Supporting Information

Palladium-Catalyzed Selective Cross-Addition of Triisopropylsilylacetylene to Internal and Terminal Unactivated Alkynes

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General. Spectroscopic measurements were carried out with the following instruments: Bruker DPX-400 and DRX-500 (^1H NMR and ^{13}C NMR), JEOL FT/IR-350 (FT-IR). Shimadzu GCMS-QP5050A (MS). Alkynes were purchased from Aldrich and TCI and used without further purification. The complexes **1** and **2** were prepared according to literature methods.^{1,2}

General procedure for the cross-addition of triisopropylsilylacetylene (TIPSA) to alkynes. To a solution of **1a** (0.01 mmol, 10 mg) in toluene (2.0 ml) were added TIPSA (0.50 mmol) and an alkyne (0.50 mmol) under nitrogen atmosphere in a pressure vial. The reaction mixture was stirred at 110 °C and was periodically monitored by GC analysis. After either of TIPSA or the other alkyne was completely consumed, the mixture was cooled to room temperature and was filtered through a short silica gel column using ether as an eluent. Solvents were removed under reduced pressure, and the products were purified by silica gel column chromatography using hexane as an eluent. The structure and stereochemistry of products were determined by NMR spectra and NOE experiments.

[(*E*)-3-Ethylhex-3-en-1-ynyl]triisopropylsilane (3a**).** ^1H NMR (400 MHz, CDCl_3) δ 0.99 (t, $J = 7.5$ Hz, 3H), 1.03-1.13 (m, 24H), 2.10 (quint, $J = 7.5$, 2H), 2.14 (q, $J = 7.5$, 2H), 5.88 (t, $J = 7.5$, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 11.4, 13.1, 13.8, 18.7, 21.4, 23.9, 86.8, 109.4, 124.5, 139.5; IR (neat) 3100-2780, 2139, 1683, 1463, 1381, 994, 918 cm^{-1} ; MS (EI)

m/z 59 (68), 73 (32), 151 (57), 179 (40), 221 (100), 264 (M , 10); HRMS (ESI) calcd for $C_{17}H_{32}Si$: 264.2268; found: 264.2270.

Triisopropyl[(*E*)-3-propylhept-3-en-1-ynyl]silane (3b). 1H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, $J = 7.5$ Hz, 3H), 0.92 (t, $J = 7.5$ Hz, 3H) 1.04-1.12 (m, 21H), 1.39 (sext, $J = 7.5$ Hz, 2H), 1.57 (sext, $J = 7.5$, 2H), 2.06 (q, $J = 7.5$ Hz, 2H), 2.11 (t, $J = 7.5$ Hz, 2H), 5.92 (t, $J = 7.5$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.4, 13.6, 13.9, 18.7, 21.5, 22.5, 30.4, 32.6, 86.5, 109.8, 123.5, 138.70; IR (neat) 2760-3100, 2140, 1463, 1381, 994, 883 cm^{-1} ; MS (EI) m/z 59 (88), 73 (34), 179 (47), 249 (100), 292 (M , 8); HRMS (ESI) calcd for $C_{19}H_{36}Si$: 292.2581; found: 292.2580.

[(*E*)-3,4-Diphenylbut-3-en-1-ynyl]triisopropylsilane (3c). 1H NMR (400 MHz, $CDCl_3$) δ 1.03-1.19 (m, 21H), 7.00-7.44 (m, 11H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.4, 18.7, 91.0, 109.8, 124.5, 127.6, 127.7, 128.1, 128.3, 129.1, 129.3, 136.1, 136.8, 137.6; IR (neat) 2780-3000, 3000-3150, 2135, 1598, 1463 cm^{-1} ; MS (EI) m/z 59 (90), 73 (45), 245 (88), 247 (55), 317 (100), 360 (M , 70); HRMS (ESI) calcd for $C_{25}H_{32}Si$: 360.2268; found: 360.2272.

