^1H and ^{13}C NMR spectra of (2'S,4'S)-lysergic acid 2,4-dimethylazetidine (LSZ)

Darcy C. Burns, Timothy E. Burrow and Stephen J. Chapman*

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Acquisition Parameters

Acquire Date: 2014-08-18T19:47:10
 Spect Frequency: 699.81 MHz
 Nucleus: ^1H
 Pulse Program: s2pul
 Pulse Width: 3.6 μsec
 Number of Points: 50223
 Acquisition Time: 4.5 s
 Number of Scans: 64
 Relaxation Delay: 5s
 Sweep Width: 11160.7 Hz
 Temperature: 27.1 $^{\circ}\text{C}$
 Solvent: dmso_insert

Processing Parameters

Phase: Manual
 Ph0: 100.74
 Ph1: -8.94
 Baseline: Whittaker
 Line Broadening: 0.22 Hz

Comment

20140818_D700_NMRLQ-V5481-B-
 ISO_SC_DCB

CSICOMP NMR Facility
 operator: Dr. D.C. Burns
 sample: E3 LSZ

^1H NMR (700 MHz, DMSO- d_6) δ 10.78 (s, 1H), 7.20 (dd, J = 7.2, 1.3 Hz, 1H), 7.13 – 6.97 (m, 3H), 6.25 (s, 1H), 4.66 – 4.58 (m, 1H), 4.35 (dt, J = 7.9, 6.2 Hz, 1H), 4.22 (s, 2H), 3.51 (dd, J = 14.5, 5.6 Hz, 1H), 3.46 (dtd, J = 7.1, 5.3, 2.9 Hz, 1H), 3.26 – 3.15 (m, 1H), 3.08 (dd, J = 11.0, 5.0 Hz, 1H), 2.67 (t, J = 10.8 Hz, 1H), 2.58 – 2.51 (m, 4H), 1.97 (dddd, J = 26.4, 11.1, 8.3, 5.4 Hz, 2H), 1.44 (d, J = 6.2 Hz, 3H), 1.35 (d, J = 6.3 Hz, 3H), 1.11 (s, 0H).

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Solvent: dms_o_insert

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20140818_vnmrs_700_20140818_D700_NMRLQ-V5481-B-ISO_SC_DCB-PROTON_01_E3 LSZ

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Number of Scans: 64

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Temperature: 27.1 $^{\circ}\text{C}$

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Acquisition Parameters

Acquire Date: 2014-08-18T19:57:52

Spect Frequency: 175.98 MHz

Nucleus: ^{13}C

Pulse Program: s2pul

Pulse Width: 3.5667 μsec

Number of Points: 65536

Acquisition Time: 1.5729 s

Number of Scans: 1024

Relaxation Delay: 0.2s

Sweep Width: 41666.7 Hz

Temperature: 27.1 $^{\circ}\text{C}$

Solvent: dmso_insert

Processing Parameters

Phase: Manual

Ph0: 58.02

Ph1: -41.55

Line Broadening: 0.64 Hz

Comment

20140818_D700_NMRLQ-V5481-B-
ISO_SC_DCB

CSICOMP NMR Facility
operator: Dr. D.C. Burns
sample: E3 LSZ

^{13}C NMR (176 MHz, dmso- d_6) δ 173.37, 170.71, 135.22, 133.83, 126.85, 125.72, 122.33, 119.41, 119.23, 111.12, 109.97, 108.44, 71.98, 62.41, 55.74, 54.81, 53.52, 42.98, 39.52, 31.26, 26.39, 22.51, 20.10.

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Acquisition Parameters

Acquire Date:

2015-01-19T20:57:16

Spect Frequency: [699.8052679,
699.8052679] MHz

Nucleus [f1,f2]: [1H, 1H]

Pulse Program: gCOSY (gCOSY)

90° Pulse Width: 7.9 µsec

Number of Points [f1,f2]: [1024,
1024]

Acquisition Time: 0.1196032 s

Number of Scans: 4

Relaxation Delay: 0.8803968s

Receiver Gain: 40

Sweep Width [f1,f2]:

[8561.64383562,
8561.64383562] Hz

Temperature: 25 °C

Solvent: dmso_insert

System: tuxedosam-vnmrs700

Probe: HCN_COLD

Processing Parameters

Phase: NoPC

Processed by: Dr Timothy
Burrow

Script: teb_tidy2D 20150202

Comment

CSICOMP NMR Facility
operator: Dr. D.C. Burns
sample: E2 AL-LAD

Acquisition Parameters

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Acquisition Time: 0.1196032 s

Number of Scans: 4

Relaxation Delay: 0.8803968s

Receiver Gain: 40

Sweep Width [f1,f2]:

[8561.64383562,
8561.64383562] Hz

Temperature: 25 °C

Solvent: dmso_insert

System: tuxedosam-vnmrs700

Probe: HCN_COLD

Processing Parameters

Phase: NoPC

Processed by: Dr Timothy
Burrow

Script: teb_tidy2D 20150202

Comment

CSICOMP NMR Facility

operator: Dr. D.C. Burns

sample: E2 AL-LAD

Acquisition Parameters

Acquire Date:

2015-01-19T19:27:44

Spect Frequency: [175.9809733,
699.8052679] MHz

Nucleus [f1,f2]: [13C, 1H]

Pulse Program: gc2hsqcse
(gc2hsqcse)

90° Pulse Width: 7.9 μ sec

Number of Points [f1,f2]: [512,
786]

Acquisition Time: 0.0918048 s

Number of Scans: 8

Relaxation Delay: 0.9081952s

Receiver Gain: 20

Sweep Width [f1,f2]:

[35195.7765068, 8561.64383562]
Hz

Temperature: 25 °C

Solvent: dmsd_insert

System: tuxedosam-vnmrs 700

Probe: HCN_COLD

Processing Parameters

Phase: Manual

Ph0: 101.38

Ph1: -4.86

Gaussian Windowing: 80.00 Hz

Processed by: Dr Timothy

Burrow

Script: teb_tidy2D 20150202

Comment

20140818_D700_NMRLQ-V5481-
B-ISO_SC_DCB

CSICOMP NMR Facility

operator: Dr. D.C. Burns

sample: E3 LSZ

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20150119_vnmrs_700_20140818_D700_NMRLQ-V5481-B-ISO_SC_DCB-gc2hsqcse_01

Unknown

Acquisition Parameters

Acquire Date:

2015-01-19T19:27:44

Spect Frequency: [175.9809733,
699.8052679] MHz

Nucleus [f1,f2]: [13C, 1H]

Pulse Program: gc2hsqcse
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90° Pulse Width: 7.9 μ sec

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Solvent: dmsd_insert

System: tuxedosam-vnmrs 700

Probe: HCN_COLD

Processing Parameters

Phase: Manual

Ph0: 101.38

Ph1: -4.86

Gaussian Windowing: 80.00 Hz

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Burrow

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operator: Dr. D.C. Burns

sample: E3 LSZ

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90° Pulse Width: 7.9 μ sec

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Number of Scans: 8

Relaxation Delay: 0.9081952s

Receiver Gain: 20

Sweep Width [f1,f2]:

[35195.7765068, 8561.64383562]
Hz

Temperature: 25 °C

Solvent: dms_o_insert

System: tuxedosam-vnmrs 700

Probe: HCN_COLD

Processing Parameters

Phase: Manual

Ph0: 101.38

Ph1: -4.86

Gaussian Windowing: 10.00 Hz

Processed by: Dr Timothy

Burrow

Script: teb_tidy2D 20150202

Comment

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