

Supplementary Information

Synthesis and Evaluation of Novel Caged DNA Alkylating Agents Bearing 3,4-Epoxy piperidine Structure

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Contents:

Result of agarose gel shift assay of compound **4a-4d** and **3** in the presence of radical scavenger (Fig. S1).

¹H and ¹³C NMR spectra of compounds **2a-2d**, **4a-4d** and **5a**, **5b**.

UV-absorption spectra of compound **3** and **4a-4d**.

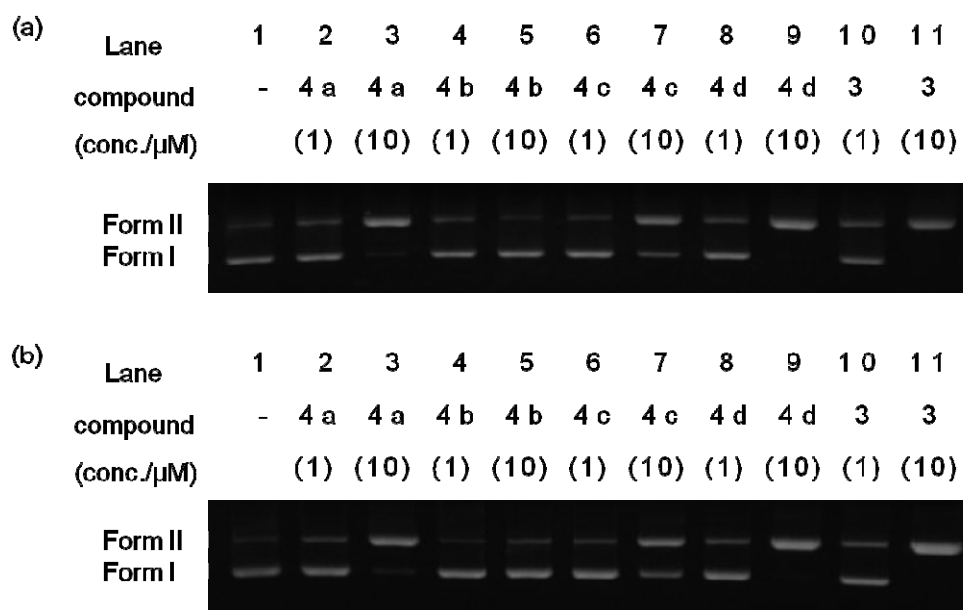
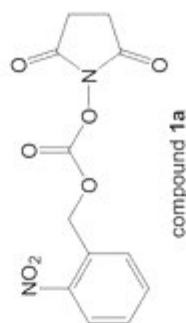
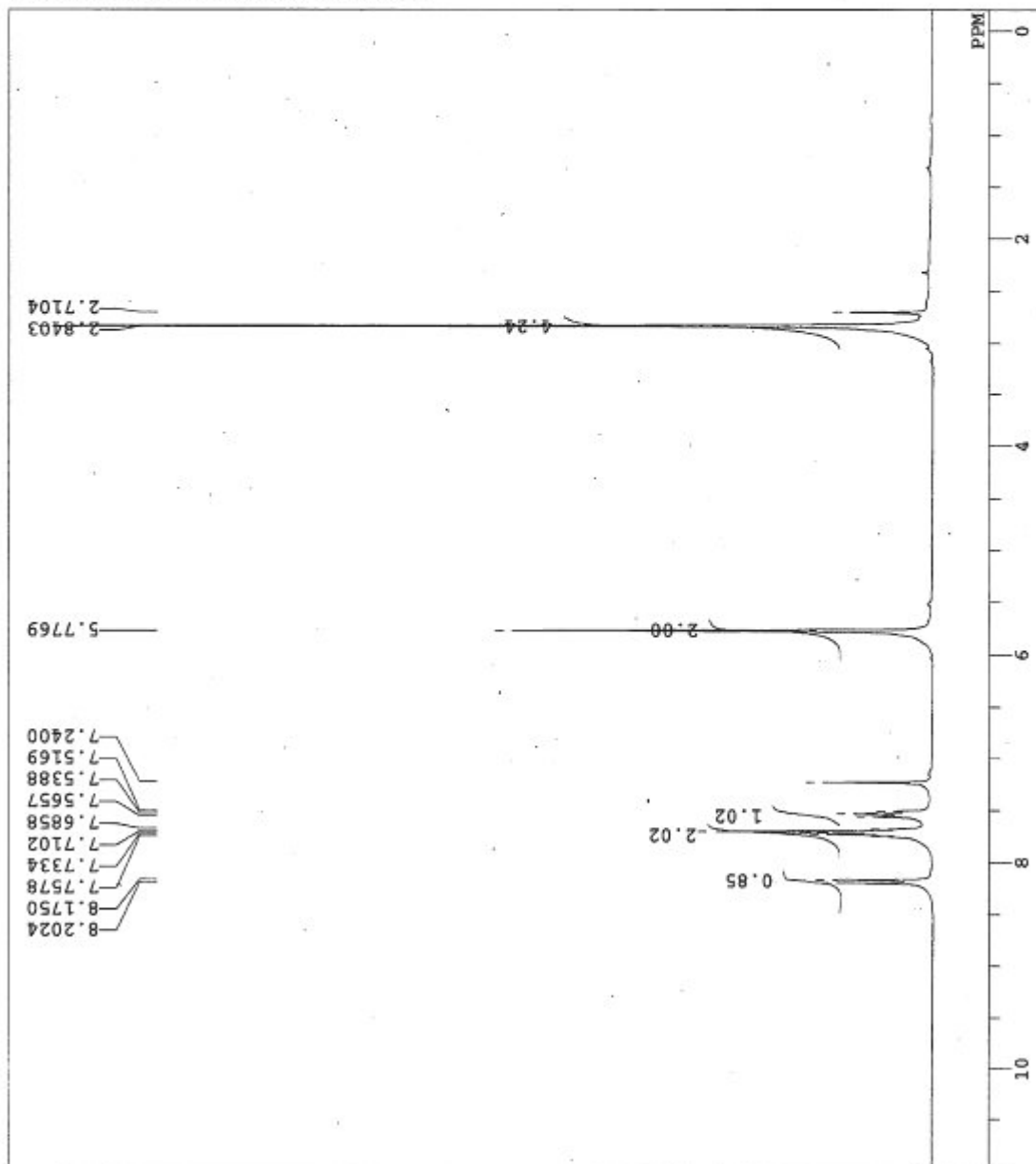


