

Supplemental data

In vitro antitubercular activity of extract and constituents from the stem bark of *Distemonanthus benthamianus* Baill. (Ceasalpinaceae)

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Abstract

A new C-glycosylflavone, apigenin 7-methyl ether 6-C-[β -xylopyranosyl-(1 \rightarrow 3)- β -glucopyranoside] named distemonanthoside (**1**) was isolated from the stem bark of *Distemonanthus benthamianus*, along with six known compounds, sitosterol 3-O- β -D-glucopyranoside (**2**), 4-methoxygallic acid (**3**), syringic acid (**4**), quercetin (**5**), 6"-O-acetylvitexin (**6**), quercetin 3-O- β -D-glucopyranoside (**7**). The structures of those compounds and others were determined through spectral analyses. Compounds **1**, **2**, **3** and **5** were tested against a clinical isolate strain of *Mycobacterium tuberculosis* AC 45; they exhibited good to moderate antitubercular activities with MIC values ranged from 31.25 to 125 μ g/ml.

Keywords: Ceasalpinaceae; *Distemonanthus benthamianus*; flavonoids; distemonanthoside; antitubercular activity; phenolic acid

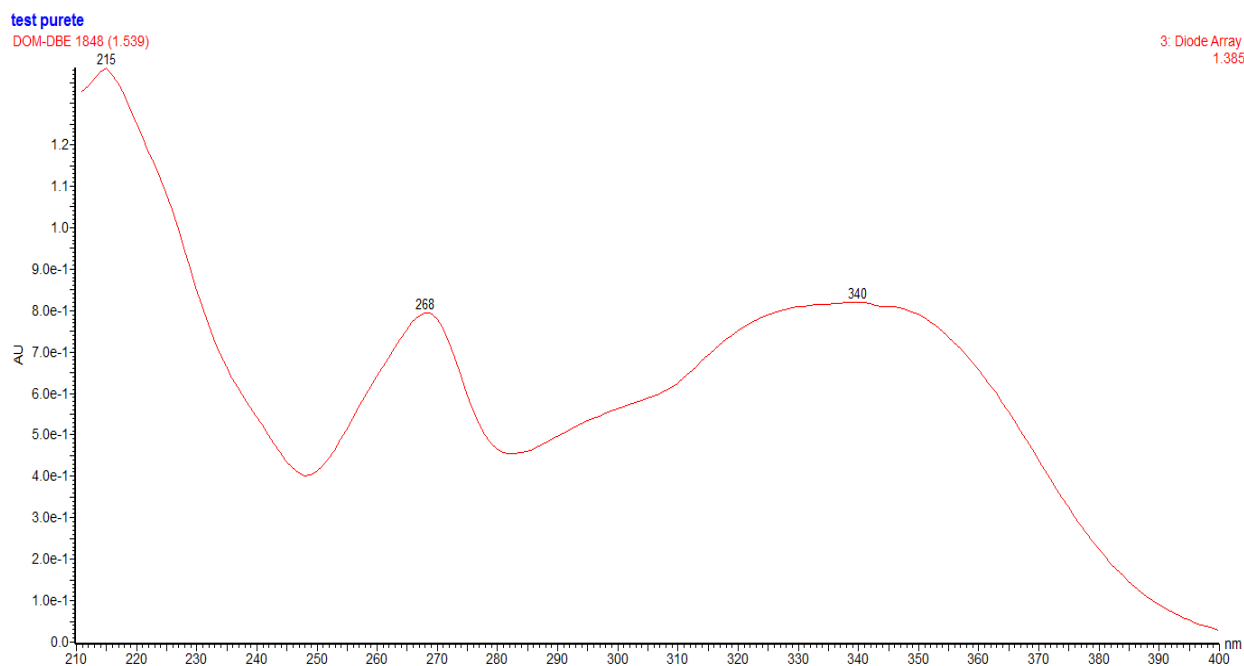


Fig.S1. UV spectrum of compound 1

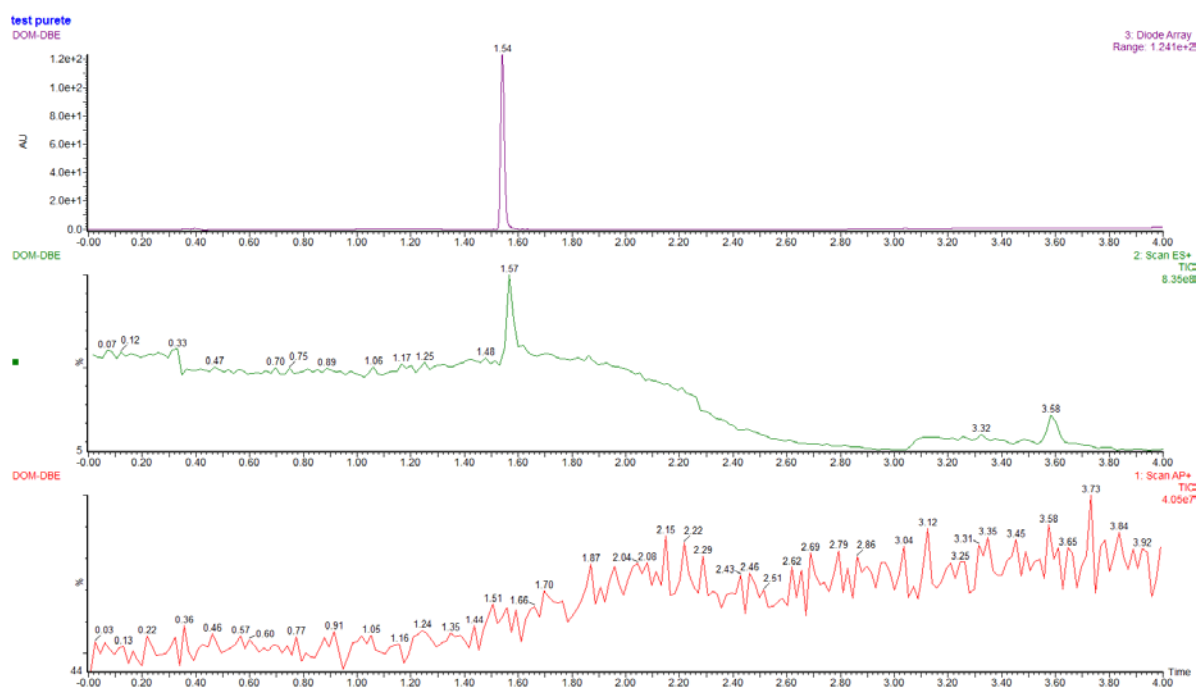
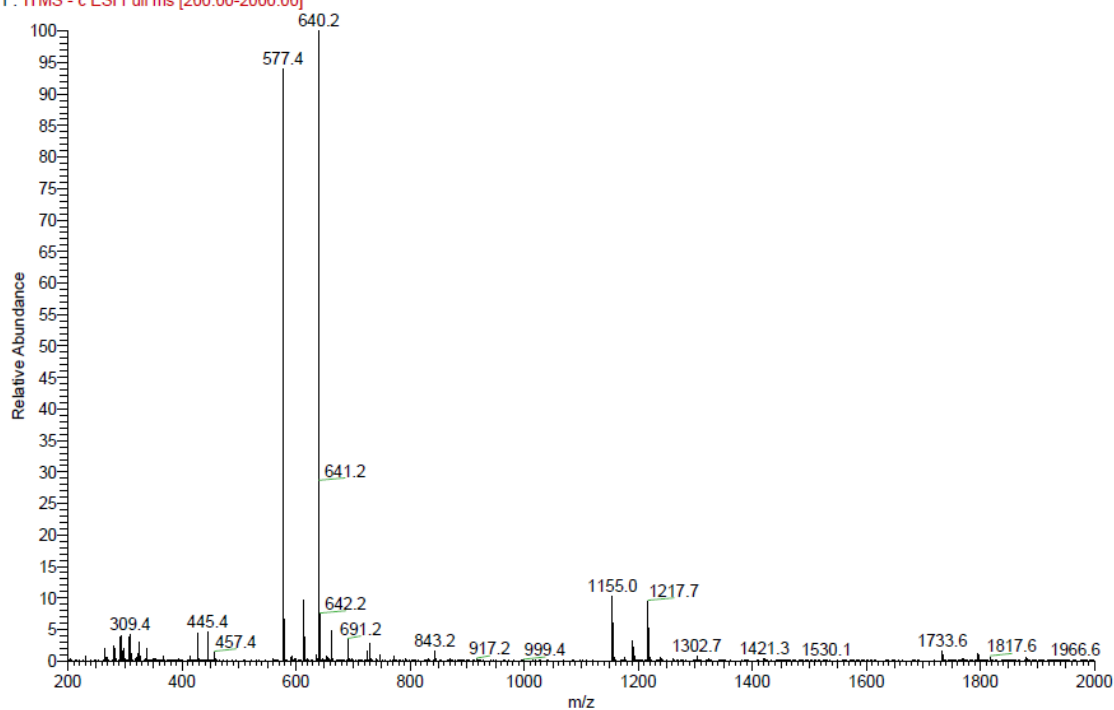