Triisopropyl[(*Z*)-5-methoxy-3-(methoxymethyl)pent-3-en-1-ynyl]silane (3d). 1H NMR (500 MHz, $CDCl_3$) δ 1.02-1.14 (m, 21H), 3.35 (s, 3H), 3.36 (s, 3H), 4.02 (s, 2H), 4.10 (d, $J = 8.1$ Hz, 2H), 6.21 (t, $J = 8.1$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.2, 18.6, 57.9, 58.3, 68.4, 70.2, 90.3, 107.1, 123.1, 138.1; IR (neat) 2650-3100, 2143, 1630, 1463, 1107 cm^{-1} ; MS (EI) m/z 43 (44), 45 (43), 59 (54), 75 (100), 105 (61), 145 (39), 264 ($M - CH_3OH$, 2); HRMS (ESI) calcd for $C_{17}H_{32}NaO_2Si$ [$M + Na$] $^+$: 319.2064; found: 319.2064.

Triisopropyl[(*E*)-3-phenylpent-3-en-1-ynyl]silane (3e). 1H NMR (400 MHz, $CDCl_3$) δ 1.05-1.11(m, 21H), 1.84 (d, $J = 7.4$ Hz, 3H), 6.35 (q, $J = 7.4$, 1H), 7.20-7.44(m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.4, 15.6, 18.7, 87.6, 109.1, 124.8, 127.2, 128.0, 128.9, 135.0, 137.1; IR (neat) 2780-3120, 2136, 1464 cm^{-1} ; MS (EI) m/z 59 (53), 99 (55), 185 (63), 199 (31), 213 (30), 255 (100), 298 (M , 19); HRMS (ESI) calcd for $C_{20}H_{30}Si$: 298.2111; found: 298.2110.

(*E*)-3-Methyl-5-(triisopropylsilyl)pent-2-en-4-yn-1-ol (3f). ^1H NMR (400 MHz, CDCl_3) δ 1.05-1.10 (m, 21H), 1.57 (br s, 1H), 1.84 (dt, $J = 1.5, 0.8$ Hz, 3H), 4.22 (d, $J = 6.8$ Hz, 2H), 6.05 (tq, $J = 6.8, 1.5$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 11.2, 17.6, 18.6, 59.1, 88.5, 109.4, 121.1, 135.9; IR (neat) 3060-3650, 2780-3060, 2142, 1631, 1464, 1011, 882, 806 cm^{-1} ; MS (EI) m/z 61 (53), 75 (68), 139 (34), 167 (28), 209 (100), 252 (*M*, 2); HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{28}\text{NaOSi}$ [$M + \text{Na}$] $^+$: 275.1802; found: 275.1801.

(*Z*)-2-[(Triisopropylsilyl)ethynyl]but-2-en-1-ol (3f'). ^1H NMR (400 MHz, CDCl_3) δ 1.06-1.10 (m, 21H), 1.61 (br s, 1H), 1.76 (dt, $J = 7.3, 0.7$ Hz, 3H), 4.19 (m, 2H), 6.12 (qt, $J = 7.3, 1.1$ Hz, 1H); ^{13}C NMR (400 MHz, CDCl_3) δ 11.2, 13.9, 18.6, 59.7, 90.1, 106.4, 123.9, 134.9; IR (neat) 3070-3660, 2760-3070, 2139, 1464, 996, 883, 817 cm^{-1} ; MS (EI) 45 (39), 61 (57), 75 (74), 103 (57), 131 (100), 191 (50), 252 (*M*, 3); HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{28}\text{NaOSi}$ [$M + \text{Na}$] $^+$: 275.1802; found: 275.1801.

(*E*)-3-Methyl-5-(triisopropylsilyl)pent-2-en-4-ynoic acid methyl ester (3g). ^1H NMR (500 MHz, CDCl_3) δ 1.07-1.11 (m, 21H), 2.31 (d, $J = 1.5$ Hz, 3H), 3.71 (s, 3H), 6.11 (q, 1.5 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 11.5, 18.7, 51.2, 96.4, 108.8, 124.3, 138.2, 166.5. MS (EI) m/z 59 (49), 75 (41), 89 (39), 167 (39), 237 (100), 280 (*M*, 1).

