Supporting Information

Cross Metathesis with Strained Exocyclic Enones: Synthesis of

3-Alkylideneoxetan-2-ones from 3-Methyleneoxetan-2-ones

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General Experimental. Melting points were determined in open Pyrex capillary tubes and are uncorrected. ^1H NMR spectra were recorded at 300 MHz, at 400 MHz and/or at 500 MHz with tetramethylsilane (TMS) as an internal standard. Chemical shifts are reported in units of parts per million (ppm). IR spectra were recorded on an FT-IR spectrometer. GC/MS spectra were obtained on a gas chromatograph equipped with a HP-1 methyl silicon column and detected on a low-resolution 5970 series mass selective detector. High resolution mass spectra were obtained on a JMS-AX505HA spectrometer. Column chromatography was performed using silica gel, 40 microns flash silica. Thin layer chromatography was performed on silica gel (Silica Gel 60 F₂₅₄) glass plates, and the compounds were visualized by UV and 2.5% *p*-anisaldehyde in H₂SO₄, acetic acid and ethanol solution.

Deuterated chloroform was dried over 3Å molecular sieves. Dichloromethane was freshly distilled from calcium hydride. But-3-enyloxy-*tert*-butyl-diphenyl-silane¹ and 4-benzhydryl-3-methyleneoxetane-2-one (**3**)² were prepared using literature procedures.

General cross-metathesis protocol. The olefin cross partner (1.5 equiv) was added to a solution of **3** (1 equiv) under N₂ in CH₂Cl₂ (0.3 N-0.4 N in lactone). Catalyst **1** or **2** (0.03-0.05 equiv) was added and the resultant solution was heated at reflux for 12-24 h. The reaction was monitored by ¹H NMR. Upon consumption of **1**, the solution was cooled and concentrated, and the brown residue was purified by flash chromatography on silica gel.

Acetic acid 3-(2-benzhydryl-4-oxooxetan-3-ylidene)propyl ester (4a**).**

Purification by flash chromatography on silica gel (petroleum ether/EtOAc 95:5) provided **4a** as a clear oil (0.27 g, 81%): IR (KBr) 3030, 1809, 1738, 1496, 1452, 1363, 1240, 1151, 1093 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.35-7.23 (m, 10H), 5.51 (d, *J* = 9.2 Hz, 1H), 5.16 (t, *J* = 7.8 Hz, 1H), 4.20 (d, *J* = 9.3 Hz, 1H), 4.03 (t, *J* = 6.3 Hz, 2H), 2.69 (m, 2H), 2.00 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.8, 163.3, 139.7, 139.3, 138.5, 133.2, 129.0, 128.9, 128.8, 128.4, 127.8, 127.3, 79.3, 62.4, 54.9, 28.5, 20.9; MS (EI) *m/z* 336 (M⁺), 276, 249, 167 (100), 152, 127, 115, 91, 77; Anal. Calcd for C₂₁H₂₀O₄: C, 74.98; H, 5.99. Found: C, 74.62; H, 5.94.

Acetic acid 4-(2-benzhydryl-4-oxooxetan-3-ylidene)butyl ester (4b).

Purification by flash chromatography on silica gel (petroleum ether/EtOAc 93:7) provided **4b** as a clear oil (0.30 g, 87%): IR (KBr) 2956, 1809, 1736, 1496, 1452, 1365, 1244, 1072 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.45-7.14 (m, 10H), 5.49 (d, $J = 9.3$ Hz, 1H), 5.14 (t, $J = 8.0$ Hz, 1H), 4.20 (d, $J = 9.3$ Hz, 1H), 3.98 (t, $J = 6.4$ Hz, 2H), 2.45 (m, 2H), 2.02 (s, 3H), 1.65 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.2, 163.5, 139.8, 139.4, 137.2, 136.8, 129.1, 129.0, 128.8, 128.4, 127.8, 127.3, 79.2, 63.2, 55.0, 27.7, 25.6, 21.1; MS (EI) m/z 350 (M^+), 332, 290, 272, 249, 167 (100), 152, 141, 77; HRMS (FAB) calcd for $\text{C}_{22}\text{H}_{23}\text{O}_4$ ($\text{M}^+ + \text{H}$) m/z 351.1596. Found: 351.1580.