Fig.S2. UPLC chromatogram of compound 1

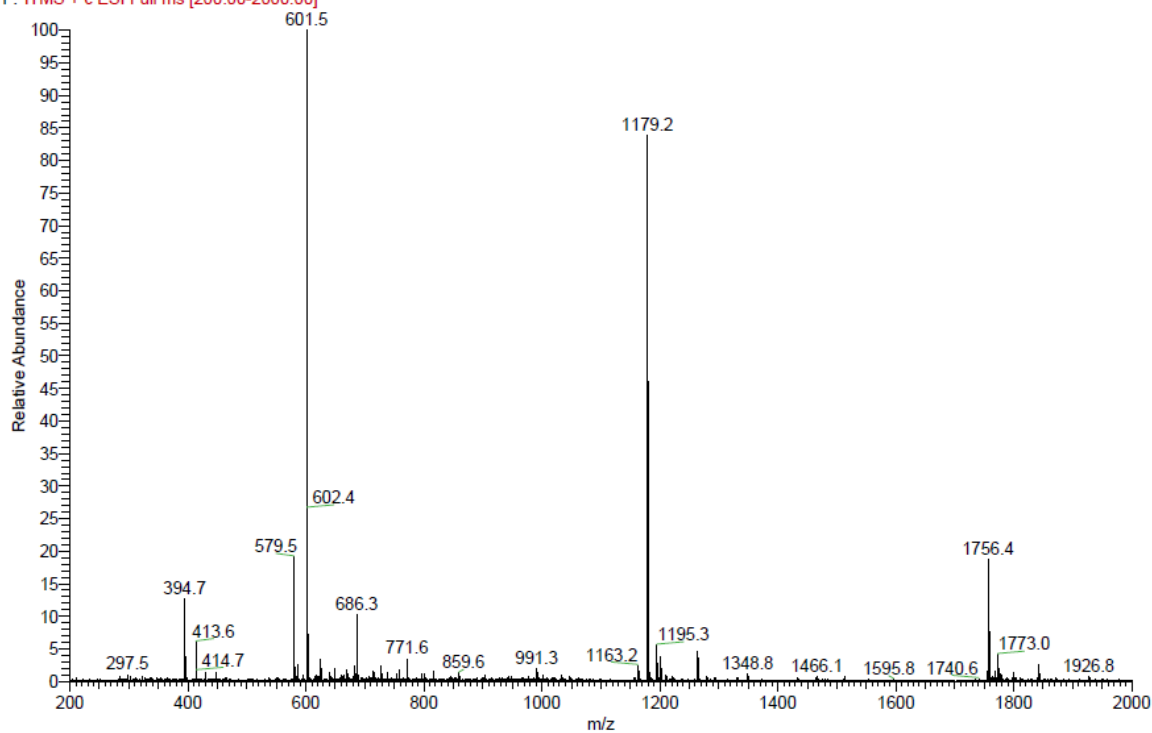
150917 EM 665 Ko neg #87 RT: 1.00 AV: 1 NL: 7.93E4

F: ITMS - c ESI Full ms [200.00-2000.00]

**Fig. S3** ESI-MS spectra of compound 1 (Negative mode)

150917 EM 665 Ko #87 RT: 1.00 AV: 1 NL: 9.98E4

F: ITMS + c ESI Full ms [200.00-2000.00]

