Supporting Information (2) for

Total Synthesis of the Proposed Structure for Pyragonicin

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----- ACQUISITION PARAMETERS -----
Derived from: 043-NO-130A-1-IR-single pu
File Name      = 043-NO-130A-1-IR-sing
Author         = hchohnoh
Sample ID      = hk
Content        = NO-130A-1-cdcl3-sym-P
Creation Date  = 2-MAR-2004 22:05:47
Revision Date  = 9-MAR-2004 22:58:05
Spec Site     = ECA0500

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Spec Type	=	DELTA2 NMR
Data Format	=	ID COMPLEX
Dimensions	=	X
Dim Title	=	1H
Dim Size	=	26214
Field Strength	=	14.09656928[T] (600 [M
X_acq_duration	=	3.96868016[s]
X_domain	=	1H
X_offset	=	600.1723046 [MHz]
X_offset	=	5 [ppm]
X_points	=	32768
X_prescans	=	1
X_resolution	=	0.23196151 [Hz]
X_sweep	=	8.25627477 [kHz]
ir_domain	=	1H
ir_freq	=	600.1723046 [MHz]
ir_offset	=	5 [ppm]
ir1_domain	=	1H
ir1_freq	=	600.1723046 [MHz]
ir1_offset	=	5 [ppm]
Mod return	=	1
Scans	=	16
Total_scans	=	16
X_90_width	=	7.65 [us]
X_acq_time	=	3.96868016 [s]
X_angle	=	45 [deg]
X_atn	=	4.7 [db]
X_pulse	=	3.825 [us]
ir1_mode	=	Off
ir1_offset	=	Off
Dance_presat	=	PULSE
initial_wait	=	1[s]
relaxation_delay	=	2[s]
repetition_time	=	3.96868016 [s]

X : narts ner Million : 1H

----- PROCESSING PARAMETERS -----

dc_balance : 0.0 [Hz] : 0.0 [s]
sweep : 5.0 [Hz] : 0.0 [s]
t1_rho2 : 0.0 [s] : 80 [s] : 100 [s]
t1_rho2 : 1 : TRUE
t1_rho2 : 1 : TRUE
macbump :
peak_pick : 0 [Hz] : 50 [Hz] : peaks
reference : 77.083 [ppm] : 77 [ppm]
base_correct : None : 0

----- ACQUISITION PARAMETERS -----

Derived from: 043-NO-130A-1-cdcl3-th5-13
File Name : 043-NO-130A-1-cdcl3-t
Author : hkoashino
Sample ID : hko
Content : NO-130A-1-cdcl3-th5-t
Creation Date : 9-MAR-2004 18:42:04
Revision Date : 9-MAR-2004 22:42:42
Spec Site : ECA600

Spec Type : DELTA2-NMR
Data Format : ID REAL

Dimensions : 1D
Dim 1 Size : 13107
Dim 2 Size : 13107
Field Strength : 14.09636928 [T] (600 [M]
X_acq_duration : 0.393216 [s]
X_domain : 13C
X_freq : 150.91343039 [MHz]
X_offset : 100 [ppm]
X_points : 16384
X_prescans : 4
X_resolution : 2.54313151 [Hz]
X_sweep : 41.66666667 [kHz]
Xir_domain : 1H
Xir_freq : 600.1723046 [MHz]
Xir_offset : 4 [ppm]
Mod_return : 1
Scans : 16000
Total_scans : 16000

X_90_width : 9.45 [us]
X_acq_time : 0.393216 [s]
X_angle : 45 [deg]
X_atn : 7.8 [dB]
X_pulse : 4.725 [us]
Xir_atn_dec : 20.3 [dB]
Xir_atn_no : 20.3 [dB]
Xir_noise : VALTZ
Decoupling : TRUE
Initial_wait : 1 [s]
Nuc : 13C
Relaxation_delay : 1.1 [s]
Repetition_time : 1.493216 [s]

