Supporting Information

Novel Functionalizations of [60]Fullerene-Fused Lactones

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2b: ^1H NMR (300 MHz, $\text{CS}_2/\text{CDCl}_3$) δ 3.86 (q, $J = 7.1$ Hz, 1H), 2.97 (br s, 1H), 2.12 (s, 3H), 1.89 (d, $J = 7.1$ Hz, 3H); ^1H NMR (400 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 6.83 (d, $J = 1.8$ Hz, 1H), 3.70 (dq, $J = 7.0, 1.8$ Hz, 1H), 1.97 (s, 3H), 1.76 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$) (all 1C unless indicated) δ 156.64, 153.23, 152.80, 149.37, 147.09, 146.40, 145.99, 145.40, 145.37, 145.32, 145.30, 145.28, 145.23, 145.12, 145.09, 145.05, 144.95 (2C), 144.89, 144.79, 144.56, 144.36, 144.34 (2C), 144.25, 144.22 (2C), 144.13, 144.03, 143.92, 143.86, 143.44, 142.09, 142.03, 141.75 (2C), 141.74 (2C), 141.68 (2C), 141.40 (2C), 141.32 (4C), 140.99, 140.97, 140.81, 140.60, 139.19, 138.70, 138.54, 138.51, 137.97, 137.58, 136.66, 134.31, 105.66, 96.77 (sp^3 -C of C_{60}), 72.53 (sp^3 -C of C_{60}), 56.47, 23.96, 12.78; FT-IR ν/cm^{-1} (KBr) 2920 (s), 2850 (m), 1427 (m), 1375 (w), 1179 (w), 1153 (w), 1104 (s), 997 (m), 921 (m), 765 (w), 724 (w), 570 (w), 523 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ (log ϵ) 255 (5.09), 312 (4.55), 428 (3.47), 692 (2.63); MS (-APCI) m/z 808 (M^+).

2c: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 7.99-7.93 (m, 2H, Ar), 7.51-7.31 (m, 4H), 5.15 (s, 0.1H, *trans* isomer), 4.91 (s, 0.9H, *cis* isomer), 2.00 (s, 2.7H, *cis* isomer), 1.82 (s, 0.3H, *trans* isomer); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent, *cis* isomer) (all 1C unless indicated) δ 155.68, 152.62, 152.35, 149.01, 146.73, 146.01, 145.59, 145.07, 145.02 (2C), 144.91, 144.87, 144.78 (2C), 144.72, 144.66, 144.57 (3C), 144.45, 144.15, 143.97, 143.92 (2C), 143.88 (2C), 143.83, 143.74, 143.65, 143.53, 143.49, 143.03, 141.71, 141.62, 141.38, 141.36 (2C), 141.34 (2C), 141.19, 141.07, 141.05, 140.97, 140.93 (3C), 140.73, 140.57, 140.45, 140.13, 138.54, 138.21, 138.18, 138.13, 137.48, 137.32, 136.33, 134.07, 133.85, 130.35 (2C, aryl C), 127.19 (2C, aryl C), 126.98 (aryl C), 105.33, 96.50 (sp^3 -C of C_{60}), 73.16 (sp^3 -C of C_{60}), 67.57, 23.99; FT-IR ν/cm^{-1} (KBr) 2922 (m), 2854 (w), 1536 (w), 1493 (w), 1453 (m), 1429 (m), 1380 (w), 1215 (w), 1179 (w), 1131 (m), 1102 (s), 1016 (s), 961 (m), 903 (m), 880 (w), 846 (w), 746 (w), 698 (s), 595 (w), 576 (m), 551 (w), 525 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ (log ϵ) 257 (4.83), 313 (4.38), 428 (3.10), 692 (2.14); MS (-APCI) m/z 870 (M^+).

