

Supporting Information for

Bionectriol A, a Polyketide Glycoside from the Fungus *Bionectria* sp.

Associated with the Fungus-Growing Ant, *Apterostigma dentigerum*

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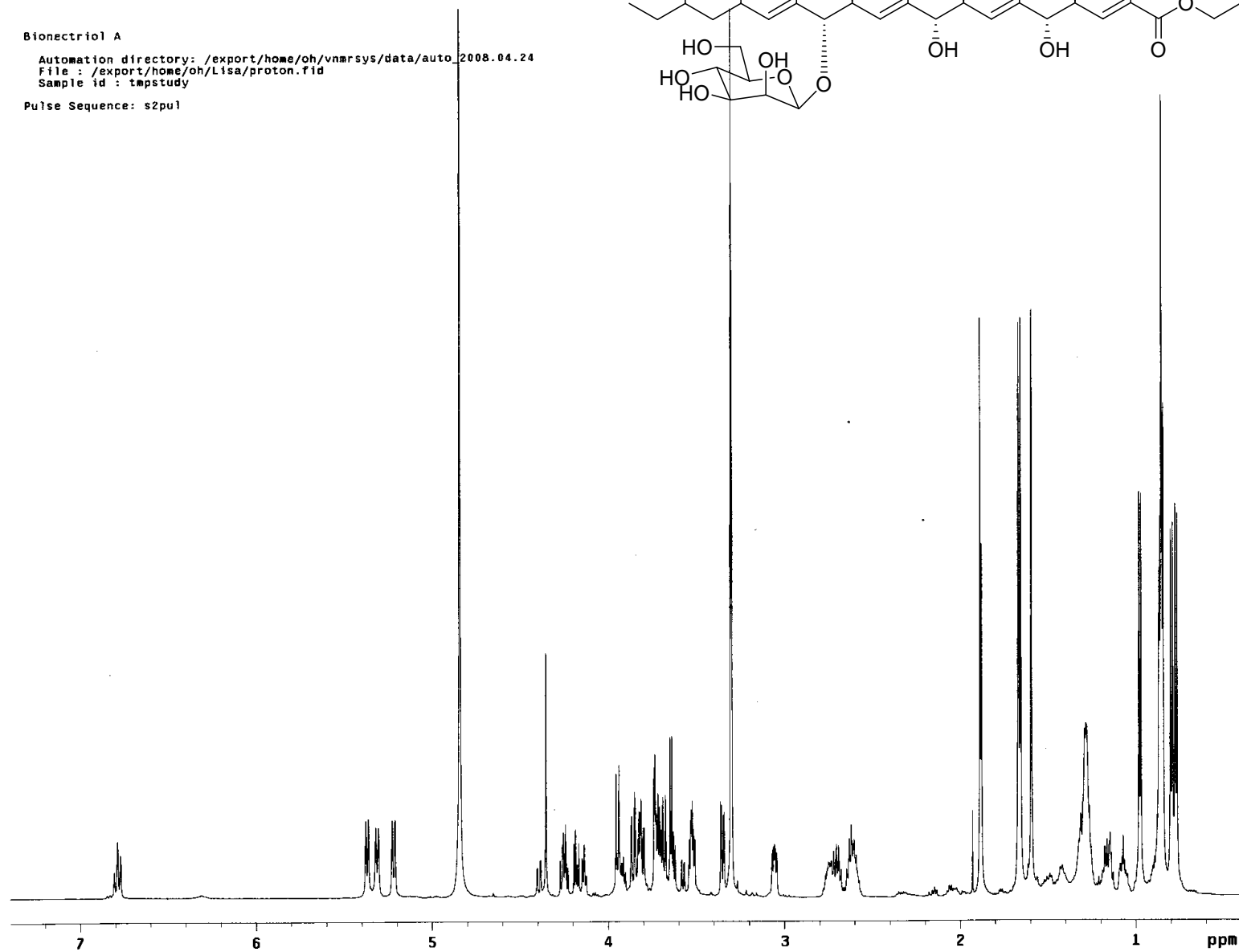
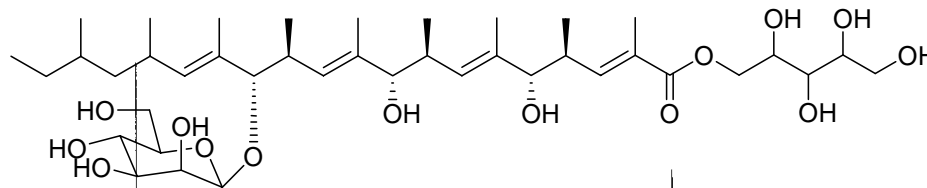
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^1H NMR spectrum of bionectriol A (1) in CD_3OD

