Supporting Information

Manuscript Title:

Dual role of alkynyl bromides in one-step synthesis of bromo-substituted alkynyl sulfides

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1) Characterization Data

(4-bromobutyl)(phenylethynyl)sulfane (2a): yellow oil,

isolated yield 92% (74.2 mg); ^1H NMR (500 MHz, CDCl_3) δ : 7.42-7.40 (m, 2H), 7.29-7.28 (m, 3H), 3.45 (t, $J = 6.3$ Hz, 2H), 2.82 (t, $J = 6.8$ Hz, 2H), 2.08-2.02 (m, 2H), 2.00-1.95 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 131.38, 128.25, 128.04, 123.32, 93.30, 78.86, 34.70, 32.87, 30.94, 27.68; HRMS (ESI, m/z) calcd for $[\text{C}_{12}\text{H}_{13}\text{BrS}]^+\text{H}^+$: 268.9994; found 269.0000.

(4-bromobutyl)((4-fluorophenyl)ethynyl)sulfane (2b):

yellow oil, isolated yield 76% (65.4 mg); ^1H NMR (500 MHz, CDCl_3) δ : 7.41-7.38 (m, 2H), 7.01-6.98 (m, 2H), 3.46 (t, $J = 6.3$ Hz, 2H), 2.82 (t, $J = 7.0$ Hz, 2H), 2.08-2.03 (m, 2H), 2.01-1.95 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 162.35 (d, $J = 248.0$ Hz), 133.48 (d, $J = 8.1$ Hz), 119.39 (d, $J = 3.5$ Hz), 115.56 (d, $J = 22.1$ Hz), 92.12, 78.52, 34.66, 32.91, 30.92, 27.67; HRMS (ESI, m/z) calcd for $[\text{C}_{12}\text{H}_{12}\text{BrFS}]^+\text{H}^+$: 286.9900; found 286.9900.

(4-bromobutyl)((2-fluorophenyl)ethynyl)sulfane (2c): Pale

yellow oil, isolated yield 81% (69.8 mg); ^1H NMR (500 MHz, CDCl_3) δ : 7.39 (td, $J = 7.5$ Hz, 1.5 Hz, 1H), 7.29-7.24 (m, 1H), 7.09-7.04 (m, 2H), 3.46 (t, $J = 6.3$ Hz, 2H), 2.85 (t, $J = 6.8$ Hz, 2H), 2.09-2.03 (m, 2H), 2.01-1.97 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 162.63 (d, $J = 249.8$ Hz), 133.08, 129.63 (d, $J = 8.0$ Hz), 123.87 (d, $J = 3.6$

Hz), 115.39 (d, $J = 20.8$ Hz), 111.93 (d, $J = 15.8$ Hz), 86.58, 84.49 (d, $J = 2.8$ Hz), 34.69, 32.91, 30.89, 27.58; HRMS (ESI, m/z) calcd for $[C_{12}H_{12}BrFS]H^+$: 286.9900; found 286.9895.

(4-bromobutyl)((4-chlorophenyl)ethynyl)sulfane (2d):

yellow oil, isolated yield 95% (86.4 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.33 (d, $J = 8.5$ Hz, 2H), 7.26 (d, $J = 8.5$ Hz, 2H), 3.46 (t, $J = 6.5$ Hz, 2H), 2.82 (t, $J = 6.8$ Hz, 2H), 2.07-2.02 (m, 2H), 2.00-1.95 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 133.96, 132.55, 128.57, 121.76, 92.15, 80.15, 34.64, 32.88, 30.88, 27.66; HRMS (ESI, m/z) calcd for $[C_{12}H_{12}BrClS]H^+$: 302.9604; found 302.9601.

((2-bromo-4-chlorophenyl)ethynyl)(4-bromobutyl)sulfane (2e):

yellow oil, isolated yield 90% (103.1 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.57 (d, $J = 2.0$ Hz, 1H), 7.33 (d, $J = 8.0$ Hz, 1H), 7.22 (dd, $J = 8.0$ Hz, 2.0 Hz, 1H), 3.46 (t, $J = 6.3$ Hz, 2H), 2.87 (t, $J = 6.5$ Hz, 2H), 2.09-2.01 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 133.95, 133.17, 132.09, 127.43, 125.26, 124.05, 91.11, 85.67, 34.81, 32.89, 30.93, 27.77; HRMS (ESI, m/z) calcd for $[C_{12}H_{11}Br_2ClS]H^+$: 380.8710; found 380.8703.

