SUPPORTING INFORMATION

A Simple, Two-step, Site-Specific Preparation of Fluorinated Naphthalene and Phenanthrene Derivatives from Fluorobromo-substituted Alkenes

Yi Wang, Jianjun Xu, and Donald J. Burton*

Department of Chemistry, University of Iowa, Iowa City, Iowa 52242

donald-burton@uiowa.edu

Supporting Information Available: Experimental procedure for the synthesis of **4e-f**, **7a**, **7c**, **8b**, **8d-e**, **8g-8h**, **9-12**, **14-15**, **17-20** and their characterization by ^1H , ^{19}F , ^{13}C NMR and HRMS; Copies of ^1H , ^{19}F and ^{13}C NMR of compounds **4d-f**, **5e**, **7c**, **8a-8b**, **8d-8e**, **8g-8h**, **9-12**, **14-15**, **17**, and **19-20**; ORTEP Plots of **5e** and **20**; Complete X-ray crystallographic data of compound **5e** and **20** (CIFs). This material is available free of charge *via* the Internet at <http://pubs.acs.org>.

Table of Contents

General Procedures.....	S4
(<i>E</i>)-2-Fluoro-1-(naphthalene-1-yl)-oct-1-en-3-yne (4e).....	S4
(<i>E</i>)-2-Fluoro-1-(naphthalen-1-yl)-4-phenylbut-1-en-3-yne (4f).....	S5
General procedure for the preparation of 1-bromo-1-fluoroalkenes.....	S5
1-[(<i>Z</i>)-2-Bromo-2-fluorovinyl]-4-fluorobenzene and 1-[(<i>E</i>)-2-bromo-2-fluorovinyl]-4-fluorobenzene (7a).....	S6
1-[(<i>Z</i>)-2-Bromo-2-fluorovinyl]-3,5-difluorobenzene and 1-[(<i>E</i>)-2-bromo-2-fluorovinyl]-3,5-difluorobenzene (7c).....	S6
1-Pentyl-3,7-difluoronaphthalene (8b).....	S6
1-Pentyl-3-fluoro-7-(trifluoromethyl)naphthalene (8d).....	S6
1-Decyl-3-fluoro-7-(trifluoromethyl)naphthalene (8e).....	S7
1-Butyl-3, 6, 8-trifluoronaphthalene (8g).....	S7
1-Pentyl-3,6,8-trifluoronaphthalene (8h).....	S7
(<i>Z</i>)- and (<i>E</i>)-1-Bromo-1-fluoro-2-(3-trifluoromethyl)phenylethene (9).....	S7
(<i>Z</i>)- and (<i>E</i>)-1-Bromo-1-fluoro-2-(3-fluoro)phenylethene (10).....	S8
Mixture of 1-butyl-3-fluoro-6-(trifluoromethyl)naphthalene (11a) and 1-butyl-3-fluoro-8-(trifluoromethyl)naphthalene (11b).....	S8
Mixture of 1-butyl-3-fluoro-6-fluoronaphthalene (12a) and 1-butyl-3-fluoro-8-fluoronaphthalene (12b).....	S8
1,1-Diphenyl-2-fluorooct-1-en-3-yne (14).....	S8
2-Fluoro-4-butyl-1-phenyl-naphthalene (15).....	S9
1-Butyl-4-fluoronaphthalene (17).....	S9
2-[(<i>Z</i>)-2-Bromo-2-fluorovinyl]naphthalene and 2-[(<i>E</i>)-2-bromo-2-fluorovinyl]naphthalene (18).....	S9
2-Fluoro-4-butyl-phenanthrene (19).....	S10
2-Fluoro-4-decyl-phenanthrene (20).....	S10
Reference.....	S10
¹ H, ¹⁹ F and ¹³ C NMR spectra of 4d	S11
¹ H, ¹⁹ F and ¹³ C NMR spectra of 4e	S14
¹ H, ¹⁹ F and ¹³ C NMR spectra of 4f	S17

^1H , ^{19}F and ^{13}C NMR spectra of 5e	S20
^1H and ^{19}F NMR spectra of 7c	S23
^1H , ^{19}F and ^{13}C NMR spectra of 8a	S25
^1H , ^{19}F and ^{13}C NMR spectra of 8b	S28
^1H , ^{19}F and ^{13}C NMR spectra of 8d	S31
^1H , ^{19}F and ^{13}C NMR spectra of 8e	S34
^1H , ^{19}F and ^{13}C NMR spectra of 8g	S37
^1H , ^{19}F and ^{13}C NMR spectra of 8h	S40
^1H and ^{19}F NMR spectra of 9	S43
^1H and ^{19}F NMR spectra of 10	S45
^1H , ^{19}F and ^{13}C NMR spectra of 11a and 11b	S47
^1H and ^{19}F NMR spectra of 12a and 12b	S50
^1H , ^{19}F and ^{13}C NMR spectra of 14	S53
^1H , ^{19}F and ^{13}C NMR spectra of 15	S56
^1H , ^{19}F and ^{13}C NMR spectra of 17	S59
^1H , ^{19}F and ^{13}C NMR spectra of 19	S62
^1H , ^{19}F and ^{13}C NMR spectra of 20	S65
ORTEP Plots of 5e and 20	S68

General procedures. ^1H , ^{19}F and ^{13}C NMR spectra of the final products were recorded on a 300 MHz or 400 MHz spectrometer. Chemical shifts have been reported in ppm relative to internal tetramethylsilane and CFCl_3 respectively. Unless noted otherwise, CDCl_3 was used as the NMR lock solvent. Low Resolution Mass Spectra were obtained at 70 eV in the electron impact mode, using a DB-1 column (0.25 mm ID $\times$ 15 m). The reported fragment peaks correspond to the most abundant ions, in addition to the parent ion(s) and other ions that can be utilized to elucidate the structure. Pre-chromatography of the reaction mixture prior to MS analysis: 30 mL of the reaction mixture was dissolved in 2 mL acetone. The solution was filtered with a micro column packed with silica gel. The filtered solution was further diluted with acetone to the required concentration. High resolution mass spectra (HRMS) were obtained by the University of Iowa High Resolution Mass Spectrometry Facility. Column chromatography was carried out using silica gel (silica gel 60, particle size 0.063-0.200 mm, 70-230 mesh ASTM). Thin layer chromatography was carried out using 40 $\times$ 80 mm PolyGram Sil G/UV₂₅₄ plates. All melting points were obtained in a 1.2 mm capillary tube and were uncorrected. All solvents were stored in a brown bottles capped with rubber septa and sealed with copper wire and Para film. N-Methyl-2-pyrrolidinone (NMP) was dried over CaH_2 overnight, and then distilled at reduced pressure. Tetrahydrofuran (THF) was obtained by distillation from sodium benzophenone ketyl under N_2 atmosphere. $\text{PdCl}_2(\text{PPh}_3)_2$ was prepared by Negishi's procedure (King, A. O.; Negishi, E.; Villani, F. J., Jr.; Silveira, A., Jr. *J. Org. Chem.* **1978**, *43*, 358). CuI was purified by reported procedure (Kauffman, G. D.; Fang, L.Y. *Inorg. Synth.* **1983**, *22*, 101). All aldehydes were purchased from vendors and used without further purification. N_2 was used without further purification.