043-NO-130A-1-cdcl3-th5-13C-single pulse dec8
NO-130A-1-cdcl3-th5-temp25single pulse decoupled gated NOE

X : marts per Million : 13C

----- PROCESSING PARAMETERS -----

sinbell1_auto
f1 : 1 : TRUE
[transpose]
zerofill : 4
sinbell1_auto
f1 : 1 : TRUE
ppm
abs
thresh : 1 : 1
symmetrize : Cozy : 24
[transpose]

----- ACQUISITION PARAMETERS -----

File Name = 043-NO-130A-1_dqf_cos
Author = hkoshino
Sample ID = hk
Content = NO-130A-1-cdd13-grad1
Creation Date = 3-MAR-2004 03:26:34
Revision Date = 3-MAR-2004 03:19:52
Spec Site = ECA600

Spec Type = DELTA2 NMR
Data Format = 2D REAL REAL
Dimensions = X Y
Dia File = 1H 1H
Dia Size = 1024, 2048
Dia Units = [ppm] [ppm]
Field Strength = 14.09636928 [T] (600 [M
X_acq_duration = 0.2131968 [s]
X_domain = 1H
X_freq = 600.1723046 [MHz]
X_offset = 3.8 [ppm]
X_points = 1280
X_prescans = 4
X_resolution = 4.69050192 [Hz]
X_sweep = 6.00384246 [kHz]
Y_domain = 1H
Y_freq = 600.1723046 [MHz]
Y_offset = 3.8 [ppm]
Y_points = 512
Y_prescans = 0
Y_resolution = 9.37830116 [Hz]
Y_sweep = 4.80169019 [kHz]
Y_domain = 1H
Y_freq = 600.1723046 [MHz]
Y_offset = 5 [ppm]
Y1_domain = 1H
Y1_freq = 600.1723046 [MHz]
Y1_offset = 5 [ppm]
Mod_return = 1
Scans = 16
Total_scans = 8192
X_acq_time = 0.2131968 [s]
X_atn = 4.7 [dB]
X_pulse = 7.65 [us]
Y_acq_time = 0.10662912 [s]
Y_offset = 0.6 [ppm]
Y1_offset = 0.6 [ppm]
Y1_offset = 0.6 [ppm]
Dante_preset = FALSE
Grad_1 = 1 [ms]
Grad_2_amp = 10 [%]
Grad_2_amp = 1 [ms]
Grad_2_amp = 7.5 [%]

043-NO-130A-1-1H-single_pulse.6

043-NO-130A-1_dqf_cosy_pfg.2
NO-130A-1-cdd13-gradient absolute value DQF Cosy

X : parts per Million : 1H

----- PROCESSING PARAMETERS -----

exp : 10.0 [Hz] : 0.0 [s]
taperoids : 0 [%] : 80 [%] : 100 [%]
zerofill : 1
fit : 1 : TRUE
ppm
machinephase
[transposed]
exp : 50.0 [Hz] : 0.0 [s]
taperoids : 0 [%] : 80 [%] : 100 [%]
zerofill : 2
fit : 1 : TRUE
ppm
machinephase