Acetic acid 5-(2-benzhydryl-4-oxooxetan-3-ylidene)pentyl ester (4c). Purification by flash chromatography on silica gel (petroleum ether/EtOAc 93:7) provided **4c** as a clear oil (0.29 g, 79%, *Z* isomer): IR (KBr) 2924, 1799, 1730, 1496, 1456, 1362, 1250, 1097, 1070, 1024 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.24 (m, 10H), 5.49 (d, $J = 9.1$ Hz, 1H), 5.16 (t, $J = 7.9$ Hz, 1H), 4.20 (d, $J = 9.1$ Hz, 1H), 4.02 (t, $J = 6.4$ Hz, 2H), 2.41 (m, 2H), 2.04 (s, 3H), 1.55 (m, 2H), 1.38 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.2, 163.7, 139.9, 139.5, 137.7, 136.8, 129.0,

129.0, 128.8, 128.5, 127.7, 127.3, 79.2, 64.1, 55.0, 28.7, 28.0, 25.3, 21.1; MS (EI) m/z 364 (M^+), 346, 249, 167 (100), 115, 91, 77; Anal. Calcd for $C_{23}H_{24}O_4$: C, 75.80; H, 6.64. Found: C, 75.54; H, 6.25. (20 mg, 6%, E isomer): IR (KBr) 2931, 1813, 1734, 1496, 1454, 1365, 1244, 1041 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.34-7.23 (m, 10H), 6.26 (t, $J = 7.6$ Hz, 1H), 5.68 (d, $J = 8.3$ Hz, 1H), 4.27 (d, $J = 8.3$ Hz, 1H), 3.94 (t, $J = 6.2$ Hz, 2H), 2.05 (s, 3H), 1.45-1.22 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 164.1, 140.3, 139.3, 136.7, 135.4, 129.3, 128.8, 128.8, 128.5, 127.8, 127.4, 80.1, 63.9, 55.0, 28.2, 28.1, 24.9, 21.1; MS (EI) m/z 364 (M^+), 346, 286, 258, 167 (100), 141, 115, 91, 77, 53; HRMS (FAB) calcd for $C_{23}H_{23}O_4$ ($M^+ - H$) m/z 363.1596. Found: 363.1602.

Acetic acid 9-(2-benzhydryl-4-oxooxetan-3-ylidene)nonyl ester (4d).

Purification by flash chromatography on silica gel (petroleum ether/EtOAc 95:5) provided **4d** as a clear oil (0.20 g, 80%): IR (KBr) 2929, 2856, 1809, 1736, 1496, 1452, 1365, 1244, 1068 cm^{-1} ; 1H NMR (500 MHz, $CDCl_3$) δ 7.36-7.22 (m, 10H), 5.48 (d, $J = 9.2$ Hz, 1H), 5.17 (ddd, $J = 8.0, 8.0, 1.0$ Hz, 1H), 4.19 (d, $J = 9.2$ Hz, 1H), 4.05 (t, $J = 6.7$ Hz, 2H), 2.35 (m, 2H), 2.04 (s, 3H), 1.61 (m, 2H), 1.28-1.22 (m, 10H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.2, 163.7, 139.9, 139.5, 138.6, 136.1, 128.9, 128.7, 128.4, 127.6, 127.2, 79.0, 64.6, 55.0, 29.1, 29.0, 28.8, 28.7, 25.9, 21.1; MS (EI) m/z 376 ($M^+ - CO_2$), 219, 205, 167 (100), 152, 115, 91; Anal. Calcd for $C_{27}H_{32}O_4$: C, 77.11; H, 7.67. Found: C, 76.90; H, 7.92.

4-Benzhydryl-3-benzylideneoxetan-2-one (4e). Purification by flash chromatography on silica gel (petroleum ether/EtOAc 93:7) provided **4e** as a white solid (0.11 g, 55%): mp 156-157 °C; IR (KBr) 1789, 1678, 1454, 1213, 1066 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.76-7.73 (m, 2H), 7.38-7.24 (m, 13H), 5.72 (s, 1H), 5.57 (dd, J = 9.5, 1.1 Hz, 1H), 4.28 (d, J = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.9, 139.9, 139.5, 135.5, 134.2, 132.9, 130.9, 130.5, 129.2, 129.2, 129.0, 128.9, 128.5, 127.9, 127.4, 78.1, 55.4; MS (EI) m/z 326 (M^+), 282, 279, 265, 220, 202, 191, 167 (100), 165, 152, 115, 103, 77, 51; Anal. Calcd for $\text{C}_{23}\text{H}_{18}\text{O}_2$: C, 84.64; H, 5.56. Found: C, 84.50; H, 5.52.

