

SUPPLEMENTARY INFORMATION

Subtle Structural Changes in Octupolar Merocyanine Dyes Influence the Photosensitized Production of Singlet Oxygen

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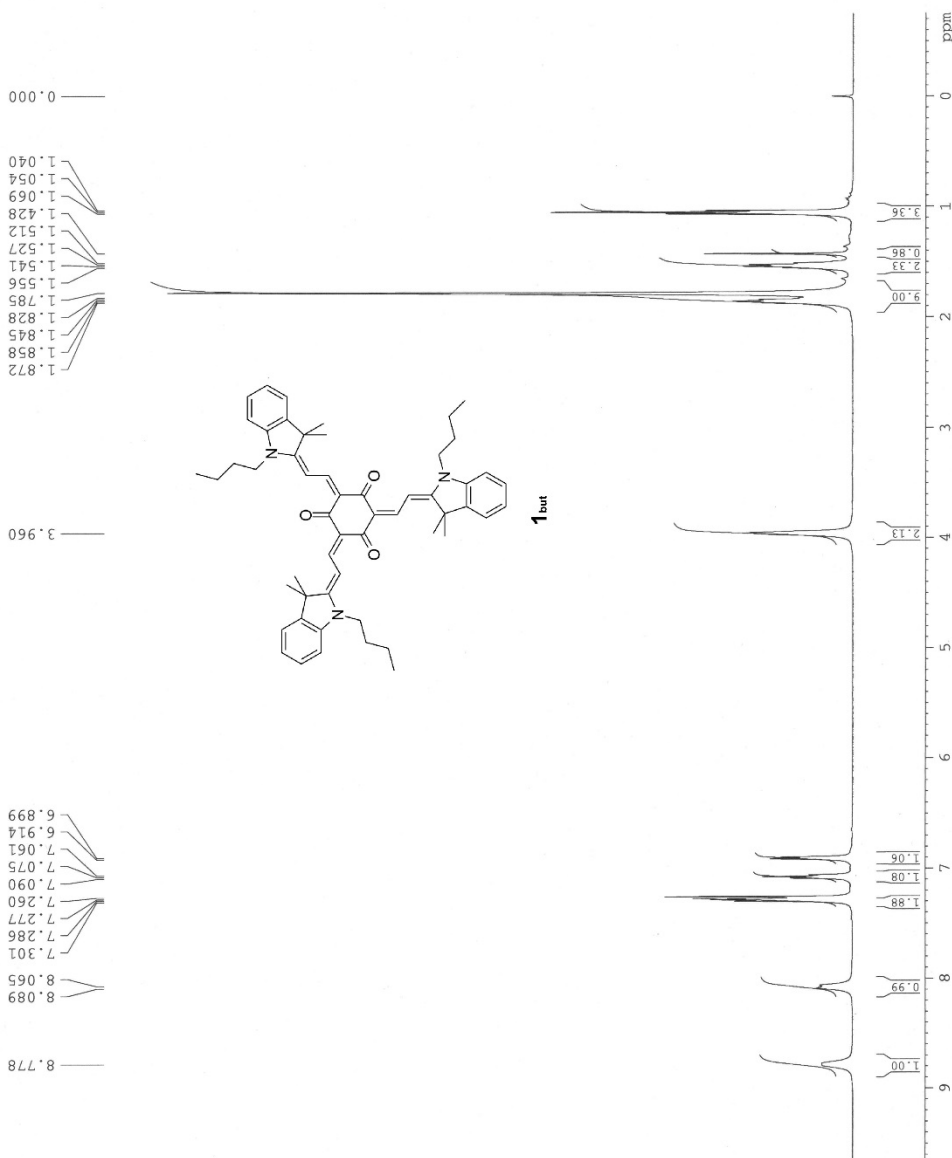


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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140304
Time 15.43
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171993 sec
RG 327
DM 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330685 MHz

F2 - Processing parameters
SI 32768
SF 500.1300261 MHz
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SSB 0
LB 0 Hz
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PROCNO    1

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PROBHD    5 mm TEI 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT    CDCl3
NS         31000
DS         4
SWH         32679.73 Hz
FIDRES     0.498653 Hz
AQ         1.0027508 sec
RG         32768
DW         15.300 usec
DE         7.10 usec
TE         303.10 K
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TD0        1