Triisopropyl(3-methylene-1-nonynyl)silane (3h). ^1H NMR (400 MHz, CDCl_3) δ 0.88 (t, $J = 6.9$, 3H), 1.03-1.14 (m, 21H), 1.21-1.37 (m, 6H), 1.49-1.59 (m, 2H), 2.15 (dt, $J = 1.4, 7.4$ Hz, 2H), 5.22 (dt, $J = 2.1, 1.4$ Hz, 1H), 5.34 (d, $J = 2.1$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 11.3, 14.1, 18.6, 22.6, 28.0, 28.5, 31.7, 37.3, 90.0, 107.7, 121.3, 132.2; IR (neat) 2780-3080, 2143, 1605, 1463, 995, 883 cm^{-1} ; MS (EI) m/z 59 (64), 137 (26), 249 (100), 292 (*M*, 1); HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{36}\text{Si}$: 292.2581; found: 292.2584.

Triisopropyl(3-methylene-1-octynyl)silane (3i). ^1H NMR (500 MHz, CDCl_3) δ 0.89 (t, $J = 7.0$, 3H), 1.01-1.14 (m, 21H), 1.24-1.37 (m, 4H), 1.51-1.59 (m, 2H), 2.15 (dt, $J = 1.4, 7.5$ Hz, 2H), 5.22 (dt, $J = 2.1, 1.4$ Hz, 1H), 5.34 (d, $J = 2.1$ Hz, 1H); ^{13}C NMR (125 MHz,

CDCl₃) δ 11.3, 14.0, 18.6, 22.5, 27.7, 31.0, 37.2, 90.0, 107.7, 121.4, 132.2; IR (neat) 2770-3080, 2143, 1607, 1464, 995, 885; MS (EI) m/z 43 (26), 59 (54), 137 (29), 165 (25), 235 (100), 278 (*M*, 1); HRMS (ESI) calcd for C₁₈H₃₄Si: 278.2424; found: 278.2430.

Triisopropyl(3-methylene-1-decynyl)silane (3j). ¹H NMR (400 MHz, CDCl₃) δ 0.88 (t, *J* = 6.9, 3H), 1.05-1.12 (m, 21H), 1.21-1.37 (m, 8H), 1.49-1.60 (m, 2H), 2.15 (dt, *J* = 1.4, 7.5 Hz, 2H), 5.21 (dt, *J* = 2.1, 1.4 Hz, 1H), 5.34 (d, *J* = 2.1 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 11.3, 14.1, 18.6, 22.7, 28.0, 28.8, 29.1, 31.8, 37.3, 90.0, 107.7, 121.3, 132.2; IR (neat) 2780-3080, 2143, 1606, 1463, 995, 884 cm⁻¹; MS (EI) m/z 41 (56), 43 (72), 59 (89), 73 (39), 137 (48), 263 (100), 306 (*M*, 0.2); HRMS (ESI) calcd for C₂₀H₃₈Si: 306.2737; found: 306.2741.

(4,4-Dimethyl-3-methylene-1-pentynyl)triisopropylsilane (3k). ¹H NMR (400 MHz, CDCl₃) δ 1.06-1.12 (m, 21H), 1.15 (s, 9H), 5.27 (d, *J* = 1.5 Hz), 5.35 (d, *J* = 1.5 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 11.4, 18.7, 28.9, 35.8, 90.7, 107.1, 118.2, 142.0; IR (neat) 2780-3080, 2150, 1601, 1464 cm⁻¹; MS (EI) m/z 41 (43), 43 (44), 59 (77), 123 (46), 151 (76), 165 (65), 221 (100), 264 (*M*, 5); HRMS (ESI) calcd for C₁₇H₃₂Si: 264.2268; found: 264.2269.

5-Methylene-7-(triisopropylsilyl)hept-6-yn-1-ol (3l). ¹H NMR (500 MHz, CDCl₃) δ 1.02-1.14 (m, 21H), 1.54-1.70 (m, 5H), 2.20 (dt, *J* = 1.3, 6.7 Hz, 2H), 3.64 (t, *J* = 6.3 Hz, 2H), 5.24 (dt, *J* = 2.0, 1.3 Hz, 1H), 5.37 (d, *J* = 2.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 11.2, 18.6, 24.0, 31.8, 36.8, 62.6, 90.2, 107.4, 121.7, 131.6; IR (neat) 3050-3600, 2780-3050, 2143, 1607, 1463, 1065, 994, 885 cm⁻¹; MS (EI) m/z 61 (83), 75 (100), 103 (73), 131 (49), 177 (44), 237 (*M* - *i*-Pr, 29); HRMS (ESI) calcd for C₁₇H₃₂NaOSi [*M* + Na]⁺: 303.2115; found: 303.2114.