3b: ^1H NMR (300 MHz, $\text{CS}_2/\text{CDCl}_3$) δ 6.38 (d, $J = 3.9$ Hz, 0.78H, *cis* isomer), 6.21 (d, $J = 1.5$ Hz, 0.22H, *trans* isomer), 4.15-4.00 (m, 1H, *cis* and *trans* isomers), 3.43 (br s, 0.22H, *trans* isomer), 3.33 (br s, 0.78H, *cis* isomer), 1.95 (d, $J = 7.4$ Hz, 0.66H, *trans* isomer), 1.92 (d, $J = 7.1$ Hz, 2.34H, *cis* isomer); MS (-APCI) m/z 794 (M^+).

3c: ^1H NMR (300 MHz, $\text{CDCl}_3/\text{CS}_2$) δ 7.91-7.83 (m, 2H, *cis* and *trans* isomers), 7.47-7.42 (m, 1H, *cis* and *trans* isomers), 7.38-7.30 (m, 2H, *cis* and *trans* isomers), 6.57 (s, 0.58H, *trans* isomer), 6.56 (d, $J = 3.7$ Hz, 0.42H, *cis* isomer), 5.25 (s, 0.58H, *trans* isomer), 5.11 (d, $J = 3.7$ Hz, 0.42H, *cis* isomer), 3.61 (br s, 0.42H, *cis* isomer), 3.45 (br s, 0.58H, *trans* isomer); MS (-APCI) m/z 856 (M^+).

4b: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 2.38 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 2C unless indicated) δ 148.19, 146.83 (1C), 146.75 (1C), 146.08 (1C), 145.29, 145.04, 144.92, 144.89, 144.75, 144.68, 144.47, 144.41, 144.16, 144.08, 143.88, 143.82, 143.23, 143.20, 141.72, 141.54, 141.45 (4C), 141.09, 141.03, 140.91, 140.77, 140.43, 139.27, 138.56, 135.85, 134.87, 103.48 (1C), 98.37 (1C, sp^3 -C of C_{60}), 76.12 (1C, sp^3 -C of C_{60}), 11.23

(1C), 10.42 (1C); FT-IR ν/cm^{-1} (KBr) 2919 (m), 2850 (w), 1537 (w), 1461 (w), 1428 (s), 1380 (w), 1269 (w), 1217 (w), 1181 (s), 1123 (m), 1046 (w), 1010 (m), 975 (s), 958 (w), 933 (w), 766 (m), 597 (w), 574 (m), 565 (w), 525 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$) 254 (4.97), 314 (4.46), 426 (3.29), 691 (2.25); MS (-APCI) m/z 790 (M^+).

4c: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 7.55 (d, $J = 8.0$ Hz, 2H), 7.37 (t, $J = 7.3$ Hz, 2H), 7.29 (t, $J = 7.4$ Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 2C unless indicated) δ 150.67 (1C), 148.09, 146.74 (1C), 146.01 (1C), 144.98, 144.83, 144.81, 144.66, 144.64, 144.62, 144.45, 144.41, 143.96, 143.83 (4C), 143.73, 143.12, 143.07, 141.62, 141.44, 141.40 (4C), 141.06, 141.00, 140.85, 140.62, 140.31, 138.96, 138.56, 135.89, 134.50, 131.65 (1C, aryl C), 129.45 (aryl C), 127.79 (aryl C), 126.94 (1C, aryl C), 110.71 (1C), 99.63 (1C, sp^3 -C of C_{60}), 75.84 (1C, sp^3 -C of C_{60}), 11.99 (1C); FT-IR ν/cm^{-1} (KBr) 2921 (m), 2851 (w), 1463 (m), 1432 (w), 1377 (w), 1240 (m), 1181 (w), 1117 (w), 1032 (m), 1013 (w), 984 (w), 964 (w), 842 (w), 817 (w), 751 (m), 700 (m), 575 (m), 553 (w), 526 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$) 255 (4.89), 314 (4.35), 426 (3.20), 693 (2.01); MS (-APCI) m/z 852 (M^+).

