**Palladium-Catalyzed Allylalkynylation of Benzyne: a Highly
Efficient Route to Substituted 1-Allyl-2-alkynylbenzenes**

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Supporting Information

Experimental Section

General procedure for the allylalkynylation of benzyne **1 with allylic chlorides **2**, and alkynylstannanes **3**:** A 25-ml round-bottom side-arm flask containing Pd(dba)₂/dppe (0.0500 mmol), CsF (3.00 mmol) was evacuated and purged with nitrogen gas three times. To the flask were then added benzyne precursor (**1**) (1.00 mmol), an allyl chloride (**2**) (1.20 mmol), alkynylstannane (**3**) (1.20 mmol) and CH₃CN (3.0 ml) via syringes. The reaction mixture was allowed to stir at 40 °C for 10 h. At the end of the reaction, the reaction mixture was diluted with CH₂Cl₂, filtered through Celite and silica gel. The filtrate was concentrated and the residue was purified through a silica gel column using hexane as eluent to give pure **4**.

Expremental procedure for the cyclization of 1-(1-hexynyl)-2-(2-methylallyl)benzene (4b**) with 1-iodonaphthalene.** A 10-ml sealed flask containing Pd(OAc)₂(0.0500 mmol), PPh₃(0.100 mmol), and Tl(OAc) (1.2 mmol) was evacuated and purged with nitrogen gas three times. To the flask were then added 1-(1-hexynyl)-2-(2-methylallyl)benzene (**4b**) (1.00 mmol), 1-iodonaphthalene (1.00 mmol) and DMF (3.0 ml) via syringes. The solution was stirred at 120 °C for 10 h and. At the end of the reaction, the reaction mixture was filtered through a Celite and silica gel pad and washed with 50ml of ether. The filtrate was washed with water, dried with MgSO₄ and concentrated in vacuo. The residue was purified through a silica gel column using hexane as eluent to give pure **5**.

Spectral data of compounds **4a-p**, **5** and **11** or **12**, and ¹H NMR Spectra of all compounds are listed bellow:

1-(2-Allylphenyl)-1-hexyne (4a**):** colorless oil; ¹H NMR (600MHz, CDCl₃): δ 7.40 (d, *J* = 7.2 Hz, 1 H), 7.21 - 7.14 (m, 3 H), 6.19 – 6.01 (m, 1 H), 5.11 - 5.06 (m, 2 H), 3.56 (d, *J* = 6.6 Hz, 2 H), 2.46 (t, *J* = 6.6 Hz, 2 H), 1.63 – 1.49 (m, 4 H), 0.97 (t, *J* =

7.2 Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 141.68, 136.77, 132.11, 128.57, 127.65, 125.91, 123.48, 115.70, 94.32, 79.03, 38.74, 30.88, 21.99, 19.21, 13.63; HRMS: calcd for $\text{C}_{15}\text{H}_{18}$ 198.1409, found 198.1404.

1-(1-Hexynyl)-2-(2-methylallyl)benzene (4b): colorless oil; ^1H NMR (600MHz, CDCl_3): δ 7.40 (d, $J = 7.2$ Hz, 1 H), 7.21 - 7.13 (m, 3 H), 4.82 (s, 1 H), 4.67 (s, 1 H), 3.52 (s, 2 H), 2.44 (t, $J = 6.6$ Hz, 2 H), 1.73 (s, 3 H), 1.62 – 1.48 (m, 4 H), 0.96 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 144.72, 141.34, 132.09, 128.97, 127.45, 125.87, 123.98, 111.74, 93.94, 79.27, 42.42, 30.89, 22.31, 21.99, 19.20, 13.62; HRMS: calcd for $\text{C}_{16}\text{H}_{20}$ 212.1565, found 212.1566.

