Supporting Information

[60]Fullerene-Fused Lactones: Mn(III) Acetate-Mediated Synthesis and Novel Reductive Ring Opening

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Synthesis of C₆₀-Fused Lactones 2a-c from the Reactions of C₆₀ with Carboxylic Acids 1a-1c and Mn(OAc)₃·2H₂O in the Presence of DMAP.

To a 50-mL three-neck flask equipped with a reflux condenser, argon inlet and outlet, and a magnetic stirrer was charged with C₆₀ (28.8 mg, 0.04 mmol), Mn(OAc)₃·2H₂O (21.4 mg, 0.08 mmol), 4-(dimethylamino)pyridine (DMAP) (4.9 mg, 0.04 mmol). After they were completely dissolved in *o*-dichlorobenzene (7 mL) by sonication, 100 equiv. of **1a** (100 equiv. of **1b** or 20 equiv. of **1c**) was added. The resulting solution was deoxygenated with argon for 10 min, and then the mixture was heated with stirring in an oil bath preset at 140 °C under argon atmosphere for a designated time (monitored by TLC). The reaction mixture was filtered through a silica gel plug in order to remove any insoluble material. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C₆₀, then with carbon disulfide/toluene as the eluent to give C₆₀-fused lactone **2a** (**2b**, or **2c**).

2a: ¹H NMR (300 MHz, ODCB-*d*₄) δ 4.65 (s, 2H); ¹³C NMR (75 MHz, ODCB-*d*₄) (all 2C unless indicated) δ 173.40 (CO, 1C), 153.28, 148.53 (1C), 147.90 (1C), 146.74, 146.68, 146.55, 146.49, 146.40, 145.67, 145.57, 145.54, 145.52, 145.41, 144.80, 144.74, 144.61, 144.52, 143.09, 142.95, 142.85, 142.43, 142.38, 142.32 (4C), 141.99, 141.51, 140.39, 139.92, 137.87, 135.44, 98.37 (sp³-C of C₆₀, 1C), 62.06 (sp³-C of C₆₀, 1C), 40.67 (CH₂); FT-IR ν/cm⁻¹ (KBr) 2921 (w), 2859 (w), 1790 (s), 1509 (m), 1430 (w), 1403 (w), 1270 (w), 1220 (w), 1193 (m), 1168 (w), 1112 (w), 1000 (s), 953 (m), 843 (w), 772 (w), 719 (w), 576 (w), 562 (w), 526 (s); UV-vis (CHCl₃) λ_{max}/nm (log ε) 256 (4.95), 316 (4.49), 418 (3.44), 686 (2.57); MS (APCI) *m/z* 778.

2c: ¹H NMR (300 MHz, CS₂/CDCl₃) δ 7.65 (d, *J* = 7.2 Hz, 2H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 5.84 (s, 1H); ¹³C NMR (75 MHz, CS₂/CDCl₃ with Cr(acac)₃ as relaxation reagent) (all 1C unless indicated) δ 173.46 (CO), 153.95, 150.21, 148.04, 147.46, 146.45, 146.35, 146.27, 146.20, 146.09, 146.07 (3C), 146.03, 146.00, 145.93, 145.85, 145.14 (3C), 145.10, 145.05, 145.03, 144.99 (2C), 144.86, 144.80 (2C), 144.38, 144.30, 144.19, 144.12, 143.96, 143.87, 142.65 (2C), 142.49,

142.46 (2C), 142.04 (2C), 141.96, 141.94, 141.89, 141.85, 141.81, 141.71, 141.50, 141.32, 141.17, 140.92, 140.05, 139.62, 139.51, 139.47, 137.61, 136.95, 136.18, 134.73, 134.19, 129.61 (aryl C, 2C), 129.24 (aryl C, 2C), 128.57 (aryl C), 96.15 (sp³-C of C₆₀), 68.28 (sp³-C of C₆₀), 56.70 (CH); FT-IR ν/cm^{-1} (KBr) 2919 (w), 2854, 1784 (s), 1510 (w), 1453 (w), 1429 (w), 1219 (w), 1183 (m), 1104 (w), 1018 (m), 991 (s), 963 (w), 727 (w), 698 (m), 562 (w), 545 (w), 526 (s); UV-vis (CHCl₃) $\lambda_{\text{max}}/\text{nm}$ (log ϵ) 256 (4.98), 317 (4.55), 417 (3.45), 688 (2.44); MS (APCI) m/z 854.