5-Methylene-7-(triisopropylsilyl)hept-6-ynoic acid methyl ester (3m). ¹H NMR (500 MHz, CDCl₃) δ 1.06-1.10 (m, 21H), 1.90 (quint, *J* = 7.4 Hz, 2H), 2.21 (dt, *J* = 1.3, 7.3 Hz, 2H), 2.34 (t, *J* = 7.5 Hz, 2H), 3.67 (s, 3H), 5.25 (d, *J* = 1.9 Hz, 1H), 5.39 (dt, *J* = 1.9, 1.3 Hz,

1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.2, 18.6, 23.1, 32.9, 36.3, 51.4, 90.6, 106.9, 122.4, 130.8, 173.8; IR (neat) 2780-3080, 2143, 1742, 1606, 1462, 995, 884 cm^{-1} ; MS (EI) m/z 59 (100), 75 (70), 91 (51), 223 (90), 235 (51), 265 ($M - i\text{-Pr}$, 85), HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{32}\text{NaO}_2\text{Si}$ [$M + \text{Na}$] $^+$: 331.2064; found: 331.2062.

5-Methylene-7-(triisopropylsilyl)hept-6-ynenitrile (3n). ^1H NMR (500 MHz, CDCl_3) δ 1.03-1.13 (m, 21H), 1.94 (quint, $J = 7.1$ Hz, 2H), 2.34 (dt, $J = 1.4, 7.1$ Hz, 2H), 2.38 (t, $J = 7.1$ Hz, 2H), 5.34 (d, $J = 1.7$ Hz, 1H), 5.45 (dt, $J = 1.7, 1.4$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.2, 15.9, 18.6, 23.6, 35.6, 91.6, 106.0, 119.4, 123.6, 129.2; IR (neat) 2780-3070, 2248, 2144, 1607, 1463, 995, 884 cm^{-1} ; MS (EI) m/z 43 (19), 59 (26), 190 (18), 232 ($M = i\text{-Pr}$, 100); HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{29}\text{NNaSi}$ [$M + \text{Na}$] $^+$: 298.1961; found: 298.1960.

References

- 1) Tsukada, N.; Mitsuboshi, T.; Setoguchi, H.; Inoue, Y. *J. Am. Chem. Soc.* **2003**, *125*, 12102-12103.
- 2) Tsukada, N.; Tamura, O.; Inoue, Y. *Organometallics* **2002**, *21*, 2521-2528.

H1-NMR

Current Data Parameters
 NAME: adduct (3-hexyne)
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060601
 Time: 15.57
 INSTRUM: gpc400
 PROBRD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TO: 65536
 SOLVENT: CDCl3
 NS: 8
 DS: 2
 SMH: 8223.695 Hz
 FIDRES: 0.125493 Hz
 AQ: 3.9846397 sec
 RG: 181
 DW: 60.800 usec
 DE: 4.50 usec
 TE: 683.2 K
 D1: 2.00000000 sec
 MCREST: 0.00000000 sec
 MCMRK: 0.01500000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 10.50 usec
 PL1: -6.00 dB
 SF01: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300110 MHz
 WDM: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 33.00 cm
 CY: 20.00 cm
 F1P: 10.000 ppm
 F1: 4001.30 Hz
 F2P: -0.500 ppm
 F2: -200.07 Hz
 PPMCH: 0.31818 ppm/cm
 HZCH: 127.31409 Hz/cm

H1-NMR

Current Data Parameters
NAME adduct(4-octyne)
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060629
Time 17.01
INSTRUM gp400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8233.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DM 60.800 usec
DE 4.50 usec
TE 297.2 K
D1 2.00000000 sec
WCRES1 0.00000000 sec
NMRRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.50 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300341 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 33.00 cm
CY 20.00 cm
FLP 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PRNCH 0.31818 ppm/cm
HZCH 127.31410 Hz/cm