1-(1-Hexynyl)-2-[(E)-1-methyl-2-butenyl]benzene (4c): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 7.41 (d, $J = 7.0$ Hz, 1 H), 7.22 - 7.13 (m, 3 H), 5.68 - 5.62 (m, 1 H), 5.49 - 5.41 (m, 1 H), 3.77 - 3.74 (m, 1 H), 2.40 (t, $J = 6.4$ Hz, 2 H), 1.77 (d, $J = 6.8$ Hz, 3H), 1.71 – 1.56 (m, 4 H), 1.35 (d, $J = 7.6$ Hz, 3 H), 0.95 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3): δ 142.75, 135.45, 131.21, 127.71, 127.08, 126.78, 126.09, 124.07, 93.71, 78.82, 42.45, 30.92, 22.37, 21.96, 20.86, 17.26, 13.63; HRMS: calcd for $\text{C}_{17}\text{H}_{22}$ 226.1721, found 226.1718.

1-[2-(2-Cyclohexenyl)phenyl]-1-hexyne (4d): colorless oil; ^1H NMR (600MHz, CDCl_3): δ 7.36 (d, $J = 7.2$ Hz, 1 H), 7.20 - 7.09 (m, 3 H), 5.92 – 5.89 (m, 1 H), 5.69 - 5.67 (m, 1 H), 3.94 – 3.92 (m, 1 H), 2.43 (t, $J = 6.6$ Hz, 2 H), 2.08 – 2.06 (m, 3 H), 1.60 – 1.48 (m, 8 H), 0.94 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 147.84, 132.06, 130.00, 128.51, 127.13, 127.48, 125.62, 123.10, 94.12, 78.99, 39.28, 30.85, 25.08, 21.94, 21.03, 19.20, 13.61; HRMS: calcd for $\text{C}_{18}\text{H}_{22}$ 238.1721, found 238.1723.

1-(2-Phenyl-1-ethynyl)-2-[(E)-3-phenyl-2-propenyl]benzene (4e): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 7.41 - 7.22 (m, 14 H), 6.56 – 6.39 (m, 2 H), 3.80 (d, $J = 6.6$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3): δ 139.31, 137.41, 136.57, 132.09, 131.04,

130.04, 129.73, 128.64, 128.45, 127.60, 127.08, 126.09, 126.73, 125.69, 92.86, 79.11, 36.63; HRMS: calcd for C₂₃H₁₈ 294.1409, found 294.1413.

1-(1-Hexynyl)-4,5-dimethyl-2-(2-methylallyl)benzene (4f): colorless oil; ¹H NMR (600MHz, CDCl₃): δ 7.18 (s, 1 H), 6.95 (s, 1 H), 4.80 (s, 1 H), 4.69 (s, 1 H), 3.45 (s, 2 H), 2.44 (t, *J* = 6.6 Hz, 2 H), 2.22 (s, 3H), 2.20 (s, 3H), 1.73 (s, 3 H), 1.61 – 1.48 (m, 4 H), 0.96 (t, *J* = 7.2 Hz, 3 H); ¹³C NMR (150 MHz, CDCl₃): δ 145.15, 138.66, 136.20, 134.06, 132.98, 130.23, 121.14, 111.37, 92.70, 79.38, 41.97, 30.97, 22.26, 21.97, 19.63, 19.19, 19.05, 13.62; HRMS: calcd for C₁₈H₂₄ 240.1878, found 240.1881.

5-(1-Hexynyl)-6-(2-methylallyl)indane (4g): colorless oil; ¹H NMR (600MHz, CDCl₃): δ 7.27 (s, 1 H), 7.06 (s, 1 H), 4.81 (s, 1 H), 4.69 (s, 1 H), 3.50 (s, 2 H), 2.88 – 2.84 (m, 2 H), 2.44 (t, *J* = 6.6 Hz, 2 H), 2.06 – 2.04 (m, 2 H), 1.74 (s, 3 H), 1.61 – 1.49 (m, 4 H), 0.96 (t, *J* = 7.2 Hz, 3 H); ¹³C NMR (150 MHz, CDCl₃): δ 145.25, 144.03, 141.83, 139.26, 127.67, 124.81, 121.46, 111.41, 92.55, 79.85, 42.31, 32.75, 32.26, 30.97, 25.38, 22.28, 21.96, 19.19, 13.62; HRMS: calcd for C₁₉H₂₄ 252.1878, found 252.1880.