Synthesis of C₆₀-Fused Lactones 2a-2c from the Reactions of C₆₀ with Carboxylic Acid Anhydrides 3a-3c and Mn(OAc)₃·2H₂O in the Presence of DMAP.

A mixture of C₆₀ (28.8 mg, 0.04 mmol), carboxylic acid anhydride **3a** (**3b** or **3c**) (0.8 mmol), Mn(OAc)₃·2H₂O (21.4 mg, 0.08 mmol) and DMAP (4.9 mg, 0.04 mmol) was dissolved in *o*-dichlorobenzene (7 mL) and heated with stirring in an oil bath preset at 100 °C. The reaction was monitored by TLC and stopped at the designated time. The reaction mixture was filtered through a silica gel plug in order to remove any insoluble material. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C₆₀, then with carbon disulfide/toluene as the eluent to afford C₆₀-fused lactone **2a** (**2b** or **2c**).

Synthesis of C₆₀-Fused Lactones 2a-2c from the Reactions of C₆₀ with Malonic Acids 4a-4c and Mn(OAc)₃·2H₂O.

A mixture of C₆₀ (28.8 mg, 0.04 mmol) and Mn(OAc)₃·2H₂O (21.4 mg, 0.08 mmol) was dissolved in *o*-dichlorobenzene (8 mL). After malonic acid **4a** (**4b** or **4c**) (20 equiv., dissolved in 1 mL of DMF) was added, the resulting solution was heated with vigorous stirring in an oil bath preset at 80 or 25 °C under argon atmosphere. The reaction was monitored by TLC and stopped at the designated time. The reaction mixture was passed through a silica gel plug in order to remove any insoluble material. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C₆₀, then with

carbon disulfide/toluene as the eluent to afford C₆₀-fused lactone **2a** (**2b** or **2c**).

Reaction of C₆₀-Fused Lactones **2a-2c** with Methylmagnesium Bromide in THF.

Lactone **2a** (**2b** or **2c**, 0.025 mmol) was suspended in freshly distilled anhydrous tetrahydrofuran (25 mL) with the help of sonication for 30 min. To the suspension was added methylmagnesium bromide (95 μ L $\times$ 3.16 M, 0.30 mmol), the reaction mixture was stirred at room temperature for 10 min (the solution turned dark green), and then acidified with 400 μ L of acetic acid. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide/acetic acid as the eluent to afford unreacted lactone and ring-opened product **5a** (**5b** or **5c**).

5a: ¹H NMR (300 MHz, CS₂/DMSO-*d*₆) δ 12.08 (s, 1H), 6.87 (s, 1H), 4.33 (s, 2H); ¹³C NMR (75 MHz, CS₂/DMSO-*d*₆ with Cr(acac)₃ as relaxation reagent) (all 2C unless indicated) δ 170.76 (CO, 1C), 154.35, 153.64, 146.54 (1C), 146.38, 146.29 (1C), 145.43, 145.40, 145.22 (4C), 145.19, 145.02, 144.63, 144.43, 144.41, 144.37, 143.91, 143.68, 142.30, 141.61, 141.57, 141.30, 141.15, 141.06, 140.82, 140.69, 140.65, 139.22, 139.17, 136.03, 135.82, 60.58 (sp³-C of C₆₀, 1C), 58.59 (sp³-C of C₆₀, 1C), 48.38 (CH₂, 1C); FT-IR ν /cm⁻¹ (KBr) 2958 (m), 2924 (s), 2854 (m), 1730 (s), 1460 (m), 1424 (w), 1382 (w), 1275 (s), 1186 (w), 1124 (m), 1072 (m), 997 (w), 808 (w), 742 (w), 575 (w), 525 (s); UV-vis (CHCl₃) λ_{max} /nm (log ϵ) 255 (4.81), 315 (4.33), 432 (3.53), 694 (3.02); MS (APCI) *m/z* 779 (M-1).