(4-bromobutyl)((4-bromophenyl)ethynyl)sulfane (2f):

Pale yellow oil, isolated yield 86% (89.8 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.42 (d, $J = 8.0$ Hz, 2H), 7.26 (d, $J = 8.5$ Hz, 2H), 3.46 (t, $J = 6.5$ Hz, 2H), 2.82 (t, $J = 7.0$ Hz,

2H), 2.07-2.02 (m, 2H), 2.00-1.94 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 132.73, 131.49, 122.22, 122.16, 92.23, 80.40, 34.63, 32.88, 30.88, 27.66; HRMS (ESI, m/z) calcd for $[\text{C}_{12}\text{H}_{12}\text{Br}_2\text{S}]\text{H}^+$: 346.9099; found 346.9101.

(4-bromobutyl)((2-bromophenyl)ethynyl)sulfane (2g) :

yellow oil, isolated yield 85% (88.7 mg); ^1H NMR (500 MHz, CDCl_3) δ : 7.55 (dd, J = 8.0 Hz, 1.0 Hz, 1H), 7.41 (dd, J = 8.0 Hz, 2.0 Hz, 1H), 7.23 (td, J = 7.5 Hz, 1.0 Hz, 1H), 7.12 (td, J = 7.8 Hz, 1.5 Hz, 1H), 3.46 (t, J = 6.3 Hz, 2H), 2.86 (t, J = 6.5 Hz, 2H), 2.09-2.02 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ : 132.66, 132.25, 128.89, 126.94, 125.39, 124.83, 91.99, 84.42, 34.77, 32.96, 30.94, 27.74; $[\text{C}_{12}\text{H}_{12}\text{Br}_2\text{S}]\text{H}^+$: 346.9099; found 346.9093.

3-(((4-bromobutyl)thio)ethynyl)benzonitrile (2h) :

Pale yellow oil, isolated yield 86% (75.9 mg); ^1H NMR (500 MHz, CDCl_3) δ : 7.66 (t, J = 1.5 Hz, 1H), 7.60 (dt, J = 8.0, 1.3 Hz, 1H), 7.56 (dt, J = 8.0, 1.5 Hz, 1H), 7.42 (t, J = 7.8 Hz, 1H), 3.47 (t, J = 6.5 Hz, 2H), 2.86 (t, J = 7.0 Hz, 2H), 2.07-2.03 (m, 2H), 2.02-1.96 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 135.07, 134.30, 130.93, 129.15, 124.80, 117.94, 112.65, 91.01, 82.60, 34.58, 32.80, 30.78, 27.63; HRMS (ESI, m/z) calcd for $[\text{C}_{13}\text{H}_{12}\text{BrNS}]\text{H}^+$: 293.9947; found 293.9945.

(4-bromobutyl)((4-nitrophenyl)ethynyl)sulfane (2i) :

yellow oil, isolated yield 91% (85.7 mg); ^1H NMR (500 MHz, CDCl_3) δ : 8.17 (d, J = 9.0 Hz, 2H), 7.50 (d, J = 9.0 Hz, 2H), 3.48 (t, J = 6.3 Hz, 2H), 2.89 (t, J = 6.8 Hz, 2H), 2.10-2.05 (m, 2H), 2.04-1.98 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 146.41, 131.28, 130.20, 123.61, 92.28, 86.56, 34.75, 32.80, 30.80, 27.69; $[\text{C}_{12}\text{H}_{12}\text{BrNO}_2\text{S}]\text{H}^+$: 313.9845; found 313.9836.