(E)-2-Fluoro-1-(naphthalene-1-yl)-oct-1-en-3-yne (4e) (not separated from the corresponding reduced products): A mixture of $\text{PdCl}_2(\text{PPh}_3)_2$ (0.028 g, 0.04 mmol), Et_3N (5 mL), 1-hexyne 0.123 g, 1.5 mmol) and CuI (0.002 g, 0.01 mmol) was reacted with 492 mg of a mixture of (Z)-1-bromo-1-fluoro-2-(naphthalene-1-yl)ethene **2** and the corresponding reduced products **3** (containing 1 mmol of **2**) for 63 h. After silica gel column chromatography (ethyl acetate: hexanes = 3:97, R_f = 0.33), 0.26 g of a mixture of **4e** and reduced products was obtained as a colorless oil (couldn't be completely separated). The weight percentage of **4e** was 86%, yield 89%. ^{19}F NMR (CDCl_3) of **4e**: δ -98.4 (dt, $^3J_{\text{FH}(\text{cis})}$ = 16.5 Hz, J = 5.1 Hz, 1 F) ppm; (Z)-reduced product: δ -123.8 (dd, $^2J_{\text{FH}}$ = 83.2 Hz, $^3J_{\text{FH}(\text{trans})}$ = 42.8 Hz) ppm; (E)-reduced product: δ -124.2

(dd, $^2J_{\text{FH}} = 86.3$ Hz, $^3J_{\text{FH(cis)}} = 16.3$ Hz) ppm; ^1H NMR of the **4e** (CDCl_3) δ 7.96-8.01 (m, 1 H), 7.92 (d, $J = 7.3$ Hz, 1 H), 7.84-7.87 (m, 1 H), 7.80 (d, $J = 8.1$ Hz, 1 H), 7.42-7.55 (m, 3 H), 7.12 (d, $^3J_{\text{HF(cis)}} = 15.4$ Hz, 1 H), 6.89 (dd, $^2J_{\text{HF}} = 83.3$ Hz, $^3J_{\text{HH}} = 5.5$ Hz), 6.30 (dd, $^3J_{\text{HF(trans)}} = 42.6$ Hz, $^3J_{\text{HH}} = 5.5$ Hz), 2.36 (td, $J = 6.9, 5.1$ Hz, 2 H), 1.45-1.52 (m, 2 H), 1.30-1.42 (m, 2 H), 0.88 (t, $J = 7.2$ Hz, 3 H) ppm; ^{13}C NMR (CDCl_3) of the **4e** and the reduced products: δ 148.8 (d, $^1J_{\text{CF}} = 269.7$ Hz), 142.7 (d, $^1J_{\text{CF}} = 234.3$ Hz), 133.5, 131.7, 131.6, 129.3 (d, $J = 8.8$ Hz), 128.6, 128.4, 128.1, 127.7, 127.6, 126.2, 125.15 (d, $J = 2.7$ Hz), 125.9, 125.7, 125.4, 125.2, 123.9, 123.8, 112.8 (d, $J = 33.2$ Hz), 107.6, 98.1 (d, $J = 5.0$ Hz), 72.5 (d, $J = 41.5$ Hz), 29.8, 21.8, 19.1 (d, $J = 2.4$ Hz), 13.5 ppm; GC-MS m/z (relative intensity) of **4e**: 254 ($\text{M}^+ + 2$, 1), 253 (19), 252 (M^+ , 98), 233 (4), 224 (5), 223 (27), 221 (29), 220 (34), 210 (41), 209 (99), 208 (56), 207 (99), 202 (29), 196 (93), 189 (48), 184 (37), 183 (100), 170 (15), 165 (12), 163 (12); the reduced products: 173 ($\text{M}^+ + 1$, 10), 172 (M^+ , 82), 171 (100), 170 (67), 153 (7), 152 (37), 151 (16), 150 (12), 139 (4), 126 (5), 125 (4), 99 (3), 98 (4), 87 (4), 86 (10), 85 (22), 76 (12), 75 (11), 63 (10); HRMS calcd 252.1314 for $\text{C}_{18}\text{H}_{17}\text{F}$, found 252.1309.

(E)-2-Fluoro-1-(naphthalen-1-yl)-4-phenylbut-1-en-3-yne (4f): A mixture of $\text{PdCl}_2(\text{PPh}_3)_2$ (0.14 g, 0.20 mmol), Et_3N (15 mL), phenylacetylene (1.256 g, 5.0 mmol), CuI (0.01 g, 0.05 mmol) was reacted with 2.46 g of a mixture of (*Z*)-1-bromo-1-fluoro-2-(naphthalen-1-yl)ethene **2** and the corresponding reduced products **3** (containing 5.0 mmol **2**) for 42 h. Silica gel column chromatography (ethyl acetate: hexanes = 3:97, $R_f = 0.39$) followed by recrystallization from hexanes/ether gave 0.92 g of a white solid (68% yield), mp: 69-71 °C; ^{19}F NMR (CDCl_3) δ -100.8 (d, $^3J_{\text{FH(cis)}} = 15.2$ Hz, 1 F) ppm; ^1H NMR (CDCl_3) δ 8.00 (dm, $J = 7.4$ Hz, 2 H), 7.80- 7.87 (m, 2 H), 7.46- 7.55 (m, 3 H), 7.37- 7.40 (m, 2 H), 7.24 – 7.33 (m, 4 H) ppm; ^{13}C NMR (CDCl_3) δ 142.3 (d, $^1J_{\text{CF}} = 235.5$ Hz), 133.5, 131.5, 129.3, 129.0 (d, $J = 8.6$ Hz), 128.7, 128.5, 128.3, 126.3, 125.9, 125.1, 123.6, 121.09, 121.06, 114.8, 114.4, 95.7 (d, $J = 6.0$ Hz), 81.0 (d, $J = 41.4$ Hz) ppm; GC-MS m/z (relative intensity) 273 ($\text{M}^+ + 1$, 9), 272 (M^+ , 45), 271 (45), 270 (100), 268 (23), 257 (32), 250 (21), 244 (9), 224 (5), 135 (42), 125 (12), 122 (25); HRMS calcd 272.1001 for $\text{C}_{20}\text{H}_{13}\text{F}$, found 272.0997.

