Supporting Information

Diterpenes from the Endangered Goldenrod
Solidago shortii

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SI Figure 1. Selected 2D NMR Correlations for Compound 4.

SI Figure 2. Selected 2D NMR Correlations for Compound 5.

SI Figure 3. Selected 2D NMR Correlations for Compound **6**.

SepFraction CP2905 H2 in MeOD (1.7mm Tube)

Current Data Parameters
 NAME SF_CP2905_H2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130115
 Time 16.25
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4079740 sec
 RG 256
 DW 52.000 usec
 DE 6.00 usec
 TE 299.0 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 2.00 dB
 SFO1 600.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 600.1300072 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 5.00

SepFraction CP 2905 H2 in MeOD

Current Data Parameters
 NAME SF_CP2905_H2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130115
 Time 16.34
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG cosygpcqf
 TD 2048
 SOLVENT MeOD
 NS 8
 DS 16
 SWH 3687.316 Hz
 FIDRES 1.800447 Hz
 AQ 0.2778944 sec
 RG 256
 DW 135.600 usec
 DE 6.00 usec
 TE 299.0 K
 d0 0.00000300 sec
 D1 1.27021003 sec
 d13 0.00000400 sec
 D16 0.00025000 sec
 INO 0.00027120 sec

===== CHANNEL f1 =====
 NUC1 1H
 P0 14.90 usec
 P1 14.90 usec
 PL1 2.00 dB
 SFO1 600.1320920 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPZ1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 600.1321 MHz
 FIDRES 14.403577 Hz
 SW 6.144 ppm
 FnMODE QF

F2 - Processing parameters
 SI 1024
 SF 600.1300058 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 10.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 600.1300055 MHz
 WDW
 SSB 0
 LB 0 Hz
 GB 0

SepFraction CP 2905 H2 in MeOD

Current Data Parameters
NAME SF_CP2905_H2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130116
Time 2.47
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG hsqcetgpsisp.2.moj
TD 4096
SOLVENT MeOD
NS 8
DS 32
SWH 3687.316 Hz
FIDRES 0.900224 Hz
AQ 0.5556032 sec
RG 2048
DW 135.600 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
CNST17 -0.5000000
d0 0.00000300 sec
D1 0.90546268 sec
d4 0.00172414 sec
d11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086000 sec
DELTA 0.00123180 sec
DELTA1 0.00120800 sec
DELTA2 0.00147014 sec
DELTA3 0.00135600 sec
IN0 0.00001655 sec
ST1CNT 0

===== CHANNEL f1 =====
NUC1 1H
P1 14.90 usec
p2 29.80 usec
PL1 2.00 dB
SFO1 600.1320920 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 13.00 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 65.00 usec
PL0 120.00 dB
PL2 -4.00 dB
PL12 9.00 dB
SFO2 150.9148810 MHz
SP3 1.80 dB
SP7 1.80 dB
SPNAM3 Crp60,0.5,20.1
SPNAM7 Crp60comp.4
SPOAL3 0.500
SPOAL7 0.500
SPOFFS3 0 Hz
SPOFFS7 0 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 10.05 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 200
SFO1 150.9149 MHz
FIDRES 151.057404 Hz
SW 200.189 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300072 MHz

SepFraction CP 2905 H2 in MeOD

Current Data Parameters
NAME SF_CP2905_H2
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130115
Time_ 20.53
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG inv4gplprnd
TD 4096
SOLVENT MeOD
NS 64
DS 32
SWH 3687.316 Hz
FIDRES 0.900224 Hz
AQ 0.5556032 sec
RG 4096
DW 135.600 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.03001201 sec
d2 0.00344828 sec
D6 0.06600000 sec
d13 0.00000300 sec
D16 0.00025000 sec
INO 0.00001185 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.90 usec
p2 29.80 usec
PL1 2.00 dB
SFO1 600.1320920 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 13.00 usec
PL2 -4.00 dB
SFO2 150.9178390 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 200
SFO1 150.9178 MHz
FIDRES 210.970459 Hz
SW 279.583 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.130063 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9026512 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction CP 2905 H2 in MeOD

Current Data Parameters
 NAME SF_CP2905_H2
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130115
 Time 17.30
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG roesyph
 TD 2048
 SOLVENT MeOD
 NS 24
 DS 16
 SWH 3687.316 Hz
 FIDRES 1.800447 Hz
 AQ 0.2778944 sec
 RG 256
 DW 135.600 usec
 DE 6.00 usec
 TE 299.0 K
 d0 0.00012211 sec
 D1 1.41316402 sec
 d12 0.00002000 sec
 IN0 0.00027120 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 ^1H
 P1 14.90 usec
 P15 250000.00 usec
 PL1 2.00 dB
 PL11 19.20 dB
 SFO1 600.1320920 MHz

F1 - Acquisition parameters
 TD 256
 SFO1 600.1321 MHz
 FIDRES 14.403577 Hz
 SW 6.144 ppm
 FnMODE States-TPPI

F2 - Processing parameters
 SI 1024
 SF 600.1300072 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States-TPPI
 SF 600.1300072 MHz
 WDW
 SSB 2
 LB 0 Hz
 GB 0

SepFraction 20478 in MeOD (1mm Tube)

Current Data Parameters
 NAME SF_20478
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130401
 Time 14.23
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4079740 sec
 RG 2048
 DW 52.000 usec
 DE 6.00 usec
 TE 299.0 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 2.00 dB
 SFO1 600.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 600.1300072 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 10.00

SepFraction 20478 in MeOD

Current Data Parameters

NAME SF_20478
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130401
Time 16.01
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG cosygpcqf
TD 2048
SOLVENT MeOD
NS 8
DS 16
SWH 4664.179 Hz
FIDRES 2.277431 Hz
AQ 0.2197028 sec
RG 2048
DW 107.200 usec
DE 6.00 usec
TE 299.0 K
d0 0.00000300 sec
D1 1.32755399 sec
d13 0.00000400 sec
D16 0.00025000 sec
IN0 0.00021440 sec

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

NUC1 1H
P0 18.00 usec
P1 18.00 usec
PL1 2.00 dB
SFO1 600.1324386 MHz

===== GRADIENT CHANNEL =====

GPNAME1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

TD 256
SFO1 600.1324 MHz
FIDRES 18.219450 Hz
SW 7.772 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300052 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 10.00