5b: ¹H NMR (300 MHz, CS₂/CDCl₃) δ 6.93 (s, 1H), 4.49 (q, *J* = 7.2 Hz, 1H), 2.48 (d *J* = 7.2 Hz, 3H); ¹³C NMR (75 MHz, CS₂/acetone-*d*₆ with Cr(acac)₃ as relaxation reagent) (all 1C unless indicated) δ 174.27 (CO), 154.83, 154.16, 154.14, 153.39, 147.84, 147.57, 146.71 (3C), 146.68 (2C), 146.53, 146.50 (2C), 146.46, 146.40, 146.23, 146.20, 145.91, 145.89, 145.76, 145.72, 145.71, 145.70, 145.64 (2C), 145.19, 145.07, 144.87 (2C), 143.56 (3C), 142.91, 142.88 (4C), 142.60 (2C), 142.41 (2C), 142.38, 142.36, 142.07, 142.01, 141.96, 141.89, 141.85, 141.79, 140.61, 140.55, 140.33, 140.21, 137.49, 137.26, 137.10, 136.71, 66.53 (sp³-C of C₆₀), 56.77 (sp³-C of C₆₀), 52.19 (CH), 15.70 (CH₃); FT-IR ν /cm⁻¹ (KBr) 2949 (m), 2919 (m), 2862 (w), 1703 (s), 1458 (m), 1425 (m), 1377 (w), 1264 (w), 1218 (m), 1185 (m), 1137 (w),

1111 (w), 972 (w), 846 (w), 764 (w), 553 (w), 527 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \varepsilon$) 256 (4.89), 315 (4.41), 433 (3.61), 692 (2.75); MS (APCI) m/z 793 (M-1).

5c: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 7.80 (d, $J = 7.5$ Hz, 2H), 7.44 (t, $J = 7.3$ Hz, 2H), 7.37 (t, $J = 7.1$ Hz, 1H), 6.98 (s, 1H), 5.56 (s, 1H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 1C unless indicated) δ 171.65 (CO), 153.74, 153.17, 153.13, 152.20, 146.14, 145.90, 145.87 (2C), 145.52, 145.50, 145.05, 145.02 (3C), 144.83 (2C), 144.76; 144.74, 144.57 (2C), 144.25, 144.11, 144.01 (2C), 143.97 (2C), 143.93 (2C), 143.51 (2C), 143.25, 143.19, 141.84 (2C), 141.21 (3C), 141.12, 140.95, 140.82, 140.75 (2C), 140.71, 140.69, 140.27 (2C), 140.23 (2C), 140.18, 140.08, 138.83, 138.78, 138.05, 137.91, 136.64, 135.62, 135.54, 135.16, 133.64, 129.68 (aryl C, 2C), 127.60 (aryl C, 2C), 127.31 (aryl C), 66.14 ($\text{sp}^3\text{-C}$ of C_{60}), 62.59 (CH), 57.04 ($\text{sp}^3\text{-C}$ of C_{60}); FT-IR ν/cm^{-1} (KBr) 2954 (s), 2923 (s), 2860 (m), 1707 (s), 1494 (w), 1456 (m), 1425 (m), 1382 (w), 1268 (w), 1186 (m), 1074 (w), 1032 (w), 844 (w), 701 (s), 578 (w), 527 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \varepsilon$) 257 (4.84), 317 (4.40), 431 (3.65), 693 (2.53); MS (APCI) m/z 855 (M-1).

Monoalkylation of C_{60} with Zn and *tert*-Butyl Bromoacetate.¹

Into a 50 mL three-neck flask were added C_{60} (72.0 mg, 0.10 mmol), *tert*-butyl bromoacetate (738 μL , 5.0 mmol), and 20 mL of DMF. Under an argon flow, the mixture was heated with stirring in an oil bath preset at 50 $^\circ\text{C}$, and then Zn dust (0.65 g, 10.0 mmol, having been successively washed with 1×2 mL 3% HCl, 3×5 mL distilled H_2O , 2×5 mL THF, and 1×5 mL DMF) was rinsed into the reaction mixture with 2 mL of DMF. The resulting mixture was stirred vigorously, and the color turned to deep black. After 15 min (TLC monitoring), the mixture was poured into 100 mL of H_2O containing 2 mL of AcOH, and 150 mL of toluene was added. The mixture was shaken, the layers were separated, and the upper (toluene) layer was further washed with H_2O (2×75 mL) and dried with anhydrous Na_2SO_4 . After being filtered and concentrated, the concentrated solution was applied to a silica gel column

and eluted with carbon disulfide to produce unreacted C₆₀ (34.4 mg, 48%), then with carbon disulfide/toluene as the eluent to obtain the monoalkylated product **6** (9.4 mg, 11%).