General procedure for the preparation of 1-bromo-1-fluoroalkenes: A 50 mL dry three necked flask equipped with stirring bar, cold water condenser and N_2 tee was charged with 10 mL of freshly distilled THF, PPh_3 (5.24 g, 20 mmol), aldehyde (10 mmol) and finally CFBr_3 (14 mmol). The mixture was refluxed for about 6 h. When the reaction was completed, the mixture

was cooled to room temperature, poured into 100 mL of hexane and filtered. After the solvent of the filtrate was removed by rotary evaporation, the residue was subject to chromatography and pure product was obtained.

1-[(Z)-2-Bromo-2-fluorovinyl]-4-fluorobenzene and 1-[(E)-2-bromo-2-fluorovinyl]-4-fluorobenzene (7a)¹: Similarly, reaction of 4-fluorobenzaldehyde (2.14 mL, 20 mmol), CFBr₃ (2.4 mL, 24 mmol), PPh₃ (10.48 g, 40 mmol) and 20 mL of freshly distilled THF gave 1.65 g of a colorless oil (38% yield), *E/Z* = 49/51. ¹⁹F NMR (CDCl₃) δ -66.0 (d, ³*J*_{FH(cis)} = 15.2 Hz), -69.8 (dm, ³*J*_{FH(trans)} = 33.6 Hz), -112.9 (s, ArF), -113.2 (s, ArF) ppm; ¹H NMR (CDCl₃) δ 7.45-6.96 (m), 6.59 (d, ³*J*_{FH(cis)} = 15.0 Hz), 5.91 (d, ³*J*_{FH(trans)} = 32.5 Hz) ppm;

1-[(Z)-2-Bromo-2-fluorovinyl]-3,5-difluorobenzene and 1-[(E)-2-bromo-2-fluorovinyl]-3,5-difluorobenzene (7c): Similarly, the reaction of 3,5-difluorobenzaldehyde (0.71 g, 5 mmol), CFBr₃ (0.49 mL, 5 mmol), PPh₃ (2.62 g, 10 mmol) and 10 mL freshly distilled THF gave 0.68 g of colorless oil (65% yield), *E/Z* = 57/43. ¹⁹F NMR (CDCl₃) δ -62.2 (d, ³*J*_{FH(cis)} = 13.1 Hz), -64.5 (d, ³*J*_{FH(trans)} = 31.3 Hz), -109.9 (m, ArF) ppm; ¹H NMR (CDCl₃) δ 7.05 (m), 6.59 (d, ³*J*_{FH(cis)} = 14.5 Hz), 5.94 (d, ³*J*_{FH(trans)} = 31.2 Hz) ppm; HRMS calcd 237.9428 for C₈H₄⁸¹BrF₃, found 237.9427.

1-Pentyl-3,7-difluoronaphthalene (8b): Colorless oil; ¹⁹F NMR (CDCl₃) δ -115.8 (m, 1 F), -117.1 (m, 1 F) ppm; ¹H NMR (CDCl₃) δ 7.73 (dd, *J* = 9.0, 5.7 Hz, 1 H), 7.59 (dd, *J* = 11.1, 2.4 Hz, 1 H), 7.30-7.22 (m, 2 H), 7.13 (dd, *J* = 9.6, 2.4 Hz, 1 H), 2.96 (t, *J* = 7.8 Hz, 2 H), 1.75-1.70 (m, 2 H), 1.43-1.37 (m, 4 H), 0.91 (t, *J* = 7.1 Hz, 3 H) ppm; ¹³C NMR (CDCl₃) δ 160.2 (dd, *J* = 242.7, 2.8 Hz), 159.8 (dd, *J* = 243.1, 2.8 Hz), 141.7 (dd, *J* = 8.1, 5.8 Hz), 131.5 (dd, *J* = 9.4, 0.7 Hz), 130.2 (dd, *J* = 8.9, 5.6 Hz), 129.8 (dd, *J* = 8.3, 0.7 Hz), 116.9 (d, *J* = 4.7 Hz), 116.7 (d, *J* = 4.9 Hz), 109.0 (dd, *J* = 20.3, 0.8 Hz), 107.8 (dd, *J* = 21.4, 2.2 Hz), 32.9 (d, *J* = 1.4 Hz), 31.9, 29.9, 22.6, 14.0 ppm; HRMS calcd 234.1220 for C₁₅H₁₆F₂, found 234.1216.

1-Pentyl-3-fluoro-7-(trifluoromethyl)naphthalene (8d): Colorless oil; ¹⁹F NMR (CDCl₃) δ -62.5 (s, 3 F), -112.2 (t, *J* = 9.3 Hz, 1 F) ppm; ¹H NMR (CDCl₃) δ 8.35 (s, 1 H), 7.94 (d, *J* = 8.7 Hz, 1 H), 7.71 (d, *J* = 8.6 Hz, 1 H), 7.41 (dd, *J* = 9.3, 2.5 Hz, 1 H), 7.27 (dd, *J* = 9.4, 2.5 Hz, 1 H), 3.14 (t, *J* = 7.8 Hz, 2 H), 1.84-1.79 (m, 2 H), 1.50-1.44 (m, 4 H), 0.98 (t, *J* = 7.0 Hz, 3 H) ppm; ¹³C NMR (CDCl₃) δ 161.5 (d, *J* = 247.4 Hz), 143.8 (d, *J* = 8.8 Hz), 136.3 (d, *J* = 8.9 Hz), 129.2 (d, *J* = 5.6 Hz), 128.0, 126.8 (qd, *J* = 31.8, 2.5 Hz), 124.5 (q, *J* = 270.3 Hz), 122.2 (q, *J* = 2.6 Hz), 121.8 (dq, *J* = 4.5, 1.5 Hz), 117.3 (d, *J* = 25.0 Hz), 109.2 (d, *J* = 20.4 Hz), 32.6 (d, *J* = 1.5 Hz),

31.7, 30.1, 22.5, 14.0 ppm; GC-MS m/z (relative intensity): 43 (18), 159 (13), 170 (11), 201 (14), 227 (100), 228 (70), 284 (34); HRMS calcd 284.1188 for $C_{16}H_{16}F_4$, found 284.1190.