5-(1-Hexynyl)-6-(2-methylallyl)-1,3-benzodioxole (4h): colorless oil; ¹H NMR (400MHz, CDCl₃): δ 6.81 (s, 1 H), 6.64 (s, 1 H), 5.89 (s, 2H), 4.77 (s, 1 H), 4.66 (s, 1 H), 3.39 (s, 2 H), 2.38 (t, *J* = 6.6 Hz, 2 H), 1.70 (s, 3 H), 1.60 – 1.49 (m, 4 H), 0.93 (t, *J* = 7.2 Hz, 3 H); ¹³C NMR (100 MHz, CDCl₃): δ 147.30, 145.56, 144.87, 136.18, 116.72, 111.69, 111.46, 109.11, 101.03, 92.35, 79.25, 42.31, 33.34, 22.09, 19.16, 13.94, 13.57; HRMS: calcd for C₁₇H₂₀O₂ 256.1463, found 256.1467.

1-(2-Methylallyl)-2-(1-propynyl)benzene (4i): colorless oil; ¹H NMR (500MHz, CDCl₃): δ 7.46 (d, *J* = 7.2 Hz, 1 H), 7.28 - 7.20 (m, 3 H), 4.89 (s, 1 H), 4.76 (s, 1 H), 3.58 (s, 2 H), 2.14 (s, 3 H), 1.79 (s, 3 H); ¹³C NMR (125 MHz, CDCl₃): δ 144.70, 141.42, 132.08, 128.95, 127.50, 125.88, 123.92, 111.82, 89.34, 78.50, 42.42, 22.25, 4.36; HRMS: calcd for C₁₃H₁₄ 170.1096, found 170.1095.

1-(3-Methoxy-1-propynyl)-2-(2-methylallyl)benzene (4j): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 7.44 (d, J = 8.0 Hz, 1 H), 7.27 - 7.14 (m, 3 H), 4.81 (s, 1 H), 4.65 (s, 1 H), 4.34 (s, 3H), 3.51 (s, 2 H), 3.44 (s, 3H), 1.71 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3): δ 144.38, 141.76, 132.39, 129.11, 128.44, 125.98, 122.59, 112.03, 88.47, 85.15, 60.42, 57.50, 42.42, 22.31; HRMS: calcd for $\text{C}_{14}\text{H}_{16}\text{O}$ 200.1201, found 200.1203.

1-(2-Methylallyl)-2-(2-phenyl-1-ethynyl)benzene (4k): colorless oil; ^1H NMR (600 MHz, CDCl_3): δ 7.54 - 7.52 (m, 3 H), 7.35 - 7.20 (m, 6 H), 4.85 (s, 1 H), 4.74 (s, 1 H), 3.61 (s, 2 H), 1.77 (s, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 144.48, 141.70, 132.18, 131.45, 129.17, 128.15, 126.08, 123.52, 123.19, 112.06, 92.97, 88.32, 42.65, 22.36; HRMS: calcd for $\text{C}_{18}\text{H}_{16}$ 232.1252, found 232.1249.

1-[2-(4-Bromophenyl)-1-ethynyl]-2-(2-methylallyl)benzene (4l): colorless oil; ^1H NMR (600 MHz, CDCl_3): δ 7.50 - 7.23 (m, 8 H), 4.82 (s, 1 H), 4.69 (s, 1 H), 3.59 (s, 2 H), 1.75 (s, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 144.36, 141.72, 132.18, 131.78, 131.45, 131.61, 129.32, 128.59, 126.15, 122.43, 122.36, 112.13, 91.85, 89.45, 42.65, 22.37; HRMS: calcd for $\text{C}_{18}\text{H}_{15}\text{Br}$ 310.0357, found 310.0357.

2-2-[2-(2-Methylallyl)phenyl]-1-ethynylthiophene (4m): colorless oil; ^1H NMR (600 MHz, CDCl_3): δ 7.45 (d, J = 7.2 Hz, 1H), 7.25 - 7.16 (m, 5 H), 6.97 (d, J = 5.4 Hz, 1 H), 4.80 (s, 1 H), 4.69 (s, 1 H), 3.52 (s, 2 H), 1.71 (s, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 144.38, 141.61, 131.96, 131.55, 129.31, 128.48, 127.13, 126.12, 123.50, 122.85, 112.16, 92.02, 86.16, 42.71, 22.35; HRMS: calcd for $\text{C}_{16}\text{H}_{14}\text{S}$ 238.0816, found 238.0816.

