	114.7(5)		
C(2)-C(20)-H(20)	124.7		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **6j**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ... \quad + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	72(1)	58(1)	41(1)	-1(1)	18(1)	10(1)
O(1)	81(3)	76(3)	74(3)	-8(3)	-13(2)	12(3)
O(2)	65(3)	122(4)	63(3)	-8(3)	1(2)	24(3)
O(3)	78(3)	79(3)	73(3)	5(2)	43(2)	16(2)
C(1)	59(4)	33(4)	38(3)	-4(2)	13(3)	7(3)
C(2)	52(4)	36(4)	37(3)	0(3)	3(3)	4(3)
C(3)	50(4)	63(4)	43(4)	-2(3)	13(3)	4(3)
C(4)	47(4)	58(5)	32(3)	-9(3)	12(3)	6(4)
C(5)	58(4)	34(4)	39(3)	4(2)	8(3)	-6(3)
C(6)	47(4)	42(5)	35(3)	-1(3)	13(3)	2(3)
C(7)	73(4)	49(4)	45(3)	10(4)	10(3)	-13(4)
C(8)	64(4)	57(4)	52(4)	4(4)	3(3)	7(5)
C(9)	42(4)	81(5)	42(3)	15(5)	-7(3)	7(5)
C(10)	56(5)	61(5)	52(4)	0(4)	11(3)	0(4)
C(11)	51(4)	58(5)	56(4)	5(3)	13(3)	12(4)
C(12)	51(4)	65(4)	38(3)	2(4)	1(3)	-11(4)
C(13)	48(4)	47(5)	51(4)	5(3)	2(3)	0(3)
C(14)	49(4)	67(5)	29(3)	-1(3)	9(3)	6(4)
C(15)	62(4)	62(4)	30(3)	8(3)	18(3)	4(3)
C(16)	63(4)	48(4)	36(3)	-9(3)	10(3)	4(3)
C(17)	69(4)	77(5)	41(4)	-3(3)	2(3)	10(4)
C(18)	67(5)	91(6)	67(4)	-11(4)	18(4)	23(4)
C(19)	38(4)	81(5)	76(4)	-11(4)	2(4)	12(4)
C(20)	50(4)	51(3)	51(3)	7(4)	-11(3)	6(4)
C(21)	86(6)	131(8)	105(6)	-19(5)	-42(4)	29(6)
C(22)	58(4)	135(7)	87(5)	-17(4)	5(4)	21(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3}) for compound **6j.**

	x	y	z	U(eq)
H(21A)	15820	745	1611	163
H(21B)	15333	309	827	163
H(21C)	14579	-71	1510	163
H(22A)	3332	4036	-1087	140
H(22B)	4562	4685	-767	140
H(22C)	4231	3179	-576	140
H(20)	6264	3237	-400	500
H(18)	5920	2473	-2646	500
H(11)	11534	158	-376	500
H(15)	10972	-960	-2113	500
H(10)	13575	-7	449	500
H(12)	10385	4184	-1579	500
H(17)	8183	1735	-2516	500
H(8)	13091	3806	1190	500
H(7)	11052	4153	427	500
H(13)	12112	3298	-2341	500
H(16)	9587	-84	-1222	500