1-Decyl-3-fluoro-7-(trifluoromethyl)naphthalene (8e): Colorless oil; ^{19}F NMR ($CDCl_3$) δ -62.5 (s, 3 F), -112.2 (t, J = 9.4 Hz, 1 F) ppm; 1H NMR ($CDCl_3$) δ 8.36 (s, 1 H), 7.93 (d, J = 8.6 Hz, 1 H), 7.71 (dd, J = 8.7, 1.3 Hz, 1 H), 7.40 (dd, J = 9.3, 2.4 Hz, 1 H), 7.27 (dd, J = 9.6, 2.4 Hz, 1 H), 3.13 (t, J = 7.8 Hz, 2 H), 1.81 (m, 2 H), 1.52-1.34 (m, 14 H), 0.95 (t, J = 6.7 Hz, 3 H) ppm; ^{13}C NMR ($CDCl_3$) δ 161.5 (d, J = 297.3 Hz), 143.8 (d, J = 8.6 Hz), 136.2 (d, J = 10.0 Hz), 129.1 (d, J = 5.5 Hz), 128.0, 126.8 (qd, J = 31.8, 3.4 Hz), 124.5 (q, J = 270.3 Hz), 122.1 (q, J = 2.9 Hz), 121.7 (q, J = 2.2 Hz), 117.2 (d, J = 25.0 Hz), 109.2 (d, J = 20.3 Hz), 32.6 (d, J = 1.4 Hz), 31.9, 30.4, 29.58, 29.55, 29.49, 29.41, 29.3, 22.7, 14.1 ppm; HRMS calcd 354.1971 for $C_{21}H_{26}F_4$, found 354.1972.

1-Butyl-3, 6, 8-trifluoronaphthalene (8g): Colorless oil; ^{19}F NMR ($CDCl_3$) δ -107.9 (m, 1 F), -112.9 (q, J = 8.5 Hz, 1 F), -113.6 (td, J = 9.7, 3.0 Hz, 1 F) ppm; 1H NMR ($CDCl_3$) δ 7.24-7.17 (m, 2 H), 7.03 (dd, J = 9.7, 1.6 Hz, 1 H), 6.90 (ddd, J = 13.5, 8.6, 2.6 Hz, 1 H), 3.11 (td, J = 7.7, 4.0 Hz, 1 H), 1.69-1.63 (m, 2 H), 1.48-1.40 (m, 2 H), 0.96 (t, J = 7.2 Hz, 3 H) ppm; ^{13}C NMR ($CDCl_3$) δ 161.2 (dd, J = 246.9, 1.7 Hz), 160.8 (dd, J = 255.9, 13.0 Hz), 160.1 (dd, J = 246.2, 13.5 Hz), 142.5 (ddd, J = 8.6, 5.3, 1.4 Hz), 137.5 (td, J = 10.7, 6.8 Hz), 117.4 (ddd, J = 24.8, 2.6, 1.2 Hz), 116.8 (dm, J = 12.1 Hz), 108.8 (ddd, J = 21.1, 5.3, 3.6 Hz), 107.6 (dt, J = 20.4, 4.9 Hz), 101.8 (td, J = 28.0, 2.6 Hz), 36.0 (dd, J = 11.4, 1.1 Hz), 33.9 (d, J = 3.5 Hz), 22.7, 13.9 ppm; HRMS calcd 238.0969 for $C_{14}H_{13}F_3$, found 238.0968.

1-Pentyl-3,6,8-trifluoronaphthalene (8h): Colorless oil; ^{19}F NMR ($CDCl_3$) δ -108.0 (m, 1 F), -112.9 (q, J = 8.5 Hz, 1 F), -113.6 (td, J = 9.3, 3.3 Hz, 1 F) ppm; 1H NMR ($CDCl_3$) δ 7.25-7.18 (m, 2 H), 7.03 (dd, J = 9.5, 2.6 Hz, 1 H), 6.91 (ddd, J = 13.5, 8.8, 2.6 Hz, 1 H), 3.11 (td, J = 7.7, 3.9 Hz, 2 H), 1.71-1.63 (m, 2 H), 1.43-1.33 (m, 4 H), 0.91 (t, J = 7.1 Hz, 3 H) ppm; ^{13}C NMR ($CDCl_3$) δ 161.2 (dd, J = 247.0, 1.7 Hz), 160.8 (dd, J = 256.3, 13.4 Hz), 160.1 (dd, J = 246.3, 13.5 Hz), 142.5 (ddd, J = 6.7, 5.2, 1.7 Hz), 137.5 (td, J = 10.7, 6.7 Hz), 117.4 (ddd, J = 24.8, 2.6, 1.3 Hz), 116.8 (d, J = 12.3 Hz), 108.8 (ddd, J = 21.1, 5.3, 3.6 Hz), 107.6 (dt, J = 20.4, 4.9 Hz), 101.8 (td, J = 28.0, 2.6 Hz), 36.3 (dd, J = 11.4, 1.1 Hz), 31.8, 31.4 (d, J = 3.6 Hz), 22.5, 14.0 ppm; HRMS calcd 252.1126 for $C_{15}H_{15}F_3$, found 252.1126.

(Z)- and (E)-1-Bromo-1-fluoro-2-(3-trifluoromethyl)phenylethene (9): A round-bottomed flask was charged with stirring bar, PPh_3 (2.62 g, 10 mmol) and nitrogen tee. Freshly distilled

THF (15 mL), CFBr_3 (0.70 mL, 7 mmol) and $m\text{-CF}_3\text{C}_6\text{H}_4\text{CHO}$ (0.67 mL, 5 mmol) were added subsequently. After the mixture was refluxed for 6 h, it was cooled to room temperature and poured into 100 mL of hexane. The mixture was filtered through Celite 545[®] and the filtrate was concentrated by rotary evaporation. The residue was purified by column chromatography (100% hexanes as eluent) and 0.84 g of a colorless oil was obtained (62% yield), $Z/E = 48:52$. ^{19}F NMR (CDCl_3) δ -63.37 (s), -63.43 (s), -63.5 (d, $^3J_{\text{FH(cis)}} = 14.6$ Hz), -66.2 (d, $^3J_{\text{FH(trans)}} = 31.6$ Hz) ppm; ^1H NMR (CDCl_3) δ 7.73-7.46 (m), 6.69 (d, $^3J_{\text{FH(cis)}} = 14.4$ Hz), 6.04 (d, $^3J_{\text{FH(trans)}} = 32.0$ Hz) ppm; HRMS calcd 269.9490 for $\text{C}_9\text{H}_5^{81}\text{BrF}_4$, found 269.9492.