**Fig. S4** ESI-MS spectra of compound 1 (Positive mode)

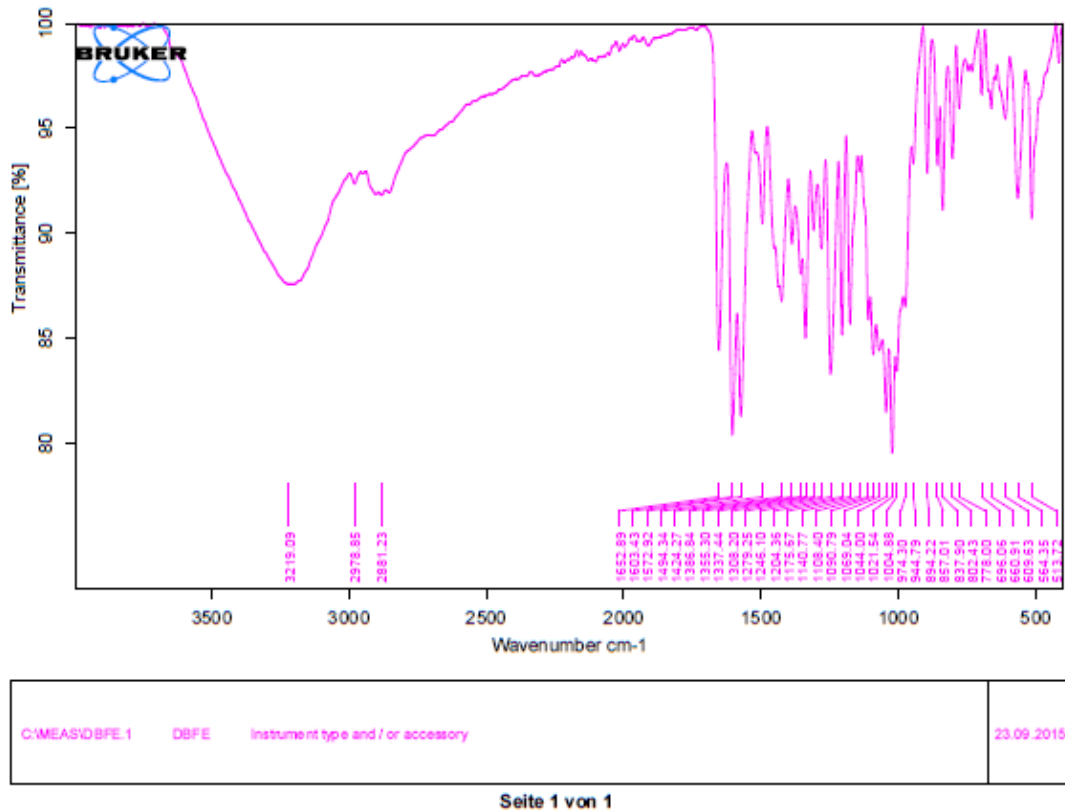


Fig. S5 IR spectrum of compound 1

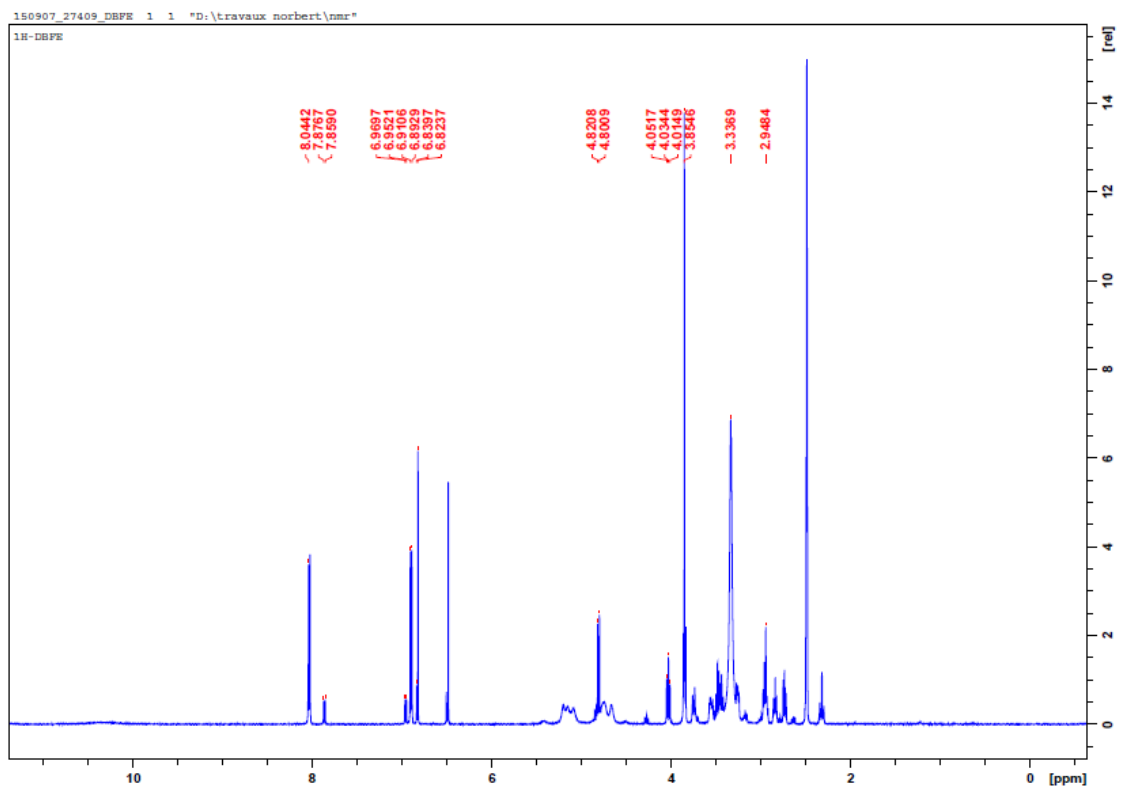
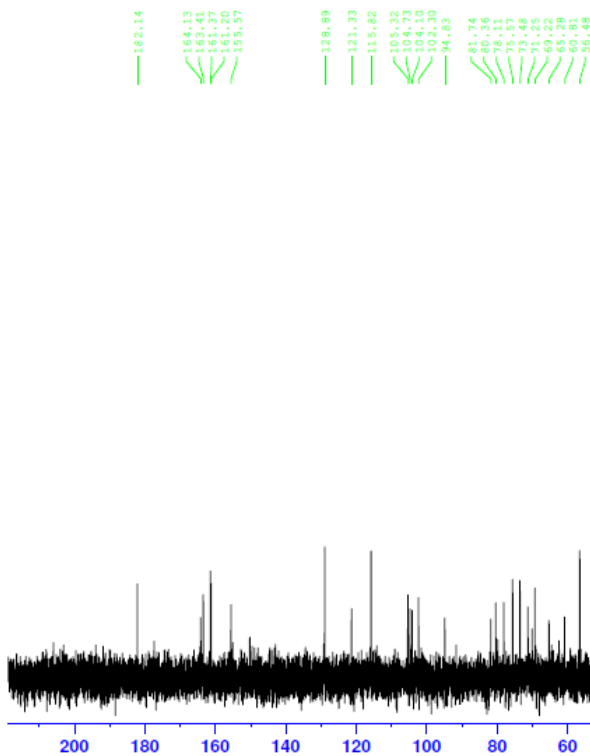