4d: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 7.47 (d, $J = 2.7$ Hz, 1H), 6.21 (d, $J = 2.7$ Hz, 1H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 2C unless indicated) δ 148.39, 146.72 (1C), 146.12 (1C), 146.00 (1C), 144.96, 144.82, 144.76, 144.67, 144.60, 144.40, 143.93, 143.87, 143.84 (4C), 143.74, 143.24, 143.12, 142.98, 141.61, 141.58, 141.40, 141.36, 141.01, 140.88, 140.86, 140.60, 140.38, 139.24, 138.50, 135.90, 134.51, 103.84 (1C), 100.65 (1C, sp^3 -C of C_{60}), 71.79 (1C, sp^3 -C of C_{60}); FT-IR ν/cm^{-1} (KBr) 2919 (m), 2850 (w), 1507 (m), 1463 (w), 1428 (m), 1242 (w), 1179 (m), 1152 (s), 1065 (w), 1037 (w), 978 (m), 940 (w), 920 (w), 838 (w), 788 (w), 765 (w), 716 (s), 599 (w), 571 (w), 526 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$) 255 (4.93), 314 (4.41), 427 (3.22), 690 (2.28); MS (-APCI) m/z 762 (M^+).

4e: ^1H NMR (300 MHz, $\text{CS}_2/\text{acetone}-d_6$) δ 7.03 (q, $J = 1.4$ Hz, 1H), 2.36 (d, $J = 1.4$ Hz, 3H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 2C unless indicated) δ 147.49, 146.69 (1C), 145.94 (1C), 144.92, 144.83, 144.79, 144.67, 144.64, 144.56, 144.40, 144.26, 144.09, 143.88, 143.77, 143.73, 143.06, 143.05, 141.76, 141.60, 141.35 (5C), 140.99, 140.93, 140.80, 140.64, 140.31, 139.21, 138.46, 135.70, 134.82, 110.51 (1C), 100.09 (1C, sp^3 -C of C_{60}), 74.72 (1C, sp^3 -C of C_{60}), 9.94 (1C); FT-IR ν/cm^{-1} (KBr) 2919 (m), 2850 (w), 1536 (w), 1505 (m), 1460 (w), 1426 (m), 1216 (w), 1181 (w), 1115 (s), 994 (m), 940 (w), 913 (w), 838 (w), 765 (w), 637 (w), 596 (w), 575 (w), 554 (w), 525 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$) 256 (4.88), 314 (4.35), 426 (3.18), 691 (2.28); MS (-APCI) m/z 776 (M^+).

4f: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 7.71 (d, $J = 8.1$ Hz, 2H), 7.51 (s, 1H), 7.37-7.26 (m, 3H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 2C unless indicated) δ 147.22, 146.50 (1C), 145.80 (1C), 144.78, 144.64 (4C), 144.53, 144.44 (4C), 144.21, 143.83, 143.80, 143.62, 143.56, 143.51, 142.85 (4C), 141.58 (1C), 141.41, 141.23 (4C), 141.15, 140.87, 140.82, 140.70, 140.34, 140.08, 138.67, 138.42, 135.60, 134.50, 130.59 (1C, aryl C), 127.66 (aryl C), 127.56 (aryl C), 126.78 (1C, aryl C), 116.80 (1C), 101.67 (1C, sp^3 -C of C_{60}), 73.46 (1C, sp^3 -C of C_{60}); FT-IR ν/cm^{-1} (KBr) 2920 (w), 2851 (w), 1536 (w), 1488 (w), 1465 (w), 1428

(m), 1216 (w), 1181 (w), 1130 (s), 1017 (w), 981 (m), 939 (w), 923 (w), 880 (m), 853 (w), 756 (m), 694 (s), 668 (w), 650 (w), 602 (w), 565 (w), 522 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$) 256 (4.86), 313 (4.35), 425 (3.15), 692 (2.30); MS (-APCI) m/z 838 (M^+).