(Z)- and (E)-1-Bromo-1-fluoro-2-(3-fluoro)phenylethene (10): Colorless oil; ^{19}F NMR (CDCl_3) δ -111.0 (d, $^3J_{\text{cis(HF)}} = 13.6$ Hz), -108.6 (d, $^3J_{\text{trans(HF)}} = 26.5$ Hz), -62.0 (m) ppm; ^1H NMR (CDCl_3) δ 7.34-6.93 (m), 6.61 (d, $^3J_{\text{cis(HF)}} = 14.7$ Hz), 5.94 (d, $^3J_{\text{trans(HF)}} = 32.1$ Hz) ppm; HRMS calcd 219.9522 for $\text{C}_8\text{H}_5^{81}\text{BrF}_2$, found 219.9521.

Mixture of 1-butyl-3-fluoro-6-(trifluoromethyl)naphthalene (11a) and 1-butyl-3-fluoro-8-(trifluoromethyl)naphthalene (11b) (ratio of **11a:11b** = 20:1, determined by ^{19}F NMR): Colorless oil; ^{19}F NMR (CDCl_3) δ -54.3 (s, CF_3 in **11b**), -62.9 (s, CF_3 in **11a**), -113.6 (t, $J = 10.1$ Hz, ArF in **11a**), -116.2 (t, $J = 9.2$ Hz, ArF in **11b**) ppm; ^1H NMR of **11a** (CDCl_3) δ 8.12 (dm, $J = 8.4$ Hz, 1 H), 8.07 (s, 1 H), 7.61 (dd, $J = 8.8, 1.6$ Hz, 1 H), 7.39 (dd, $J = 9.2, 2.4$ Hz, 1 H), 7.23 (dd, $J = 9.6, 2.4$ Hz, 1 H), 3.08 (t, $J = 7.9$ Hz, 2 H), 1.77-1.69 (m, 2 H), 1.51-1.42 (m, 2 H), 0.98 (t, $J = 7.4$ Hz, 3 H) ppm; ^{13}C NMR of **11a** (CDCl_3) δ 160.8 (d, $J = 246.3$ Hz), 142.8 (d, $J = 8.4$ Hz), 133.8 (d, $J = 9.9$ Hz), 130.3, 128.4 (q, $J = 31.9$), 125.7 (m), 125.2 (d, $J = 1.3$ Hz), 124.2 (q, $J = 270.6$ Hz), 120.5 (m), 118.1 (d, $J = 24.9$ Hz), 110.0 (d, $J = 20.4$ Hz), 32.58 (d, $J = 1.5$ Hz), 32.56, 22.7, 13.9 ppm; HRMS calcd 270.1032 for $\text{C}_{15}\text{H}_{14}\text{F}_4$, found 270.1030.

Mixture of 1-butyl-3,6-difluoronaphthalene (12a) and 1-butyl-3,8-difluoronaphthalene (12b) (ratio of **12a:12b** = 1:1.5, determined by ^{19}F NMR): Colorless oil; ^{19}F NMR (CDCl_3) δ -112.9 (dm, $J = 13.8$ Hz, 8-F in **12b**), -114.3 (t, $J = 9.6$ Hz, 6-F in **12a**), -115.12 (t, $J = 9.2$ Hz, 3-F in **12b**), -115.13 (t, $J = 9.3$ Hz, 3-F in **12a**) ppm; ^1H NMR (CDCl_3) δ 7.99 (dd, $J = 9.2, 5.6$ Hz, ArH in **12a**), 7.53 (dd, $J = 8.2, 1.0$ Hz, ArH in **12b**), 7.40-7.19 (m), 7.09-7.04 (m), 3.15 (td, $J = 7.8, 3.6$ Hz, benzylic H in **12b**), 3.03 (t, $J = 7.9$ Hz, benzylic H in **12a**), 1.74-1.66 (m), 1.48-1.42 (m), 0.97 (t, $J = 7.4$ Hz, CH_3 in **12a**), 0.96 (t, $J = 7.4$ Hz, CH_3 in **12b**) ppm; HRMS calcd 220.1064 for $\text{C}_{14}\text{H}_{14}\text{F}_2$, found 220.1063.

1,1-Diphenyl-2-fluorooct-1-en-3-yne (14): Sonogashira reaction of 1-bromo-1-fluoro-2,2-

diphenylethene with *n*-hexyne: PdCl₂(PPh₃)₂ (50 mg, 0.07 mmol), CuI (40 mg, 0.21 mmol), 5 mL of CH₃CN and 0.45 g 1-bromo-1-fluoro-2,2-diphenylethene (1.62 mmol) were added to a round bottom flask. Then *n*-hexyne (0.23 mL, 2.01 mmol) and Et₃N (0.45 mL, 3.23 mmol) were added. The mixture was stirred at 50 °C for 12 h. Then it was cooled to room temperature and poured into 50 mL of hexane and filtered. After removal of solvent in filtrate, the residue was purified on silica gel (hexane as eluent) and 0.41 g of a yellow oil was obtained (yield: 91%). ¹⁹F NMR (CDCl₃) δ -104.9 (t, *J* = 5.4 Hz) ppm; ¹H NMR (CDCl₃) δ 7.39-7.24 (m, 10 H), 2.30 (td, *J* = 6.9, 5.0 Hz, 2 H), 1.48-1.22 (m, 4 H), 0.85 (t, *J* = 7.3 Hz, 3 H) ppm; ¹³C NMR (CDCl₃) δ 138.9 (d, *J* = 245.2 Hz), 137.7, 136.7(d, *J* = 3.3 Hz), 130.4 (d, *J* = 3.0 Hz), 129.93, 129.88, 128.0, 127.9, 127.7, 127.6, 97.6 (d, *J* = 6.2 Hz), 73.8 (d, *J* = 40.4 Hz), 29.9 (d, *J* = 1.8 Hz), 21.7, 19.1 (d, *J* = 2.2 Hz), 13.5 ppm; HRMS calcd 278.1471 for C₂₀H₁₉F, found 278.1473.