Fig. S1. Plasmid relaxation assay with caged DNA alkylating agents **4a-4d** and **3** in the presence of glycerol (a) or NaN₃ (b).

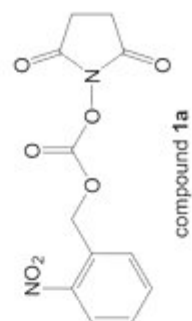
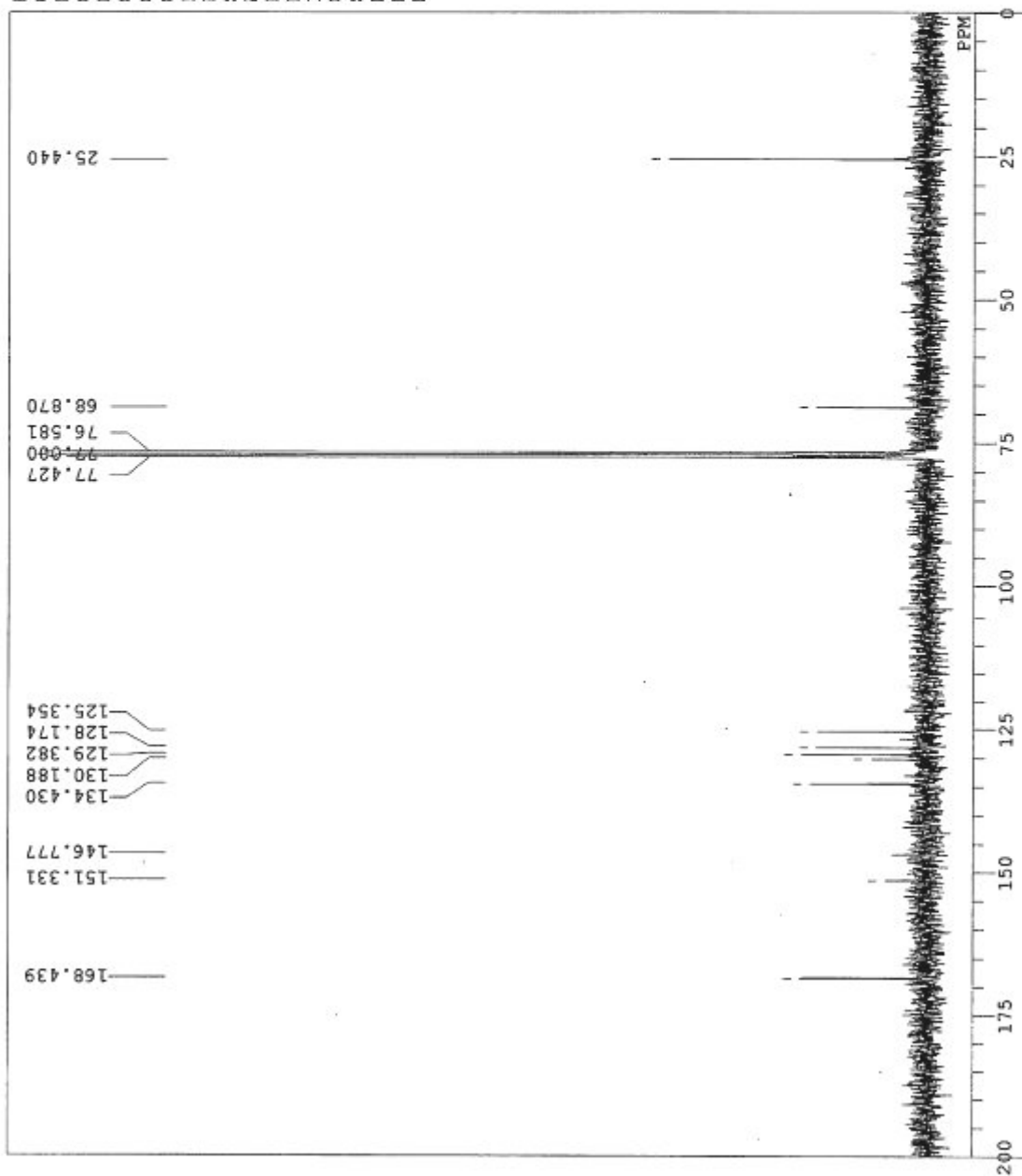