5b: ^1H NMR (300 MHz, $\text{CS}_2/\text{DMSO}-d_6$) δ 9.35 (s, 1H), 8.94 (br s, 1H), 5.97-5.85 (m, 1H), 5.22 (d, $J = 17.9$ Hz, 1H), 5.11 (d, $J = 10.3$ Hz, 1H), 4.49 (s, 2H), 4.04-4.00 (m, 2H); ^{13}C NMR (75 MHz, $\text{CS}_2/\text{DMSO}-d_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent) (all 2C unless indicated) δ 170.89 (1C, CONH), 154.71, 152.93, 146.92 (1C), 146.45 (1C), 145.07 (4C), 144.78, 144.70, 144.60, 144.48, 144.45, 143.97, 143.93 (6C), 143.61, 143.30, 141.55, 141.21, 141.16, 141.01, 140.98, 140.75, 140.49, 140.45, 139.82, 138.42, 138.04, 135.14, 134.75, 133.33 (1C), 114.82 (1C), 86.46 (1C, $sp^3\text{-C}$ of C_{60}), 62.84 (1C, $sp^3\text{-C}$ of C_{60}), 44.16 (1C), 41.23 (1C); FT-IR ν/cm^{-1} (KBr) 3434 (s), 2922 (m), 2851 (w), 1626 (s), 1565 (m), 1426 (m), 1261 (w), 1181 (w), 1158 (w), 1107 (m), 1034 (s), 1002 (w), 921 (m), 752 (s), 572 (w), 527 (s); UV-vis (CHCl_3) $\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$) 254 (4.93), 314 (4.26), 430 (3.14), 694 (2.29); MS (-APCI) m/z 834 (M^+-1).

¹H NMR (300 MHz, CS₂/o-C₆D₄Cl₂) of compound **2a**

Current Data Parameters
 NAME f1b05053001
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050530
 Time 11.14
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CSO6
 NS 32
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 287.4
 CW 63.400 usec
 DE 6.00 usec
 TE 296.6 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321009 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300898 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.245 ppm
 F2P 2405.75 Hz
 F3P -0.342 ppm
 MCHW 0.39051 ppm/cm
 MZCX 117.20363 Hz/cm

Current Data Parameters
NAME 1f05060701
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050608
Time 8.00
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15317
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 5792.6
DM 22.050 usec
DE 6.00 usec
TE 299.9 K
D1 2.00000000 sec
d11 0.03000000 sec
wDREST 0.00000000 sec
wDNRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 3.00 usec
PL1 -1.00 dB
SFO1 75.476051 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SFO2 300.1315007 MHz

F2 - Processing parameters
SI 131072
SF 75.4678215 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 203.201 ppm
F1 15335.17 Hz
F2P -4.453 ppm
F2 -336.02 Hz
SFOCM 9.43881 ppm/cm
AQCM 712.32672 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-*d*₆) of compound 2a

¹H NMR (400 MHz, CS₂/DMSO-d₆) of compound **2b**

Current Data Parameters
 NAME 1fb05092101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050922
 Time 11.30
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.9715922 sec
 RG 287.4
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 -1.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300396 MHz
 WDW EN
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 9.000 ppm
 F1 3601.17 Hz
 F2 -0.500 ppm
 F2 -200.06 Hz
 PPMCM 0.47500 ppm/cm
 HZCM 190.06177 Hz/cm

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **2c**

Current Data Parameters
 NAME 1105050202
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050602
 Time 11.04
 INSTRUM av300
 PROBO 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 362
 DW 83.400 usec
 DE 6.00 usec
 TE 296.8 K
 D1 2.0000000 sec
 MCOREST 0.0000000 sec
 MCNMRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321009 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300025 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 9.092 ppm
 F1 2728.90 Hz
 F2P -0.344 ppm
 F2 -103.32 Hz
 PPMCM 0.42894 ppm/cm
 HZCM 128.73714 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-*d*₆) of compound **2c**