(4-bromobutyl)((3-nitrophenyl)ethynyl)sulfane (2j) :

yellow oil, isolated yield 85% (80.1 mg); ^1H NMR (500 MHz, CDCl_3) δ : 8.23 (t, J = 1.8 Hz, 1H), 8.13 (dd, J = 8.5, 2.5 Hz, 1H), 7.69 (dt, J = 7.5, 1.3 Hz, 1H), 7.48 (t, J = 8.0 Hz, 1H), 3.48 (t, J = 6.3 Hz, 2H), 2.88 (t, J = 7.0 Hz, 2H), 2.10-2.04 (m, 2H), 2.03-1.98 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 148.02, 136.68, 129.28, 125.83, 125.08, 122.48, 91.09, 82.94, 34.67, 32.80, 30.86, 27.71; HRMS (ESI, m/z) calcd for $[\text{C}_{12}\text{H}_{12}\text{BrNO}_2\text{S}]\text{H}^+$: 313.9845; found 313.9836.

1-(4-(((4-bromobutyl)thio)ethynyl)phenyl)ethan-1-one (2k):

(2k): Pale yellow solid, isolated yield 92% (85.8 mg); mp: 35.8-36.6 °C; ^1H NMR (500 MHz, CDCl_3) δ : 7.89 (d, J = 8.5 Hz, 2H), 7.46 (d, J = 8.5 Hz, 2H), 3.47 (t, J = 6.5 Hz, 2H), 2.86 (t, J = 6.8 Hz, 2H), 2.59 (s, 3H), 2.09-2.05 (m, 2H), 2.04-1.98 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 197.15, 135.67, 130.91, 128.19, 128.14, 92.95, 83.49, 34.69, 32.84, 30.82, 27.64, 26.53; HRMS (ESI, m/z) calcd for $[\text{C}_{14}\text{H}_{15}\text{BrOS}]\text{H}^+$:

311.0100; found 311.0093.

Pale yellow solid, isolated yield 88% (86.3 mg); mp: 52.8-54.0 °C; ¹H NMR (500

MHz, CDCl₃) δ: 7.96 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 3.91 (s, 3H), 3.47

(t, *J* = 6.3 Hz, 2H), 2.85 (t, *J* = 6.8 Hz, 2H), 2.09-2.04 (m, 2H), 2.03-1.96 (m, 2H);

¹³C NMR (125 MHz, CDCl₃) δ: 166.42, 130.78, 129.42, 128.95, 127.95, 92.93, 83.01,

52.15, 34.69, 32.83, 30.85, 27.66; HRMS (ESI, *m/z*) calcd for [C₁₄H₁₅BrO₂S]⁺:

327.0049; found 327.0040.

(2m): yellow oil, isolated yield 63% (56.5 mg); ¹H NMR (500 MHz, CDCl₃) δ: 7.37

(d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 8.5 Hz, 2H), 3.80 (s, 3H), 3.46 (t, *J* = 6.5 Hz, 2H),

2.80 (t, *J* = 6.8 Hz, 2H), 2.06-2.02 (m, 2H), 1.99-1.94 (m, 2H); ¹³C NMR (125 MHz,

CDCl₃) δ: 159.59, 133.34, 115.38, 113.88, 93.05, 76.83, 55.25, 34.74, 32.97, 30.97,

27.65; HRMS (ESI, *m/z*) calcd for [C₁₃H₁₅BrOS]⁺: 299.0100; found 299.0094.

isolated yield 73% (61.9 mg); ¹H NMR (500 MHz, CDCl₃) δ: 7.31 (d, *J* = 8.0 Hz, 2H),

7.10 (d, *J* = 8.0 Hz, 2H), 3.45 (t, *J* = 6.5 Hz, 2H), 2.80 (t, *J* = 7.0 Hz, 2H), 2.34 (s, 3H),

2.07-2.02 (m, 2H), 2.00-1.94 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ: 138.28, 131.44,

129.01, 120.20, 93.34, 77.78, 34.68, 32.95, 30.94, 27.64, 21.45; HRMS (ESI, *m/z*)

calcd for $[C_{13}H_{15}BrS]H^+$: 283.0151; found 283.0150.