H1-NMR

Current Data Parameters
NAME: adduct (aipmylactyl)enol
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060703
Time: 13:17:10
INSTRUM: spect
PROBHD: 5 mm DNP HX/13
PULPROG: zg30
TD: 65536
SOLVENT: DMS-d6
NS: 8
DS: 2
SWH: 823.865 Hz
FIDRES: 0.02483 Hz
AQ: 3.584837 sec
RG: 64
DM: 60.800 usec
DE: 4.50 usec
TE: 296.2 K
O1: 2.00000000 sec
MCREST: 0.00000000 sec
MCNMR: 0.01000000 sec

***** CHANNEL f1 *****
NUC1: 1H
P1: 10.50 usec
PL1: -6.00 dB
SFO1: 400.1324710 MHz

F2 - Processing parameters
SI: 32768
SF: 400.1300984 MHz
WDW: 0
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.00

10 NMR Plot Parameters
CX: 33.00 cm
CY: 20.00 cm
ZP: 10.00000 mm
F1: 4001.30 Hz
FAP: -0.000 ppm
F2: -200.07 Hz
PPHCH: 0.31818 ppm/cm
HZCM: 127.31412 Hz/cm

H1-NMR

Current Data Parameters
 Name: 4-methoxy-2-butyn-1-ol
 Date: 20071415
 Time: 14:40
 Instrument: spect
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TO: 2930
 SOLVENT: CDCl3
 NS: 2
 DS: 4
 SWH: 8233.665 Hz
 FIDRES: 0.125483 Hz
 AQ: 3.884587 sec
 ZG: 1.000000 sec
 DE: 683.2 K
 TE: 2.0000000 sec
 AQC: 0.0000000 sec
 ACQ: 0.0150000 sec
 ***** CHANNEL f1 *****
 NUC1: 1H
 P1: 18.50 usec
 PL1: -2.50 dB
 SFO1: 400.132470 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.132470 MHz
 WHW: 400.132470 MHz
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00
 1D NMR plot parameters
 CX: 33.00 cm
 CY: 20.00 cm
 CZ: 10.00 cm
 F1: 400.132470 MHz
 F2: -200.07 Hz
 PPMCH: 0.31618 ppm/cm
 XZCH: 127.31499 Hz/cm

H1-NMR

Current Data Parameters
 Name: adduct (1-phenyl-1-propyne)
 EPRNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
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 Time: 16.06
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 PROBR40: 5 mm QNP 1H/13
 PULPROG: zg30
 TO: 65535
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8223.566 Hz
 FIDRES: 0.125483 Hz
 AQ: 3.9846387 sec
 RG: 64
 DM: 60.800 usec
 DE: 19.000 usec
 TE: 300.2 K
 O1: 2.00000000 sec
 MCPRST: 0.00000000 sec
 MCNMR: 0.01500000 sec
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 NUC1: 1H
 P1: 12.00 usec
 PL1: -6.00 dB
 SFO1: 400.1324710 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.1300348 MHz
 MCN: 1
 SCB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00
 LO NMR plot parameters
 CX: 33.00 cm
 CY: 20.00 cm
 CLP: 10.000000 mm
 F1: 4001.30 Hz
 F2: -200.07 Hz
 PRNOM: 0.31818 ppm/cm
 HZCM: 127.31410 Hz/cm

H1-NMR

Current Data Parameters
 NAME adduct (2-butyn-1-ol) B
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070422
 Time 15.50
 INSTRUM dp400
 PROBRG 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SMH 8223.685 Hz
 FIDRES 0.123483 Hz
 AQ 3.9846387 sec
 RG 203.2
 DM 60.800 uSAC
 DE 4.50 uSAC
 TE 294.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCNMR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 uSAC
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F3 - Processing parameters
 SF 400.1300650 MHz
 ST 32768
 WDM 100
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 33.00 cm
 CY 20.00 cm
 FIP 10.000 ppm
 FI 4001.30 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMM 0.31818 ppm/cm
 HZCM 127.31409 Hz/cm

H1-NMR

Current Data Parameters
 Name: 3f
 Sample: 1
 P1: 1.00
 P2: 1.00

F2 - Acquisition Parameters

Date: 20070422
 Time: 14:55
 INSTRUM: spect
 P1: 1.00
 P2: 1.00
 P3: 1.00
 P4: 1.00
 P5: 1.00
 P6: 1.00
 P7: 1.00
 P8: 1.00
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 P80: 1.00
 P81: 1.00
 P82: 1.00
 P83: 1.00
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 P90: 1.00
 P91: 1.00
 P92: 1.00
 P93: 1.00
 P94: 1.00
 P95: 1.00
 P96: 1.00
 P97: 1.00
 P98: 1.00
 P99: 1.00
 P100: 1.00

