Supporting Information

Synthesis of poly-functionalized benzofurans via one-pot domino oxidation/[3+2] cyclization reactions of a hydroquinone ester and ynamides

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1. General

$^1$H NMR and $^{13}$C NMR were recorded on a Bruker-400 MHz spectrometer. Proton chemical shifts are reported in ppm downfield from tetramethylsilane or from the residual solvent as internal standard in CDCl$_3$ (δ 7.26 ppm). Carbon chemical shifts were internally referenced to the deuterated solvent signals in CDCl$_3$ (δ 77.0 ppm). High-resolution mass spectra were recorded on a Thermo Scientific LTQ Orbitrap ESI ion trap mass spectrometer. Reagents obtained from commercial sources are used without further purification and all solvents were purified and dried according to standard methods prior to use, unless stated otherwise.

2. Preparation of ynamides

**General procedure for the preparation of ynamides 1.** Based on the literature procedures,$^{1,2}$ amide (3.0-4.0 mmol), CuCl$_2$ (26.9 mg, 0.20 mmol), and Na$_2$CO$_3$ (212.0 mg, 2.0 mmol) were combined in a 50 mL three-neck round-bottom flask. The flask was purged with O$_2$ for 10 min and connected with a balloon filled with O$_2$. A solution of pyridine (160.0 μL, 2.0 mmol) in 8.0 mL dry toluene was added to the reaction flask via a syringe and the flask was heated to 70 °C. A solution of alkyne (1.0 mmol) in 5.0 mL dry toluene was added to the flask slowly over a period of 3-4 h. After complete addition of the alkyne, the reaction mixture was allowed to stir at 70 °C for another 10 h. After cooling to room temperature, the crude mixture was filtered through a pad of Celite, concentrated by rotary evaporation, and purified by flash chromatography to provide the desired product, which was later stored in the freezer.

**Procedure for a 6 mmol-scale reaction for the synthesis of 1h.** Methyl indole-3-carboxylate (3.15 g, 18.0 mmol), CuCl$_2$ (161.4 mg, 1.2 mmol), and Na$_2$CO$_3$ (1.27 g, 12.0 mmol) were combined in a 250 mL three-neck round-bottom flask. The flask was purged with O$_2$ for 10 min and connected with a balloon filled with O$_2$. A solution of pyridine (966.7 μL, 12.0 mmol) in 45.0 mL dry toluene was added to the reaction flask via a syringe and the flask was heated to 70 °C. A solution of 1-heptyne (577.1 mg, 6.0 mmol) in 30.0 mL dry toluene was added to the flask slowly over a period of 4 h. After complete addition of the alkyne, the reaction mixture was allowed to stir at 70 °C for another 20 h. After cooling to room temperature, the crude mixture was filtered through a pad of Celite, concentrated by rotary evaporation, and purified by flash chromatography to provide 1h (1.10 g, 68%).

Ynamides 1a,$^1$ 1b,$^1$ 1c,$^2$ 1d,$^1$ 1e,$^1$ and 1g$^1$ are known compounds and characterizations are the same as reported.

1-(Hept-1-yn-1-yl)azetidin-2-one (1f)

![1f](synthesis of 1f)

Synthesized by the general procedure; 138.7 mg (84%).

Yellow oil. $^1$H NMR (400 MHz, CDCl3): δ = 0.87 (t, J = 6.8 Hz, 3H, CH$_3$), 1.23-1.36 (m, 4H, CH$_2$×2), 1.45-1.52 (m, 2H, CH$_2$), 2.25 (t, J = 7.2Hz, 2H, CH$_2$), 2.97 (t, J = 4.7 Hz, 2H, CH$_2$), 3.55 (t, J = 4.8 Hz, 2H, CH$_2$) ppm; $^{13}$C NMR (100 MHz, CDCl3): δ = 13.9, 18.3, 22.1, 28.4,
30.9, 37.4, 42.8, 69.9, 70.2, 167.2 ppm. HRMS (ESI): calcd. for C_{16}H_{16}NO ([M + H]^+) 166.1226, found 166.1228.