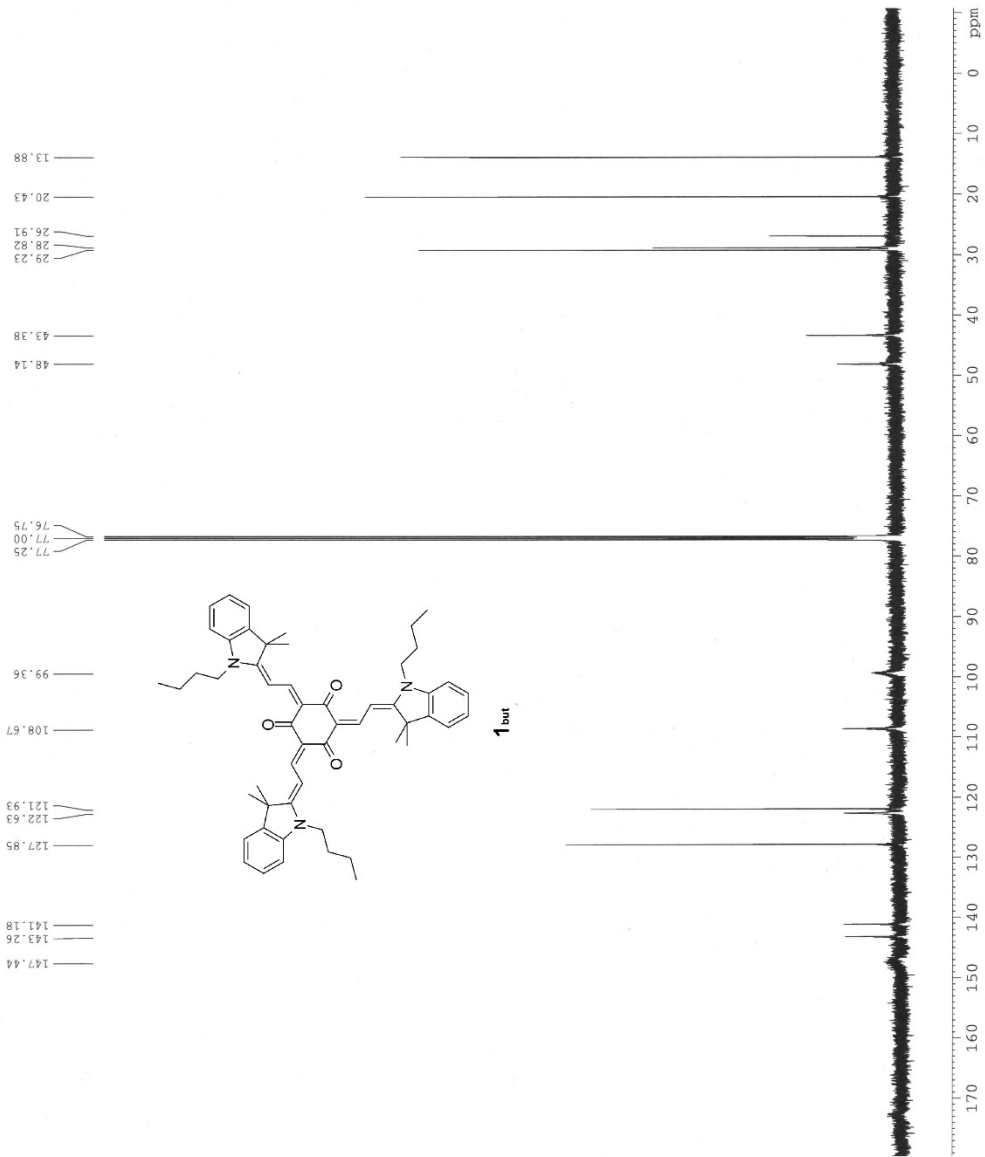
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NUC1       13C
P1         5.00 usec
PL1        3.00 dB
SFO1       125.7703643 MHz

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NUC2       1H
PCPD2      98.00 usec
PL2         3.00 dB
PL12        23.00 dB
PL13        32.00 dB
SFO2       500.1320005 MHz

F1 - Acquisition parameters
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TD          128
SFO1        500.132 MHz
FIDRES      7.812500 Hz
AQC         1.0000000 sec
PQ         0
PC          1.40

F2 - Processing parameters
SI          262144
SF          125.7577941 MHz
RG          0
SSB         0
LB          0.50 Hz
GB          0
PC          1.40