Current Data Parameters
 NAME 11005082901
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050930
 Time 8.54
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 15590
 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 2.0000000 sec
 d11 0.0300000 sec
 MCREST 0.0000000 sec
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 3.00 usec
 PL1 -1.00 dB
 SF01 75.4756051 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 80.00 usec
 PL2 -3.00 dB
 PL12 16.00 dB
 SF02 300.1315007 MHz

F2 - Processing parameters
 SI 131072
 SF 75.4678484 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 205.784 ppm
 F1 15530.83 Hz
 F2P -5.292 ppm
 F2 -399.35 Hz
 PPKCM 9.59480 ppm/cm
 HZCM 724.09918 Hz/cm

¹H NMR (300 MHz, CS₂/o-C₆D₄Cl₂) of compound **3a**

Current Data Parameters
 NAME 1f005053002
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050530
 Time 11:22
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT C6D6
 NS 32
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 256
 CW 83.400 usec
 DE 6.00 usec
 TE 295.6 K
 D1 2.0000000 sec
 WDEFT 0.0000000 sec
 WDWK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321309 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300163 MHz
 WDW no
 SSB 0
 -B 0.00 Hz
 GB 0
 -C 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 ZP 8.26200m
 F1 2485.53 Hz
 F2 -0.31000m
 F2 -92.95 Hz
 -F2M 0.39051 ppm/cm
 -ZCM 117.20383 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-*d*₆) of compound **3a**

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Current Data Parameters
NAME      J160506201
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20050903
Time      7.35
INSTRUM   av300
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg
TD         65536
SOLVENT    DMSO
NS         14653
DS         4
SWH        22675.736 Hz
FIDRES     0.346004 Hz
AQ         1.4451188 sec
RG          40
W2         7298.2
WDW         22.050 usec
SSB         6.00 usec
GB          0
TE         301.1 K
D1         2.0000000 sec
D11        0.0300000 sec
ICREST     0.0000000 sec
ICWRRK     0.0150000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         3.00 usec
PL1        -1.00 dB
SFO1       75.4766951 MHz

===== CHANNEL f2 =====
CPOPRG2    waitz16
NUC2       1H
PCPD2      80.00 usec
PL2        -3.00 dB
PL12       16.00 dB
SFO2       300.1315007 MHz

F2 - Processing parameters
SI         131072
SF         75.4678195 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
FIP        204.544 ppm
F1         15436.52 Hz
F2         -1.121 ppm
F3         -84.63 Hz
F4         9.34825 ppm/cm
ZDCH       705.50684 Hz/cm
    
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¹H NMR (300 MHz, CS₂-CDCl₃) of compound **3b**

¹H NMR (300 MHz, CS₂-CDCl₃) of compound **3c**

Current Data Parameters
 NAME J1605083002
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20050830
 Time 11.17
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl₃
 NS 128
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.183959 Hz
 AQ 2.7329011 sec
 RG 512
 DW 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321009 MHz
 F2 - Processing parameters
 S1 16384
 SF 300.1300199 MHz
 WDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 22.00 cm
 CI 0.00 cm
 FIP 8.562 ppm
 F1 2569.86 Hz
 F2 -0.469 ppm
 F2 -140.78 Hz
 PPMCM 0.41049 ppm/cm
 HZCM 123.20167 Hz/cm

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **4a**

Current Data Parameters
NAME jfb05090903
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050909
Time 17.16
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.162959 Hz
AQ 2.7329011 sec
RG 645.1
DM 83.400 usec
DE 6.00 usec
TE 298.2 K
D1 2.0000000 sec
MCREST 0.0000000 sec
MCMRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 7.50 usec
PL1 -3.00 dB
SF01 300.1321009 MHz

