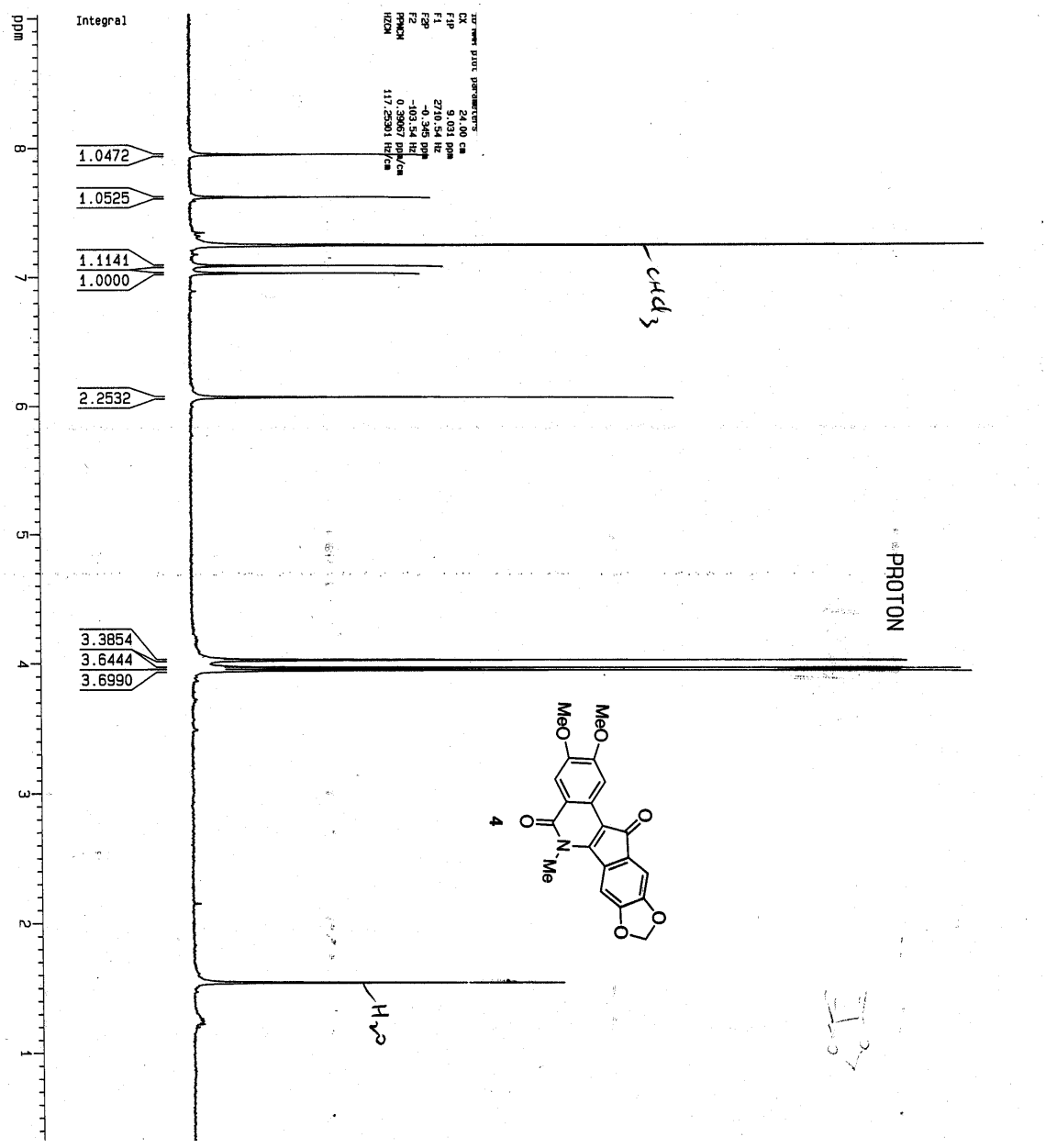
Supporting Information

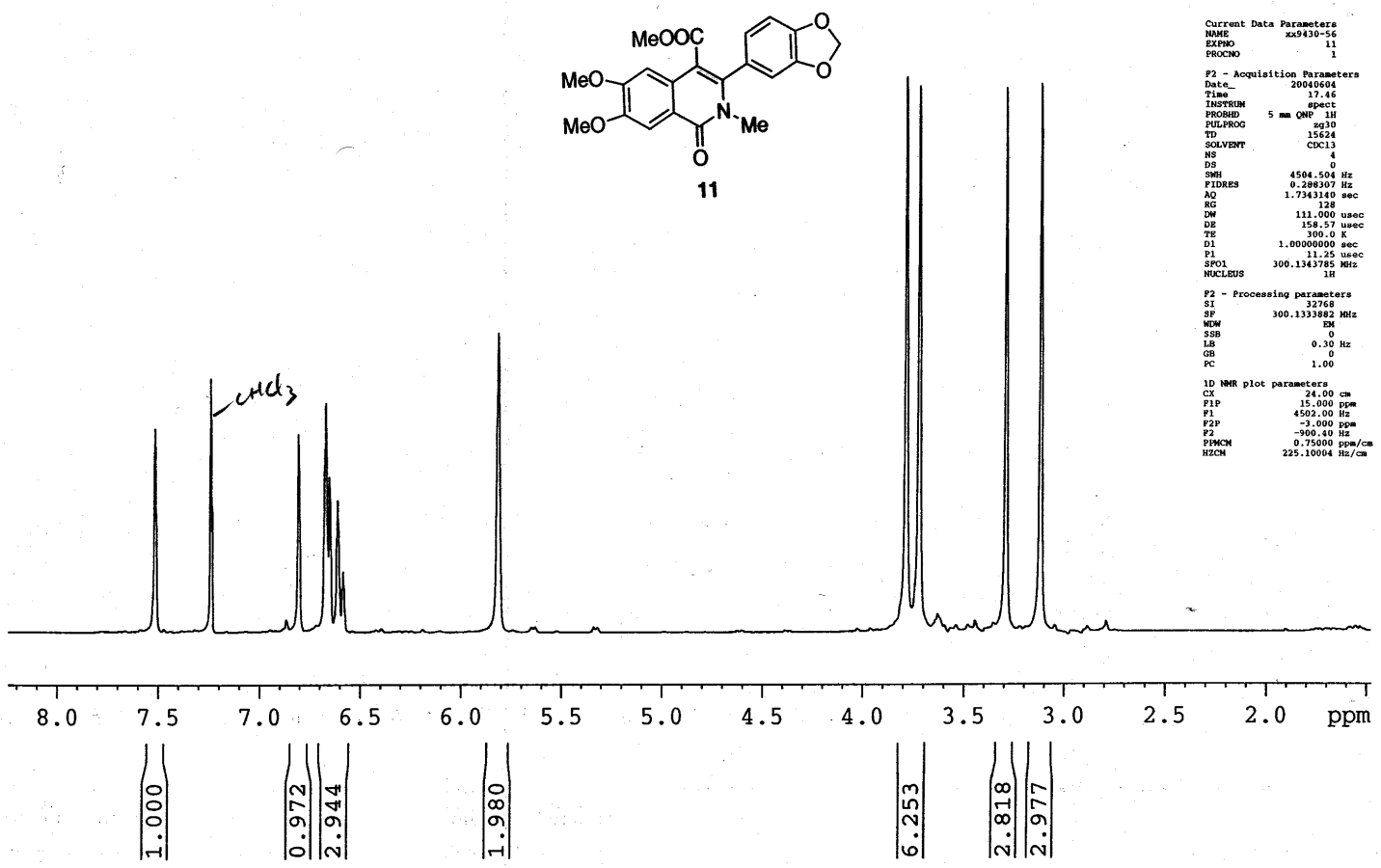
A Facile Method to Transform trans-4-Carboxy-3,4-dihydro-3-phenyl-1(2H)-isoquinolones to Indeno[1,2-c]isoquinolines