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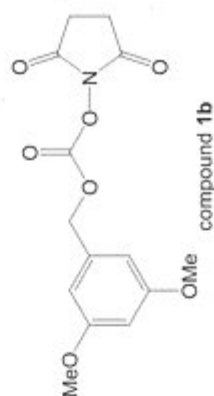
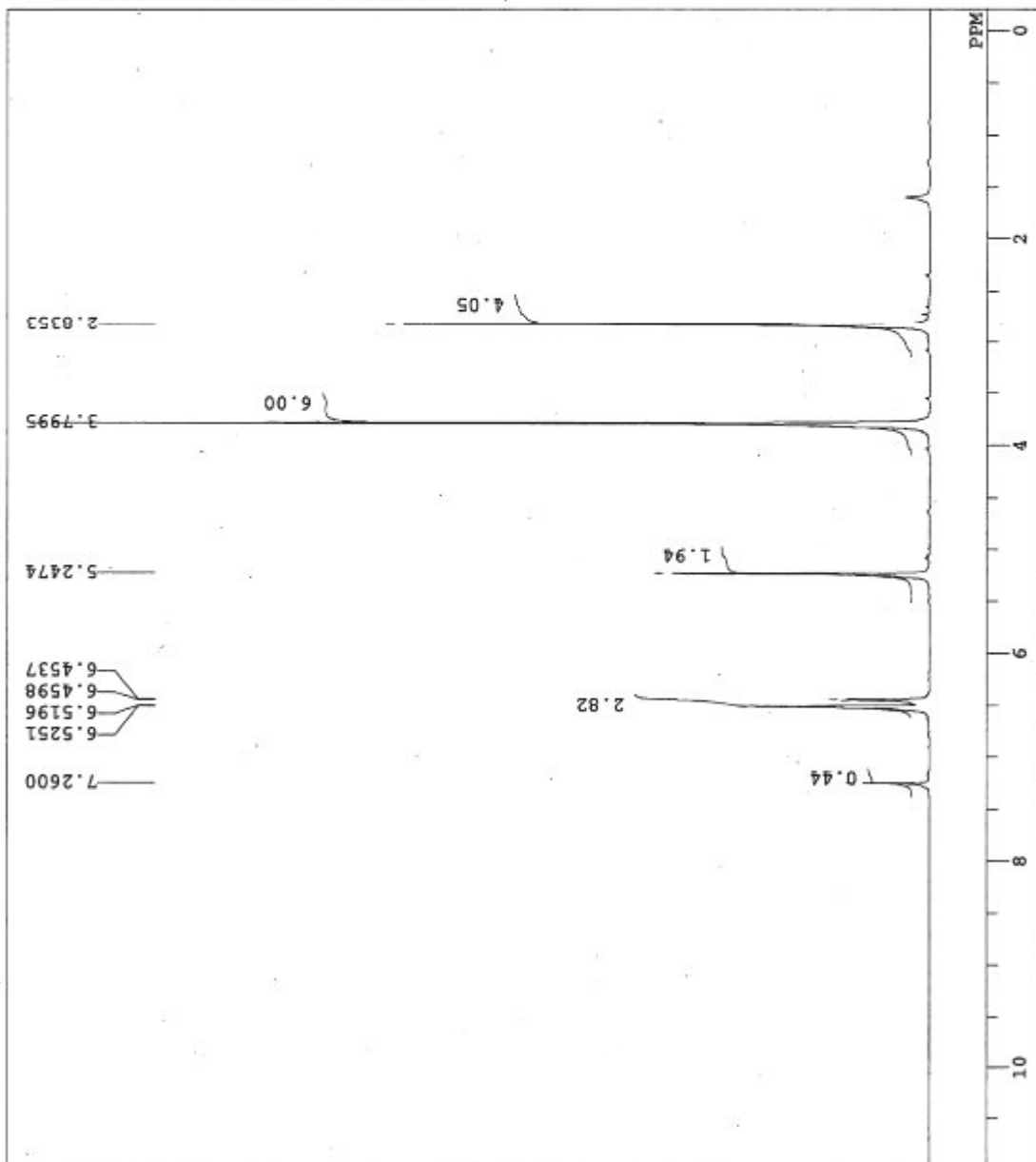
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RGAIN 26