F2 - Processing Parameters

SI: 32768
 SF: 400.130077 MHz
 KW: 1.00
 SSF: 1.00
 SSB: 0.00 Hz
 CB: 0
 PC: 1.00

10 NMR plot parameters

CX: 33.00 cm
 CY: 20.00 cm
 FL: 10.000 ppm
 F2: 4001.30 Hz
 F3: -0.500 ppm
 F4: -200.07 Hz
 F5: 0.31618 ppm/cm
 F6: 127.31409 Hz/cm

NMR

Current Data Parameters
NAME n
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060725
Time 14.18
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 36.9
DM 48.400 usec
DE 6.00 usec
TE 295.2 K
D1 2.0000000 sec
NOREST 0.0000000 sec
NORMK 0.01500000 sec

***** CHANNEL f1 *****

NUC1 1H
P1 9.20 usec
PL1 -6.00 dB
SFO1 500.130095 MHz

F2 - Processing parameters

SI 32768
SF 500.1300043 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CV 33.00 cm
CY 15.00 cm
F1P 10.000 ppm
F1 500.130 Hz
F2P -260.07 Hz
F2 0.31818 ppm/cm
PCNOM 159.13228 Hz/cm

7.32489
7.31060
7.29623
7.28211
7.27842
6.78329
6.76815
6.75307
6.73802
6.27260
6.14613
6.11273
6.10977
6.10684
6.10401
6.09928
6.06898
5.94294

3.85568
3.81507
3.80727
3.77572
3.76797
3.75076
3.73521
3.72699
3.71143
3.67091
3.56241
2.43705
2.30860
2.30550
2.30092
2.29821
2.16501
2.15091
2.06969
2.05531
1.72237
1.21215
1.20896
1.20255
1.15628
1.12644
1.11704
1.10922
1.08690
1.08411
1.06791
1.05119
1.04647
1.03215
0.99842
0.96461
0.95121
0.66205
0.13510
0.07610
0.00024

H1-NMR

Current Data Parameters
 NAME: adduct (1-octyne)
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20070423
 Time: 13.02
 INSTRUM: gp400
 PROBRD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 ID: 65536
 SOLVENT: CDCl3
 NS: 8
 DS: 2
 SWH: 8223.685 Hz
 FIDRES: 0.125483 Hz
 AQ: 3.9846387 sec
 RG: 228.1
 DM: 60.800 usec
 DE: 4.50 usec
 TE: 294.2 K
 O1: 2.00000000 sec
 WPREST: 0.00000000 sec
 MCHMK: 0.01500000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 10.50 usec
 PL1: -6.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300102 MHz
 WDM: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 33.00 cm
 CY: 20.00 cm
 FLIP: 10.000 ppm
 F1: 4001.30 Hz
 F2P: -0.500 ppm
 F2: -200.07 Hz
 PRNCH: 0.31818 ppm/cm
 MZCH: 127.31409 Hz/cm

NMR

Current Data Parameters
NAME: adduct(1-pentyl)
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20070422
Time: 15.23
INSTRUM: drx500
PROBHD: 5 mm Multinuc1
PULPROG: zg30
TO: 65536
SOLVENT: CDCl3
NS: 8
DS: 2
SWH: 10330.578 Hz
FIDRES: 0.157632 Hz
AQ: 3.1719923 sec
RG: 35.9
DN: 48.400 usec
DE: 6.00 usec
TE: 294.8 K
O1: 2.00000000 sec
MCREST: 0.00000000 sec
MCMRK: 0.01500000 sec

***** CHANNEL f1 *****
NUC1: 1H
P1: 9.20 usec
PL1: -6.00 dB
SFO1: 500.1300895 MHz

F2 - Processing parameters
SI: 32768
SF: 500.1300163 MHz
WDW: no
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.00

10 NMR plot parameters
CX: 33.00 cm
CY: 15.00 cm
F1P: 10.000 ppm
F1: 5001.30 Hz
F2P: -0.500 ppm
F2: -250.07 Hz
PNUC1: 0.31818 ppm/cm
HZCM: 159.13228 Hz/cm