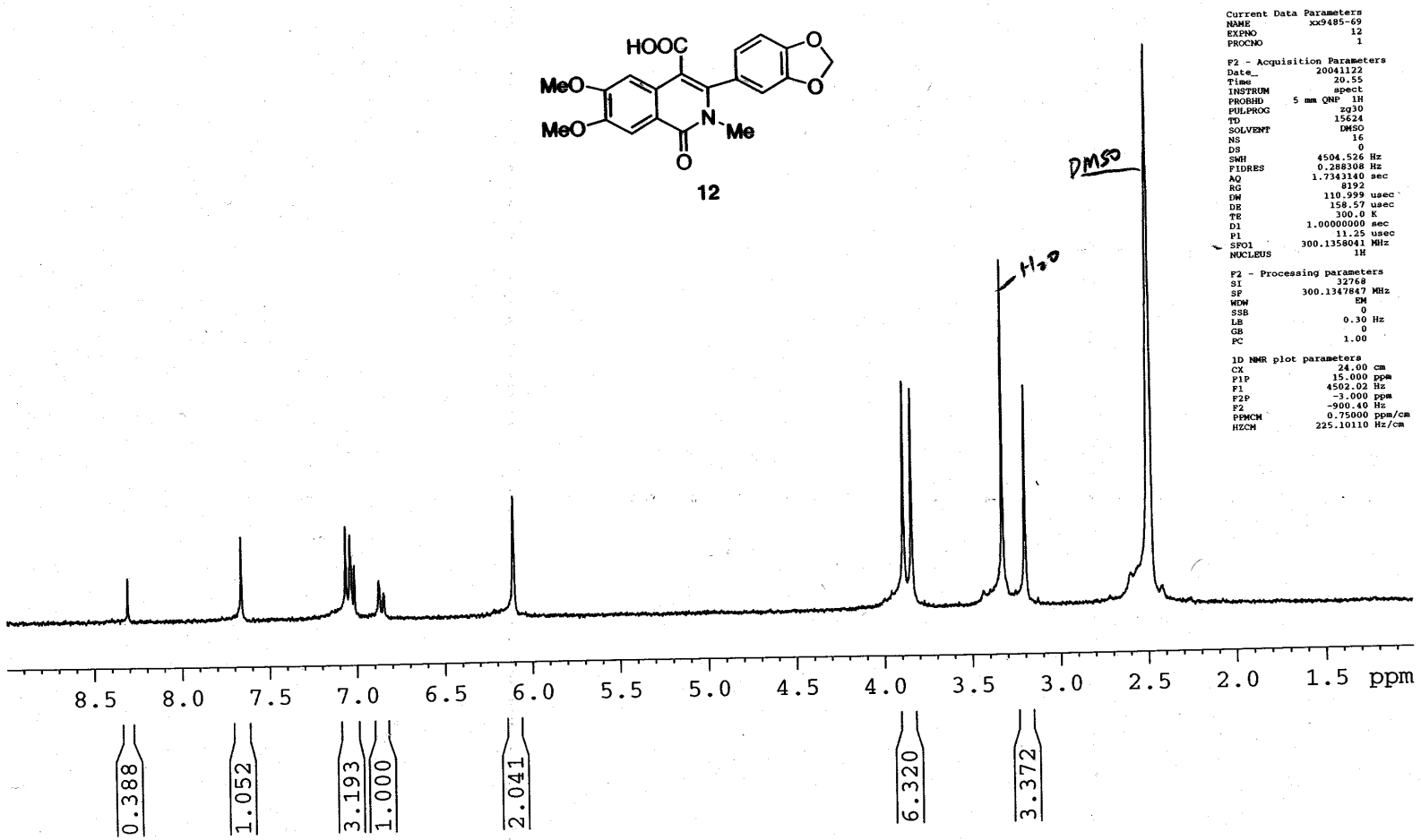
Xiangshu Xiao and Mark Cushman*

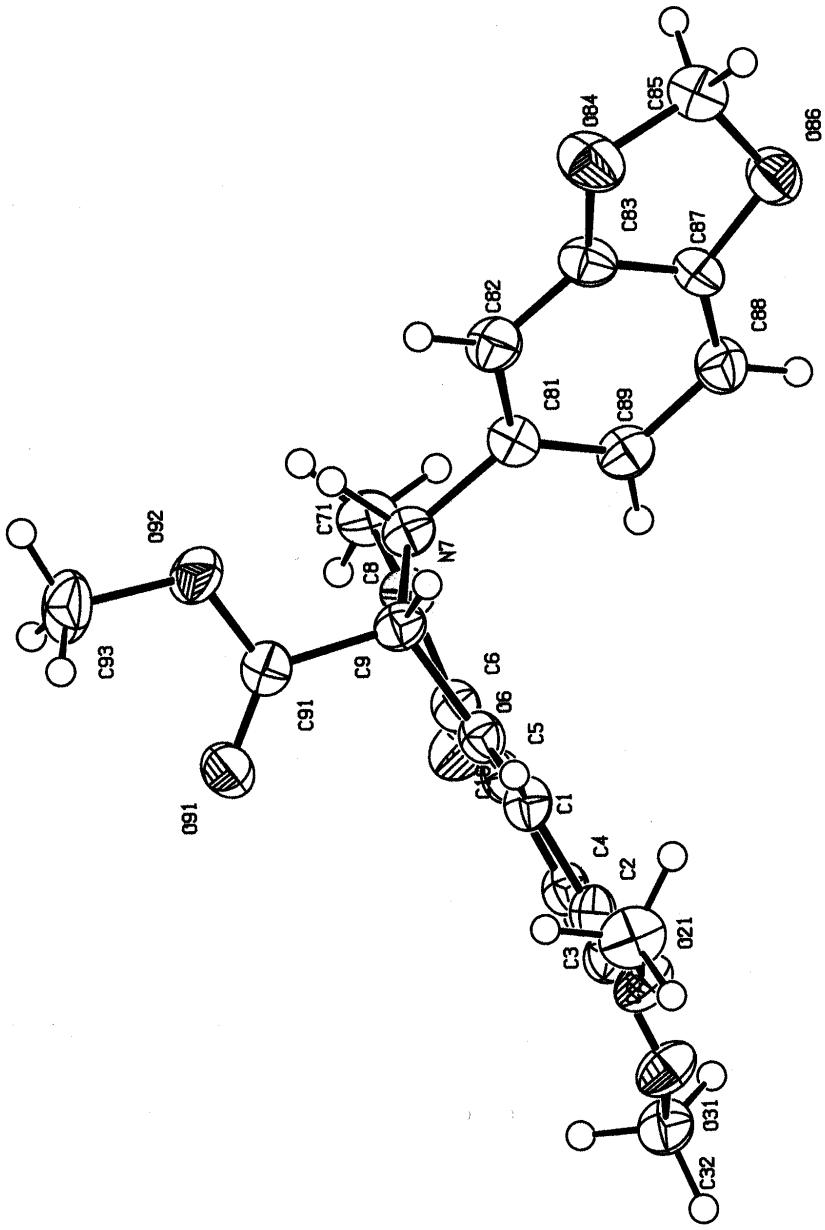
Department of Medicinal Chemistry and Molecular Pharmacology and the Purdue Cancer Center, School of Pharmacy and Pharmaceutical Sciences, Purdue University, West Lafayette, IN 47907, USA

Corresponding Author: Phone number: 765-494-1465; fax number: 765-494-6790, e-mail: cushman@pharmacy.purdue.edu


Integral
1.0472
1.0525
1.1141
1.0000
2.2532
3.3854
3.6444
3.6990
PROTON
MeO
MeO
O
O
N
Me
4


MeOOC
MeO
MeO
N
Me
O
O
O
11
CHCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.000
0.972
2.944
1.980
6.253
2.818
2.977
Current Data Parameters
NAME xx9430-56
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040604
Time 17.46
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 15624
SOLVENT CDCl3
NS 4
DS 0
SWH 4504.504 Hz
FIDRES 0.288307 Hz
AQ 1.7343140 sec
RG 128
DW 111.000 usec
DE 158.57 usec
TE 300.0 K
D1 1.00000000 sec
P1 11.25 usec