1-(1-Hexynyl)-4-methyl-2-(2-methylallyl)benzene (4n): colorless oil; ^1H NMR (600MHz, CDCl_3): δ 7.43 (d, J = 7.2 Hz, 1 H), 7.25 - 7.16 (m, 3 H), 5.38 (s, 1 H), 5.29 (s, 1 H), 4.82 (s, 1 H), 4.70 (s, 1 H), 3.50 (s, 2 H), 1.99 (s, 3H), 1.73 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 144.47, 141.59, 132.13, 129.16, 128.21, 126.97, 126.01,

123.13, 121.57, 111.96, 94.18, 87.29, 42.53, 23.49, 22.30; HRMS: calcd for C₁₅H₁₆ 196.1252, found 196.1250.

1-[2-(1-Cyclohexenyl)-1-ethynyl]-2-(2-methylallyl)benzene (4o): colorless oil; ¹H NMR (600MHz, CDCl₃): δ 7.40 (d, *J* = 7.2 Hz, 1 H), 7.21 - 7.14 (m, 3 H), 6.29 (t, *J* = 2 Hz, 1 H), 4.81 (s, 1 H), 4.69 (s, 1 H), 3.51 (s, 2 H), 2.23 – 2.13 (m, 4 H), 1.72 (s, 3H), 1.68 – 1.60 (m, 4H); ¹³C NMR (150 MHz, CDCl₃): δ 144.61, 141.29, 134.77, 131.93, 129.02, 127.75, 125.93, 123.61, 120.87, 111.87, 94.89, 85.62, 42.50, 29.22, 25.72, 22.31, 21.49; HRMS: calcd for C₁₈H₂₀ 236.1565, found 236.1568.

1-(2-Allylphenyl)-1-hexyne (4p): colorless oil; ¹H NMR (400MHz, CDCl₃): δ 7.60 – 7.56 (m, 3 H), 7.41 - 7.27 (m, 6 H), 6.19 – 6.02 (m, 1 H), 5.21 - 5.07 (m, 2 H), 3.70 (d, *J* = 6.8 Hz, 2 H); ¹³C NMR (100 MHz, CDCl₃): δ 141.97, 136.52, 132.15, 131.45, 128.78, 128.50, 128.38, 128.32, 126.09, 123.42, 122.70, 116.01, 93.26, 88.04, 38.83; HRMS: calcd for C₁₇H₁₄ 218.1096, found 218.1097.

13-Butyl-7a-methyl-7a,8-dihydro-7H-indeno[2,1-b]phenanthrene (5): colorless oil; ¹H NMR (500 MHz, CDCl₃): δ 8.21 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 8 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1 H), 7.48 - 7.25 (m, 7 H), 3.48 – 3.42 (m, 1 H), 3.27 – 3.20 (m, 1 H), 3.01 – 2.88 (m, 4 H), 1.27 – 1.08 (m, 4 H), 0.88 (s, 3 H), 0.66 (t, *J* = 7.0 Hz, 3 H); ¹³C NMR (125 MHz, CDCl₃): δ 148.73, 146.52, 139.29, 134.49, 134.37, 133.56, 130.75, 130.45, 128.60, 127.40, 127.04, 126.60, 126.45, 126.08, 125.70, 125.54, 124.81, 124.35, 46.99, 44.23, 42.89, 32.91, 30.86, 22.64, 21.70, 13.76; HRMS: calcd for C₂₆H₂₆ 338.2034, found 338.2036.