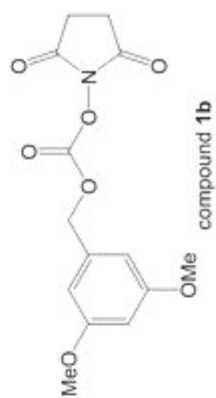
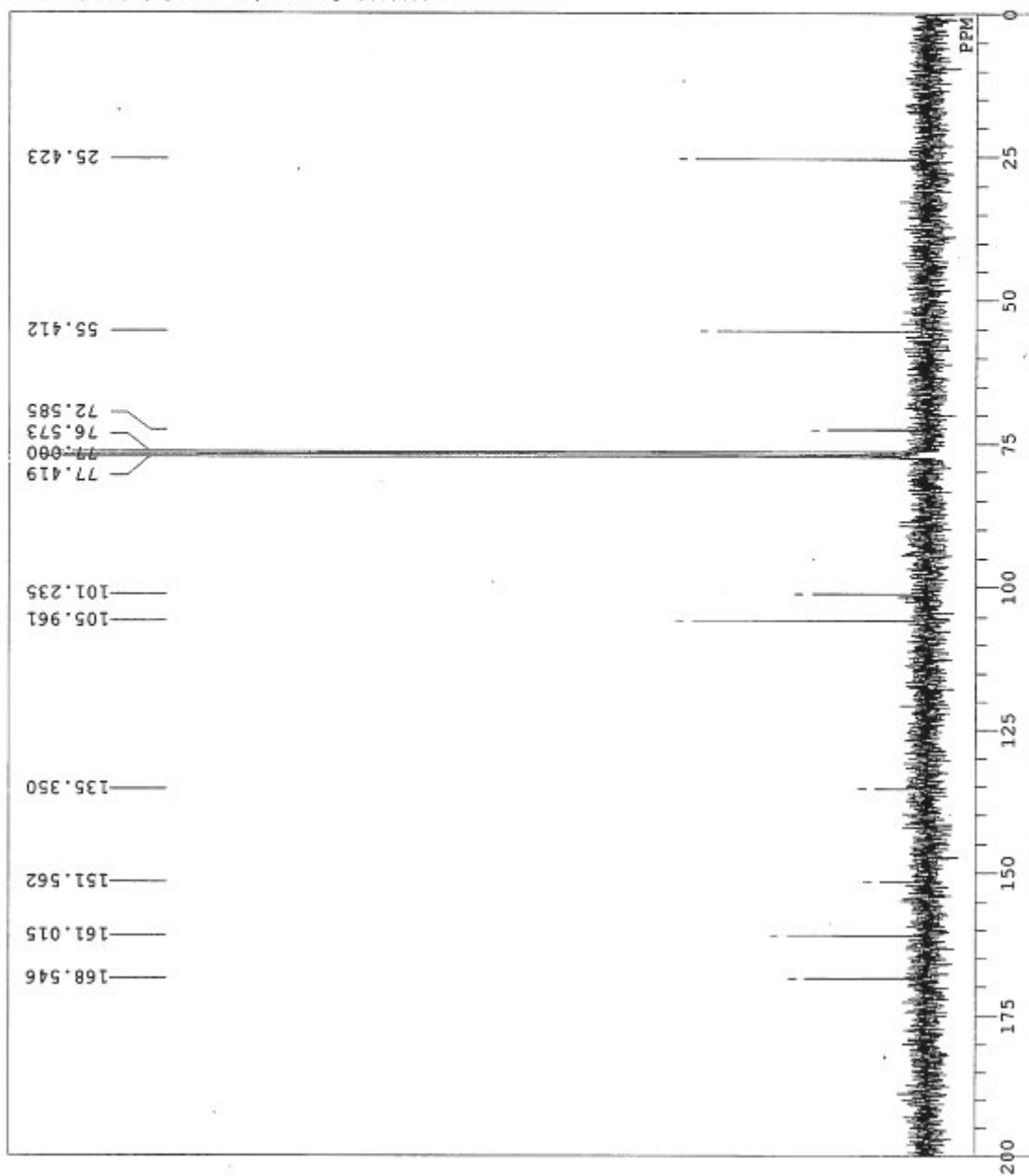
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PD 1.5440 sec
PWL 5.80 usec
IRNUC 1H
CTEMP 20.7 C
SLVNT CDCL3
EXREF 7.26 ppm
BF 1.20 Hz
RGAIN 19