Bionectriol A

Automation directory: /export/home/oh/vnmrsys/data/aut_2008.04.24
File: /export/home/oh/Lisa/proton.fid
Sample id: tmpstudy

Pulse Sequence: s2pu1

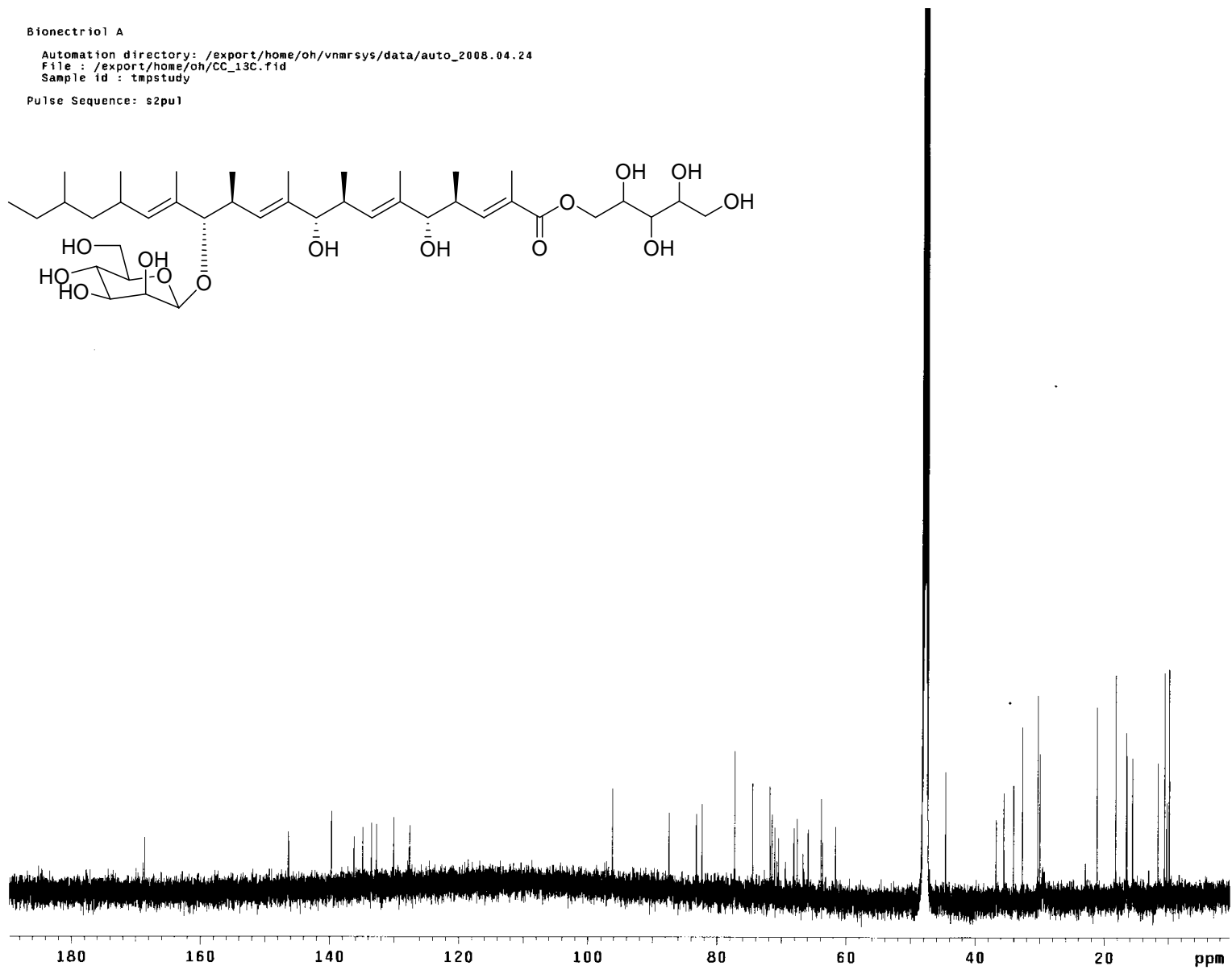
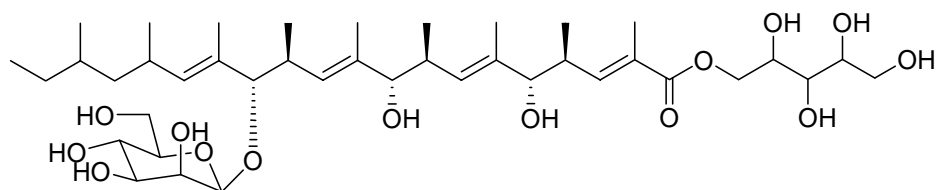