----- ACQUISITION PARAMETERS -----

File Name = 043-NO-130A-1-hsac_to
Author = hkoishino
Sample ID = hK
Content = NO-130A-1-cdcl3-fg2hx
Creation Date = 4-MAR-2004 02:01:16
Revision Date = 4-MAR-2004 01:54:35
Spec Site = ECA600
Spec Type = DELTA2 NMR
Data Format = 2D COMPLEX COMPLEX
Dimensions = X Y
Dim Title = 1H 13C
Dim Size = 819, 1024
Dim Units = [ppm], [ppm]
Field strength = 14.0863928 [T] (600 [M
X_acq_duration = 0.17053744 [s]
X_domain = 1H
X_freq = 600.1723046 [MHz]
X_offset = 3.8 [ppm]
X_points = 1024
X_prescans = 4
X_resolution = 5.8631274 [Hz]
X_sweep = 6.00384246 [kHz]
Y_domain = 13C
Y_freq = 150.91343039 [MHz]
Y_offset = 80 [ppm]
Y_points = 512
Y_prescans = 0
Y_resolution = 47.17693237 [Hz]
Y_sweep = 24.15458937 [kHz]
F1_domain = 1H
F1_freq = 600.1723046 [MHz]
F1_offset = 5 [ppm]
Mod_return = 1
Scans = 16
Total_scans = 8192
X_acq_time = 0.17053744 [s]
X_atn = 4.7 [dB]
X_pulse = 7.65 [us]
X_spinlock_atn = 10.7 [dB]
X_spinlock_pulse = 15.3 [us]
Y_acq_time = 21.1968 [ms]
Y_atn = 7.8 [dB]
Y_pl_correction = 360
Y_pulse = 20 [us]
Y_atn_dec = 19.3 [dB]
MPP8 = Off
T1_mode = FALSE
Decoupling = TRUE

043-NO-130A-1-1H-single_pulse5

043-NO-130A-1-hsac_toesy_dec_phase_pfgzz2
NO-130A-1-cdcl3-fg2hx5-temp25_50ms-absorption_hsqc_toes

HSQC toesy

X : parts per Million : 1H

(Billions)

043-NO-130A-1-1hmqc_dplfsc_dec.4
NO-130A-1-cdcl3-temp25-fg2hx5-absorption HMQC with X-decoupling

HMQC

X : parts per Million : 1H

----- PROCESSING PARAMETERS -----
sweep : 10.0 [Hz] : 0.0 [s]
trapzoid3 : 0 [%] : 80 [%] : 100 [%]
zerofill : 1
fft : 1 : TRUE
ppm
naechinphase
phase : 0 : 0 : 3.80977 [ppm]
phase : -4 : 100 : 3.80977 [ppm]
[transposel]
sweep : 50.0 [Hz] : 0.0 [s]
trapzoid3 : 0 [%] : 80 [%] : 100 [%]
zerofill : 2
fft : 1 : TRUE

----- ACQUISITION PARAMETERS -----
File Name : 043-NO-130A-1-1hmqc_dp
Author : hkoishino
Sample ID : hko
Content : NO-130A-1-cdcl3-temp2
Creation Date : 3-MAR-2004 15:48:33
Revision Date : 9-MAR-2004 22:43:54
Spec Site : ECA600
Spec Type : DELTA2 NMR
Data Format : 2D COMPLEX COMPLEX
Dimensions : X Y
Dim Title : 1H 13C
Dim Size : 819, 1024
Dim Units : [ppm] [ppm]
Field strength : 14.09363928 [T] (600 [M
X_acq_duration : 0.17055744 [s]
X_domain : 1H
X_freq : 600.1723046 [MHz]
X_offset : 3.8 [ppm]
X_points : 1024
X_prescans : 4
X_resolution : 5.8631274 [Hz]
X_sweep : 6.00384246 [kHz]
Y_domain : 150.91343039 [MHz]
Y_freq : 80 [ppm]
Y_offset : 512
Y_prescans : 0
Y_resolution : 47.17693237 [Hz]
Y_sweep : 24.15458937 [kHz]
Trl_domain : 1H
Trl_freq : 600.1723046 [MHz]
Trl_offset : 5 [ppm]
Mod_return : 1
Scans : 16
Total_scans : 8192

X_acq_time : 0.17055744 [s]
X_atn : 4.7 [db]
X_pulse : 7.65 [us]
Y_acq_time : 21.1968 [ms]
Y_atn : 7.8 [db]
Y_pl_correction : -360
Y_pulse : 20 [us]
irr_atn_dec : 19.3 [db]
irr_noise : MPF8
Trl_mode : Off
Pulse_program : FALSE
Decoupling : TRUE
Grad_1 : 1 [ms]
Grad_1_amp : 10 [%]