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POINT 32768
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PW1 4.50 usec
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SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 26



E:\NMR Data\200909-200912\091

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBPRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PWL
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

Mon Dec 28 13:12:09 2009

1H

NON

300.40 MHz

130.00 KHz

1150.00 Hz

32768

6006.01 Hz

16

5.4559 sec

1.5440 sec

5.80 usec

1H

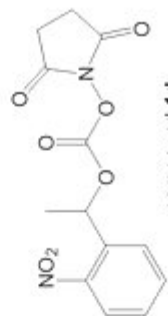
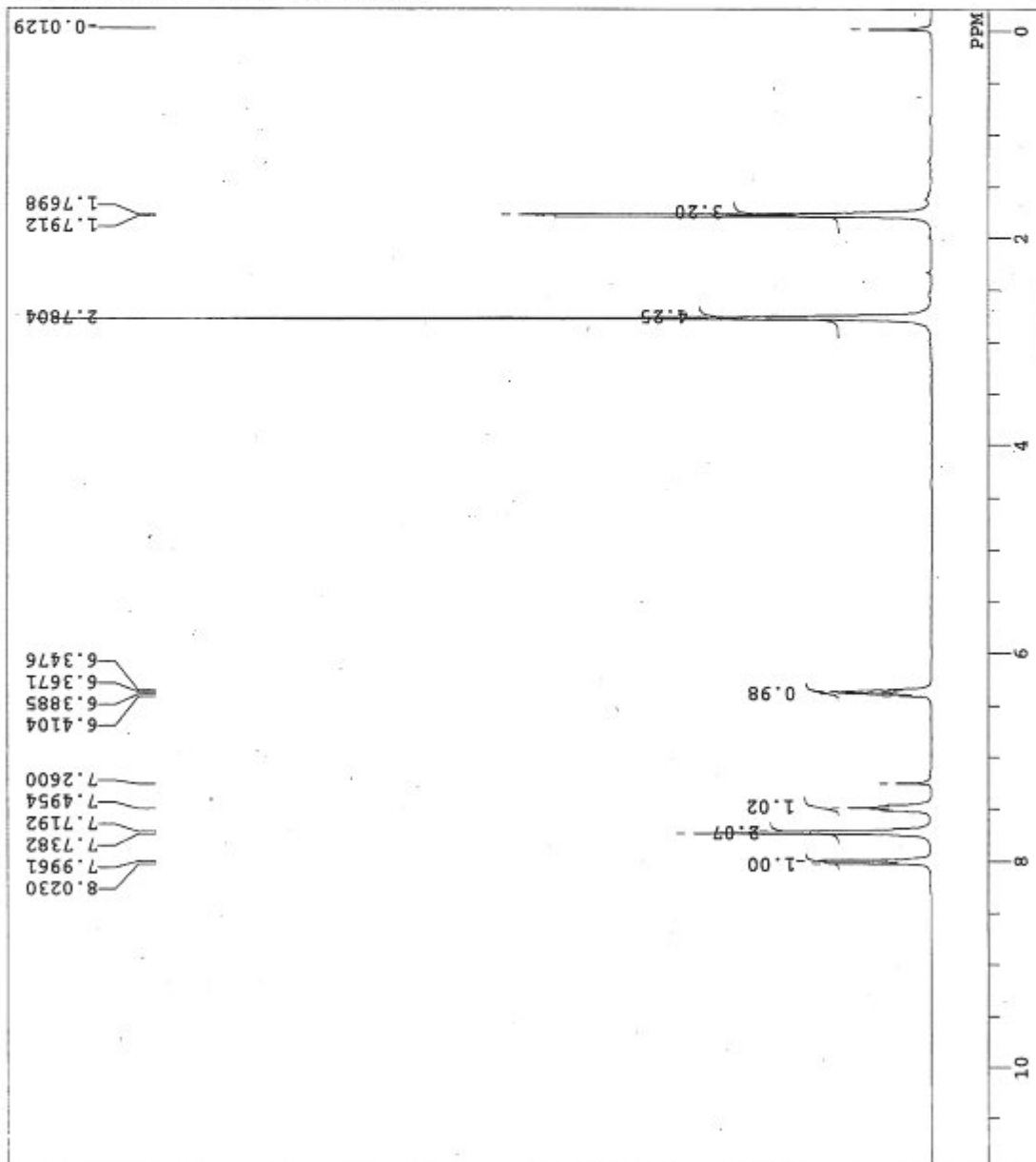
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CDCL3