¹³C NMR spectrum of bionectriol A (1) in CD₃OD

Bionectriol A

Automation directory: /export/home/oh/vnmrsys/data/auto_2008.04.24
File : /export/home/oh/cc_13c.fid
Sample id : tmpstudy

Pulse Sequence: s2pu1



gCOSY NMR spectrum of bionectriol A (1) in CD₃OD

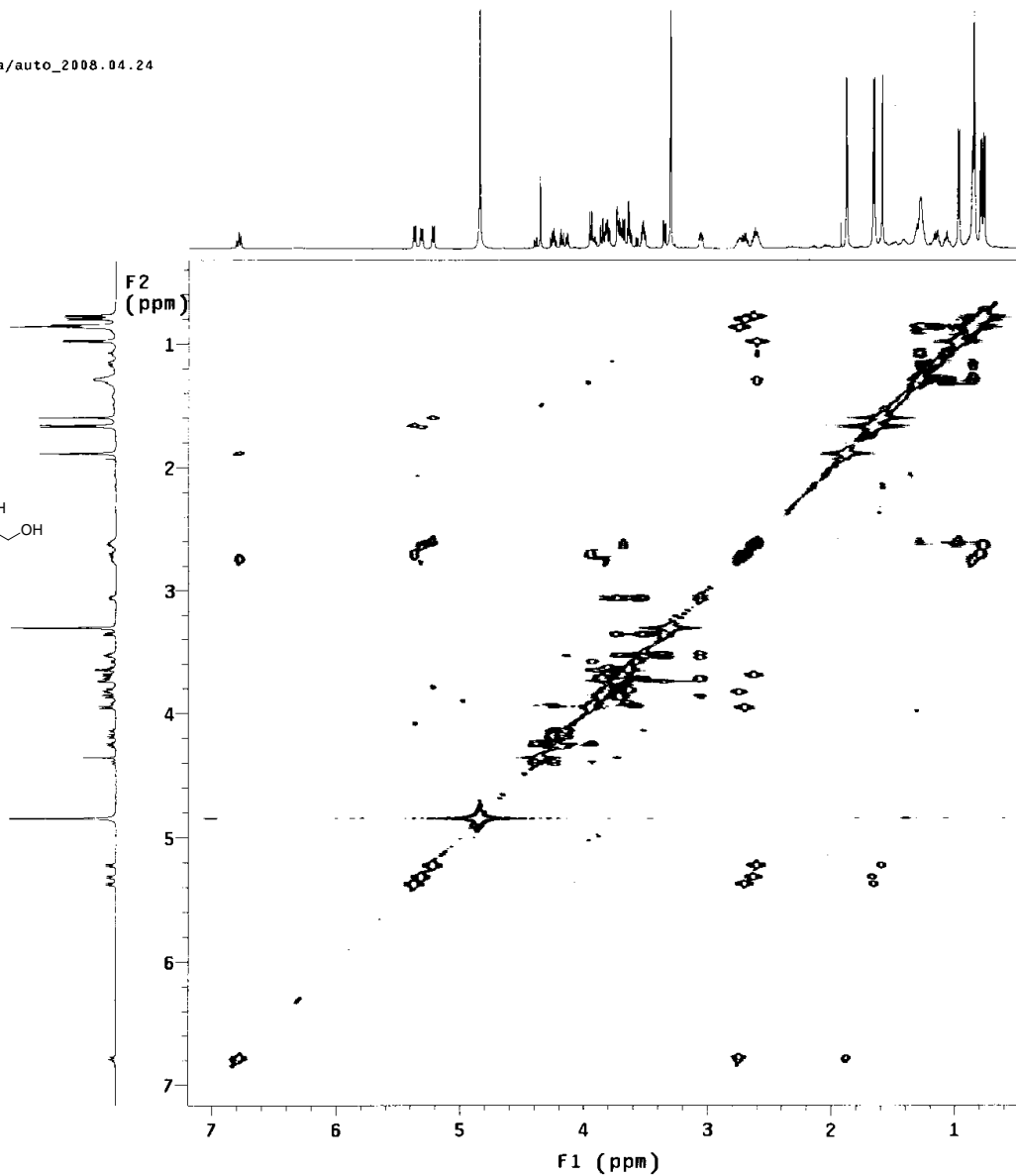
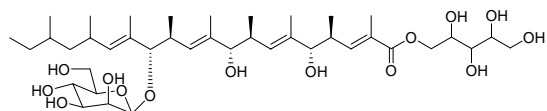
STANDARD 1H OBSERVE - profile

Automation directory: /export/home/oh/vnmrsys/data/auto_2008.04.24
 File : /export/home/oh/Lisa/COSY.fid
 Sample id : tmpstudy

Pulse Sequence: gCOSY

Solvent: cd3od
 Temp: 25.0 C / 298.1 K
 Operator: freinkma
 File: COSY
 VNMR5-600 "nmr"

Relax. delay 1.301 sec
 Acq. time 0.213 sec
 Width 4807.7 Hz
 2D Width 4807.7 Hz
 16 repetitions
 128 increments
 OBSERVE H1, 599.7703395 MHz
 DATA PROCESSING
 Sine bell 0.106 sec
 F1 DATA PROCESSING
 Sine bell 0.053 sec
 FT size 2048 x 2048
 Total time 52 min, 58 sec