5.34410
5.33990
5.21444
5.21677
5.21645
5.21450
5.21198

2.16523
2.15023
2.12526
1.96767
1.95313
1.93817
1.91448
1.90566
1.29969
1.29756
1.29162
1.28426
1.08878
1.09237
1.08551
1.08049
1.07706
1.07016
0.90329
0.88945
0.87528

H1-NMR

Current Data Parameters

NAME adduct (1-nonynyl)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070426
Time 13.46
INSTRUM dp400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 143.7
DM 60.800 usec
DE 4.50 usec
TE 294.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCNRC 0.01500000 sec

***** CHANNEL f1 *****

NUC1 1H
P1 10.50 usec
PL1 -6.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters

SI 32768
SF 400.1300112 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

10 NMR plot parameters

CX 33.00 cm
CY 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCH 0.31818 ppm/cm
HZCH 127.31409 Hz/cm

H1-NMR

5.35440
5.35059
5.26707
5.26321

1.55053
1.15135
1.14557
1.05952
1.03164

Current Data Parameters
NAME adduct13-3-dimethyl-1-butynol
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060720
Time 18.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
ZGPG30
TO 65530
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.895 Hz
FIDRES 0.124833 Hz
AQ 3.584633 sec
RG 287.4
DM 60.800 usec
DE 4.50 usec
TE 296.2 K
NUC1 13C
NUC2 1H
ACQRES 0.00000000 sec
MCOREST 0.01500000 sec
MCORX 0.01500000 sec
***** CHANNEL f1 *****
NUC1 1H
P1 10.50 usec
PL1 -6.00 dB
SFO1 400.132710 MHz
F2 - Processing parameters
SI 32768
SF 400.132710 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 NMR D10 parameters
CT 33.00 cm
CY 20.00 cm
F1P 10.000 ppm
F1 400.132710 MHz
F2P -0.500 ppm
F2 -200.07 Hz
PNUCH 0.31818 ppm/cm
HCHN 127.3109 Hz/cm

H1-NMR

Current Data Parameters
 NAME adduct (5-hexyne-1-ol)
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20070426
 Time 13.13
 INSTRUM spect
 PROBP0 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 8223.695 Hz
 FIDRES 0.125493 Hz
 AQ 3.9846397 sec
 RG 161.3
 DW 60.800 usec
 DE 4.50 usec
 TE 294.2 K
 D1 2.00000000 sec
 MCHEST 0.00000000 sec
 MCMK 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL 0.00 dB
 SF01 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 33.00 cm
 CY 20.00 cm
 F1P 16.000 ppm
 F1 4001.30 Hz
 F2P 101.580 ppm
 F2 -200.13 Hz
 BRNCH 0.3118 ppm/cm
 HZCM 127.31409 Hz/cm

NMR

Current Data Parameters
NAME: adduct (5-hexenyl-tri1)
EXPNO: 1
PROCNO: 1

ppm

TIPS

7.2659

5.4520
5.4466
5.3387
5.3358

2.3898
2.3756
2.3614
2.3517
2.3375
2.3234
1.9448
1.9353
1.9211

1.0679
1.0784
1.0709

-0.0001

F2 - Acquisition Parameters
Date_: 20070422
Time: 14.54
INSTRUM: dr4500
PROBHD: 5 mm Multic1
PULPROG: zg30
TD: 65536
SOLVENT: CDCl3
NS: 2
DS: 2
SWH: 10330.578 Hz
FIDRES: 0.157632 Hz
AQ: 3.171933 sec
RG: 80.6
DM: 48.400 usec
DE: 15.000 usec
TE: 294.2 K
D1: 2.00000000 sec
MCREST: 0.00000000 sec
MCWPR: 0.01500000 sec

***** CHANNEL f1 *****
NUC1: 13C
P1: 9.20 usec
PL1: -6.00 dB
SFO1: 500.130085 MHz

F2 - Processing parameters
SI: 32768
SF: 500.130019 MHz
WDW: 0
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CY: 15.00 cm
CX: 15.00 cm
FIP: 10.000 ppm
F1: 5001.30 Hz
F2: -500.07 Hz
PWRCH: 0.31618 dBm/cm
H2OCH: 159.13288 Hz/cm