F1 - Processing parameters

SI 1024
MC2 QF
SF 600.1300050 MHz
WDW
SSB 0
LB 0 Hz
GB 0

SepFraction 20478 in MeOD

Current Data Parameters
 NAME SF_20478
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130401
 Time 14.36
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG hsqcetgpsisp.2.moj
 TD 4096
 SOLVENT MeOD
 NS 16
 DS 32
 SWH 4664.179 Hz
 FIDRES 1.138716 Hz
 AQ 0.4392484 sec
 RG 2048
 DW 107.200 usec
 DE 6.00 usec
 TE 299.0 K
 CNST2 145.0000000
 CNST17 -0.5000000
 d0 0.00000300 sec
 D1 1.02015102 sec
 d4 0.00172414 sec
 d11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.00086000 sec
 DELTA 0.00123800 sec
 DELTA1 0.00120800 sec
 DELTA2 0.00147014 sec
 DELTA3 0.00135600 sec
 IN0 0.00001655 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 1H
 P1 18.00 usec
 p2 36.00 usec
 PL1 2.00 dB
 SFO1 600.1324386 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 13.00 usec
 P14 500.00 usec
 P24 2000.00 usec
 PCPD2 65.00 usec
 PL0 120.00 dB
 PL2 -4.00 dB
 PL12 9.00 dB
 SFO2 150.9148810 MHz
 SP3 1.80 dB
 SP7 1.80 dB
 SPNAM3 Crp60,0.5,20.1
 SPNAM7 Crp60comp.4
 SPOAL3 0.500
 SPOAL7 0.500
 SPOFFS3 0 Hz
 SPOFFS7 0 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 40.00 %
 GPZ2 10.05 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 200
 SFO1 150.9149 MHz
 FIDRES 151.057404 Hz
 SW 200.189 ppm
 FMODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 600.1300051 MHz

SepFraction 20478 in MeOD

Current Data Parameters
NAME SF_20478
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20130401
Time 20.21
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG inv4gplprnd
TD 4096
SOLVENT MeOD
NS 128
DS 32
SWH 4664.179 Hz
FIDRES 1.138716 Hz
AQ 0.4392484 sec
RG 4096
DW 107.200 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.14470005 sec
d2 0.00344828 sec
D6 0.06600000 sec
d13 0.00000300 sec
D16 0.00025000 sec
INO 0.00001185 sec

===== CHANNEL f1 =====
NUC1 1H
P1 18.00 usec
p2 36.00 usec
PL1 2.00 dB
SFO1 600.1324386 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 13.00 usec
PL2 -4.00 dB
SFO2 150.9178390 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 167
SFO1 150.9178 MHz
FIDRES 225.636856 Hz
SW 279.583 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.130052 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9026163 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20478 in MeOD

Current Data Parameters

NAME SF_20478
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130401
Time 16.57
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG roesyph
TD 2048
SOLVENT MeOD
NS 24
DS 16
SWH 4664.179 Hz
FIDRES 2.277431 Hz
AQ 0.2197028 sec
RG 2048
DW 107.200 usec
DE 6.00 usec
TE 299.0 K
d0 0.00009174 sec
D1 1.47050798 sec
d12 0.00002000 sec
IN0 0.00021440 sec
ST1CNT 0

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

NUC1 1H
P1 18.00 usec
P15 250000.00 usec
PL1 2.00 dB
PL11 19.20 dB
SFO1 600.1324386 MHz

F1 - Acquisition parameters

TD 256
SFO1 600.1324 MHz
FIDRES 18.219450 Hz
SW 7.772 ppm
FnMODE States-TPPI

F2 - Processing parameters

SI 1024
SF 600.1300053 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 600.1300046 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20479 in MeOD (1.7mm Tube)

Current Data Parameters
 NAME SF_20479
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130304
 Time 13.07
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4079740 sec
 RG 2048
 DW 52.000 usec
 DE 6.00 usec
 TE 299.0 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 2.00 dB
 SFO1 600.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 600.1300072 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 10.00

SepFraction 20479 in MeOD

Current Data Parameters

NAME SF_20479
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130304
Time 14.38
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG cosygpcqf
TD 2048
SOLVENT MeOD
NS 8
DS 16
SWH 3531.073 Hz
FIDRES 1.724157 Hz
AQ 0.2901884 sec
RG 2048
DW 141.600 usec
DE 6.00 usec
TE 298.9 K
d0 0.00000300 sec
D1 1.25792205 sec
d13 0.00000400 sec
D16 0.00025000 sec
IN0 0.00028320 sec

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

NUC1 1H
P0 12.90 usec
P1 17.50 usec
PL1 2.00 dB
SFO1 600.1320329 MHz

===== GRADIENT CHANNEL =====

GPNAME1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

TD 256
SFO1 600.132 MHz
FIDRES 13.793256 Hz
SW 5.884 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300060 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 10.00

F1 - Processing parameters

SI 1024
MC2 QF
SF 600.1300064 MHz
WDW
SSB 0
LB 0 Hz
GB 0

SepFraction 20479 in MeOD

Current Data Parameters
 NAME SF_20479
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130304
 Time 13.16
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG hsqcetgpsisp.2.moj
 TD 4096
 SOLVENT MeOD
 NS 16
 DS 32
 SWH 3531.073 Hz
 FIDRES 0.862078 Hz
 AQ 0.5801852 sec
 RG 2048
 DW 141.600 usec
 DE 6.00 usec
 TE 298.9 K
 CNST2 145.0000000
 CNST17 -0.5000000
 d0 0.00000300 sec
 D1 0.88088667 sec
 d4 0.00172414 sec
 d11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.00086000 sec
 DELTA 0.00123700 sec
 DELTA1 0.00120800 sec
 DELTA2 0.00147014 sec
 DELTA3 0.00135600 sec
 IN0 0.00001655 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 1H
 P1 17.50 usec
 p2 35.00 usec
 PL1 2.00 dB
 SFO1 600.1320329 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 13.00 usec
 P14 500.00 usec
 P24 2000.00 usec
 PCPD2 65.00 usec
 PL0 120.00 dB
 PL2 -4.00 dB
 PL12 9.00 dB
 SFO2 150.9148810 MHz
 SP3 1.80 dB
 SP7 1.80 dB
 SPNAM3 Crp60,0.5,20.1
 SPNAM7 Crp60comp.4
 SPOAL3 0.500
 SPOAL7 0.500
 SPOFFS3 0 Hz
 SPOFFS7 0 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 40.00 %
 GPZ2 10.05 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 200
 SFO1 150.9149 MHz
 FIDRES 151.057404 Hz
 SW 200.189 ppm
 FnmODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 600.1300047 MHz