2-Fluoro-4-butyl-1-phenyl-naphthalene (15): A solution of 0.40 g enyne (1.44 mmol), 0.03 mL of DBU (0.20 mmol) in 4 mL NMP was heated at reflux temperature under N₂. After 3 h, the mixture was cooled to room temperature and poured onto silica gel (hexane as eluent) and 0.26 g of a colorless oil was afforded (yield: 65%). ¹⁹F NMR (CDCl₃) δ -116.9 (d, *J* = 9.9 Hz) ppm; ¹H NMR (CDCl₃) δ 8.07 (dm, *J* = 8.2 Hz, 1 H), 7.68 (dm, *J* = 8.3 Hz, 1 H), 7.51-7.40 (m, 7 H), 7.22 (d, *J* = 10.5 Hz, 1 H), 3.11 (t, *J* = 7.8 Hz, 2 H), 1.84-1.74 (m, 2 H), 1.57-1.44 (m, 2 H), 1.00 (t, *J* = 7.3 Hz, 3 H) ppm; ¹³C NMR (CDCl₃) δ 156.5 (d, *J* = 242.3 Hz), 141.5 (d, *J* = 8.8 Hz), 133.9, 133.8 (d, *J* = 7.5 Hz), 130.9 (d, *J* = 0.9 Hz), 129.1, 128.3, 127.6, 126.4 (d, *J* = 6.4 Hz), 124.6 (d, *J* = 2.4 Hz), 124.0 (d, *J* = 1.6 Hz), 121.9 (d, *J* = 5.1 Hz), 115.8 (d, *J* = 26.6 Hz), 32.7 (d, *J* = 1.4 Hz), 32.6, 22.8, 14.0 ppm; HRMS calcd 278.1471 for C₂₀H₁₉F, found 278.1468.

1-Butyl-4-fluoronaphthalene (17): Colorless oil; ¹⁹F NMR (CDCl₃) δ -126.8 (dd, *J* = 10.0, 6.6 Hz) ppm; ¹H NMR (CDCl₃) δ 8.13-7.99 (m, 2 H), 7.56-7.48 (m, 2 H), 7.19 (dd, *J* = 7.7, 5.6 Hz, 1 H), 7.03 (dd, *J* = 10.5, 7.8 Hz, 1 H), 3.00 (t, *J* = 7.7 Hz, 2 H), 1.74-1.64 (m, 2 H), 1.49-1.37 (m, 2 H), 0.96 (t, *J* = 7.2 Hz, 3 H) ppm; ¹³C NMR (CDCl₃) δ 157.4 (d, *J* = 247.7 Hz), 134.7 (d, *J* = 4.4 Hz), 132.9 (d, *J* = 4.2 Hz), 126.5, 125.6 (d, *J* = 1.9 Hz), 125.2 (d, *J* = 8.0 Hz), 123.98 (d, *J* = 15.9 Hz), 123.96 (d, *J* = 2.9 Hz), 121.1 (d, *J* = 5.7 Hz), 108.8 (d, *J* = 9.7 Hz), 33.0 (d, *J* = 0.9 Hz), 32.4, 22.8, 14.0 ppm; HRMS calcd 202.1158 for C₁₄H₁₅F, found 202.1161.

2-[(Z)-2-Bromo-2-fluorovinyl]naphthalene and 2-[(E)-2-bromo-2-fluorovinyl]naphthalene (18)¹: Similarly, the reaction of 2-naphthaldehyde (1.56 g, 10 mmol), CBrF₃ (1.20 mL, 12 mmol), PPh₃ (5.24 g, 20 mmol) and 10 mL of THF gave 1.05 g of a white solid (42% yield), *E/Z* = 47:53,

mp: 61-62 °C; ^{19}F NMR (CDCl_3) δ -65.2 (d, $^3J_{\text{FH(cis)}} = 15.3$ Hz), -67.9 (d, $^3J_{\text{FH(trans)}} = 32.3$ Hz) ppm; ^1H NMR (CDCl_3) δ 8.00 (s), 7.90-7.85 (m), 7.65 (dd, $J = 8.7, 2.0$ Hz), 7.61 (dd, $J = 8.7, 1.8$ Hz), 7.57-7.52 (m), 6.88 (d, $^3J_{\text{FH(cis)}} = 15.0$ Hz), 6.20 (d, $^3J_{\text{FH(trans)}} = 33.0$ Hz) ppm; ^{13}C NMR (CDCl_3) δ 135.2 (d, $J = 313.8$ Hz), 134.1 (d, $J = 329.3$ Hz), 133.3, 133.1, 132.8, 132.6 (d, $J = 1.8$ Hz), 130.0 (d, $J = 4.8$ Hz), 128.9 (d, $J = 8.1$ Hz), 128.3, 128.1, 128.03, 127.99, 127.8 (d, $J = 3.9$ Hz), 127.66, 127.60, 127.4 (d, $J = 7.2$ Hz), 126.4, 125.8 (d, $J = 2.5$ Hz), 125.6 (d, $J = 7.4$ Hz), 113.2 (d, $J = 6.0$ Hz), 111.8 (d, $J = 23.9$ Hz) ppm; HMRS calcd 249.9793 for $\text{C}_{12}\text{H}_8^{79}\text{BrF}$, found 249.9800.

2-Fluoro-4-butyl-phenanthrene (19): Colorless oil; ^{19}F NMR (CDCl_3) δ -117.2 (t, $J = 9.2$ Hz) ppm; ^1H NMR (CDCl_3) δ 8.67 (d, $J = 8.3$ Hz, 1 H), 7.89 (dd, $J = 7.6, 1.9$ Hz, 1 H), 7.71 (d, $J = 8.7$ Hz, 1 H), 7.62 (td, $J = 7.0, 1.9$ Hz, 1 H), 7.61 (d, $J = 8.7$ Hz, 1 H), 7.57 (td, $J = 7.0, 1.3$ Hz, 1 H), 7.38 (dd, $J = 8.7, 2.9$ Hz, 1 H), 7.27 (dd, $J = 9.9, 2.9$ Hz, 1 H), 3.42 (t, $J = 8.0$ Hz, 1 H), 1.95-1.85 (m, 2 H), 1.60-1.52 (m, 2 H), 1.03 (t, $J = 7.3$ Hz, 3 H) ppm; ^{13}C NMR (CDCl_3) δ 160.1 (d, $J = 244.5$ Hz), 143.6 (d, $J = 7.5$ Hz), 135.5 (d, $J = 8.8$ Hz), 133.0 (d, $J = 1.1$ Hz), 130.8, 128.9, 128.1, 127.5 (d, $J = 3.7$ Hz), 126.8, 126.3 (d, $J = 2.1$ Hz), 126.0, 125.7, 118.3 (d, $J = 22.5$ Hz), 111.3 (d, $J = 19.5$ Hz), 37.9 (d, $J = 1.1$ Hz), 32.6, 22.9, 14.0 ppm; HRMS calcd 252.1314 for $\text{C}_{18}\text{H}_{17}\text{F}$, found 252.1312.