(2o): yellow oil, isolated yield 73% (68.1 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.33

(d, J = 8.0 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 3.45 (t, J = 6.5 Hz, 2H), 2.80 (t, J = 6.8

Hz, 2H), 2.56 (t, J = 7.5 Hz, 2H), 2.06-2.02 (m, 2H), 2.00-1.94 (m, 2H), 1.65-1.59 (m,

2H), 0.92 (t, J = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 143.07, 131.46, 128.43,

120.45, 93.39, 77.78, 37.88, 34.70, 32.94, 30.94, 27.65, 24.28, 13.71; HRMS (ESI,

m/z) calcd for $[C_{15}H_{19}BrS]H^+$: 311.0464; found 311.0465.

(2p): yellow oil, isolated yield 74% (75.3 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.33

(d, J = 8.0 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 3.45 (t, J = 6.5 Hz, 2H), 2.80 (t, J = 6.8

Hz, 2H), 2.58 (t, J = 7.8 Hz, 2H), 2.07-2.02 (m, 2H), 2.00-1.94 (m, 2H), 1.62-1.56 (m,

2H), 1.34-1.27 (m, 4H), 0.88 (t, J = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ :

143.32, 131.47, 128.36, 120.39, 93.38, 77.76, 35.78, 34.69, 32.93, 31.35, 30.94, 30.86,

27.64, 22.46, 13.97; HRMS (ESI, m/z) calcd for $[C_{17}H_{23}BrS]H^+$: 339.0777; found

339.0772.

(2q): yellow solid, isolated yield 92% (95.2 mg); mp: 38.8-40.0 °C; 1H NMR (500

MHz, $CDCl_3$) δ : 7.57 (d, J = 7.5 Hz, 2H), 7.53 (t, J = 8.0 Hz, 2H), 7.48 (d, J = 8.5 Hz,

2H), 7.43 (t, $J = 7.8$ Hz, 2H), 7.35 (t, $J = 7.3$ Hz, 1H), 3.46 (t, $J = 6.3$ Hz, 2H), 2.83 (t, $J = 6.8$ Hz, 2H), 2.09-2.05 (m, 2H), 2.03-1.98 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 140.75, 140.22, 131.85, 128.81, 127.59, 126.93 (2C), 122.19, 93.19, 79.53, 34.74, 32.95, 30.94, 27.68; HRMS (ESI, m/z) calcd for $[\text{C}_{18}\text{H}_{17}\text{BrS}]^+$: 345.0307; found 345.0314.

(4-bromobutyl)(naphthalen-1-ylethynyl)sulfane (2r) :

yellow oil, isolated yield 73% (69.8 mg); ^1H NMR (500 MHz, CDCl_3) δ : 8.28 (d, $J = 8.0$ Hz, 1H), 7.83 (t, $J = 8.0$ Hz, 1H), 7.79 (d, $J = 8.5$ Hz, 1H), 7.64 (dd, $J = 7.0, 0.5$ Hz, 1H), 7.56 (td, $J = 7.5, 1.5$ Hz, 1H), 7.50 (td, $J = 7.5, 1.0$ Hz, 1H), 7.40 (t, $J = 7.8$ Hz, 1H), 3.46 (t, $J = 6.3$ Hz, 2H), 2.89 (t, $J = 6.5$ Hz, 2H), 2.11-2.01 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ : 133.25, 133.10, 130.27, 128.51, 128.26, 126.75, 126.38, 126.04, 125.18, 120.96, 91.47, 83.65, 34.96, 32.94, 30.98, 27.81; HRMS (ESI, m/z) calcd for $[\text{C}_{16}\text{H}_{15}\text{BrS}]^+$: 319.0151; found 319.0142.

2-(((4-bromobutyl)thio)ethynyl)thiophene (2s) :

yellow oil, isolated yield 75% (61.9 mg); ^1H NMR (500 MHz, CDCl_3) δ : 7.26 (d, $J = 5.0$ Hz, 1H), 7.22 (d, $J = 3.5$ Hz, 1H), 6.96 (dd, $J = 5.0, 3.5$ Hz, 1H), 3.45 (t, $J = 6.5$ Hz, 2H), 2.81 (t, $J = 6.8$ Hz, 2H), 2.06-2.01 (m, 2H), 1.98-1.92 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 132.95, 127.77, 126.90, 123.42, 85.93, 83.34, 34.94, 32.87, 30.92, 27.67;

HRMS (ESI, m/z) calcd for $[C_{10}H_{11}BrS_2]^+$: 274.9558; found 274.9552.