4-Benzhydryl-3-butylideneoxetan-2-one (4f). Purification by flash chromatography on silica gel (petroleum ether/EtOAc 99:1) provided **4f** as a clear oil (0.25 g, 86%): IR (KBr) 1795, 1454, 1095 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.17 (m, 10H), 5.46 (d, J = 9.1 Hz, 1H), 5.16 (t, J = 7.9 Hz, 1H), 4.18 (d, J = 9.1 Hz, 1H), 2.33 (m, 2H), 1.32 (m, 2H), 0.82 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.8, 139.9, 139.5, 138.5, 136.2, 128.9, 128.6, 128.4, 127.6, 127.1, 79.0, 55.0, 30.9, 22.0, 13.4; MS (EI) m/z 292 (M^+), 249, 186, 167 (100), 165, 152, 129, 115, 83, 55; Anal. Calcd for $\text{C}_{20}\text{H}_{20}\text{O}_2$: C, 82.16; H, 6.89. Found: C, 82.53; H, 6.55.

4-Benzhydryl-3-(3-bromopropylidene)-oxetan-2-one (4g). Purification

by flash chromatography on silica gel (petroleum ether/EtOAc 96:4) provided **4g** as a clear oil (0.32 g, 89%): IR (KBr) 3027, 2958, 1810, 1716, 1600, 1494, 1452, 1357, 1303, 1268, 1218, 1068 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.37-7.23 (m, 10H), 5.52 (d, J = 9.2 Hz, 1H), 5.23 (t, J = 7.4 Hz, 1H), 4.24 (d, J = 9.2 Hz, 1H), 3.33 (t, J = 6.4 Hz, 2H), 2.96 (m, 1H), 2.88 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.3, 139.6, 139.2, 138.7, 134.1, 129.1, 129.0, 128.8, 128.5, 127.9, 127.4, 79.3, 54.9, 31.5, 30.9; MS (EI) m/z 358, 356 (M^+), 249, 189, 167 (100), 165, 115, 91, 77, 53; HRMS (FAB) calcd for $\text{C}_{19}\text{H}_{17}\text{BrO}_2$ (M^+) m/z 357.0490. Found: 357.0494.

4-Benzhydryl-3-(2-chloroethylidene)oxetan-2-one (4h). Purification by

flash chromatography on silica gel (petroleum ether/EtOAc 98.5:1.5) provided **4h** as a white solid (0.19 g, 74%): mp 123-124 $^{\circ}\text{C}$; IR (KBr) 3028, 1807, 1716, 1493, 1450, 1132, 1070 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.38-7.21 (m, 10H), 5.54 (d, J = 9.5 Hz, 1H), 5.23 (t, J = 7.8 Hz, 1H), 4.30-4.21 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.4, 139.4, 139.2, 138.8, 130.8, 129.2, 129.0, 129.0, 128.3, 128.0, 127.5, 79.2, 54.6, 38.2; MS (EI) m/z 298 (M^+), 262, 249, 167 (100), 152, 115, 91, 77; Anal. Calcd for $\text{C}_{18}\text{H}_{15}\text{ClO}_2$: C, 72.36; H, 5.06. Found: C, 72.75; H, 5.43.

4-Benzhydryl-3-[3-(*tert*-

butyldiphenylsilyloxy)propylidene]oxetan-2-one (4i). Purification by flash chromatography on silica gel (petroleum ether/EtOAc 96:4) provided **4i** as a clear waxy, solid (0.25 g, 79%, *Z* isomer): IR (KBr) 3030, 2929, 2856, 1813, 1714, 1427, 1111 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 7.60-7.59 (m, 4H), 7.44-7.36 (m, 6H), 7.32-7.21 (m, 10H), 5.47 (d, $J = 9.5$ Hz, 1H), 5.41 (t, $J = 7.5$ Hz, 1H), 4.19 (d, $J = 9.5$ Hz, 1H), 3.68-3.60 (m, 2H), 2.64-2.60 (m, 2H), 1.01 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 163.7, 140.0, 139.4, 137.5, 135.7, 135.6, 133.6, 133.6, 129.9, 129.9, 129.0, 128.9, 128.8, 128.4, 127.9, 127.8, 127.3, 79.3, 62.4, 55.0, 32.4, 27.0, 19.4; MS (EI) m/z 374, 257, 167 (100), 152, 129, 115, 91; HRMS (FAB) calcd for $\text{C}_{35}\text{H}_{37}\text{O}_3\text{Si}$ ($\text{M}^+ + \text{H}$) m/z 533.2512. Found: 533.2524. (30 mg, 9%, *E* isomer): IR (KBr) 2927, 1817, 1427, 1111 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.59 (m, 4H), 7.47-7.38 (m, 6H), 7.33-7.24 (m, 10H), 6.37 (t, $J = 7.6$ Hz, 1H), 5.59 (d, $J = 7.8$ Hz, 1H), 4.22 (d, $J = 7.8$ Hz, 1H), 3.52-3.45 (m, 2H), 1.63-1.58 (m, 2H), 1.01 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.9, 140.3, 139.3, 137.8, 135.7, 135.7, 133.5, 133.5, 133.1, 130.0, 129.2, 128.9, 128.9, 128.8, 128.7, 128.0, 127.7, 127.4, 80.0, 62.1, 54.9, 31.8, 27.0, 19.4; MS (EI) m/z 264 ($\text{M}^+ - \text{CH}_2\text{OTBDPS}$), 249, 167 (100), 165, 115, 97, 77, 51; HRMS (FAB) calcd for $\text{C}_{35}\text{H}_{37}\text{O}_3\text{Si}$ ($\text{M}^+ + \text{H}$) m/z 533.2512. Found: 533.2515.