SepFraction 20479 in MeOD

Current Data Parameters
 NAME SF_20479
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130304
 Time 19.00
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG inv4gplprnd
 TD 4096
 SOLVENT MeOD
 NS 192
 DS 32
 SWH 3531.073 Hz
 FIDRES 0.862078 Hz
 AQ 0.5801852 sec
 RG 4096
 DW 141.600 usec
 DE 6.00 usec
 TE 299.0 K
 CNST2 145.0000000
 d0 0.00000300 sec
 D1 1.00543594 sec
 d2 0.00344828 sec
 D6 0.06600000 sec
 d13 0.00000300 sec
 D16 0.00025000 sec
 INO 0.00001185 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 17.50 usec
 p2 35.00 usec
 PL1 2.00 dB
 SFO1 600.1320329 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P3 13.00 usec
 PL2 -4.00 dB
 SFO2 150.9178390 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 186
 SFO1 150.9178 MHz
 FIDRES 226.849960 Hz
 SW 279.583 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 600.1300051 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 150.9026376 MHz
 WDW
 SSB 2
 LB 0 Hz
 GB 0

SepFraction 20479 in MeOD

Current Data Parameters

NAME SF_20479
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130304
Time 15.33
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG roesyph
TD 2048
SOLVENT MeOD
NS 24
DS 16
SWH 3531.073 Hz
FIDRES 1.724157 Hz
AQ 0.2901884 sec
RG 2048
DW 141.600 usec
DE 6.00 usec
TE 299.0 K
d0 0.00012646 sec
D1 1.40087605 sec
d12 0.00002000 sec
IN0 0.00028320 sec
ST1CNT 0

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

NUC1 1H
P1 17.50 usec
P15 250000.00 usec
PL1 2.00 dB
PL11 19.20 dB
SFO1 600.1320329 MHz

F1 - Acquisition parameters

TD 256
SFO1 600.132 MHz
FIDRES 13.793256 Hz
SW 5.884 ppm
FnMODE States-TPPI

F2 - Processing parameters

SI 1024
SF 600.1300060 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 600.1300061 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20318 in MeOD (1mm Tube)

Current Data Parameters
 NAME SF_20318
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121031
 Time_ 14.43
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4079740 sec
 RG 2048
 DW 52.000 usec
 DE 20.00 usec
 TE 299.0 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 2.00 dB
 SFO1 600.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 600.1300072 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 10.00

SepFraction 20318 in MeOD

Current Data Parameters

NAME SF_20318
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121031
Time 15.42
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG cosygpcqf
TD 2048
SOLVENT MeOD
NS 8
DS 16
SWH 3654.971 Hz
FIDRES 1.784654 Hz
AQ 0.2803532 sec
RG 2048
DW 136.800 usec
DE 6.00 usec
TE 572.2 K
d0 0.00000300 sec
D1 1.26611400 sec
d13 0.00000400 sec
D16 0.00025000 sec
IN0 0.00027360 sec

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

NUC1 1H
P0 14.00 usec
P1 14.00 usec
PL1 2.00 dB
SFO1 600.1320966 MHz

===== GRADIENT CHANNEL =====

GPNAME1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

TD 256
SFO1 600.1321 MHz
FIDRES 14.277229 Hz
SW 6.090 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300051 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 10.00

F1 - Processing parameters

SI 1024
MC2 QF
SF 600.1300052 MHz
WDW
SSB 0
LB 0 Hz
GB 0

SepFraction 20318 in MeOD

Current Data Parameters
NAME SF_20318
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121031
Time 14.57
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG hsqcetgpsisp.2.moj
TD 4096
SOLVENT MeOD
NS 8
DS 32
SWH 3654.971 Hz
FIDRES 0.892327 Hz
AQ 0.5605196 sec
RG 2048
DW 136.800 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
CNST17 -0.5000000
d0 0.00000300 sec
D1 0.89809018 sec
d4 0.00172414 sec
d11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086000 sec
DELTA 0.00123000 sec
DELTA1 0.00120800 sec
DELTA2 0.00147014 sec
DELTA3 0.00135600 sec
IN0 0.00001655 sec
ST1CNT 0

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
p2 28.00 usec
PL1 2.00 dB
SFO1 600.1320966 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 13.00 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 65.00 usec
PL0 120.00 dB
PL2 -4.00 dB
PL12 9.00 dB
SFO2 150.9148810 MHz
SP3 1.80 dB
SP7 1.80 dB
SPNAM3 Crp60,0.5,20.1
SPNAM7 Crp60comp.4
SPOAL3 0.500
SPOAL7 0.500
SPOFFS3 0 Hz
SPOFFS7 0 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 10.05 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 200
SFO1 150.9149 MHz
FIDRES 151.057404 Hz
SW 200.189 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300046 MHz

SepFraction 20318 in MeOD

Current Data Parameters
NAME SF_20318
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121031
Time 18.56
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG inv4gplprnd
TD 4096
SOLVENT MeOD
NS 128
DS 32
SWH 3654.971 Hz
FIDRES 0.892327 Hz
AQ 0.5605196 sec
RG 4096
DW 136.800 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.02263904 sec
d2 0.00344828 sec
D6 0.06600000 sec
d13 0.00000300 sec
D16 0.00025000 sec
INO 0.00001185 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
p2 28.00 usec
PL1 2.00 dB
SFO1 600.1320966 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 12.50 usec
PL2 -4.00 dB
SFO2 150.9178390 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 200
SFO1 150.9178 MHz
FIDRES 210.970459 Hz
SW 279.583 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300022 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9025988 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20318 in MeOD

Current Data Parameters

NAME SF_20318
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121031
Time 16.38
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG roesyph
TD 2048
SOLVENT MeOD
NS 16
DS 16
SWH 3654.971 Hz
FIDRES 1.784654 Hz
AQ 0.2803532 sec
RG 2048
DW 136.800 usec
DE 6.00 usec
TE 299.0 K
d0 0.00012389 sec
D1 1.40906799 sec
d12 0.00002000 sec
IN0 0.00027360 sec
ST1CNT 0

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

NUC1 1H
P1 14.00 usec
P15 250000.00 usec
PL1 2.00 dB
PL11 19.20 dB
SFO1 600.1320966 MHz

F1 - Acquisition parameters

TD 256
SFO1 600.1321 MHz
FIDRES 14.277229 Hz
SW 6.090 ppm
FnMODE States-TPPI

F2 - Processing parameters

SI 1024
SF 600.1300047 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 600.1300057 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20322 in MeOD (1.7mm Tube)

Current Data Parameters
 NAME SF_20322
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20121102
 Time 16.06
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4079740 sec
 RG 2048
 DW 52.000 usec
 DE 20.00 usec
 TE 299.1 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 2.00 dB
 SFO1 600.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 600.1300072 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 10.00

SepFraction 20322 in MeOD

Current Data Parameters

NAME SF_20322
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121102
Time 16.18
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG cosygpcf
TD 2048
SOLVENT MeOD
NS 8
DS 16
SWH 3687.316 Hz
FIDRES 1.800447 Hz
AQ 0.2778944 sec
RG 1024
DW 135.600 usec
DE 6.00 usec
TE 299.0 K
d0 0.00000300 sec
D1 1.26816201 sec
d13 0.00000400 sec
D16 0.00025000 sec
IN0 0.00027120 sec

