Opening of Aryl-Substituted Epoxides to form Quaternary Stereogenic Centers:

Synthesis of (-)-Mesembrine

Douglass F. Taber and Yigang He

Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716

Supporting Information

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Experimental Section

General. ^1H and ^{13}C NMR were recorded as solutions in CDCl_3 at 400 and 100 (or 90) MHz, respectively. ^{13}C NMR multiplicities were determined with the aid of a JVERT sequence, differentiating the signals for methylene and quaternary carbons as "u" from methyl and methine carbons as "d". The infrared (IR) spectra were determined as neat oils. R_f values indicated refer to thin-layer chromatography on 2.5×10 cm, 250- μm analytical plates coated with silica gel GF and developed in the solvent indicated. Flash column chromatography was performed with 35-60 μ silica gel following the procedure of Still. Where specified, TLC mesh silica gel was employed, following the procedure described by Taber. Solvents are referred as volume/volume mixture. PE is petroleum ether. EtOAc is ethyl acetate. MTBE is methyl tert-butyl ether. "Wet ether" is the organic layer after partitioning between ether and deionized water. THF and diethyl ether were distilled from sodium/benzophenone under N_2 and used immediately. CH_2Cl_2 was distilled from CaH_2 under N_2 . All reactions were carried out in flame-dried glassware under a positive pressure of N_2 unless otherwise indicated. The alkenes were prepared by adding the corresponding ketone to the appropriate Grignard reagent, followed by *p*-toluenesulfonic acid-catalyzed dehydration of the product alcohol.

Alcohol (6c): Clear oil (86% yield), TLC R_f = 0.63 (PE: MTBE, 1:1). IR (neat, cm^{-1}): 3464, 2935, 1638, 1609, 1514, 1251, 1184, 1038; ^1H NMR (400 MHz, CDCl_3) δ 7.32 (m, 2H), 6.88 (m, 2H), 5.25 (m, 1H), 4.92 (d, J = 26.8 Hz, 1H), 4.88 (d, J =19.6 Hz, 1H), 3.98 (t, J =3.2 Hz, 1H), 3.78 (s, 3H), 1.30-2.65 (m, 11H); ^{13}C NMR (CDCl_3 , 100 MHz) δ u: 157.9, 136.8, 117.1, 44.9, 41.4, 28.3, 27.2, 21.1, 20.1; d: 134.6, 128.1, 114.0, 74.1, 55.2; HRMS calcd for $\text{C}_{16}\text{H}_{23}\text{O}_2$ ($\text{M}+\text{H}$) 247.1698, found 247.1696.

Alcohol (6e): Clear oil (88% yield from **10**), TLC R_f = 0.56 (PE: EtOAc, 1:1). IR (neat, cm^{-1}): 3515 (s), 2954 (s), 1638 (w), 1587 (w), 1516 (s), 1463 (m), 1258 (s), 1150 (s), 1028 (s); ^1H NMR (400 MHz, CDCl_3) δ 6.82-6.98 (m, 3H), 4.73 (t, J = 2.0 Hz, 1H), 4.56 (s, 1H), 4.19 (t, J =3.6 Hz, 1H), 3.99 (m, 4H), 3.88 (s, 3H), 3.86 (s, 3H), 3.09 (d, J =7.6 Hz, 1H), 1.78-2.57 (m, 8H), 1.11 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ u: 148.7, 147.4, 143.1, 137.6, 114.7, 109.0, 64.7, 64.2, 45.3, 44.9, 37.1, 31.0, 26.0; d: 119.7, 111.2, 111.0, 74.9, 56.1, 55.9, 24.4; HRMS calcd for $\text{C}_{20}\text{H}_{28}\text{O}_5\text{Na}$ ($\text{M}+\text{Na}$) 371.1834, found 371.1838.