Fig. S6 ¹H NMR spectrum of compound 1

DBFE-DMSO-d6



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EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20150904
Time     6.17
INSTRUM  spect
PROBHD   5 mm PABBO BH-
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       512
DS       4
SWH      18028.846 Hz
FIDRES   0.275098 Hz
AQ       1.8175317 sec
RG       2050
DW       27.733 usec
DE       6.00 usec
TE       300.0 K
D1       0.50000000 sec
D11      0.03000000 sec
TD0      1

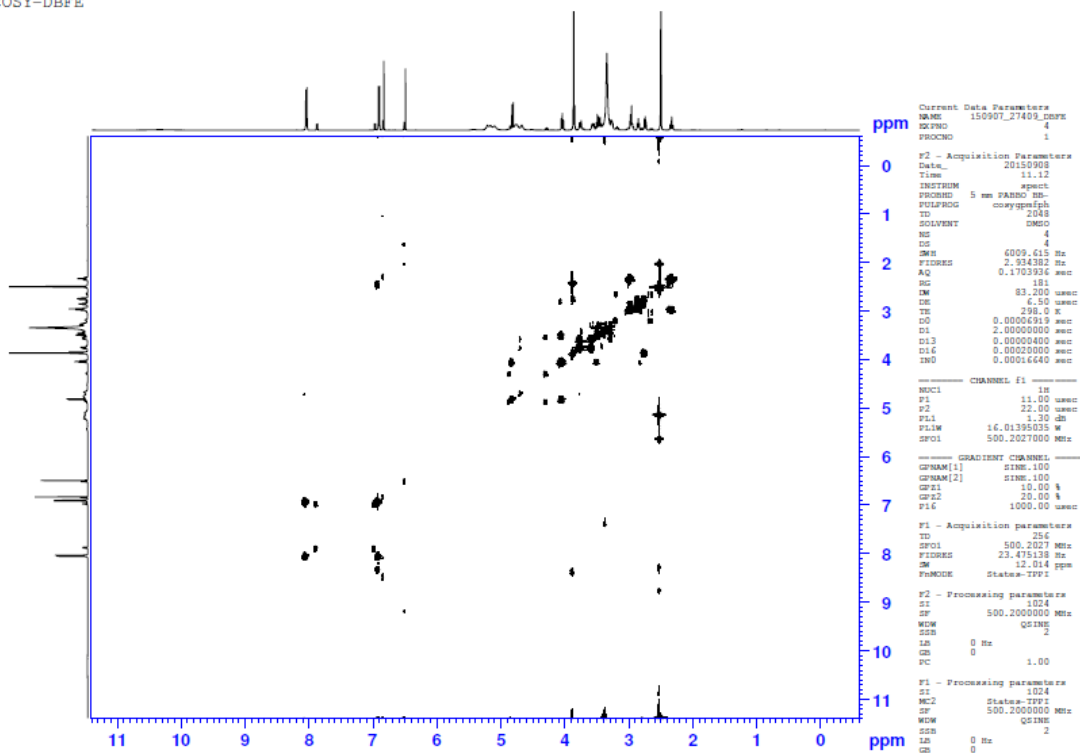
===== CHANNEL f1 =====
NUC1     13C
P1       6.70 usec
PL1      -4.00 dB
PL1W     81.39349365 W
SFO1     75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -2.00 dB
PL12     16.79 dB
PL13     16.79 dB
PL2W     18.31292915 W
PL12W    0.24196789 W
PL13W    0.24196789 W
SFO2     300.1312000 MHz