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

NUC1 1H
P0 14.70 usec
P1 14.70 usec
PL1 2.00 dB
SFO1 600.1320963 MHz

===== GRADIENT CHANNEL =====

GPNAME1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

TD 104
SFO1 600.1321 MHz
FIDRES 35.454960 Hz
SW 6.144 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300072 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 10.00

F1 - Processing parameters

SI 1024
MC2 QF
SF 600.1300072 MHz
WDW
SSB 0
LB 0 Hz
GB 0

SepFraction 20322 in MeOD

27

Current Data Parameters
NAME SF_20322
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121103
Time 4.55
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG hsqcetgpsisp.2.moj
TD 4096
SOLVENT MeOD
NS 16
DS 32
SWH 3687.316 Hz
FIDRES 0.900224 Hz
AQ 0.5556032 sec
RG 2048
DW 135.600 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
CNST17 -0.5000000
d0 0.00000300 sec
D1 0.90136671 sec
d4 0.00172414 sec
d11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086000 sec
DELTA 0.00123140 sec
DELTA1 0.00120800 sec
DELTA2 0.00147014 sec
DELTA3 0.00135600 sec
IN0 0.00001655 sec
ST1CNT 0

===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
p2 29.40 usec
PL1 2.00 dB
SFO1 600.1320963 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 13.00 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 65.00 usec
PL0 120.00 dB
PL2 -4.00 dB
PL12 9.00 dB
SFO2 150.9148810 MHz
SP3 1.80 dB
SP7 1.80 dB
SPNAM3 Crp60,0.5,20.1
SPNAM7 Crp60comp.4
SPOAL3 0.500
SPOAL7 0.500
SPOFFS3 0 Hz
SPOFFS7 0 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 10.05 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 200
SFO1 150.9149 MHz
FIDRES 151.057404 Hz
SW 200.189 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300033 MHz

SepFraction 20322 in MeOD

Current Data Parameters
 NAME SF_20322
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121102
 Time_ 20.05
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG inv4gplprnd
 TD 4096
 SOLVENT MeOD
 NS 96
 DS 32
 SWH 3687.316 Hz
 FIDRES 0.900224 Hz
 AQ 0.5556032 sec
 RG 4096
 DW 135.600 usec
 DE 6.00 usec
 TE 299.0 K
 CNST2 145.0000000
 d0 0.00000300 sec
 D1 1.02673495 sec
 d2 0.00344828 sec
 D6 0.06600000 sec
 d13 0.00000300 sec
 D16 0.00025000 sec
 INO 0.00001185 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.70 usec
 p2 29.40 usec
 PL1 2.00 dB
 SFO1 600.1320963 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P3 13.00 usec
 PL2 -4.00 dB
 SFO2 150.9178390 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 200
 SFO1 150.9178 MHz
 FIDRES 210.970459 Hz
 SW 279.583 ppm
 FnMODE QF

F2 - Processing parameters
 SI 1024
 SF 600.1300024 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 150.9027344 MHz
 WDW
 SSB 2
 LB 0 Hz
 GB 0

SepFraction 20322 in MeOD

29

Current Data Parameters

NAME SF_20322
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121102
Time 16.41
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG roesyph
TD 2048
SOLVENT MeOD
NS 24
DS 16
SWH 3687.316 Hz
FIDRES 1.800447 Hz
AQ 0.2778944 sec
RG 1024
DW 135.600 usec
DE 6.00 usec
TE 299.0 K
d0 0.00012224 sec
D1 1.41111600 sec
d12 0.00002000 sec
IN0 0.00027120 sec
ST1CNT 0

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

NUC1 1H
P1 14.70 usec
P15 250000.00 usec
PL1 2.00 dB
PL11 19.20 dB
SFO1 600.1320963 MHz

F1 - Acquisition parameters

TD 256
SFO1 600.1321 MHz
FIDRES 14.403577 Hz
SW 6.144 ppm
FnMODE States-TPPI

F2 - Processing parameters

SI 1024
SF 600.1300058 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 600.1300051 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20317 in MeOD (1mm Tube)

Current Data Parameters
NAME SF_20317
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121030
Time_ 16.12
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG zg
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079740 sec
RG 2048
DW 52.000 usec
DE 20.00 usec
TE 299.0 K
D1 1.50000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 2.00 dB
SFO1 600.1324000 MHz

F2 - Processing parameters
SI 32768
SF 600.1300072 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 10.00

SepFraction 20317 in MeOD

Current Data Parameters

NAME SF_20317
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121030
Time 16.28
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG cosygpcqf
TD 2048
SOLVENT MeOD
NS 8
DS 16
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2131460 sec
RG 2048
DW 104.000 usec
DE 6.00 usec
TE 299.0 K
d0 0.00000300 sec
D1 1.33369803 sec
d13 0.00000400 sec
D16 0.00025000 sec
INO 0.00020800 sec

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

NUC1 1H
P0 15.00 usec
P1 15.00 usec
PL1 2.00 dB
SFO1 600.1326076 MHz

===== GRADIENT CHANNEL =====

GPNAME1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

TD 256
SFO1 600.1326 MHz
FIDRES 18.780048 Hz
SW 8.011 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300056 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 10.00

F1 - Processing parameters

SI 1024
MC2 QF
SF 600.1300081 MHz
WDW
SSB 0
LB 0 Hz
GB 0

SepFraction 20317 in MeOD

Current Data Parameters
 NAME SF_20317
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121101
 Time 9.40
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG hsqcetgpsisp.2.moj
 TD 4096
 SOLVENT MeOD
 NS 32
 DS 32
 SWH 4807.692 Hz
 FIDRES 1.173753 Hz
 AQ 0.4261380 sec
 RG 2048
 DW 104.000 usec
 DE 6.00 usec
 TE 299.0 K
 CNST2 145.0000000
 CNST17 -0.5000000
 d0 0.0000300 sec
 D1 1.03243899 sec
 d4 0.00172414 sec
 d11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.00086000 sec
 DELTA 0.00123400 sec
 DELTA1 0.00120800 sec
 DELTA2 0.00147014 sec
 DELTA3 0.00135600 sec
 IN0 0.0001655 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 1H
 P1 16.00 usec
 p2 32.00 usec
 PL1 2.00 dB
 SFO1 600.1326076 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 13.00 usec
 P14 500.00 usec
 P24 2000.00 usec
 PCPD2 65.00 usec
 PL0 120.00 dB
 PL2 -4.00 dB
 PL12 9.00 dB
 SFO2 150.9148810 MHz
 SP3 1.80 dB
 SP7 1.80 dB
 SPNAM3 Crp60,0.5,20.1
 SPNAM7 Crp60comp.4
 SPOAL3 0.500
 SPOAL7 0.500
 SPOFFS3 0 Hz
 SPOFFS7 0 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 40.00 %
 GPZ2 10.05 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 118
 SFO1 150.9149 MHz
 FIDRES 256.029480 Hz
 SW 200.189 ppm
 FMODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 600.1300048 MHz