6: ¹H NMR (300 MHz, CS₂/CDCl₃) δ 6.79 (s, 1H), 4.33 (s, 2H), 1.74 (s, 9H); ¹³C NMR (75 MHz, CS₂/CDCl₃ with Cr(acac)₃ as relaxation reagent) (all 2C unless indicated) δ 168.46 (CO, 1C), 153.65, 152.81, 146.80 (1C), 146.56 (1C), 146.26, 145.68, 145.65, 145.48, 145.45, 145.12, 144.99, 144.87, 144.69 (4C), 144.63, 144.06, 143.82, 142.52, 141.86, 141.82, 141.47, 141.35, 141.24, 140.97, 140.89 (4C), 139.52, 139.46, 135.85, 135.74, 81.55 (C(CH₃)₃, 1C), 60.72 (sp³-C of C₆₀, 1C), 58.33 (sp³-C of C₆₀, 1C), 50.10 (CH₂, 1C), 27.70 (CH₃, 3C); FT-IR ν /cm⁻¹ (KBr) 2968 (w), 2924 (m), 2853 (w), 1727 (s), 1508 (w), 1459 (w), 1425 (m), 1365 (m), 1348 (w), 1258 (w), 1213 (m), 1180 (w), 1149 (s), 854 (w), 834 (w), 809 (w), 763 (w), 577 (m), 526 (s); UV-vis (CHCl₃) λ_{max} /nm (log ϵ) 256 (4.83), 319 (4.30), 432 (3.35), 705 (2.40); MS (APCI) m/z 835 (M-1).

Hydrolysis of Compound **6** with *p*-Toluenesulfonic Acid Monohydrate.

A mixture of compound **6** (14.7 mg, 0.018 mmol) and *p*-toluenesulfonic acid monohydrate (6.7 mg, 0.036 mmol) was dissolved in monochlorobenzene (20 mL) and then the mixture was heated with stirring in an oil bath preset at 130 °C. The reaction was monitored by TLC, and stopped after 40 min. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide/acetic acid as the eluent to afford product **5a** (13.6 mg, 99%).

Reference

1. Wang, Z.; Meier, M. S. *J. Org. Chem.* **2003**, *68*, 3043.

¹H NMR of **2a** in *o*-C₆D₄Cl₂

2a

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Current Data Parameters
NAME      znc030513
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20030513
Time      9.55
INSTRUM   a300
PROBHD    5 mm BBO BB-H
PULPROG   zg
TD         32768
SOLVENT    CDCl3
NS         200
DS         2
SWH         11930.472 Hz
FIDRES     0.3561918 Hz
AQ         1.3667556 sec
RG          256
DM          0
DE          41.700 usec
TE         5.00 usec
JC         300.0 K
D1         2.00000000 sec

***** CHANNEL f1 *****
NUC1       1H
P1         4.00 usec
PL         -3.00 dB
SFO1       300.1321009 MHz

F2 - Processing parameters
S1         16384
SF          300.1395615 MHz
WDW         no
SSB         0
LB          0.00 Hz
GB          0
PC          1.00

ID MR plot parameters
CX         -22.00 cm
CY          0.00 cm
ZP          0.00 cm
F1         2'01.17 Hz
F2         -2'00.200 ppm
F3         -60.03 Hz
F4         0.41818 ppm/cm
F5         125.50850 Hz/cm

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¹³C NMR of **2a** in *o*-C₆D₄Cl₂

Current Data Parameters
 NAME zhtu030513c
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030516
 Time 22.08
 INSTRUM spect
 PPRBND 5 mm BBO BB-1H
 PULPROG zgpg30
 TO 32768
 SOLVENT ocd5d4c12
 NS 44143
 DS 2
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 2896.3
 DW 27.600 usec
 DE 5.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 ¹³C
 P1 2.40 usec
 PL1 -6.00 dB
 SF01 75.4755568 MHz

***** CHANNEL f2 *****
 CDPORG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 16.00 dB
 SF02 300.1315007 MHz

F2 - Processing Parameters
 SI 131072
 SF 75.4677240 MHz
 SN 32768
 EN
 SSF 0
 LB 1.00 Hz
 GB 0
 CB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 CY 300.00 cm
 FIP 180.371 ppm
 F1 1.361216 Hz
 F2 -1.159 ppm
 F2 -87.46 Hz
 SFOH 8.25134 ppm/cm
 F2CH 622.70990 Hz/cm