SFO1 300.1343785 MHz
NUCLEUS 1H
F2 - Processing parameters
SI 32768
SF 300.1333882 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 24.00 cm
F1P 15.000 ppm
F1 4502.00 Hz
F2P -3.000 ppm
F2 -900.40 Hz
PPMCM 0.75000 ppm/cm
HZCM 225.10004 Hz/cm


HOOC
MeO
MeO
N
Me
O
O
O
O
12
DMSO
H2O
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
0.388
1.052
3.193
1.000
2.041
6.320
3.372
Current Data Parameters
NAME xx9485-69
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041122
Time 20.55
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 15624
SOLVENT DMSO
NS 16
DS 0
SWH 4504.526 Hz
FIDRES 0.288308 Hz
AQ 1.7343140 sec
RG 8192
DW 110.999 usec
DE 158.57 usec
TE 300.0 K
D1 1.00000000 sec
P1 11.25 usec
SFO1 300.1358041 MHz
NUCLEUS 1H
F2 - Processing parameters
SI 32768
SF 300.1347847 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 24.00 cm
F1P 15.000 ppm
F1 4502.02 Hz
F2P -3.000 ppm
F2 -900.40 Hz
PPMCM 0.75000 ppm/cm
HZCM 225.10110 Hz/cm



ORTEP drawing of **10**.