SepFraction 20317 in MeOD

Current Data Parameters
NAME SF_20317
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121030
Time 20.47
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG inv4gplprnd
TD 4096
SOLVENT MeOD
NS 128
DS 32
SWH 4807.692 Hz
FIDRES 1.173753 Hz
AQ 0.4261380 sec
RG 4096
DW 104.000 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.15780699 sec
d2 0.00344828 sec
D6 0.06600000 sec
d13 0.00000300 sec
D16 0.00025000 sec
INO 0.00001185 sec

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
p2 30.00 usec
PL1 2.00 dB
SFO1 600.1326076 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 12.50 usec
PL2 -4.00 dB
SFO2 150.9178390 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 176
SFO1 150.9178 MHz
FIDRES 239.739166 Hz
SW 279.583 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300040 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9025816 MHz
WDW
SSB 2
LB 0 Hz
GB 0

SepFraction 20317 in MeOD

Current Data Parameters

NAME SF_20317
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121030
Time 17.23
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG roesyph
TD 2048
SOLVENT MeOD
NS 24
DS 16
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2131460 sec
RG 2048
DW 104.000 usec
DE 6.00 usec
TE 299.0 K
d0 0.00009045 sec
D1 1.47665203 sec
d12 0.00002000 sec
IN0 0.00020800 sec
ST1CNT 0

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

NUC1 1H
P1 15.00 usec
P15 250000.00 usec
PL1 2.00 dB
PL11 18.50 dB
SFO1 600.1326076 MHz

F1 - Acquisition parameters

TD 256
SFO1 600.1326 MHz
FIDRES 18.780048 Hz
SW 8.011 ppm
FnMODE States-TPPI

F2 - Processing parameters

SI 1024
SF 600.1300049 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 600.1300059 MHz
WDW
SSB 2
LB 0 Hz
GB 0

Table 1. Crystal data and structure refinement for compound 1.

Empirical formula	C ₂₅ H ₃₆ O ₅	
Formula weight	416.54	
Crystal system	monoclinic	
Space group	<i>I</i> 2	
Unit cell dimensions	<i>a</i> = 13.9471(18) Å	$\alpha = 90^\circ$
	<i>b</i> = 8.2238(10) Å	$\beta = 93.918(3)^\circ$
	<i>c</i> = 19.675(2) Å	$\gamma = 90^\circ$
Volume	2251.4(5) Å ³	
Z, Z'	4, 1	
Density (calculated)	1.229 Mg/m ³	
Wavelength	0.71073 Å	
Temperature	100(2) K	
<i>F</i> (000)	904	
Absorption coefficient	0.084 mm ⁻¹	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.977 and 0.967	
Theta range for data collection	1.735 to 28.295°	
Reflections collected	11330	
Independent reflections	5476 [<i>R</i> (int) = 0.0346]	
Data / restraints / parameters	5476 / 1 / 277	
<i>wR</i> (<i>F</i> ² all data)	<i>wR</i> 2 = 0.1269	
<i>R</i> (<i>F</i> obsd data)	<i>R</i> 1 = 0.0507	
Goodness-of-fit on <i>F</i> ²	1.003	
Observed data [<i>I</i> > 2σ(<i>I</i>)]	4701	
Absolute structure parameter	-0.7(7)	
Largest and mean shift / s.u.	0.000 and 0.000	
Largest diff. peak and hole	0.324 and -0.200 e/Å ³	

 $wR2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$

$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for compound 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
O(1)	0.36965(14)	0.4245(2)	0.64309(9)	0.0271(5)
O(2)	0.60230(15)	0.0101(3)	0.27304(11)	0.0353(5)
O(3)	0.48214(15)	-0.1525(3)	0.30095(11)	0.0334(5)
O(4)	0.09002(13)	0.5858(2)	0.39352(9)	0.0222(4)
O(5)	0.19731(15)	0.7136(3)	0.33297(13)	0.0439(6)
C(1)	0.16580(19)	0.2556(3)	0.59000(13)	0.0217(6)
C(2)	0.2137(2)	0.2806(4)	0.66116(14)	0.0258(6)
C(3)	0.2720(2)	0.4342(4)	0.66497(14)	0.0258(6)
C(4)	0.29830(19)	0.5192(3)	0.60300(14)	0.0221(6)
C(5)	0.27653(19)	0.4474(3)	0.53106(13)	0.0189(5)
C(6)	0.19964(19)	0.5538(3)	0.49213(13)	0.0204(5)
C(7)	0.16631(18)	0.4812(3)	0.42377(13)	0.0185(5)
C(8)	0.12333(19)	0.3111(3)	0.42938(13)	0.0195(5)
C(9)	0.19888(18)	0.1932(3)	0.46474(13)	0.0182(5)
C(10)	0.23931(18)	0.2672(3)	0.53480(12)	0.0181(5)
C(11)	0.27776(19)	0.1533(3)	0.41496(14)	0.0204(6)
C(12)	0.3641(2)	0.0522(4)	0.44460(14)	0.0246(6)
C(13)	0.42711(18)	0.0030(3)	0.38910(13)	0.0215(5)
C(14)	0.50005(19)	0.0811(3)	0.36431(13)	0.0225(6)
C(15)	0.53644(19)	-0.0144(3)	0.30852(14)	0.0242(6)
C(16)	0.4113(2)	-0.1520(4)	0.35066(18)	0.0371(8)
C(17)	0.0804(2)	0.2544(4)	0.35972(14)	0.0256(6)
C(18)	0.3152(2)	0.7008(4)	0.60902(16)	0.0301(7)
C(19)	0.37306(19)	0.4594(3)	0.49712(14)	0.0234(6)
C(20)	0.1486(2)	0.0294(3)	0.47780(14)	0.0236(6)
C(21)	0.1152(2)	0.6959(3)	0.34710(14)	0.0224(6)
C(22)	0.03098(19)	0.7923(3)	0.31963(13)	0.0226(6)
C(23)	-0.0622(2)	0.7720(4)	0.35402(15)	0.0286(6)
C(24)	0.0378(2)	0.8922(3)	0.26662(13)	0.0259(6)
C(25)	0.1214(3)	0.9267(4)	0.22587(15)	0.0337(7)

Table 3. Bond lengths [Å] and angles [°] for compound 1.