F2 - Processing parameters
SI 16384
SF 300.1300305 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
FIP 8.426 ppm
F1 2528.82 Hz
F2P -0.538 ppm
F2 -161.46 Hz
PPMXX 0.40744 ppm/cm
FICH 122.28566 Hz/cm

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **4b**

2.37912
2.31162

ppm

Current Data Parameters
NAME Ifb05083004
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050830
Time 16.56
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT DMSO
NS 32
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 574.7
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SF01 300.1321009 MHz

F2 - Processing parameters
SI 16384
SF 300.1300240 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1 7.253 ppm
F2 2176.42 Hz
F3 0.231 ppm
F4 69.22 Hz
PRGCM 0.54010 ppm/cm
HZCM 102.07446 Hz/cm

Current Data Parameters
 NAME 1f00503004
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050831
 Time 8.10
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TO 65536
 SOLVENT DMSO
 NS 14581
 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
 MCKRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 3.00 usec
 PL1 -1.00 dB
 SF01 75.476051 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 75.4678496 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1p 199.243 ppm
 F1 15036.43 Hz
 F2p 7.135 ppm
 F2 -538.43 Hz
 PPMCN 9.38079 ppm/cm
 HZCM 707.94806 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-d₆) of compound **4b**

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **4c**

Current Data Parameters
 NAME jfb05090101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050901
 Time 16:58
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 512
 DM 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 MCREST 0.0000000 sec
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321009 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300302 MHz
 WDW nc
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.425 ppm
 F1 2528.49 Hz
 F2P -0.366 ppm
 F2 -109.79 Hz
 PPMH 0.39957 ppm/cm
 HZCM 119.92198 Hz/cm

¹H NMR (300 MHz, CS₂/DMSO-*d*₆) of compound **4d**

Current Data Parameters
 NAME 1f05091901
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050919
 Time 17 11
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 41
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 1024
 DM 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 MPREST 0.00000000 sec
 MCWRR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 4.00 usec
 PL1 -3.00 dB
 SF01 300.1315000 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300297 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 7.998 ppm
 F1 2400.55 Hz
 F2P -0.333 ppm
 F2 -99.91 Hz
 PPMCM 0.37869 ppm/cm
 HZCM 113.65740 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-*d*₆) of compound **4d**

Current Data Parameters
 NAME 11005091901
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050920
 Time 8.08
 INSTRUM av-300
 PROBHQ 5 mm BBO BB-1H
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 14896
 DS 4
 SWH 22675.736 Hz
 FIDRES 0.346004 Hz
 AQ 1.445188 sec
 RG 5160.6
 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
 S1 131072
 SF 75.4678574 MHz
 MDW 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 207.619 ppm
 F1 15668.59 Hz
 F2P -6.508 ppm
 F2 -491.14 Hz
 F2MCM 9.73306 ppm/cm
 F2CM 734.53284 Hz/cm

¹H NMR (300 MHz, CS₂-CD₃COCD₃) of compound **4e**

Current Data Parameters
 NAME 1:00509002
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050909
 Time 17.08
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT Acetone
 NS 32
 DS 0
 SFO1 5995.204 Hz
 FIDRES 0.182569 Hz
 AQ 2.7329011 sec
 RG 724.1
 DM 83.400 usec
 DE 6.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321009 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300188 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 FIP 7.675 ppm
 F1 2303.57 Hz
 F2 -0.394 ppm
 F2 -118.14 Hz
 PPMCM 0.36677 ppm/cm
 HZCM 110.07762 Hz/cm

Current Data Parameters
NAME 1f605082601
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050928
Time 1.17
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpgc
TD 65536
SOLVENT DMSO
NS 31744
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 9195.2
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRR 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
SP02 300.1315007 MHz

F2 - Processing parameters
SI 131072
SF 75.4678596 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 91.00 cm
F1P 207.160 ppm
F1 15633.92 Hz
F2P -5.441 ppm
F2 -410.60 Hz
PRCM 9.66366 ppm/cm
HZCM 729.25602 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-d₆) of compound **4e**