Alcohol (6f): Clear oil (88% yield from **10**), TLC R_f = 0.63 (PE: EtOAc, 1:1). IR (neat, cm^{-1}): 3506 (s), 2955 (s), 1604 (w), 1515 (s), 1496 (w), 1489 (w), 1256 (s), 1150 (s), 1029 (s); ^1H NMR (400 MHz, CDCl_3) δ 6.57-7.26 (m, 8H), 4.34 (br, 1H), 4.00 (m, 4H), 3.87 (s, 3H), 3.75 (s, 3H), 3.21 (t, J = 3.6 Hz, 1H), 2.97, 2.90 (ABq, J =13.2 Hz, 2H), 1.77-2.31 (m, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ u: 148.5, 147.4, 137.5, 136.9, 109.0, 64.7, 64.3, 46.4, 43.8, 37.3, 31.2, 25.8; d: 130.3, 127.7, 126.3, 120.0, 111.5, 110.9, 74.2, 56.0, 55.9; HRMS calcd for $\text{C}_{23}\text{H}_{28}\text{O}_5$ (M^+) 384.1937, found 384.1929.

Alcohol (6h): Clear oil (85% yield **10**), TLC R_f =0.42 (PE: EtOAc, 1:1). IR (neat, cm^{-1}): 3520 (s), 2937 (s), 1638 (w), 1586 (w), 1515 (s), 1256 (s), 1150 (s), 1029 (s); ^1H NMR (400 MHz, CDCl_3) δ 6.82-6.94 (m, 3H), 4.69 (br, 1H), 4.18 (t, J =3.6 Hz, 1H), 3.97 (m, 4H), 3.87 (s, 3H), 3.86 (s, 3H), 3.04 (d, J =7.6 Hz, 1H), 1.75-2.48 (m, 8H), 1.57 (s, 3H), 1.47 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ u: 148.5, 147.0, 137.7, 133.8, 108.9, 64.7, 64.2, 45.4, 37.0, 35.7, 31.0, 25.8; d: 119.7, 119.4, 110.8, 110.6, 74.6, 55.9, 55.8, 26.1, 18.2; HRMS calcd for $\text{C}_{21}\text{H}_{30}\text{O}_5\text{Na}$ ($M+\text{Na}$) 385.1991, found 385.1987.

Alcohols (*cis* – 6g) and (*trans* – 6g): Clear oil (52% yield from **10**), TLC R_f = 0.36 (PE: EtOAc, 1:1). IR (neat, cm^{-1}) 3517 (s), 2933 (m), 1636 (w), 1515 (s), 1256 (s), 1149 (s), 1028 (s); ^1H NMR (400 MHz, CDCl_3) δ 6.75-6.92 (m, 3H), 5.32-5.48 (m, 1H), 4.84-5.00 (m, 1H), 4.12-4.23 (m, 1H), 3.95-4.02 (m, 4H), 3.88-3.92 (m, 6H), 3.05 (m, 1H), 1.68-2.55 (m, 8H), 1.50-1.54 (m, 3H); ^{13}C NMR (CDCl_3 , 90 MHz) δ u: 148.7, 147.3, 147.2, 137.7, 137.5, 109.0, 108.9, 64.7, 64.3, 45.3, 45.0, 40.6, 37.1, 36.9, 34.5, 31.1, 30.7, 25.8, 25.5; d: 127.9, 126.7, 126.2, 125.9, 119.5, 119.4, 111.1, 110.9, 74.7, 74.5, 56.0, 55.9, 18.1, 13.2; HRMS calcd for $\text{C}_{20}\text{H}_{28}\text{O}_5\text{Na}$ ($M+\text{Na}$, 371.1834, found 371.1838.

Current Data Parameters
 NAME b0133hl
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030927
 Time 14.36
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 20.2
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300228 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME b0133c13
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030927
Time 14.42
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 201
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 11585.2
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 100.6127559 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME b0126h1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030916
 Time 18.03
 INSTRUM spect
 PROHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 10.1
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300204 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME b0126c13
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030916
 Time 18.11

INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG jvert
 TD 65536
 SOLVENT CDCl3
 NS 800
 DS 0
 SWH 27173.912 Hz
 FIDRES 0.414641 Hz
 AQ 1.2059124 sec
 RG 9195.2
 DW 18.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 6.00000000 sec
 D11 0.03000000 sec
 D13 0.00000300 sec
 D20 0.00700000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 P2 21.00 usec
 PL1 0.00 dB
 SFO1 100.6242995 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127625 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME b01303hlp
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030905
 Time 11.04
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 20.2
 DW 89.400 use
 DE 4.50 use
 TE 300.0 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 use
 PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME b01303c13
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030905
 Time 10.37
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG jmod.sb
 TD 65536
 SOLVENT CDCl3
 NS 3246
 DS 0
 SWH 21834.061 Hz
 FIDRES 0.333161 Hz
 AQ 1.5008202 sec
 RG 16384
 DW 22.900 usec
 DE 28.62 usec
 TE 300.0 K
 P1 8.00 usec
 CNST2 145.0000000
 CNST11 1.0000000
 D20 0.0068966 sec
 HL1 13 dB
 D1 5.0000000 sec
 CPDPRG waltz16
 P31 100.00 usec
 D13 0.0000040 sec
 P2 16.0 usec
 SF01 90.5648644 MHz
 NUCLEUS 13C