**Methyl 1-(hept-1-yn-1-yl)-1H-indole-3-carboxylate (1h)**

![Methyl 1-(hept-1-yn-1-yl)-1H-indole-3-carboxylate](image)

Synthesized by the general procedure; 177.7 mg (66%). Colorless solid. $^1$H NMR (400 MHz, CDCl3): $\delta = 0.95$ (t, $J = 7.1$ Hz, 3H, CH$_3$), 1.34-1.51 (m, 4H, CH$_2 \times 2$), 1.62-1.68 (m, 2H, CH$_2$), 2.47 (t, $J = 7.0$ Hz, 2H, CH$_2$), 3.92 (s, 3H, CH$_3$), 7.31-7.39 (m, 2H, ArH), 7.55 (d, $J = 8.0$ Hz, 1H, ArH), 7.89 (s, 1H, ArH), 8.16 (d, $J = 7.4$Hz, 1H, ArH) ppm; $^{13}$C NMR (100 MHz, CDCl3): $\delta = 14.0$, 18.3, 22.2, 28.4, 31.0, 51.3, 70.5, 71.8, 109.8, 111.4, 121.7, 123.3, 124.1, 125.1, 135.2, 138.5, 164.5 ppm. HRMS (ESI): calcd. for C$_{17}$H$_{20}$NO$_2$ ([M + H]^+) 270.1489, found 270.1490.

3. **Procedure for the oxidation of hydroquinone ester 5**

According to literature procedure$^3$, silver oxide (2.09 g, 9.0 mmol) and magnesium sulfate (1.08 g, 9.0 mmol) were added to a solution of methyl 2,5-dihydroxybenzoate (5) (504.5 mg, 3.0 mmol) in diethyl ether (50 mL). The reaction mixture was stirred at 25 °C for 3 h. After filtration through a pad of Celite, the filtrate was concentrated in vacuo and purified by flash chromatography to furnish the desired quinone ester 2b. Characterizations are the same as reported.

**Oxidation using O$_2$ as the oxidant.** Hydroquinone ester 5 (20.2 mg, 0.12 mmol), MgSO$_4$ (28.9 mg, 0.24 mmol) were mixed in CH$_2$Cl$_2$ (2.0 mL) under oxygen atmosphere (use of O$_2$ balloon). The reaction was stirred at room temperature (25 °C) for 8 h. TLC indicated that only small amount of 5 was oxidized, which indicated that O$_2$ is not a good oxidant for the oxidation of 5.

4. **Procedures for the one-pot domino oxidation/[3+2] cyclization**

**General procedure for the one-pot domino oxidation/[3+2] cyclization.** Hydroquinone ester 5 (20.2 mg, 0.12 mmol), Ag$_2$O (55.6 mg, 0.24 mmol) and MgSO$_4$ (28.9 mg, 0.24 mmol) were mixed in CH$_2$Cl$_2$ (2.0 mL) and stirred at room temperature (25 °C) for 2 h. Then, ynamide 1 (0.1 mmol) and Sc(OTf)$_3$ (1.0 mg, 0.002 mmol) were added to the above mixture. All the reactions finished with 5 min. The crude reaction mixture was filtered through a pad of Celite, concentrated by rotary evaporation, and purified by flash chromatography to provide the desired product 3.

**Procedure for a large scale one-pot reaction.** Hydroquinone ester 5 (1.23 g, 4.90 mmol), Ag$_2$O (3.41 g, 14.7 mmol) and MgSO$_4$ (1.77 g, 14.7 mmol) were mixed in CH$_2$Cl$_2$ (60.0 mL) and stirred at room temperature (25 °C) for 4 h. Ynamide 1h (1.10 g, 4.08 mmol) and Sc(OTf)$_3$ (20.2 mg, 0.041 mmol) were added to the above mixture. The reaction was allowed to stir for 30 min. Then, the crude reaction mixture was filtered through a pad of Celite, concentrated by rotary evaporation, and purified by flash chromatography to provide the desired product 3h (1.64 g, 92%).
Methyl 2-((N,4-dimethylphenyl)sulfonamido)-5-hydroxy-3-phenylbenzofuran-4-carboxylate (3a)