7.26 ppm

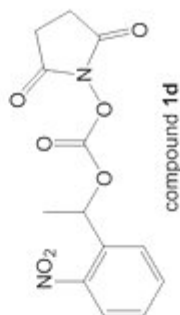
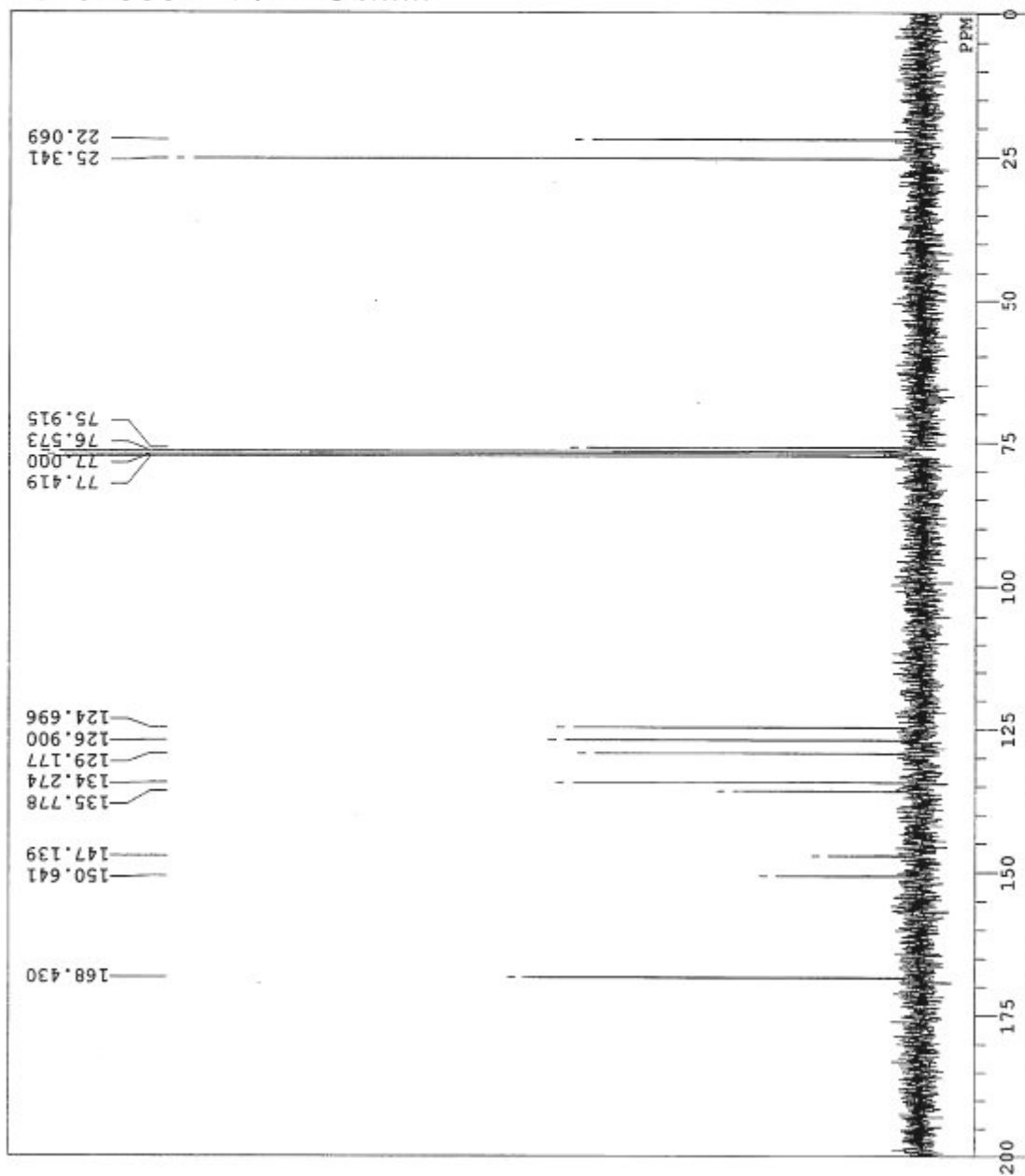