F1 - Processing parameters
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MC2         QF
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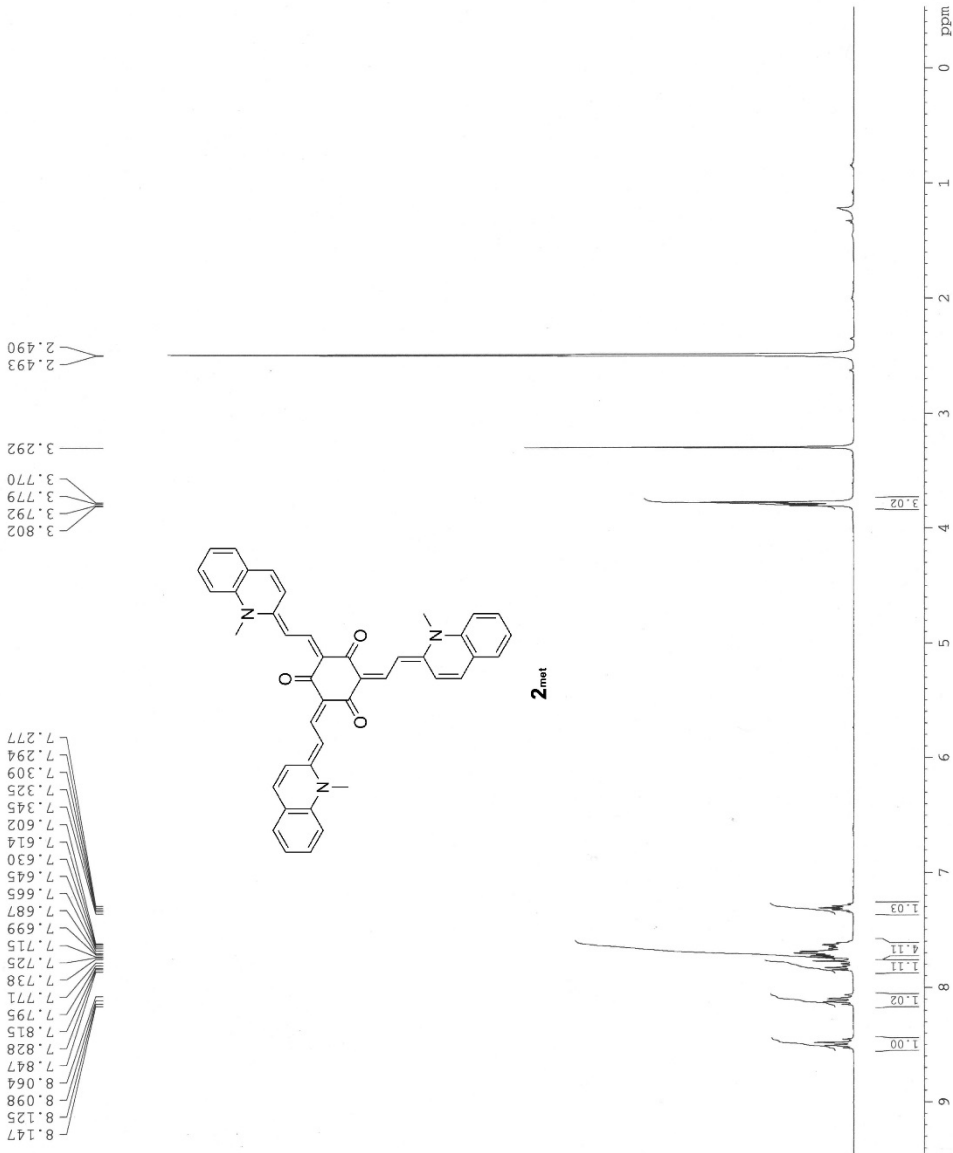


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 EXPNO 1
 PROCNO 1

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 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.171973 sec
 RG 327.4
 DM 48.400 usec
 DE 6.78 usec
 TE 303.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 5.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
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 SF 500.1300100 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00





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Current Data Parameters
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EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
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Date_     20140616
Time      15:31
INSTRUM   DRX
PROBHD    5 mm TBI LH/13
PULPROG   zgpg
TD         65536
AQ        0.00000000
RG         32000
DS         4
SMH        32679.738 Hz
FIDRES     0.498653 Hz
AQ         1.00000000 sec
RG         32768
DS         4
DE         15.300 usec
TE         7.10 usec
TE        303.0 K
TD         131072
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TD0       1