2-Fluoro-4-decyl-phenanthrene (20): White solid, mp: 42-44 °C; ^{19}F NMR (CDCl_3): δ -117.2 (t, $J = 9.7$ Hz) ppm; ^1H NMR (CDCl_3): δ 8.69 (d, $J = 8.4$ Hz, 1 H), 7.91 (dd, $J = 7.7, 1.9$ Hz, 1 H), 7.72 (d, $J = 8.8$ Hz, 1 H), 7.65-7.59 (m, 3 H), 7.40 (dd, $J = 8.7, 2.9$ Hz, 1 H), 7.29 (dd, $J = 9.8, 2.4$ Hz, 1 H), 3.43 (t, $J = 8.1$ Hz, 2 H), 1.95-1.91 (m, 2 H), 1.58-1.54 (m, 2 H), 1.42-1.30 (m, 12 H), 0.91 (t, $J = 6.9$ Hz, 3 H) ppm; ^{13}C NMR (CDCl_3): δ 160.1 (d, $J = 244.5$ Hz), 143.6 (d, $J = 7.5$ Hz), 135.5 (d, $J = 8.8$ Hz), 132.9 (d, $J = 1.1$ Hz), 130.8, 128.9, 128.1, 127.5 (d, $J = 3.7$ Hz), 126.8, 126.3 (d, $J = 2.1$ Hz), 126.0, 125.7, 118.3 (d, $J = 22.5$ Hz), 111.3 (d, $J = 19.5$ Hz), 38.26, 38.25, 31.9, 30.5, 29.8, 29.6, 29.5, 29.3, 22.7, 14.1 ppm; HRMS calcd 336.2253 for $\text{C}_{24}\text{H}_{29}\text{F}$, found 336.2244.

Reference:

1. Lei, X.; Dutheuil, G.; Pannecouke, X.; Quirion, J.-C. *Org. Lett.* **2004**, 6, 2101-2104.

wangy1147

DRX-400

CDCl3

04-Dec-02

```

===== CHANNEL F1 =====
NUC1      13C
P1         7.25 usec
SFO1      100.6231927 MHz
===== CHANNEL F2 =====
NAME      wait216
NUC2      13C
P2         75.00 usec
SFO2      400.136006 MHz
===== Processing parameters =====
SI         100.6125216 MHz
SF         400.136006 MHz
WDW         EM
SSB         0
GB         0
PC         1.00
  
```

wangy1146

```

===== CHANNEL F1 =====
NUC1 13C
P1 7.15 usec
PL1 -2.00 dB
SFO1 100.621927 MHz

===== CHANNEL F2 =====
NAME waltz16
NUC2 1H
P2 0.00 usec
PL2 0.00 dB
PL12 21.00 dB
SFO2 400.118008 MHz

===== Processing parameters =====
SI 65536
SF 100.612773 MHz
RG 32768
WDW EM
SSB 0
GB 0
PC 1.00
  
```

wangyi133 drx400

```

===== CHANNEL F1 =====
NUC1 13C
P1 7.25 uSAC
PL1 -2.00 dB
SFO1 100.6231927 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 13C
P2 75.00 uSAC
PL2 0.00 dB
SFO2 400.1318006 MHz

F2 - Processing parameters
SI 65536
SF 100.612713 MHz
WDW RM
SSB 0
GB 0
PC 1.00
  
```

wangyi135 cdc13 drx400

```

PROBHD 5 mm Multinuc1
PULPROG zgpg30
TO 65516
SOLVENT CDCl3
NS 1800
DS 64
SM 26246.719 Hz
AQ 10.460431 N
F2 1.2485298 sec
RG 7298.2
DE 14.50 usec
TE 298.0 K
D1 0.75148922 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 17.00 usec
PL1 -2.00 dB
SFO1 100.6211927 MHz

===== CHANNEL f2 =====
NAME216
CPDPRG2 waltz16
NUC2 1H
P2 12.00 usec
PL2 0.00 dB
SFO2 400.1181006 MHz

F2 - Processing parameters
SI 65516
SF 100.6127718 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.00

```

wangyi223 drx400

```

NAME      8g
EXPNO     1
PROCNO    1
F2        26246.734 Hz
AQ         0.400493 Hz
RG         1.2485298 sec
RG         1.29872
RG         1.34500 usec
DE         4.50 usec
TE         298.0 K
D1         0.7518322 sec
D11        0.10000000 sec

===== CHANNEL F1 =====
NUC1       13C
P1         7.25 usec
PL1        -2.00 dB
SFO1       100.6211927 MHz

===== CHANNEL F2 =====
NAME2      waltz16
NUC2       13C
P2         75.00 usec
PL2        0.00 dB
SFO2       400.118006 MHz

F2 - Processing parameters
SI         65536
SF         100.6121654 MHz
WDW        EM
SSB        0
GB         0.80 Hz
PC         1.00
  
```

wangyi227 drx400

```

NAME: 8h
EXPNO: 1
PROCNO: 1
PROCPS: 64
SOLVENT: DMSO
NS: 1800
DS: 4
AQ: 0.000433 Hz
RG: 1.246228 sec
RG2: 7298.2
RG3: 1.450 usec
RG4: 4.50 usec
RG5: 298.0 K
RG6: 0.75248922 sec
RG7: 0.03000000 sec
RG8:
RG9:
RG10:
RG11:
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 usec
PL1: -2.00 dB
SFO1: 100.6211927 MHz
===== CHANNEL f2 =====
NAME: waltz16
NUC2: 1H
P2: 75.10 usec
PL2: 0.00 dB
PL12: 21.00 dB
SFO2: 400.1118006 MHz
F2 - Processing parameters
SI: 65536
SF: 100.6121692 MHz
WDW: EM
SSB: 0
LB: 0.80 Hz
GB: 0
PC: 1.00
  