1-(((4-bromobutyl)thio)ethynyl)cyclohexan-1-ol (2t) :

yellow oil, isolated yield 42% (36.7mg); 1H NMR (500 MHz, $CDCl_3$) δ : 3.45 (t, J = 6.5 Hz, 2H), 2.73 (t, J = 7.0 Hz, 2H), 2.11 (s, 1H), 2.05-1.99 (m, 2H), 1.95-1.90 (m, 4H), 1.71-1.68 (m, 2H), 1.61-1.52 (m, 4H), 1.29-1.22 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 97.61, 73.63, 69.49, 39.86, 34.34, 32.98, 30.84, 27.51, 25.09, 23.29;

HRMS (ESI, m/z) calcd for $[C_{12}H_{19}BrOS]^+$: 291.0413; found 291.0407.

and

(4-chlorobutyl)(phenylethynyl)-sulfane (2u) and (4-bromobutyl)(phenylethynyl)sulfane (2a) :

2u:2a = 1.6:1; yellow oil, isolated yield 70% (74.2 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.42-7.40 (m, 3.2H), 7.29-7.28 (m, 4.8H), 3.59 (t, J = 6.0 Hz, 2H), 3.45 (t, J = 6.3 Hz, 1.2H), 2.84-2.81 (m, 3.2H), 2.07-2.03 (m, 1.2H), 1.98-1.97 (m, 5.2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 131.40 (2C), 128.26 (2C), 128.05 (2C), 123.37 (2C), 93.33, 93.29, 78.91 (2C), 44.29, 34.89, 34.73, 32.82, 30.97, 30.86, 27.70, 26.48; **2u**: MS (EI): m/z (%) = 134 (100), 224 (47) $[M^+]$, 226 (17) $[M^+]$; **2a**: MS (EI): m/z (%) = 135 (100), 268 (31) $[M^+]$, 270 (31) $[M^+]$.

and

(chloromethyl)((4-methoxyphenyl)ethynyl)sulfane (2v) and (bromomethyl)((4-methoxyphenyl)ethynyl)sulfane (2m):

2v:2m = 1.6:1; yellow oil, isolated yield 55% (74.2 mg); 1H NMR (500 MHz, $CDCl_3$) δ : 7.37 (d, J = 8.5 Hz, 3.2H), 6.82 (d, J = 9.0 Hz, 3.2H), 3.80 (s, 4.8H), 3.59 (t, J = 6.0 Hz, 2H), 3.45 (t, J = 6.5 Hz, 1.2H), 2.81-2.79 (m, 3.2H), 2.06-2.03 (m, 1.2H), 1.98-1.95 (m, 5.2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 159.66

(2C), 133.35 (2C), 115.49 (2C), 113.93 (2C), 93.11, 93.08, 76.93 (2C), 55.27, 44.33, 34.97, 34.81, 32.87, 31.03, 30.91, 27.71, 26.48; **2v**: MS (EI): m/z (%) = 164 (100), 254 (59) $[M^+]$, 256 (21) $[M^+]$; **2m**: MS (EI): m/z (%) = 164 (100), 298 (51) $[M^+]$, 300 (54) $[M^+]$.