Synthesized by the general procedure; 40.9 mg (91%).
Light yellow solid. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta = 2.45\) (s, 3H, CH\(_3\)), 2.98 (s, 3H, CH\(_3\)), 3.02 (s, 3H, CH\(_3\)), 7.02 (d, \(J = 9.0\) Hz, 1H, ArH), 7.27-7.42 (m, 7H, ArH), 7.53 (d, \(J = 9.0\) Hz, 1H, ArH), 7.61 (d, \(J = 8.3\) Hz, 2H, ArH), 10.8 (s, 1H, OH) ppm; \(^1^3\)C NMR (100 MHz, CDCl\(_3\)): \(\delta = 21.6, 37.7, 51.0, 105.1, 115.7, 118.5, 119.4, 126.0, 127.0, 127.9, 128.2, 129.1, 129.6, 133.9, 135.0, 144.1, 146.0, 148.1, 159.1, 170.0\) ppm; HRMS (ESI): calcd. for C\(_{24}\)H\(_{22}\)NO\(_6\)S ([M + H]\(^+\)) 452.1162, found 452.1163.

Methyl 2-((N,4-dimethylphenyl)sulfonamido)-5-hydroxy-3-(4-methoxyphenyl)benzofuran-4-carboxylate (3b)

Synthesized by the general procedure; 42.3 mg (88%).
Light yellow solid. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta = 2.46\) (s, 3H, CH\(_3\)), 2.97 (s, 3H, CH\(_3\)), 3.11 (s, 3H, CH\(_3\)), 3.87 (s, 3H, CH\(_3\)), 6.94 (d, \(J = 8.6\) Hz, 2H, ArH), 7.01 (d, \(J = 9.0\) Hz, 1H, ArH), 7.23-7.30 (m, 4H, ArH), 7.50 (d, \(J = 9.0\) Hz, 1H, ArH), 7.64 (d, \(J = 8.2\) Hz, 2H, ArH), 10.71 (s, 1H, OH) ppm; \(^1^3\)C NMR (100 MHz, CDCl\(_3\)): \(\delta = 29.7, 37.7, 51.2, 55.3, 105.2, 113.3, 115.6, 118.4, 119.1, 124.1, 126.2, 128.2, 129.57, 129.58, 130.1, 135.2, 144.1, 146.0, 148.2, 159.1, 170.1\) ppm; HRMS (ESI): calcd. for C\(_{25}\)H\(_{24}\)NO\(_7\)S ([M + H]\(^+\)) 482.1268, found 482.1265.

Methyl 2-((N,4-dimethylphenyl)sulfonamido)-5-hydroxy-3-pentylbenzofuran-4-carboxylate (3c)
Synthesized by the general procedure; 41.8 mg (94%).
Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$): $\delta = 0.88$ (t, $J = 6.8$ Hz, 3H, CH$_3$), 1.29-1.46 (m, 6H, CH$_2$×3), 2.46 (s, 3H, CH$_3$), 2.85 (t, $J = 7.6$ Hz, 2H, CH$_2$), 3.16 (s, 3H, CH$_3$), 4.02 (s, 3H, CH$_3$), 6.94 (d, $J = 9.0$ Hz, 1H, ArH), 7.32 (d, $J = 8.0$ Hz, 2H, ArH), 7.36 (d, $J = 9.0$ Hz, 1H, ArH), 7.68 (d, $J = 8.3$ Hz, 1H, ArH), 10.9 (s, 1H, OH) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 14.1, 21.6, 22.6, 25.9, 29.3, 32.1, 37.6, 51.9, 105.4, 115.2, 118.5, 118.6, 125.7, 128.1, 129.6, 134.7, 144.2, 146.1, 147.8, 159.2, 170.7$ ppm; HRMS (ESI): calcd. for C$_{23}$H$_{28}$NO$_6$S ([M + H]$^+$) 446.1632, found 446.1634.