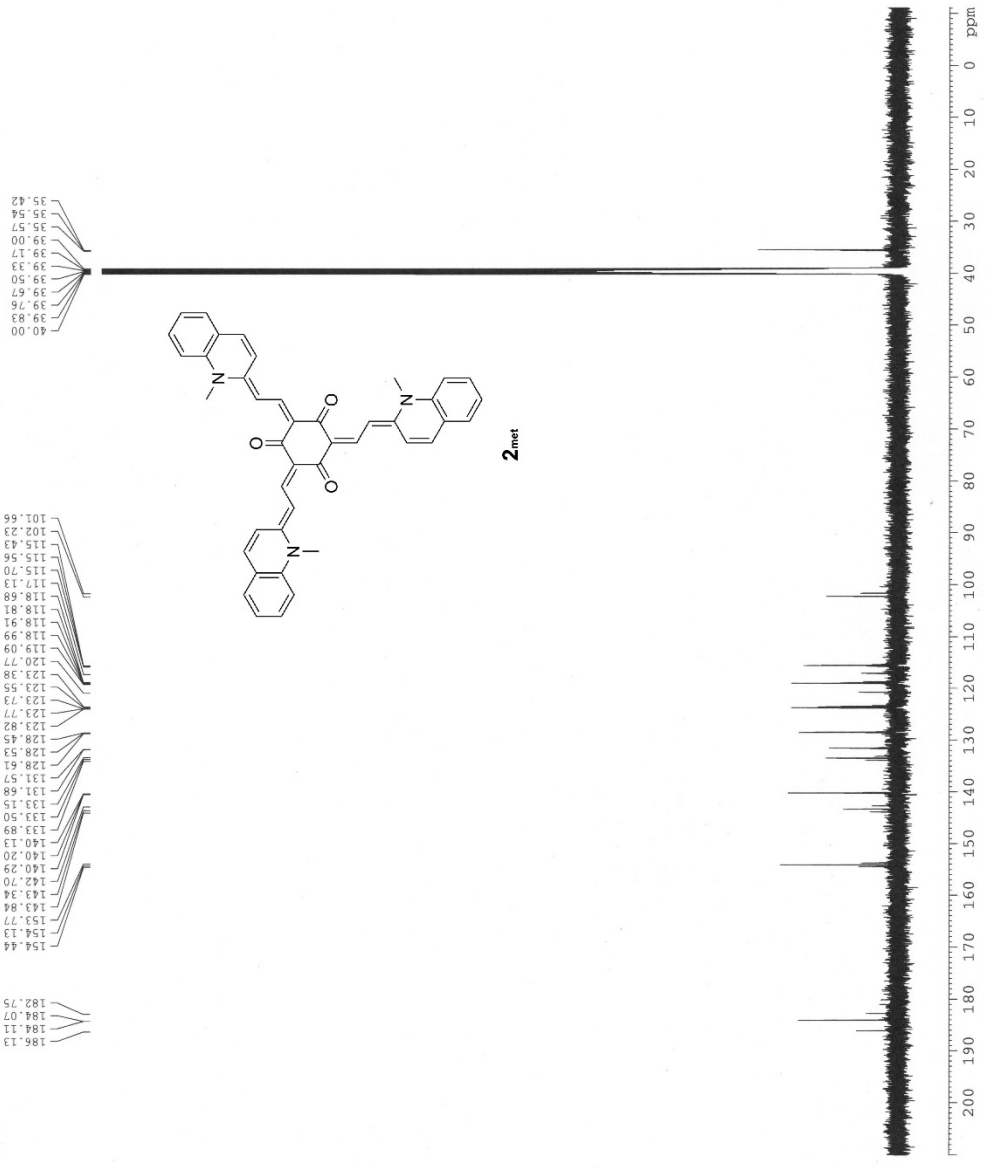
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P1         5.00 usec
PL1       -3.00 dB
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     98.00 usec
PL2       3.00 dB
PL12      3.00 dB
PL13      32.00 dB
SFO2      500.1320005 MHz

F1 - Acquisition parameters
=====
TD0       128
SFO1      500.132 MHz
FIDRES     7.812500 Hz
SW         1.999 EPM
FMODE     QF