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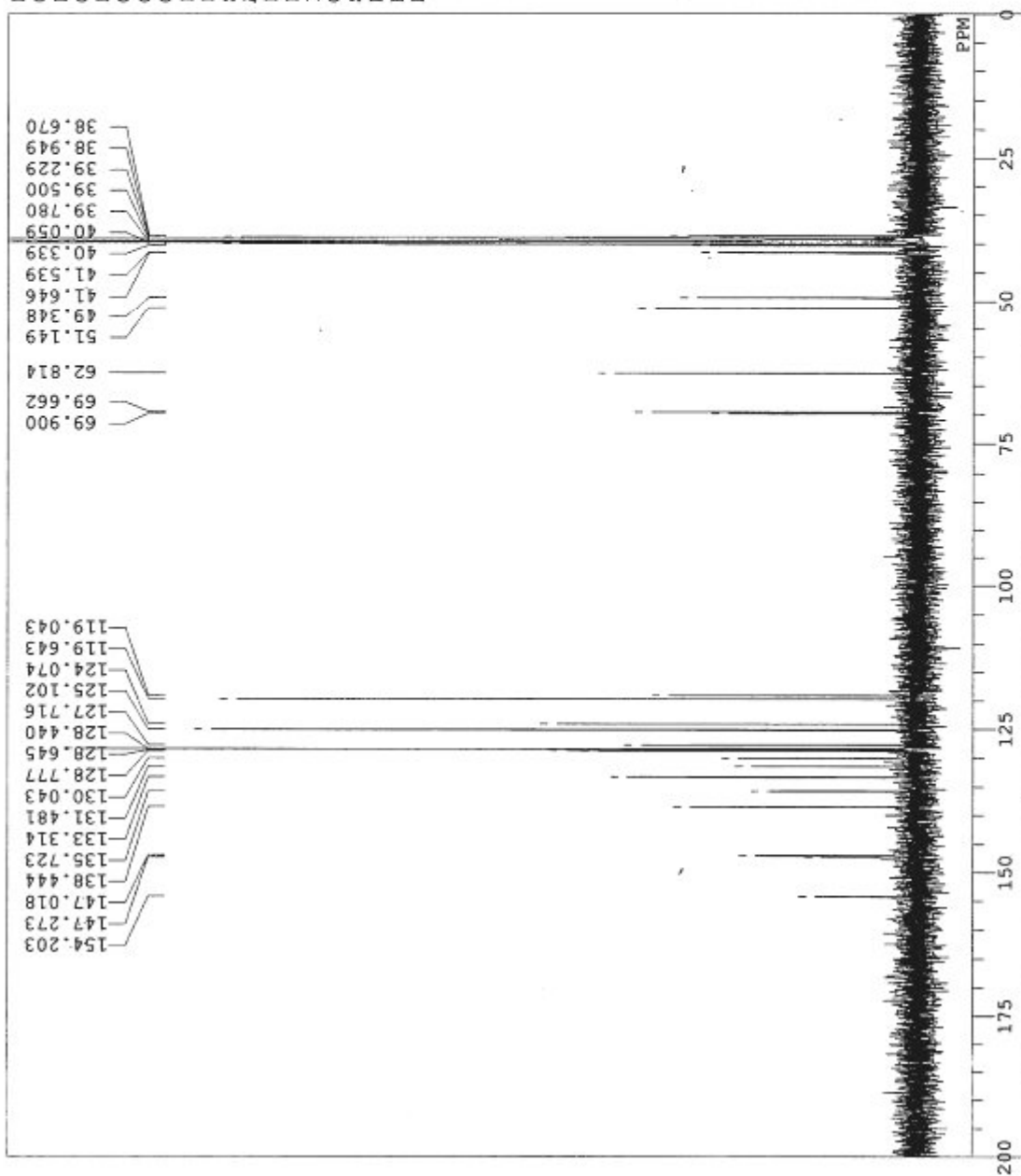