```

m-FC6H4CH=CFBr dpx300

Date: 20060617
 Time: 0.10
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 8
 DS: 4
 SWH: 6172.839 Hz
 FIDRES: 0.094190 Hz
 AQ: 5.308460 sec
 RG: 114
 DW: 81.000 usec
 DE: 6.00 usec
 TE: 297.2 K
 D1: 4.00000000 sec
 MCREST: 0.00000000 sec
 MCPRK: 0.01300000 sec
 CHANNEL f1
 NUC1: ¹H
 P1: 7.25 usec
 PL1: -3.00 dB
 SFO1: 300.1322082 MHz
 F2 - Processing parameters
 SF: 300.1298310 MHz
 WDW: EM
 SSB: 0
 LB: 0.20 Hz
 GB: 0
 PC: 0.50

wangyi530 drx400

```

--
RG      1.0384
RG      1.0384
DE      4.50 usac
TE      298.0 K
D1      0.01000000 sec
C11     0.01000000 sec

===== CHANNEL F1 =====
NUC1    13C
P1      7.75 usac
PL1     -2.00 dB
SFO1    100.6211927 MHz

===== CHANNEL F2 =====
NAME    waltz16
NUC2    13C
P2      76.00 usac
PL2     0.00 dB
SFO2    400.1318006 MHz

F2 - Processing parameters
SI      131072
SF      131072 MHz
RG      1.0384
DE      4.50 usac
TE      298.0 K
D1      0.01000000 sec
C11     0.01000000 sec
PC      0.50
  
```

wangy1533 qpx300

```

Current Data Parameters
NAME      wangy1533
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20040119
Time      11:13
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         65536
FIDRES    0.3144
AQ         0.0316
RG          327.1
DS          4
SWH         8333.336 Hz
FIDRES     0.3144 Hz
RG          327.1
RG          1.372940 sec
RG          3649.1
RG          6.000 usec
DE          8.57 K
DE          28.57 K
DI          10.0000000 sec

===== CHANNEL f1 =====
NUC1       19F
P1          13.00 usec
PL1         -4.00 dB
SFO1        282.3762178 MHz

F2 - Processing parameters
SI          327.1 MHz
SF          282.4042774 MHz
WDW         EM
SSB          0
GB          0.70 Hz
PC          1.00
  
```

wangyi533 dpx300

-112.9196
-112.9686

-114.3088
-114.3422
-114.3762

-115.0836
-115.0980
-115.1167
-115.1303
-115.1491
-115.1640

NU 1.5728140 sec
SI 3.6540
RG 6.000 usec
DE 8.57 usec
TE 298.0 K
D1 10.00000000 sec
===== CHANNEL f1 =====
NUC1 ^{19}F
P1 4.35 usec
PL1 -4.35 dB
SFO1 282.3762178 MHz
F2 - Processing parameters
SI 2622144
RG 6.000 usec
DE 8.57 usec
TE 282.4042178 MHz
SFO2 282.4042178 MHz
LB 0
GB 0
PC 1.00

wangyi431 drx400

```

===== CHANNEL F1 =====
NUC1 13C
P1 7.00 usec
PL1 -2.00 dB
SFO1 100.6213927 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 19.00 dB
PL12 21.00 dB
SFO2 400.118006 MHz

F2 - Processing parameters
SI 65536
SF 100.6127747 MHz
WDW EM
SSB 0
GB 0
PC 1.00
  
```

wangyi432 drx400

```

===== CHANNEL F1 =====
NUC1 13C
P1 7.25 usec
PL 1.00 dB
SFO1 100.621927 MHz

===== CHANNEL F2 =====
CHCPRO2 waltz16
NUC2 13C
P2 75.00 usec
PL2 0.00 dB
SFO2 400.131806 MHz

F2 - Processing parameters
SI 32768
SF 100.6127743 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.00
  
```

wangyi441 drx400

158.6787
156.2019
134.7338
134.6895
132.9616
132.9200
126.4820
125.6106
125.5917
125.2403
125.1607
124.0583
123.9735
123.9448
123.8990
121.1571
121.0999
108.8549
108.6617

77.3190
77.0015
76.6839

33.0285
33.0195
32.3675

22.7677

13.9653

```

===== CHANNEL F1 =====
NUC1      13C
P1         7.75 usec
PL1        -2.00 dB
SFO1      100.6213927 MHz

===== CHANNEL F2 =====
CPDPRG22  waltz16
NUC2      1H
P2         76.00 usec
PL2        0.00 dB
PCPD2     19.050 usec
DE        4.50 usec
TE        298.20 K
F2        0.2514832 sec
d11       0.03000000 sec

===== CHANNEL F1 =====
NUC1      13C
P1         7.75 usec
PL1        -2.00 dB
SFO1      100.6213927 MHz

===== CHANNEL F2 =====
CPDPRG22  waltz16
NUC2      1H
P2         76.00 usec
PL2        0.00 dB
PCPD2     19.050 usec
DE        4.50 usec
TE        298.20 K
F2        0.2514832 sec
d11       0.03000000 sec

F2 - Processing parameters
SI         32768
SF         100.6127764 MHz
WDW        EM
SSB        0
GB         0
PC         0.50
  
```

Current Data Parameters

PC	1.00	
CP	0	
DB	0.80 Hz	
EN		
FM	100.6128771 MHz	
FR		
SP		
ST		
SW		
SI		
SR	400.13000 MHz	
SS		
PI2	0.00 dB	
PI1	75.00 dBc	
NO		
CH	W12x15	
CM		
CH2		
SI1	100.6231957 MHz	
PL1	-2.00 dB	
PL2	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB	
PL1	7.13 dBc	
NI1		
NI2		
CH1		
SI0	100.6231957 MHz	
PL0	-2.00 dB

wangyi412 drx400

===== CHANNEL F1 =====
 NUC1 13C
 P1 7.25 usec
 PL1 -2.00 dB
 SFO1 100.6213927 MHz
 ===== CHANNEL F2 =====
 CPOPC2 waltz16
 NUC2 1H
 P1 75.00 usec
 PL2 0.00 dB
 PCPO2 0.00 dB
 F12 20.00 MHz
 SFO2 400.118006 MHz
 F2 - Processing parameters
 SI 100.6127249 MHz
 SF 100.6127249 MHz
 WDM 0
 SSB 0
 GB 0
 PC 1.00

Figure 1. ORTEP Plot of 1-Butyl-3-fluorophenanthrene **5e**

Figure 2. ORTEP Plot of 2-Fluoro-4-decyl-phenanthrene (**20**)