O(1)-C(4)	1.453(3)	C(11)-H(11A)	0.9900
O(1)-C(3)	1.459(3)	C(11)-H(11B)	0.9900
O(2)-C(15)	1.208(3)	C(12)-C(13)	1.504(4)
O(3)-C(15)	1.368(3)	C(12)-H(12A)	0.9900
O(3)-C(16)	1.437(3)	C(12)-H(12B)	0.9900
O(4)-C(21)	1.350(3)	C(13)-C(14)	1.324(4)
O(4)-C(7)	1.463(3)	C(13)-C(16)	1.490(4)
O(5)-C(21)	1.205(3)	C(14)-C(15)	1.468(4)
C(1)-C(2)	1.523(4)	C(14)-H(14)	0.9500
C(1)-C(10)	1.547(3)	C(16)-H(16A)	0.9900
C(1)-H(1A)	0.9900	C(16)-H(16B)	0.9900
C(1)-H(1B)	0.9900	C(17)-H(17A)	0.9800
C(2)-C(3)	1.501(4)	C(17)-H(17B)	0.9800
C(2)-H(2A)	0.9900	C(17)-H(17C)	0.9800
C(2)-H(2B)	0.9900	C(18)-H(18A)	0.9800
C(3)-C(4)	1.474(4)	C(18)-H(18B)	0.9800
C(3)-H(3)	1.0000	C(18)-H(18C)	0.9800
C(4)-C(18)	1.515(4)	C(19)-H(19A)	0.9800
C(4)-C(5)	1.545(4)	C(19)-H(19B)	0.9800
C(5)-C(19)	1.546(4)	C(19)-H(19C)	0.9800
C(5)-C(6)	1.546(4)	C(20)-H(20A)	0.9800
C(5)-C(10)	1.573(4)	C(20)-H(20B)	0.9800
C(6)-C(7)	1.515(3)	C(20)-H(20C)	0.9800
C(6)-H(6A)	0.9900	C(21)-C(22)	1.488(4)
C(6)-H(6B)	0.9900	C(22)-C(24)	1.336(4)
C(7)-C(8)	1.529(4)	C(22)-C(23)	1.515(4)
C(7)-H(7)	1.0000	C(23)-H(23A)	0.9800
C(8)-C(17)	1.531(4)	C(23)-H(23B)	0.9800
C(8)-C(9)	1.560(4)	C(23)-H(23C)	0.9800
C(8)-H(8)	1.0000	C(24)-C(25)	1.486(4)
C(9)-C(20)	1.548(4)	C(24)-H(24)	0.9500
C(9)-C(11)	1.557(3)	C(25)-H(25A)	0.9800
C(9)-C(10)	1.576(3)	C(25)-H(25B)	0.9800
C(10)-H(10)	1.0000	C(25)-H(25C)	0.9800
C(11)-C(12)	1.544(4)		
C(4)-O(1)-C(3)	60.81(17)	C(2)-C(1)-H(1B)	109.3
C(15)-O(3)-C(16)	108.9(2)	C(10)-C(1)-H(1B)	109.3
C(21)-O(4)-C(7)	117.0(2)	H(1A)-C(1)-H(1B)	108.0
C(2)-C(1)-C(10)	111.5(2)	C(3)-C(2)-C(1)	111.2(2)
C(2)-C(1)-H(1A)	109.3	C(3)-C(2)-H(2A)	109.4
C(10)-C(1)-H(1A)	109.3	C(1)-C(2)-H(2A)	109.4

C(3)-C(2)-H(2B)	109.4	C(1)-C(10)-C(5)	109.1(2)
C(1)-C(2)-H(2B)	109.4	C(1)-C(10)-C(9)	112.1(2)
H(2A)-C(2)-H(2B)	108.0	C(5)-C(10)-C(9)	115.0(2)
O(1)-C(3)-C(4)	59.42(16)	C(1)-C(10)-H(10)	106.7
O(1)-C(3)-C(2)	116.9(2)	C(5)-C(10)-H(10)	106.7
C(4)-C(3)-C(2)	121.5(2)	C(9)-C(10)-H(10)	106.7
O(1)-C(3)-H(3)	115.7	C(12)-C(11)-C(9)	116.2(2)
C(4)-C(3)-H(3)	115.7	C(12)-C(11)-H(11A)	108.2
C(2)-C(3)-H(3)	115.7	C(9)-C(11)-H(11A)	108.2
O(1)-C(4)-C(3)	59.78(17)	C(12)-C(11)-H(11B)	108.2
O(1)-C(4)-C(18)	112.9(2)	C(9)-C(11)-H(11B)	108.2
C(3)-C(4)-C(18)	116.7(2)	H(11A)-C(11)-H(11B)	107.4
O(1)-C(4)-C(5)	112.1(2)	C(13)-C(12)-C(11)	110.5(2)
C(3)-C(4)-C(5)	122.1(2)	C(13)-C(12)-H(12A)	109.5
C(18)-C(4)-C(5)	117.9(2)	C(11)-C(12)-H(12A)	109.5
C(4)-C(5)-C(19)	104.4(2)	C(13)-C(12)-H(12B)	109.5
C(4)-C(5)-C(6)	108.9(2)	C(11)-C(12)-H(12B)	109.5
C(19)-C(5)-C(6)	110.2(2)	H(12A)-C(12)-H(12B)	108.1
C(4)-C(5)-C(10)	111.2(2)	C(14)-C(13)-C(16)	108.6(2)
C(19)-C(5)-C(10)	112.3(2)	C(14)-C(13)-C(12)	129.7(3)
C(6)-C(5)-C(10)	109.7(2)	C(16)-C(13)-C(12)	121.7(3)
C(7)-C(6)-C(5)	112.1(2)	C(13)-C(14)-C(15)	109.2(3)
C(7)-C(6)-H(6A)	109.2	C(13)-C(14)-H(14)	125.4
C(5)-C(6)-H(6A)	109.2	C(15)-C(14)-H(14)	125.4
C(7)-C(6)-H(6B)	109.2	O(2)-C(15)-O(3)	120.8(3)
C(5)-C(6)-H(6B)	109.2	O(2)-C(15)-C(14)	131.2(3)
H(6A)-C(6)-H(6B)	107.9	O(3)-C(15)-C(14)	108.0(2)
O(4)-C(7)-C(6)	107.4(2)	O(3)-C(16)-C(13)	105.3(2)
O(4)-C(7)-C(8)	106.8(2)	O(3)-C(16)-H(16A)	110.7
C(6)-C(7)-C(8)	113.2(2)	C(13)-C(16)-H(16A)	110.7
O(4)-C(7)-H(7)	109.7	O(3)-C(16)-H(16B)	110.7
C(6)-C(7)-H(7)	109.7	C(13)-C(16)-H(16B)	110.7
C(8)-C(7)-H(7)	109.7	H(16A)-C(16)-H(16B)	108.8
C(7)-C(8)-C(17)	110.2(2)	C(8)-C(17)-H(17A)	109.5
C(7)-C(8)-C(9)	110.2(2)	C(8)-C(17)-H(17B)	109.5
C(17)-C(8)-C(9)	114.9(2)	H(17A)-C(17)-H(17B)	109.5
C(7)-C(8)-H(8)	107.1	C(8)-C(17)-H(17C)	109.5
C(17)-C(8)-H(8)	107.1	H(17A)-C(17)-H(17C)	109.5
C(9)-C(8)-H(8)	107.1	H(17B)-C(17)-H(17C)	109.5
C(20)-C(9)-C(11)	105.6(2)	C(4)-C(18)-H(18A)	109.5
C(20)-C(9)-C(8)	108.3(2)	C(4)-C(18)-H(18B)	109.5
C(11)-C(9)-C(8)	109.6(2)	H(18A)-C(18)-H(18B)	109.5
C(20)-C(9)-C(10)	109.3(2)	C(4)-C(18)-H(18C)	109.5
C(11)-C(9)-C(10)	113.9(2)	H(18A)-C(18)-H(18C)	109.5
C(8)-C(9)-C(10)	109.9(2)	H(18B)-C(18)-H(18C)	109.5