Methyl 2-((N,4-dimethylphenyl)sulfonamido)-5-hydroxy-3-(triisopropylsilyl)benzofuran-4-carboxylate (3d)

Synthesized by the general procedure; 45.4 mg (85%).
Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$): $\delta = 1.20$ (br, 18H, CH$_3$×6), 1.61-1.68 (m, 3H, CHx3), 2.48 (s, 3H, CH$_3$), 3.02 (s, 3H, CH$_3$), 3.94 (s, 3H, CH$_3$), 6.93 (d, $J = 9.0$ Hz, 1H, ArH), 7.29 (d, $J = 9.0$ Hz, 1H, ArH), 7.34 (d, $J = 8.2$ Hz, 2H, ArH), 7.71 (d, $J = 8.2$ Hz, 2H, ArH), 9.51 (s, 1H, OH) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 13.5, 20.0, 38.7, 52.8, 109.3, 110.8, 115.2, 116.9, 127.3, 129.2, 129.4, 130.0, 130.7, 133.6, 144.4, 146.8, 156.3, 170.0$ ppm; HRMS (ESI): calcd. for C$_{27}$H$_{38}$NO$_6$Si ([M + H]$^+$) 532.2184, found 532.2189.

Methyl 5-hydroxy-2-(2-oxazetidin-1-yl)-3-phenylbenzofuran-4-carboxylate (3e)

Synthesized by the general procedure; 28.8 mg (85%).
Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$): $\delta = 2.99$ (s, 3H, CH$_3$), 3.03 (t, $J = 4.8$ Hz, 2H, CH$_2$), 3.20 (t, $J = 4.7$ Hz, 2H, CH$_2$), 6.91 (d, $J = 9.0$ Hz, 1H, ArH), 7.29-7.31 (m, 2H, ArH), 7.36-7.43 (m, 3H, ArH), 7.59 (d, $J = 8.9$ Hz, 1H, ArH), 10.9 (s, 1H, OH) ppm; $^{13}$C
NMR (100 MHz, CDCl₃): δ = 38.0, 41.0, 50.8, 104.4, 108.0, 113.8, 118.2, 126.8, 127.3, 127.7, 130.2, 133.6, 145.1, 145.9, 159.5, 164.1, 170.3 ppm; HRMS (ESI): calcd. for C₁₀H₁₆NO₅ ([M + H]⁺) 338.1023, found 338.1022.

Methyl 5-hydroxy-2-(2-oxazetidin-1-yl)-3-pentylbenzofuran-4-carboxylate (3f)

Synthesized by the general procedure; 30.1 mg (91%).
Light yellow solid. ¹H NMR (400 MHz, CDCl₃): δ = 0.87 (t, J = 6.9 Hz, 3H, CH₃), 1.25-1.45 (m, 6H, CH₂×3), 2.80 (t, J = 7.6 Hz, 2H, CH₂), 3.21 (t, J = 4.7 Hz, 2H, CH₂), 3.81 (t, J = 4.6 Hz, 2H, CH₂), 3.99 (s, 3H, CH₃), 6.89 (d, J = 9.0 Hz, 1H, ArH), 7.45 (d, J = 9.0 Hz, 1H, ArH), 10.9 (s, 1H, OH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ = 14.1, 22.6, 25.1, 29.7, 31.9, 37.3, 40.9, 51.8, 105.1, 110.8, 114.1, 118.2, 126.6, 144.6, 145.6, 159.2, 164.5, 170.8 ppm; HRMS (ESI): calcd. for C₁₈H₂₂NO₅ ([M + H]⁺) 332.1492, found 332.1494.