¹³C NMR of **2a** in *o*-C₆D₄Cl₂

Current Data Parameters
 NAME zth030513c
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
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 Time_ 22.08
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 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
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 SOLVENT ccd4cl2
 NS 44143
 DS 2
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 2896.3
 DW 27.600 usec
 DE 5.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 ***** CHANNEL f1 *****
 NUC1 13C
 P1 2.40 usec
 PL1 -6.00 dB
 SF01 75.4755688 MHz
 ***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 16.00 dB
 SF02 300.1315007 MHz
 F2 - Processing parameters
 SI 32768
 SF 75.4677245 MHz
 WDW EN
 SSF 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 ID NMR plot parameters
 CX 22.00 cm
 CY 300.00 cm
 FIP 146.636 ppm
 C1 11232.35 Hz
 C2 135.128 ppm
 F2 10197.78 Hz
 SFO1 0.82312 ppm/cm
 SFO2 47.82275 Hz/cm

¹H NMR of **5a** in DMSO-*d*₆

¹³C NMR of **5a** in DMSO-*d*₆

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Current Data Parameters
NAME      Ifb05102801
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20051030
Time      8.33
INSTRUM   av300
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         39812
DS         4
SWH        22675.736 Hz
FIDRES     0.346004 Hz
AQ         1.445188 sec
RG         8192
DM         22.050 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
MCREST    0.00000000 sec
MCWRK      0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         3.00 usec
PL1        -1.00 dB
SF01       75.4768051 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -3.00 dB
PL12       15.00 dB
SF02       300.1315007 MHz

F2 - Processing parameters
SI         131072
SF         75.4678268 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         22.00 cm
CY         0.00 cm
F1P        211.608 ppm
F1         15969.59 Hz
F2P        -5.538 ppm
F2         -417.91 Hz
PPM0M      9.87025 ppm/cm
HZCM       744.88666 Hz/cm
  
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¹³C NMR of **5a** in DMSO-*d*₆

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Current Data Parameters
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EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
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Time      8.33
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PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         39812
DS         4
SWH        22675.735 Hz
FIDRES     0.346004 Hz
AQ          1.4451188 sec
RG          8192
DM          22.050 usec
DE          6.00 usec
TE          300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
MCPRST     0.00000000 sec
MCMRK      0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1          3.00 usec
PL1         -1.00 dB
SF01        75.4768051 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PL2          -3.00 dB
PL12        16.00 dB
SF02        300.1315007 MHz

F2 - Processing parameters
SI          131072
SF          75.4678288 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

1D NMR plot parameters
CX          22.00 cm
CY          146.715 ppm
F1          11072.33 Hz
F2          145.465 ppm
F2P         10826.33 Hz
PRCM        0.14798 ppm/cm
HZCM        11.16802 Hz/cm
    
```

¹³C NMR of **5a** in DMSO-*d*₆

Current Data Parameters

NAME jfb05102801

EXPNO 4

PROCNO 1

F2 - Acquisition Parameters

Date_ 20051030

Time 8.33

INSTRUM av300

PROBHD 5 mm BBO BB-1H

PULPROG zgpg

 TD 65536 | SOLVENT DMSO | NS 39812 | DS 4 | SWH 22675.736 Hz | FIDRES 0.346004 Hz | AQ 1.4451188 sec | RG 8192 | DM 22.050 usec | DE 6.00 usec | TE 300.0 K | D1 2.00000000 sec | d11 0.03000000 sec | MCREST 0.00000000 sec | MCNMRK 0.01500000 sec | ===== CHANNEL f1 ===== | NUC1 13C | P1 3.00 usec | PL1 -1.00 dB | SF01 75.4768051 MHz | ===== CHANNEL f2 ===== | CPDPRG2 waltz16 | NUC2 1H | PCPD2 80.00 usec | PL2 -3.00 dB | PL12 15.00 dB | SF02 300.1315007 MHz | F2 - Processing parameters | SI 131072 | SF 75.4678286 MHz | WDW EM | SSB 0 | LB 1.00 Hz | GB 0 | PC 1.40 | 1D NMR plot parameters | CX 22.00 cm | CY 0.00 cm | F1P 142.851 ppm | F1 10760.66 Hz | F2P 135.525 ppm | F2 10227.75 Hz | PRGM 0.33302 ppm/cm | HZCM 25.13221 Hz/cm |