C(5)-C(19)-H(19A)	109.5	C(21)-C(22)-C(23)	117.3(2)
C(5)-C(19)-H(19B)	109.5	C(22)-C(23)-H(23A)	109.5
H(19A)-C(19)-H(19B)	109.5	C(22)-C(23)-H(23B)	109.5
C(5)-C(19)-H(19C)	109.5	H(23A)-C(23)-H(23B)	109.5
H(19A)-C(19)-H(19C)	109.5	C(22)-C(23)-H(23C)	109.5
H(19B)-C(19)-H(19C)	109.5	H(23A)-C(23)-H(23C)	109.5
C(9)-C(20)-H(20A)	109.5	H(23B)-C(23)-H(23C)	109.5
C(9)-C(20)-H(20B)	109.5	C(22)-C(24)-C(25)	129.7(3)
H(20A)-C(20)-H(20B)	109.5	C(22)-C(24)-H(24)	115.1
C(9)-C(20)-H(20C)	109.5	C(25)-C(24)-H(24)	115.1
H(20A)-C(20)-H(20C)	109.5	C(24)-C(25)-H(25A)	109.5
H(20B)-C(20)-H(20C)	109.5	C(24)-C(25)-H(25B)	109.5
O(5)-C(21)-O(4)	122.2(2)	H(25A)-C(25)-H(25B)	109.5
O(5)-C(21)-C(22)	126.2(3)	C(24)-C(25)-H(25C)	109.5
O(4)-C(21)-C(22)	111.6(2)	H(25A)-C(25)-H(25C)	109.5
C(24)-C(22)-C(21)	120.9(3)	H(25B)-C(25)-H(25C)	109.5
C(24)-C(22)-C(23)	121.7(3)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 1. The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	22(1)	35(1)	24(1)	-2(1)	-3(1)	6(1)
O(2)	36(1)	39(1)	34(1)	7(1)	18(1)	9(1)
O(3)	26(1)	38(1)	37(1)	-18(1)	8(1)	-1(1)
O(4)	19(1)	25(1)	22(1)	2(1)	1(1)	4(1)
O(5)	23(1)	47(1)	63(2)	28(1)	5(1)	2(1)
C(1)	22(1)	24(1)	20(1)	-1(1)	6(1)	-1(1)
C(2)	27(1)	32(2)	19(1)	0(1)	6(1)	4(1)
C(3)	26(1)	32(2)	20(1)	-7(1)	3(1)	6(1)
C(4)	19(1)	24(1)	24(1)	-5(1)	-1(1)	3(1)
C(5)	17(1)	19(1)	21(1)	-1(1)	2(1)	0(1)
C(6)	20(1)	19(1)	22(1)	1(1)	2(1)	1(1)
C(7)	17(1)	20(1)	19(1)	1(1)	2(1)	3(1)
C(8)	17(1)	21(1)	21(1)	-2(1)	4(1)	1(1)
C(9)	19(1)	20(1)	16(1)	-1(1)	4(1)	1(1)
C(10)	18(1)	19(1)	18(1)	1(1)	4(1)	2(1)
C(11)	22(1)	20(1)	19(1)	-1(1)	4(1)	2(1)
C(12)	24(1)	28(1)	23(1)	1(1)	8(1)	7(1)
C(13)	18(1)	24(1)	22(1)	0(1)	1(1)	5(1)
C(14)	24(1)	21(1)	23(1)	-2(1)	2(1)	3(1)
C(15)	24(1)	27(1)	22(1)	4(1)	0(1)	6(1)
C(16)	30(2)	34(2)	49(2)	-17(2)	17(2)	-6(1)
C(17)	28(1)	26(1)	23(1)	-5(1)	-1(1)	2(1)
C(18)	30(2)	26(1)	33(2)	-7(1)	-4(1)	0(1)
C(19)	21(1)	24(1)	26(1)	1(1)	2(1)	-3(1)
C(20)	27(1)	20(1)	25(1)	-4(1)	5(1)	-2(1)
C(21)	23(1)	20(1)	24(1)	2(1)	-1(1)	-2(1)
C(22)	24(1)	21(1)	23(1)	-3(1)	-3(1)	0(1)
C(23)	23(1)	32(2)	31(2)	4(1)	1(1)	7(1)
C(24)	33(2)	23(1)	21(1)	-3(1)	-5(1)	2(1)
C(25)	48(2)	28(2)	26(2)	1(1)	4(1)	-2(1)

Table 5. Hydrogen coordinates and isotropic displacement parameters for compound 1.

	x	y	z	U(eq)
H(1A)	0.1153	0.3390	0.5811	0.026
H(1B)	0.1346	0.1474	0.5875	0.026
H(2A)	0.1638	0.2859	0.6946	0.031
H(2B)	0.2559	0.1868	0.6733	0.031
H(3)	0.2632	0.5048	0.7054	0.031
H(6A)	0.1437	0.5662	0.5201	0.024
H(6B)	0.2266	0.6634	0.4850	0.024
H(7)	0.2211	0.4780	0.3935	0.022
H(8)	0.0691	0.3199	0.4599	0.023
H(10)	0.2957	0.1991	0.5509	0.022
H(11A)	0.2472	0.0938	0.3755	0.024
H(11B)	0.3025	0.2572	0.3977	0.024
H(12A)	0.4020	0.1173	0.4792	0.030
H(12B)	0.3405	-0.0461	0.4672	0.030
H(14)	0.5249	0.1829	0.3801	0.027
H(16A)	0.4201	-0.2466	0.3815	0.044
H(16B)	0.3456	-0.1556	0.3281	0.044
H(17A)	0.0274	0.3266	0.3443	0.038
H(17B)	0.0562	0.1431	0.3634	0.038
H(17C)	0.1300	0.2572	0.3268	0.038
H(18A)	0.3368	0.7278	0.6561	0.045
H(18B)	0.2552	0.7587	0.5963	0.045
H(18C)	0.3645	0.7334	0.5785	0.045
H(19A)	0.3641	0.4228	0.4497	0.035
H(19B)	0.4210	0.3904	0.5218	0.035
H(19C)	0.3953	0.5724	0.4983	0.035
H(20A)	0.1405	-0.0320	0.4351	0.035
H(20B)	0.0854	0.0503	0.4950	0.035
H(20C)	0.1879	-0.0336	0.5115	0.035
H(23A)	-0.1111	0.8444	0.3325	0.043
H(23B)	-0.0517	0.7995	0.4024	0.043
H(23C)	-0.0840	0.6590	0.3494	0.043
H(24)	-0.0193	0.9498	0.2529	0.031
H(25A)	0.1562	1.0216	0.2449	0.051
H(25B)	0.0986	0.9489	0.1786	0.051
H(25C)	0.1643	0.8322	0.2273	0.051