F2 - Processing parameters
SI       32768
SF       75.4677922 MHz
WDW      EM
SSB      0
LB       0
GB       1.00 Hz
PC       1.40
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Fig. S7 ^{13}C NMR spectrum of compound 1

COSY-DBFE



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PROCNO   1

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INSTRUM  spect
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PULPROG  cosygpmph
TD       2048
SOLVENT  DMSO
NS       4
DS       4
SWH      6009.615 Hz
FIDRES   2.934382 Hz
AQ       0.1103336 sec
RG       181
DW       83.200 usec
DE       6.50 usec
TE       298.0 K
D0       0.00000019 sec
D1       2.00000000 sec
D13      0.00000400 sec
D16      0.00010000 sec
D18      0.00016440 sec
D19      0.00016440 sec

===== CHANNEL f1 =====
NUC1     1H
P1       11.00 usec
P2       22.00 usec
PL1      1.30 dB
PL1W     16.01395035 W
SFO1     500.2027000 MHz

===== GRADIENT CHANNEL =====
GPRAM[1] SIMS.100
GPRAM[2] SIMS.100
CPC1    10.00 %
CPC2    20.00 %
P16     1000.00 usec

F1 - Acquisition parameters
TD       256
SFO1     500.2027000 MHz
FIDRES   23.475138 Hz
SW       12.014 ppm
F2MODE   States-TFPI

F2 - Processing parameters
SI       1024
SF       500.2000000 MHz
WDW      QFINE
SSB      2
LB       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       1024
MC2      States-TFPI
SF       500.2000000 MHz
WDW      QFINE
SSB      2
LB       0 Hz
GB       0
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Fig. S8 ^1H - ^1H COSY spectrum of compound 1