Methyl 1-(5-hydroxy-4-(methoxycarbonyl)-3-phenylbenzofuran-2-yl)-1H-indole-3-carboxylate (3g)

Synthesized by the general procedure; 39.6 mg (90%).
Light yellow solid. ¹H NMR (400 MHz, CDCl₃): δ = 3.05 (s, 3H, CH₃), 3.86 (s, 3H, CH₃), 7.09 (d, J = 9.0 Hz, 1H, ArH), 7.16-7.19 (m, 2H, ArH), 7.28-7.34 (m, 5H, ArH), 7.42-7.44 (m, 1H, ArH), 7.60 (s, 1H, ArH), 7.67 (d, J = 9.0 Hz, 1H, ArH), 8.14-8.16 (m, 1H, ArH), 10.8 (s, 1H, OH) ppm; ¹³C NMR(100 MHz, CDCl₃): δ = 51.12, 51.26, 105.1, 110.9, 111.7, 115.7, 118.6, 121.7, 123.2, 124.2, 126.0, 126.1, 127.5, 128.4, 128.9, 132.8, 133.9, 137.5, 145.8, 146.0, 159.5, 164.7, 170.0 ppm; HRMS (ESI): calcd. for C₂₆H₂₀NO₆ ([M + H]⁺) 442.1285, found 442.1284.

Methyl 1-(5-hydroxy-4-(methoxycarbonyl)-3-pentylbenzofuran-2-yl)-1H-indole-3-carboxylate (3h)
Synthesized by the general procedure; 41.2 mg (90%); for a large scale reaction 1.64 g (92%). Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$): $\delta = 0.72$ (t, $J = 6.7$ Hz, 3H, CH$_3$), 1.05-1.12 (m, 3H, CH$_2$$\times$1.5), 1.35-1.45 (m, 3H, CH$_2$$\times$1.5), 2.64 (t, $J = 7.6$ Hz, 2H, CH$_2$), 3.96 (s, 3H, CH$_3$), 4.04 (s, 3H, CH$_3$), 7.05 (d, $J = 9.0$ Hz, 1H, ArH), 7.28-7.39 (m, 3H, ArH), 7.59 (d, $J = 9.0$ Hz, 1H, ArH), 7.96 (s, 1H, ArH), 8.24-8.27 (m, 1H, ArH), 11.0 (s, 1H, OH) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 13.8$, 22.3, 25.5, 29.5, 31.5, 51.4, 52.0, 105.4, 111.0, 111.3, 115.0, 115.7, 119.0, 121.9, 123.2, 124.3, 125.7, 126.1, 134.3, 137.8, 145.1, 146.5, 159.6, 164.9, 170.5 ppm; HRMS (ESI): calcd. for C$_{25}$H$_{26}$NO$_6$ ([M + H]$^+$) 436.1755, found 436.1777.

5. References

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[3] Y. H. Chen, D. J. Cheng, J. Zhang, Y. Wang, X. Y. Liu and B. Tan, J. Am. Chem. Soc., 2015, 137, 15062.
NAME       ynamide-1f
EXPNO      20190228
PROCNO     1
Date_      20190228
Time       19.58
INSTRUM     spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD         65536
SOLVENT    CDC13
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ          3.9846387 sec
RG          80.6
DW         60,800 usec
DE          6.50 usec
TE         293.9 K
D1         1.00000000 sec
TDO        1

-------- CHANNEL f1 ---------
NUC1       1H
P1         14.80 usec
PL1        -1.00 dB
PL1W       10.90985775 W
SF01       400.1724712 MHz
SI          32768
SF         400.1700156 MHz
WDW        no
SSB        0
LB          0.00 Hz
GB          0
PC         1.00
NAME           fanyin 5
EXPNO          20181127
PROCNO                1
Date_          20181127
Time              15.35
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65356
SOLVENT           CDCl3
NS                16
DS                2
SNH     8223.685 Hz
FIDRES     0.125483 Hz
AQ            3.9846387 sec
RG       228
DW    60.800 usec
DE        6.50 usec
TE           296.0 K
D1   1.00000000 sec
TD0                1