Table 6. Torsion angles [°] for compound 1.

C(10)-C(1)-C(2)-C(3)	52.1(3)	C(2)-C(1)-C(10)-C(5)	-68.0(3)
C(4)-O(1)-C(3)-C(2)	112.4(3)	C(2)-C(1)-C(10)-C(9)	163.5(2)
C(1)-C(2)-C(3)-O(1)	-84.3(3)	C(4)-C(5)-C(10)-C(1)	43.4(3)
C(1)-C(2)-C(3)-C(4)	-15.3(4)	C(19)-C(5)-C(10)-C(1)	160.0(2)
C(3)-O(1)-C(4)-C(18)	108.6(3)	C(6)-C(5)-C(10)-C(1)	-77.1(3)
C(3)-O(1)-C(4)-C(5)	-115.3(3)	C(4)-C(5)-C(10)-C(9)	170.3(2)
C(2)-C(3)-C(4)-O(1)	-104.7(3)	C(19)-C(5)-C(10)-C(9)	-73.1(3)
O(1)-C(3)-C(4)-C(18)	-102.2(3)	C(6)-C(5)-C(10)-C(9)	49.8(3)
C(2)-C(3)-C(4)-C(18)	153.1(3)	C(20)-C(9)-C(10)-C(1)	-44.5(3)
O(1)-C(3)-C(4)-C(5)	98.6(3)	C(11)-C(9)-C(10)-C(1)	-162.3(2)
C(2)-C(3)-C(4)-C(5)	-6.2(4)	C(8)-C(9)-C(10)-C(1)	74.3(3)
O(1)-C(4)-C(5)-C(19)	-62.9(3)	C(20)-C(9)-C(10)-C(5)	-169.9(2)
C(3)-C(4)-C(5)-C(19)	-130.1(3)	C(11)-C(9)-C(10)-C(5)	72.3(3)
C(18)-C(4)-C(5)-C(19)	70.8(3)	C(8)-C(9)-C(10)-C(5)	-51.1(3)
O(1)-C(4)-C(5)-C(6)	179.5(2)	C(20)-C(9)-C(11)-C(12)	-69.7(3)
C(3)-C(4)-C(5)-C(6)	112.2(3)	C(8)-C(9)-C(11)-C(12)	173.8(2)
C(18)-C(4)-C(5)-C(6)	-46.8(3)	C(10)-C(9)-C(11)-C(12)	50.2(3)
O(1)-C(4)-C(5)-C(10)	58.5(3)	C(9)-C(11)-C(12)-C(13)	172.0(2)
C(3)-C(4)-C(5)-C(10)	-8.8(3)	C(11)-C(12)-C(13)-C(14)	88.0(3)
C(18)-C(4)-C(5)-C(10)	-167.8(2)	C(11)-C(12)-C(13)-C(16)	-90.0(3)
C(4)-C(5)-C(6)-C(7)	-173.8(2)	C(16)-C(13)-C(14)-C(15)	0.4(3)
C(19)-C(5)-C(6)-C(7)	72.3(3)	C(12)-C(13)-C(14)-C(15)	-177.8(3)
C(10)-C(5)-C(6)-C(7)	-51.9(3)	C(16)-O(3)-C(15)-O(2)	178.3(3)
C(21)-O(4)-C(7)-C(6)	98.3(3)	C(16)-O(3)-C(15)-C(14)	-0.6(3)
C(21)-O(4)-C(7)-C(8)	-139.9(2)	C(13)-C(14)-C(15)-O(2)	-178.6(3)
C(5)-C(6)-C(7)-O(4)	176.6(2)	C(13)-C(14)-C(15)-O(3)	0.1(3)
C(5)-C(6)-C(7)-C(8)	58.8(3)	C(15)-O(3)-C(16)-C(13)	0.7(3)
O(4)-C(7)-C(8)-C(17)	55.0(3)	C(14)-C(13)-C(16)-O(3)	-0.7(3)
C(6)-C(7)-C(8)-C(17)	173.1(2)	C(12)-C(13)-C(16)-O(3)	177.7(2)
O(4)-C(7)-C(8)-C(9)	-177.13(19)	C(7)-O(4)-C(21)-O(5)	-3.3(4)
C(6)-C(7)-C(8)-C(9)	-59.0(3)	C(7)-O(4)-C(21)-C(22)	179.1(2)
C(7)-C(8)-C(9)-C(20)	172.7(2)	O(5)-C(21)-C(22)-C(24)	11.6(5)
C(17)-C(8)-C(9)-C(20)	-62.1(3)	O(4)-C(21)-C(22)-C(24)	-170.9(2)
C(7)-C(8)-C(9)-C(11)	-72.5(3)	O(5)-C(21)-C(22)-C(23)	-168.6(3)
C(17)-C(8)-C(9)-C(11)	52.7(3)	O(4)-C(21)-C(22)-C(23)	9.0(3)
C(7)-C(8)-C(9)-C(10)	53.4(3)	C(21)-C(22)-C(24)-C(25)	0.8(5)
C(17)-C(8)-C(9)-C(10)	178.6(2)	C(23)-C(22)-C(24)-C(25)	-179.1(3)

Table 7. Hydrogen bonds for compound 1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2A)...O(2)#1	0.99	2.59	3.360(3)	134.8
C(2)-H(2B)...O(2)#2	0.99	2.62	3.572(4)	161.9
C(14)-H(14)...O(1)#2	0.95	2.53	3.367(3)	146.7
C(16)-H(16B)...O(5)#3	0.99	2.34	3.180(4)	142.1

Symmetry transformations used to generate equivalent atoms:

#1 $x-1/2, y+1/2, z+1/2$ #2 $-x+1, y, -z+1$ #3 $x, y-1, z$