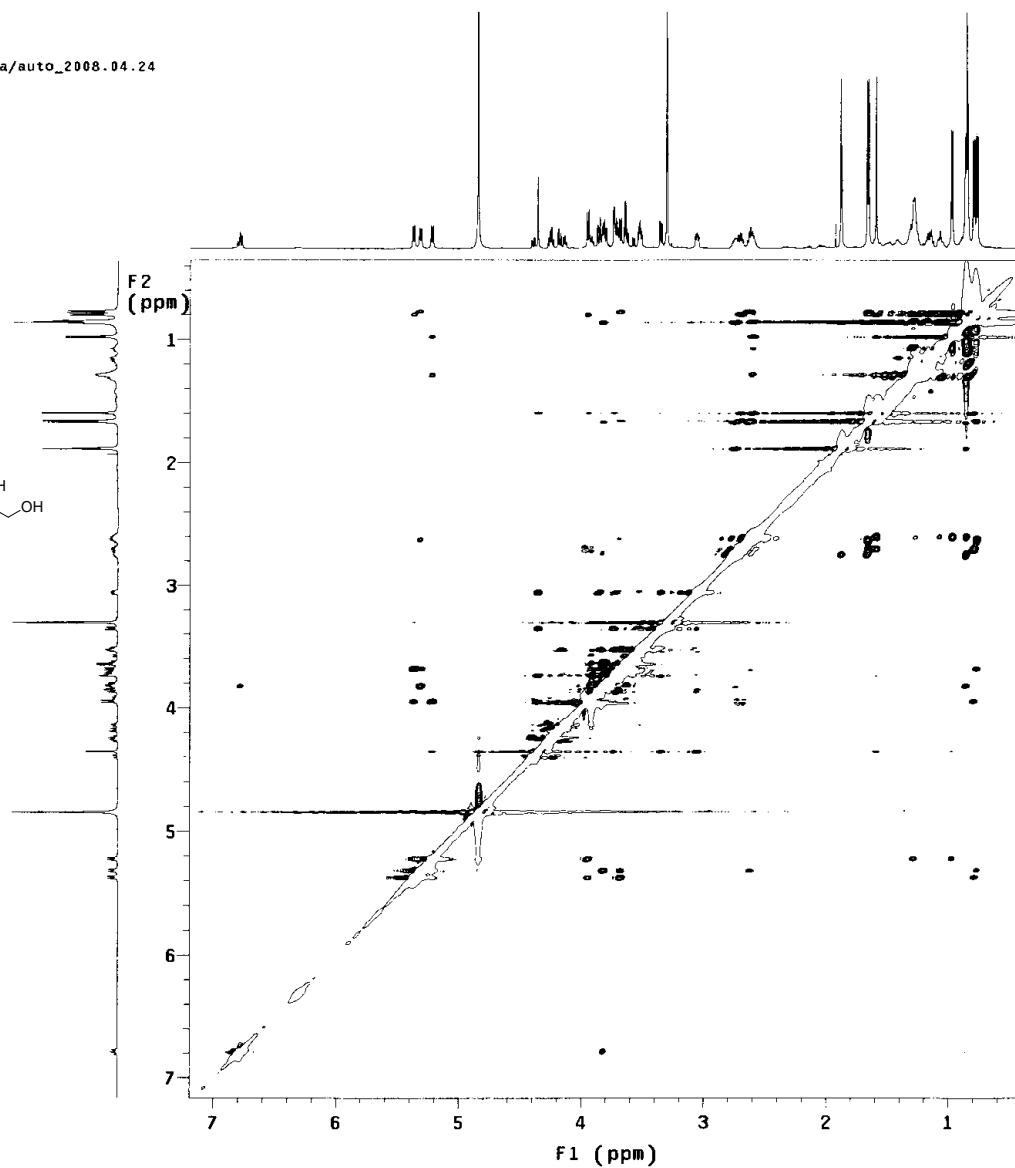
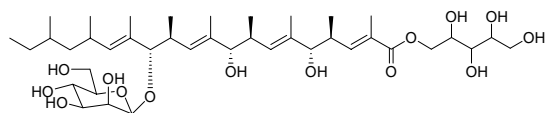
ROESY NMR spectrum of bionectriol A (1) in CD₃OD