-------- CHANNEL f1 --------
NUC1                 1H
P1            14.80 usec
PL1           -1.00 dB
PL1W        10.90985775 W
SF01       400.1724712 MHz
SI            32768
SF        400.1700153 MHz
WDW            no
SSB              0
LB            0.00 Hz
GB            0
PC        1.000000

ppm
NAME               dz01
EXPNO        2018113004
PROCNO                1
Date_          20181130
Time              22.38
INSTRUM           spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD               68536
SOLVENT        CDC13
NS                12000
DS                 4
SWH        24038.461 Hz
FIDRES    0.366798 Hz
AQ          1.3631988 sec
RG               2050
DW        20.800 usec
DE                6.50 usec
TE            295.9 K
D1       2.00000000 sec
D11     0.03000000 sec
TD0                 1

-------- CHANNEL f1 --------
NUC1                13C
P1               9.90 usec
PL1        -1.10 dB
PL1W       40.29647064 W
SF01     100.6328888 MHz

-------- CHANNEL f2 --------
CPDPRG2         waltz16
NUC2                1H
PCPD2        90.00 usec
PL2        -1.00 dB
PL12         14.68 dB
PL13        17.68 dB
PL2W    10.90985775 W
PL12W    0.29499799 W
PL13W    0.14784923 W
SF02    400.1716007 MHz
SI        32768
SF    100.6228303 MHz
WDW             no
SSB                0
LB            0.00 Hz
GB                0
PC            1.40
NAME               dz02
EXPNO        2018113002
PROCNO                1
Date_          20181130
Time              21.25
INSTRUM           spect
PROBHD ...                1093
SOLVENT           CDC13
NS                 1093
DS            4
SWH     24038.461 Hz
FIDRES          0.366798 Hz
RQ                 2050
DW               20.800 usec
DE                 6.50 usec
TE                295.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                                      1

-------- CHANNEL f1 --------
NUC1               13C
P1                 9.90 usec
PL1           -1.10 dB
PL1W      40.29647064 W
SF01           100.6328888 MHz

-------- CHANNEL f2 --------
CPDPRG2         waltz16
NUC2               1H
PCPD2            90.00 usec
PL2                 -1.00 dB
PL2W     0.29499799 W
PL3W        0.14784923 W
SF02       400.1716007 MHz
SI                32768
SF       100.6228319 MHz
NDW                   no
SSB                   no
LR                 0.00 Hz
GB                 0
PC                1.40

200  180  160  140  120  100  80  60  40  20  ppm

NAME               dz02
EXPNO        2018113002
PROCNO                1
Date_          20181130
Time              21.25
INSTRUM           spect
PROBHD ...                1093
SOLVENT           CDC13
NS                 1093
DS            4
SWH     24038.461 Hz
FIDRES          0.366798 Hz
RQ                 2050
DW               20.800 usec
DE                 6.50 usec
TE                295.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                                      1

-------- CHANNEL f1 --------
NUC1               13C
P1                 9.90 usec
PL1           -1.10 dB
PL1W      40.29647064 W
SF01           100.6328888 MHz

-------- CHANNEL f2 --------
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NUC2               1H
PCPD2            90.00 usec
PL2                 -1.00 dB
PL2W     0.29499799 W
PL3W        0.14784923 W
SF02       400.1716007 MHz
SI                32768
SF       100.6228319 MHz
NDW                   no
SSB                   no
LR                 0.00 Hz
GB                 0
PC                1.40

200  180  160  140  120  100  80  60  40  20  ppm
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EXPNO      2018121806
PROCNO     1
Date_      20181219
Time       20.52
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         15000
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         2050
DW         20.800 usec
DE         6.50 usec
TE         2956.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

------- CHANNEL f1 -------
NUC1       13C
P1         9.90 usec
PL1        -1.10 dB
PL1W       40.29647064 MHz
SFO1       100.6328888 MHz

------- CHANNEL f2 -------
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -1.00 dB
PL12       14.68 dB
PL13       17.68 dB
PL2W       10.90985775 W
PL12W      0.29499799 W
PL13W      0.14784923 W
SFO2       400.1716007 MHz
SI         32768
SP         100.6228304 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