1-[5-Methyl-2-(2-methylallyl)phenyl]-1-hexyne (11 and 12): colorless oil; ¹H NMR (600MHz, CDCl₃): δ 7.30 (d, *J* = 7.2 Hz, 1 H), 7.23 (s, 1 H), 7.08 – 6.95 (m, 4 H), 4.82 – 4.80 (m, 2 H), 4.70 – 4.67 (m, 2 H), 3.48 (m, 4 H), 2.45 – 2.42 (s, 6 H), 1.73 – 1.51 (m, 8 H), 0.97 – 0.95 (m, 6 H); ¹³C NMR (150 MHz, CDCl₃): δ 144.94, 144.88, 141.16, 138.32, 137.32, 135.33, 132.57, 131.92, 129.69, 128.87, 128.38, 126.71,

123.73, 120.99, 111.60, 111.50, 93.48, 93.05, 79.42, 79.32, 42.37, 42.01, 30.95, 30.92, 22.29, 22.26, 21.98, 21.33, 20.72, 19.19, 13.60; HRMS: calcd for C₁₇H₂₂ 226.1721, found 226.1719.

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TE 0.0 K
D1 1.00000000 sec
DELTA 0.00000000 sec
RGPRG 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 500.132987 MHz
F2 - Processing Parameters
SI 32768
SF 500.132987 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
FID 9.500 cm
F1 563.63 Hz
F2 563.63 Hz
PC 20.00 cm
PWC 0.5000 cm/cm
H2O 299.87503 Hz/cm

pgm

f2 - Acquisition Parameters
 Date 20040212

Time	0.11
MS/MS	500.1

FROM: 5 mm ONP 11/1
ON PROG 20

10	32768
501 VMAT	70613

25 26

SWH	0.389 262 Hz
FTIME	0.256030 sec

1 9530228 SEC

OM	59.600 used
OM	6.50 used

0.0 x
1 000000000 sec

MCNEST	0 00000000	sec
MCNTRK	0 01500000	sec

***** CHANNEL *****

MUC1	1H
P1	14 00 usec

Fl 1	4.00 dB
Sf 01	599 7529987 MHz

F2 - Processing Parameters

SI 32/64
Sf 509 7500304 MHz

NO	NOX
0	0.50

0	0
0 00 442	0
00	00
00	00

0.30
0.48

10 mm P10L bar amplifiers	
CX	20.00 cm

10.00 cm	10
9.500 cm	5

1 5097.62 Hz
f2p -0.500 00m

0 50000 0000 /w00 0000S 0
24 68 682-
mJHdd

0.937 ± 0.009 Hz

Current Data Parameters
NAME AS
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040209
Time 15.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256429 Hz
AQ 1.9534238 SEC
RG 655
DE 18.00 uSEC
TE 300.2 K
D1 1.00000000 SEC
MCRES1 0.00000000 SEC
MCRES2 0.01500000 SEC
***** CHANNEL f1 *****
NUC1 13C
P1 14.00 uSEC
PL1 0.00 dB
SFO1 509.7529787 MHz
F2 - Processing parameters
SI 32768
SF 509.7529787 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50
TO 1600.000000
F2 20.00 cm
CY 10.00 cm
F1F 9.300 ppm
F1 5897.63 Hz
F2F -299.88 Hz
PCPM 0.00000000
H2CH 209.07503 Hz/GC

C=C/C#Cc1ccccc1

The chemical structure shows a complex polycyclic aromatic hydrocarbon. It features a central benzene ring fused to a five-membered ring on the left and a naphthalene system on the right. The five-membered ring is labeled with the number '5' and has a substituent line extending from it. The naphthalene system has a long alkyl chain attached to one of its rings.

Current Data Parameters
NAME: 1
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20040212
Time: 0.16
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 8399.250 Hz
FIDRES: 0.245000 Hz
AQ: 1.9530228 sec
RG: 4
OW: 59.600 usec
DE: 6.50 usec
TE: 0.0 K
D1: 1.00000000 sec
DELTA: 0.00000000 sec
PCPRG2: 0.01500000 sec
MCPRG: 0.01500000 sec
***** CHANNEL f1 *****
NUC1: 1H
P1: 14.00 usec
PL1: 4.00 dB
SFO1: 500.135097 MHz
F2 - Processing parameters
SI: 32768
SF: 500.135097 MHz
WDW: no
SSB: 0 Hz
LB: 0 Hz
GB: 0 Hz
PC: 0.50
ID parameters
CX: 20.00 cm
CY: 15.00 cm
CZ: 0.500 mm
F1: 500.135097 MHz
F2: -299.88 Hz
PQCH: 0.50000 mm/cm
H2CH: 299.87500 Hz/cm