HSQC-DBFE

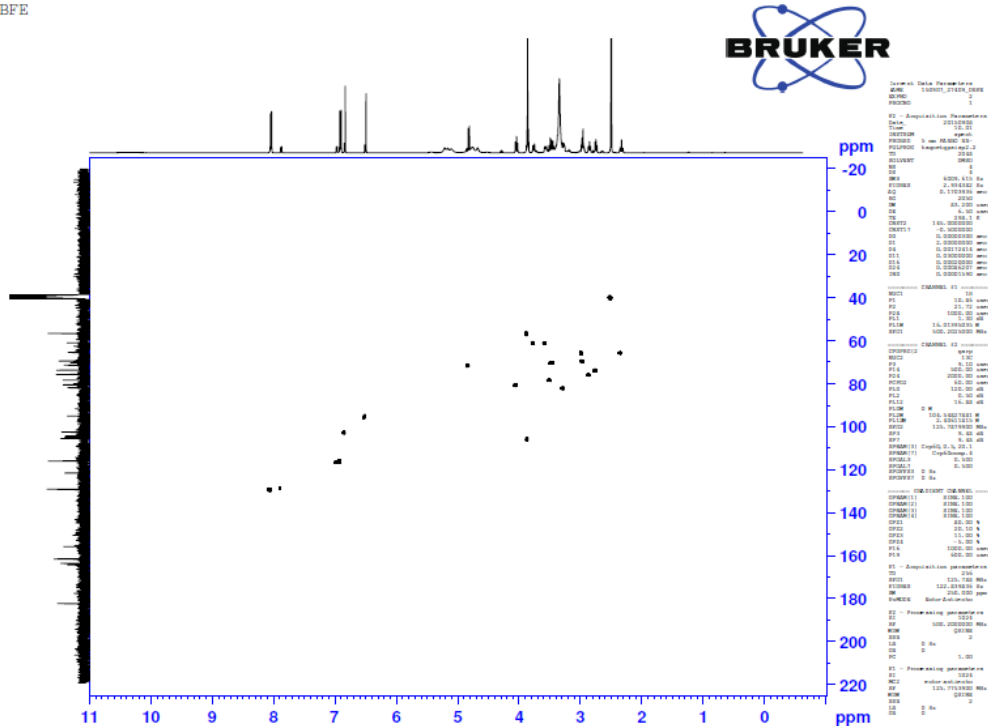


Fig. S9 HSQC spectrum of compound 1

HMBC-DBFE

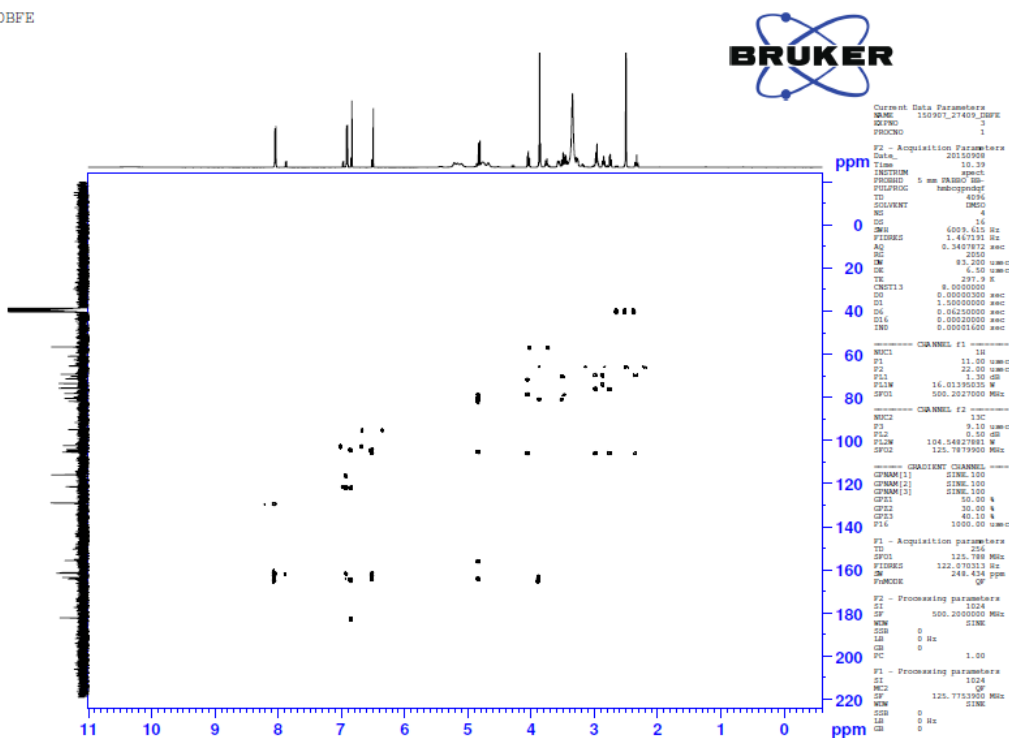


Fig. S10 HMBC spectrum of compound 1

NOESY-DBFE