3-Butylidene-4-phenethyloxetan-2-one (6).

Purification by flash chromatography on silica gel (petroleum ether/EtOAc 98:2)

provided **6** as a clear oil (0.14 g, 62%, Z isomer): ^1H NMR (400 MHz, CDCl_3) δ 7.31-7.28 (m, 2H), 7.24-7.18 (m, 3H), 5.74 (t, $J = 7.9$ Hz, 1H), 4.85 (t, $J = 6.2$ Hz, 1H), 2.83 (m, 1H), 2.74 (m, 1H), 2.45 (q, $J = 7.5$ Hz, 2H), 2.12 (m, 2H), 1.47 (sex, $J = 7.3$ Hz, 2H), 0.93 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 164.1, 140.5, 137.5, 136.6, 128.8, 128.6, 126.5, 77.8, 35.6, 31.1, 30.9, 22.2, 13.6; MS (EI) m/z 230 (M^+), 187, 125, 105, 91 (100), 70, 55; HRMS (FAB) calcd for $\text{C}_{15}\text{H}_{19}\text{O}_2$ ($\text{M}^+ + \text{H}$) m/z 231.1385. Found: 231.1400. (31 mg, 14%, E isomer): ^1H NMR (400 MHz, CDCl_3) δ 7.33-7.29 (m, 2H), 7.25-7.20 (m, 3H), 6.35 (ddd, $J = 7.8, 7.8, 1.5$ Hz, 1H), 5.0 (d, $J = 8.5$ Hz, 1H), 2.85 (m, 1H), 2.80 (m, 1H), 2.24 (m, 1H), 2.11-2.03 (m, 3H), 1.49 (sex, $J = 7.3$ Hz, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 164.3, 140.6, 137.7, 134.3, 128.8, 128.6, 126.5, 78.2, 35.3, 31.1, 30.9, 21.9, 13.9; Anal. Calcd for $\text{C}_{15}\text{H}_{18}\text{O}_2$: C, 78.23; H, 7.88. Found: C, 78.20; H, 7.69.

¹ Francesch, A.; Alvarez, R.; Lopez, S.; de Lera, A.R. *J. Org. Chem.* **1997**, 62, 310-319.

² Martinez, I.; Andrews, A. E.; Emch, J. D.; Ndakala, A. J.; Wang, J.; Howell, A. R. *Org. Lett.* **2003**, 5, 399.

7.31
7.29
7.28
7.25
7.24
7.24
7.21

5.50
5.47
5.16
5.14
5.12

4.21
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3.96

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1.65

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PROCNO 1

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Current Data Parameters
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PROCNO 1

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DS 4
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PCPD2 110.00 usec
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PL13 19.00 dB
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F2 - Processing parameters
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SF 100.6162812 MHz
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Current Data Parameters
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 DS 4
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 DE 6.00 usec
 TE 297.2 K
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 MCREST 0.00000000 sec
 MCWRK 1.00000000 sec
 ST1CNT 128

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F2 - Processing parameters
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 SF 500.1300000 MHz
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 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
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 SSB 2
 LB 0.00 Hz
 GB 0

Current Data Parameters
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 PROCNO 1

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 DS 2
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 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 101.6
 DW 89.400 usec
 DE 6.00 usec
 TE 300.0 K
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 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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 LB 0.30 Hz
 GB 0
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 PROCNO 1

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 Time 13.06
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 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 6502
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 DE 6.00 usec
 TE 300.0 K
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 PL12 19.00 dB
 PL13 19.00 dB
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F2 - Processing parameters
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Current Data Parameters
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 PROCNO 1

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 DS 4
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F2 - Processing parameters
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 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
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F1 - Processing parameters
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 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