F2 - Processing parameters
 SI 65536
 SF 90.5557462 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

Current Data Parameters
 NAME b0201h1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030905
 Time 11.10
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 20.2
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 ===
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300167 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Handwritten annotations: three sets of curly braces on the left side of the spectrum, likely indicating specific peak regions.

Current Data Parameters
 NAME b0201c13
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030905
 Time 16.38
 INSTRUM spect
 PROBD 5 mm QNP 1H
 PULPROG jmod.sb
 TD 65536
 SOLVENT CDCl3
 NS 8771
 DS 0
 SWH 21834.061 Hz
 FIDRES 0.333161 Hz
 AQ 1.5008202 sec
 RG 16384
 DW 22.900 usec
 DE 28.62 usec
 TE 300.0 K
 P1 8.00 usec
 CNST2 145.0000000
 CNST11 1.0000000
 D20 0.0068966 sec
 HL1 13 dB
 D1 5.0000000 sec
 CPDPRG waltz16
 P31 100.00 usec
 D13 0.0000040 sec
 P2 16.0 usec
 SFO1 90.5648644 MHz
 NUCLEUS 13C

F2 - Processing parameters

SI 65536
 SF 90.5557456 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

148.505
 147.361
 137.537
 136.857
 130.345
 127.678
 126.254
 119.953
 111.502
 110.933
 109.046
 77.583
 77.230
 76.877
 74.213
 64.737
 64.308
 55.984
 55.947
 46.394
 43.828
 37.321
 31.172
 25.839

Current Data Parameters
 NAME b0225h102
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030917
 Time 14.01
 INSTRUM spect
 PROBP 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 32
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300133 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

148.744
147.304
147.251
137.678
137.533
127.909
126.710
126.182
125.864
119.493
119.387
111.064
110.851
108.977
108.940

77.585
77.231
76.878
74.746
74.462
64.721
64.282
56.046
55.942
45.277
45.028
40.573
37.110
36.897
34.462
31.093
30.733
25.839
25.534
18.108
13.249

Current Data Parameters
NAME b0225c1302
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030919
Time 15:52
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod.sb
TD 65536
SOLVENT CDCl3
NS 12198
DS 0
SWH 21834.061 Hz
FIDRES 0.333161 Hz
AQ 1.5008202 sec
RG 16384
DE 22.900 usec
TE 28.62 usec
P1 300.0 K
F1 8.00 usec
CNST2 145.000000
CNST11 1.000000
D20 0.0068966 sec
HL1 13 dB
D1 5.0000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648644 MHz
NUCLEUS 13C

F2 - Processing parameters
SI 65536
SF 90.5557446 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00

Current Data Parameters
 NAME b0241h1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030929
 Time 8.02
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 20.2
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 ===
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300102 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

148.502
147.044
137.660
133.782
119.704
119.375
110.832
110.612
108.922
77.550
77.231
76.914
74.596
64.661
64.229
55.923
55.850
45.365
36.965
35.698
31.009
26.079
25.817
18.157

Current Data Parameters
NAME b0241c13
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030928
Time 16.40
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 33
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 7298.2
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 100.6127576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME b0160h1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030930
 Time 12.26

INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 10.1
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300037 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME b01229hip
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030807
 Time 9.21

INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg

TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0

SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec

RG 20.2
 DW 89.400 use
 DE 4.50 use

TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 ===
 NUC1 1H
 P1 9.00 use

PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300003 MHz

WDW EM
 SSB 0
 LB 0.00 Hz

GB 0
 PC 1.00

199.567

155.294
149.107
147.975

135.392
133.557
129.479

119.409
118.957
111.061
110.158

77.583
77.230
76.876

56.072
55.948
46.339
43.551
36.099
34.532

Current Data Parameters
NAME b01229c13
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030806
Time 7.40
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod.sb
TD 65536
SOLVENT CDCl3
NS 1534
DS 0
SWH 21834.061 Hz
FIDRES 0.333161 Hz
AQ 1.5008202 sec
RG 16384
DW 22.900 usec
DE 28.62 usec
TE 300.0 K
P1 8.00 usec
CNST2 145.000000
CNST11 1.000000
D20 0.0068966 sec
HL1 13 dB
D1 5.0000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648644 MHz
NUCLEUS 13C

F2 - Processing parameters

SI 65536
SF 90.5557516 MHz
EM 0
WDW 0
SSB 1.00 Hz
LB 0
GB 0
PC 4.00

Current Data Parameters
 NAME 101003hlmajor
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20031010
 Time 8.27
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 57
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 ===
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300085 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.00

Current Data Parameters
 NAME 101003c13major
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031010
 Time 8.05
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG jmod.sb
 TD 65536
 SOLVENT CDCl3
 NS 1265
 DS 0
 SWH 21834.061 Hz
 FIDRES 0.333161 Hz
 AQ 1.5008202 sec
 RG 16384
 DW 22.900 usec
 DE 28.62 usec
 TE 300.0 K
 F1 8.00 usec
 CNST2 145.0000000
 CNST11 1.0000000
 D20 0.0068966 sec
 HL1 13 dB
 D1 5.00000000 sec
 CPDPRG waltz16
 F31 100.00 usec
 D13 0.0000040 sec
 P2 16.0 usec
 SFO1 90.5648644 MHz
 NUCLEUS 13C

F2 - Processing parameters
 SI 65536
 SF 90.5557476 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

Current Data Parameters
 NAME b01293h1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030829
 Time 8.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 20.2
 DW 89.400 use
 DE 4.50 use
 TE 300.0 K
 D1 5.0000000 sec

===== CHANNEL f1 ===
 NUC1 1H
 P1 9.00 use
 PL1 0.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300105 MHz
 WDN EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

21.765
28.782
34.974
40.866
41.776
56.035
56.112
66.981
67.776
76.878
77.231
77.585
110.293
111.103
119.457
127.938
129.939
132.536
133.246
133.722
137.843
144.889
147.741
149.026

Current Data Parameters
NAME b01293c13
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030829
Time 7.46
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod.sb
TD 65536
SOLVENT CDCl3
NS 2565
DS 0
SWH 21834.061 Hz
FIDRES 0.333161 Hz
AQ 1.5008202 sec
RG 16384
DW 22.900 usec
DE 28.62 usec
TE 300.0 K
P1 8.00 usec
CNST2 145.0000000
CNST11 1.0000000
D20 0.0068966 sec
HL1 13 dB
D1 5.0000000 sec
CPDPRG waltz16
P31 100.00 usec
DI3 0.0000040 sec
P2 16.0 usec
SFO1 90.5648644 MHz
NUCLEUS 13C

F2 - Processing parameters
SI 65536
SF 90.5557452 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00

Current Data Parameters
 NAME b01295h1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030830
 Time 12.06
 INSTRUM spect
 PROHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 71.8
 DE 89.400 usec
 TE 4.50 usec
 D1 300.0 K
 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300170 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

(-)-Mesembrine 1

211.466

149.305
147.809
140.388

118.183
111.332
110.319

77.583
77.230
76.877
70.589

56.273
56.138
55.056
47.765
40.759
40.260
39.086
36.437
35.479
30.536

(-)-Mesembrine 1

Current Data Parameters
NAME b01295c13
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030901
Time 11.48
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod.sb
TD 65536
SOLVENT CDCl3
NS 10895
DS 0
SWH 21834.061 Hz
FIDRES 0.333161 Hz
AQ 1.5008202 sec
RG 16384
DW 22.900 usec
DE 28.62 usec
TE 300.0 K
P1 8.00 usec
CNST2 145.0000000
CNST11 1.0000000
D20 0.0068966 sec
HL1 13 dB
D1 5.0000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648644 MHz
NUCLEUS 13C

F2 - Processing parameters
SI 65536
SF 90.5557416 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00