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **4f**

Current Data Parameters
NAME 1f0506201
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050622
Time 16.32
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 5995.204 Hz
FIDRES 0.162959 Hz
AQ 2.7329011 sec
RG 455.1
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec
***** CHANNEL f1 *****
NUC1 1H
P1 4.00 usec
PL1 -3.00 dB
SF01 300.1315000 MHz
F2 - Processing parameters
SI 16384
SF 300.1300294 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
ID NMR plot parameters
CX 22.00 cm
CY 0.00 cm
FIP 8.543 deg
F1 2563.67 Hz
F2 -0.320 deg
ZD -95.19 Hz
SFOCM 0.40286 ppm/cm
HZCM 120.91167 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-d₆) of compound **4f**

```

Current Data Parameters
NAME      1f005062901
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20050630
Time      8.15
INSTRUM   av300
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         14882
DS         4
SWH        22675.736 Hz
FIDRES     0.346004 Hz
AQ         1.4451188 sec
RG         1824.6
DM         22.050 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
MGREST    0.00000000 sec
MGMR      0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         3.00 usec
PL1        -1.00 dB
SFO1       75.4768051 MHz

===== CHANNEL f2 =====
CPDPRG2    waitz16
NUC2       1H
PCPD2      80.00 usec
PL2        -3.00 dB
PL12       16.00 dB
SFO2       300.1315007 MHz

F2 - Processing parameters
SI         131072
SF         75.4678740 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        208.386 ppm
F1         15726.44 Hz
F2P        -4.754 ppm
F2         -358.81 Hz
PPMCM      9.68620 ppm/cm
HZCM       731.14783 Hz/cm
  
```

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **5a**

Current Data Parameters
 NAME 1f60410801
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041108
 Time 17.03
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 322.5
 DM 83.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1321009 MHz

F2 - Processing parameters
 S1 16384
 SF 300.1300305 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 10.056 ppm
 F1 3018.24 Hz
 F2P -0.332 ppm
 F2 -99.65 Hz
 PPMCH 0.47220 ppm/cm
 HZCM 141.72232 Hz/cm

¹H NMR (300 MHz, CS₂/DMSO-d₆) of compound **5b**

Current Data Parameters
 NAME 1f00509501
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20050905
 Time 17.31
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.162959 Hz
 AQ 2.7328011 sec
 RG 406.4
 DM 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 MCREST 0.0000000 sec
 MCWRR 0.0150000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SF01 300.1318008 MHz
 F2 - Processing parameters
 SI 16384
 SF 300.1300228 MHz
 MVM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 9.636 ppm
 F1 29982.08 Hz
 F2P -0.371 ppm
 F2 -111.25 Hz
 PPMCM 0.46848 ppm/cm
 HZCM 140.60564 Hz/cm

¹³C NMR (75 MHz, CS₂/DMSO-d₆) of compound 5b

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Current Data Parameters
NAME      J10050901
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20050905
Time      18.57
INSTRUM   av300
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg
TD         65536
SOLVENT   Acetone
NS         13960
DS         4
SMH        22675.735 Hz
FIDRES     0.346004 Hz
AQ         1.4451188 sec
RG         5792.6
DM         22.050 usec
DE         6.00 usec
TE         300.1 K
D1         2.00000000 sec
d11        0.03000000 sec
MCREST    0.00000000 sec
MCWPRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         3.00 usec
PL1        -1.00 dB
SFO1       75.4756051 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -3.00 dB
PL12       16.00 dB
SFO2       300.1315007 MHz

F2 - Processing parameters
SI         131072
SF         75.4678615 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        203.617 ppm
F1         15366.56 Hz
F2P        12.679 ppm
F2         956.85 Hz
PQCM       8.67901 ppm/cm
HZCM       654.98657 Hz/cm
    
```