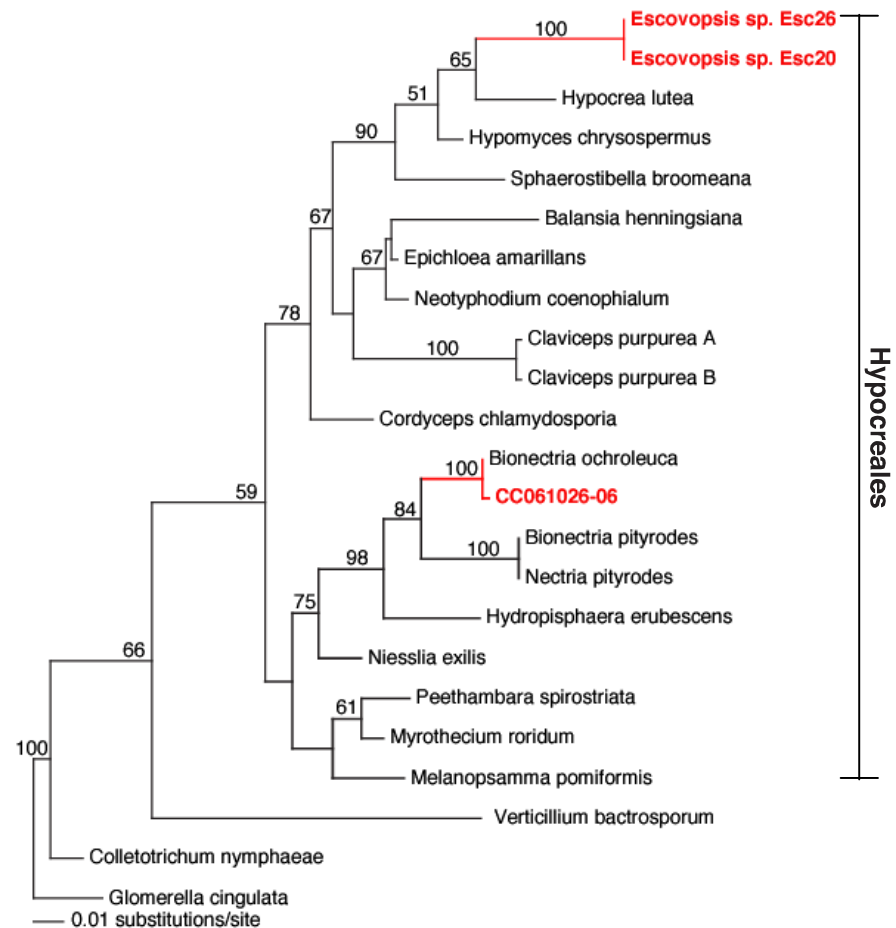
STANDARD 1H OBSERVE - profile

Automation directory: /export/home/oh/vnmrsys/data/auto_2008.04.24
 File: /export/home/oh/Lisa/ROESYf1dd
 Sample id: tmpstudy

Pulse Sequence: gBBSQZ
 Solvent: cd3od
 Temp: 25.0 C / 298.1 K
 Operator: freinkma
 File: ROESY
 VNMRS-600 "nmr"

Relax. delay 1.000 sec
 Mixing 0.200 sec
 Acq. time 0.213 sec
 Width 4807.7 Hz
 2D Width 4807.7 Hz
 32 repetitions
 2 x 128 increments
 OBSERVE H1, 599.7703395 MHz
 DATA PROCESSING
 Gauss apodization 0.098 sec
 F1 DATA PROCESSING
 Gauss apodization 0.038 sec
 FT size 2048 x 2048
 Total time 3 hr, 18 min, 17 sec





S8: Molecular phylogeny for the fungal strain CC061026-06. A maximum likelihood (ML) phylogenetic analysis of ~555 base-pairs of 28S rRNA gene sequences from 22 representative members of Hypocreomycetidae (Ascomycota), 19 of which were from the order Hypocreales. The remaining three (3) taxa were used as an outgroup for the analysis. Branch numbers represent bootstrap values for 100 pseudoreplicates under maximum likelihood analysis. Values below 50 are not included. Strong bootstrap support indicates that CC061026-06 (shown in red)

is most closely related to *Bionectria ochroleuca* and sister to *Bionectria pityrodes* and *Nectria pityrodes*. As part of this analysis we also included two strains of the pathogen known to infect the fungal gardens of *Apterotigma* ants, *Escovopsis* sp. (*Escovopsis* sp. Esc26 and *Escovopsis* sp. Esc20, also in red). Our analysis indicates that CC061026-06 is distantly related to the pathogen *Escovopsis* and thus we cannot be certain of its role in the system at this time.