F2 - Processing parameters
=====
SI         262144
SF         125.7578568 MHz
WDW        EM
SSB        0
GB         0
PC         1.40

F1 - Processing parameters
=====
SI         1024
MC2       OF
SF         500.1300000 MHz
WDW        SINE
SSB        0
GB         0.30 Hz
          0.1
  
```





E. Foronik
zesp10/Var600/2EP-138K/2EP-138K
HI
zesp10/Var600/2EP-138K/2EP-138K
HI

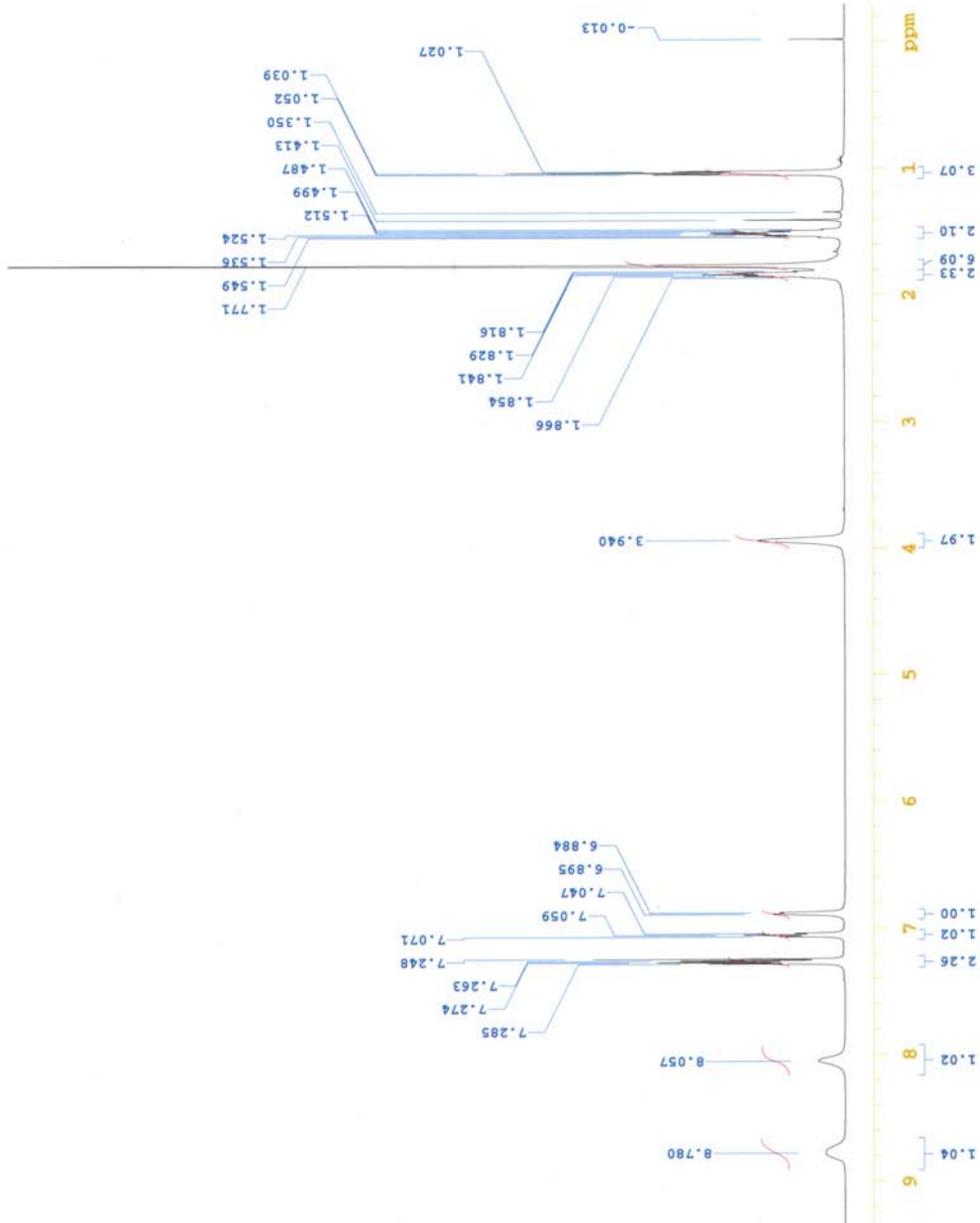
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Data Collected on:
Varian-NMR-vnmrs600
Archive directory:

Sample directory:
Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 30 2015

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: vnmr1