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F2 - Processing parameters
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WDW                      EM
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GB                      0
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Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zgpg30
 TD 32768
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 NS 171
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.916444 Hz
 AQ 0.5456539 sec
 RG 18390.4
 DW 16.650 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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 NUC1 13C
 P1 7.75 usec
 PL1 0.00 dB
 SFO1 125.7703643 MHz

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 NUC2 1H
 PCPD2 70.00 usec
 PL2 -1.00 dB
 PL12 14.69 dB
 PL13 17.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
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 SF 125.7577762 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
NAME rr2-27-4
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050314
Time 9.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl₃
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.292314 Hz
AQ 1.7105396 sec
RG 362
DW 104.400 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F2 - Processing parameters	
SI	32768
SF	125.7577762 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Current Data Parameters
 NAME rr2-141-3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051110
 Time 15.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 71.8
 DW 89.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 25.00 usec
 PL1 6.20 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440165 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME rr2-141-3
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051110
Time 15.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 136
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.30 usec
PL1 -3.00 dB
SFO1 100.6263505 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 400.1456006 MHz

F2 - Processing parameters
SI 32768
SF 100.6162782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME rr2-141-4
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051118
 Time 10.32
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 80.6
 DW 89.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 25.00 usec
 PL1 6.20 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME rr2-141-4
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051118
 Time 10.39
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 301
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.30 usec
 PL1 -3.00 dB
 SFO1 100.6263505 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 0.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SFO2 400.1456006 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162760 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
NAME rr-20-4
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050302
Time 15.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG noesyph
TD 2048
SOLVENT CDC13
NS 4
DS 4
SWH 5122.951 Hz
FIDRES 2.501441 Hz
AQ 0.2000324 sec
RG 48
DW 97.600 usec
DE 6.00 usec
TE 298.2 K
d0 0.00008232 sec
D1 2.00000000 sec
D8 0.30000001 sec
IN0 0.00019520 sec
MCREST 0.00000000 sec
MCWRK 1.00000000 sec
ST1CNT 128

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
SFO1 500.1323022 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 500.1323 MHz
FIDRES 20.011526 Hz
SW 10.243 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 500.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

4c

Current Data Parameters
NAME rr2-63-2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050525
Time 9.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG noesyph
TD 2048
SOLVENT CDCl₃
NS 4
DS 4
SWH 4084.967 Hz
FIDRES 1.994613 Hz
AQ 0.2507252 sec
RG 40
DW 122.400 usec
DE 6.00 usec
TE 300.0 K
d0 0.00011005 sec
D1 2.00000000 sec
D8 0.69999999 sec
INQ 0.00024480 sec
MCREST 0.00000000 sec
MCWRK 1.00000000 sec
STICNT 128

===== CHANNEL f1 =====
NUC1 1H
P1 9.70 usec
PL1 -2.00 dB
SFO1 400.1458419 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1458 MHz
FIDRES 15.956903 Hz
SW 10.209 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.1440000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.1440000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

Current Data Parameters
NAME RR2-32-1-1
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050324
Time 11.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG noesyph
TD 2048
SOLVENT CDC13
NS 4
DS 4
SWH 4084.967 Hz
FIDRES 1.994613 Hz
AQ 0.2507252 sec
RG 160
DW 122.400 usec
DE 6.00 usec
TE 300.0 K
d0 0.00011005 sec
D1 2.00000000 sec
D8 0.69999999 sec
INO 0.00024480 sec
MCREST 0.00000000 sec
MCWRK 1.00000000 sec
ST1CNT 128

===== CHANNEL f1 =====
NUC1 1H
P1 9.70 usec
PL1 -2.00 dB
SFO1 400.1458419 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1458 MHz
FIDRES 15.956903 Hz
SW 10.209 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.1440000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.1440000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

Current Data Parameters
NAME rr2-59-1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050516
Time 10.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG noesyph
TD 2048
SOLVENT CDCl3
NS 2
DS 4
SWH 4084.967 Hz
FIDRES 1.994613 Hz
AQ 0.2507252 sec
RG 30
DW 122.400 usec
DE 6.00 usec
TE 300.0 K
d0 0.00011005 sec
D1 2.00000000 sec
D8 0.69999999 sec
IN0 0.00024480 sec
MCREST 0.00000000 sec
MCWRK 1.00000000 sec
STCNT 128

===== CHANNEL f1 =====
NUC1 1H
P1 9.70 usec
PL1 -2.00 dB
SFO1 400.1458419 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1458 MHz
FIDRES 15.956903 Hz
SW 10.209 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.1440000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.1440000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0