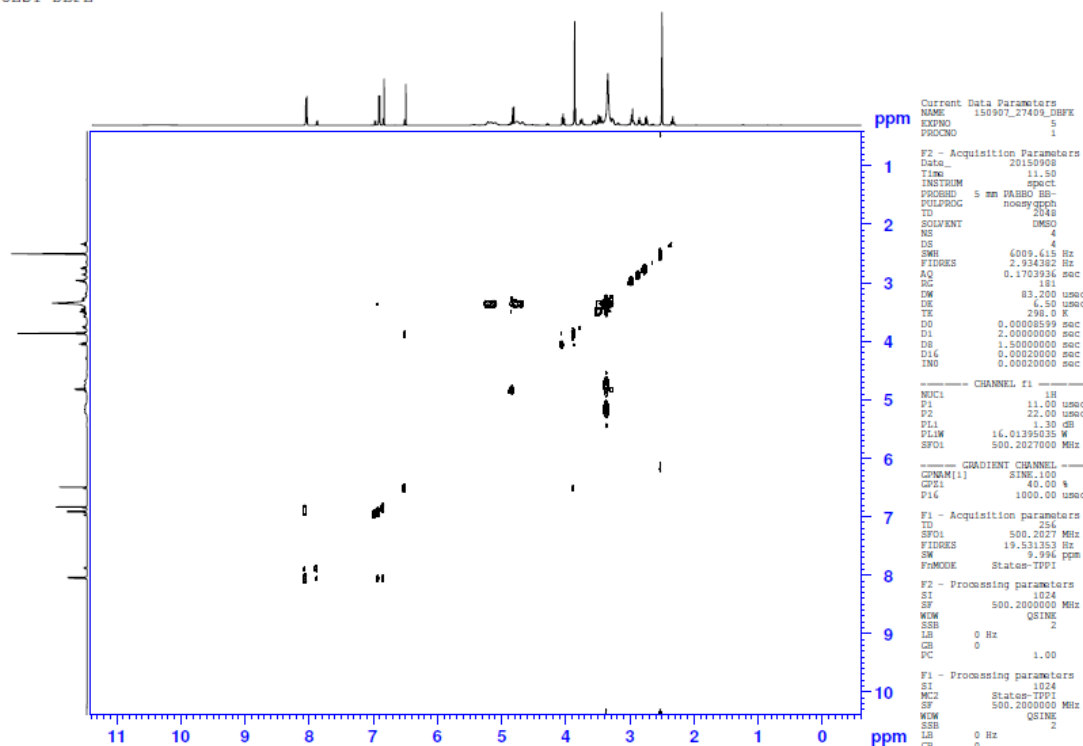


Fig. S11 NOESY spectrum of compound 1

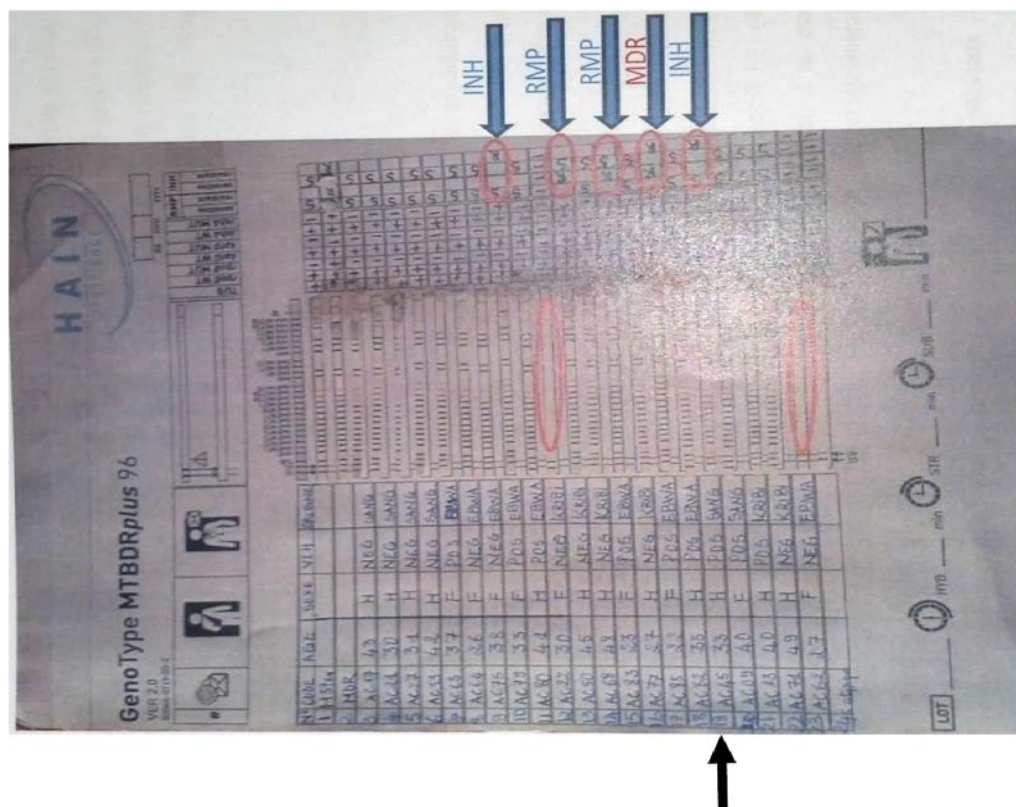


Figure S12. Genotype profile of *M. tuberculosis* codifies AC 45