2) Scanned ^1H NMR and ^{13}C NMR Spectra of All New Compounds

H-L22

NAME yangyuan130227
EXPNO 1
PROCNO 1
Date_ 20130227
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SF01 500.1330885 MHz
SI 32768
SF 500.1300114 MHz
WDW nc
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

C-L22

NAME yangyuan130227
EXPNO 2
PROCNO 1
Date_ 20130227
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
FULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 104
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 9.80 usec
PL1 2.80 dB
PL1W 52.46661758 W
SF01 125.7703643 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.89 dB
PL13 16.70 dB
PL2W 9.90558243 W
PL12W 0.32127732 W
PL13W 0.33564481 W
SF02 500.1326005 MHz
SI 32768
SF 125.7577977 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

H-L20

NAME yangyuan130226
EXPNO 9
PROCNO 1
Date 20130226
Time 16.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719823 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300124 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

C-L20

NAME yangyuan130226
EXPNO 10
PROCNO 1
Date 20130226
Time 16.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 73
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 2.80 dB
PL1W 52.46661758 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.69 dB
PL13 16.70 dB
PL2W 9.90558243 W
PL12W 0.32127732 W
PL13W 0.33564481 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578009 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

H-L41
 NAME yangyuan130316
 EXPNO 5
 PROCNO 1
 Date 20130316
 Time 11.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 80.6
 DW 48.400 usec
 DE 6.50 usec
 TE 294.7 K
 D1 1.00000000 sec
 TDO 1
 CHANNEL f1
 NUC1 1H
 P1 14.40 usec
 PL1 2.00 dB
 PL1W 9.90558243 W
 SF01 500.1330885 MHz
 ST 32768
 SF 500.1300138 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

C-L41
 NAME yangyuan130316
 EXPNO 6
 PROCNO 1
 Date 20130316
 Time 11.46
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 80
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 2050
 DW 16.800 usec
 DE 6.50 usec
 TE 295.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 CHANNEL f1
 NUC1 13C
 P1 9.80 usec
 PL1 2.80 dB
 PL1W 52.46661758 W
 SF01 125.7703643 MHz
 CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 16.89 dB
 PL13 16.70 dB
 PL2W 9.90558243 W
 PL12W 0.32127732 W
 PL13W 0.33564481 W
 SF02 500.1320005 MHz
 SF 125.7578031 MHz
 ST 32768
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

H-L15

NAME yangyuan130226
EXPNO 7
PROCNO 1
Date 20130226
Time 16.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 90.3
DW 48.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SFO1 500.130885 MHz
SI 32768
SF 500.1300067 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

C-L15

NAME yangyuan130226
EXPNO 8
PROCNO 1
Date 20130226
Time 16.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 2.80 dB
PL1W 52.46661758 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.89 dB
PL13 16.70 dB
PL2W 9.90558243 W
PL12W 0.32127732 W
PL13W 0.33564481 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578004 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

and
2u and 2a

H-J55 (1)

NAME	yangyuan140509
EXPNO	1
PROCNO	1
Date_	20140509
Time	14.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	10330.576 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	90.5
DW	48.400 usec
DE	6.50 usec
TE	297.7 K
D1	1.00000000 sec
TD0	1

===== CHANNEL f1 =====

NUC1	1H
P1	13.70 usec
PL1	1.00 dB
PL1W	12.47038937 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300205 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

and
2u and 2a

C-J55 (1)

NAME	yangyuan140509
EXPNO	2
PROCNO	1
Date_	20140509
Time	14.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	119
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	299.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

===== CHANNEL f1 =====

NUC1	13C
P1	9.00 usec
PL1	1.00 dB
PL1W	79.41143799 W
SFO1	125.7703643 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	15.93 dB
PL13	15.93 dB
PL12W	12.47038937 W
PL12W	0.40075597 W
PL13W	0.40075597 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577959 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

H-J55(2)

NAME	yangyuan140509
EXPNO	3
PROCNO	1
Date_	20140509
Time	14.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	128
DW	48.400 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TDO	1

===== CHANNEL f1 =====

NUC1	1H
P1	13.70 usec
PL1	1.00 dB
PL1W	12.47038937 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300160 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

C-J55(2)

NAME	yangyuan140509
EXPNO	4
PROCNO	1
Date_	20140509
Time	15.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	160
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	300.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

===== CHANNEL f1 =====

NUC1	13C
P1	9.00 usec
PL1	1.00 dB
PL1W	79.41143799 W
SFO1	125.7703643 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	15.93 dB
PL13	15.93 dB
PL1W	12.47038937 W
PL12W	0.40075597 W
PL13W	0.40075597 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577932 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40