VNMRS-600 "Varian-NMR"

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 4.509 sec
Width 7267.4 Hz
16 repetitions
OBSERVE HI, 599.8350742 MHz
DATA PROCESSING
Ft size 65536



E. Poronik
zesp10/Var600/2EP-138K/2EP-138K-NOESY

Sample Name:
2EP-138K
Data Collected on:
Varian-NMR-vnars600
Archive directory:

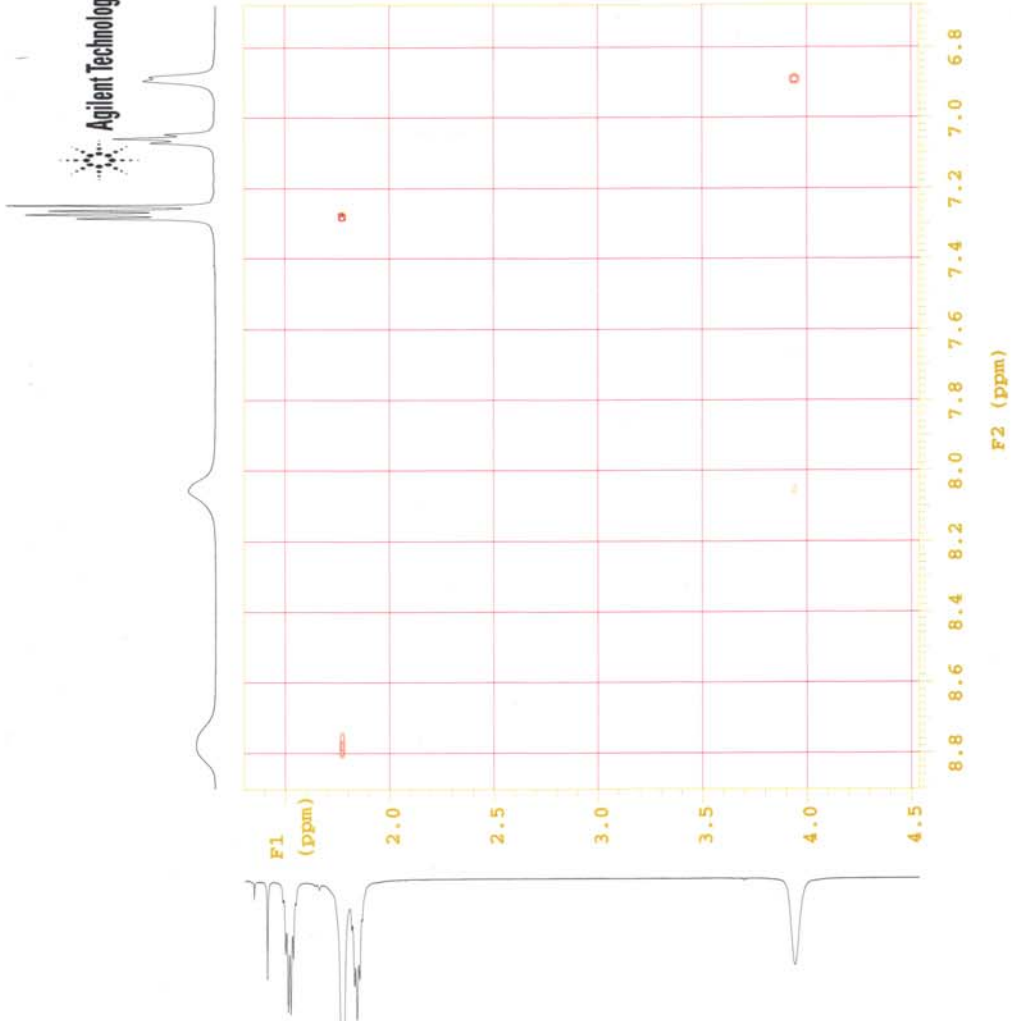
Sample directory:

File: NOESY

Pulse Sequence: NOESY

Solvent: cdcl3

Data collected on: Mar 30 2015



Crystallographic Data for **1_{met}**:

X-ray diffraction analysis was performed on **1_{met}** (see below). The structure was deposited (CCDC 1057779). It clearly resolves the configuration of double bonds as all-E isomer.