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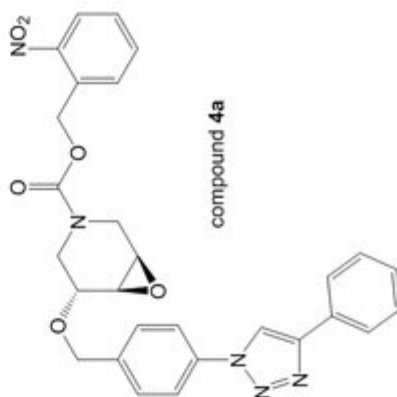
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POINT 32768
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PW1 4.50 usec
IRNUC 1H
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BF 1.20 Hz
RGAIN 26



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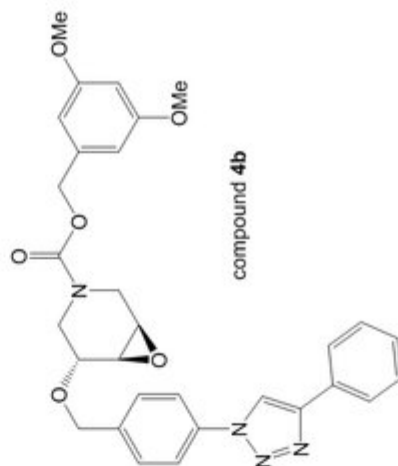
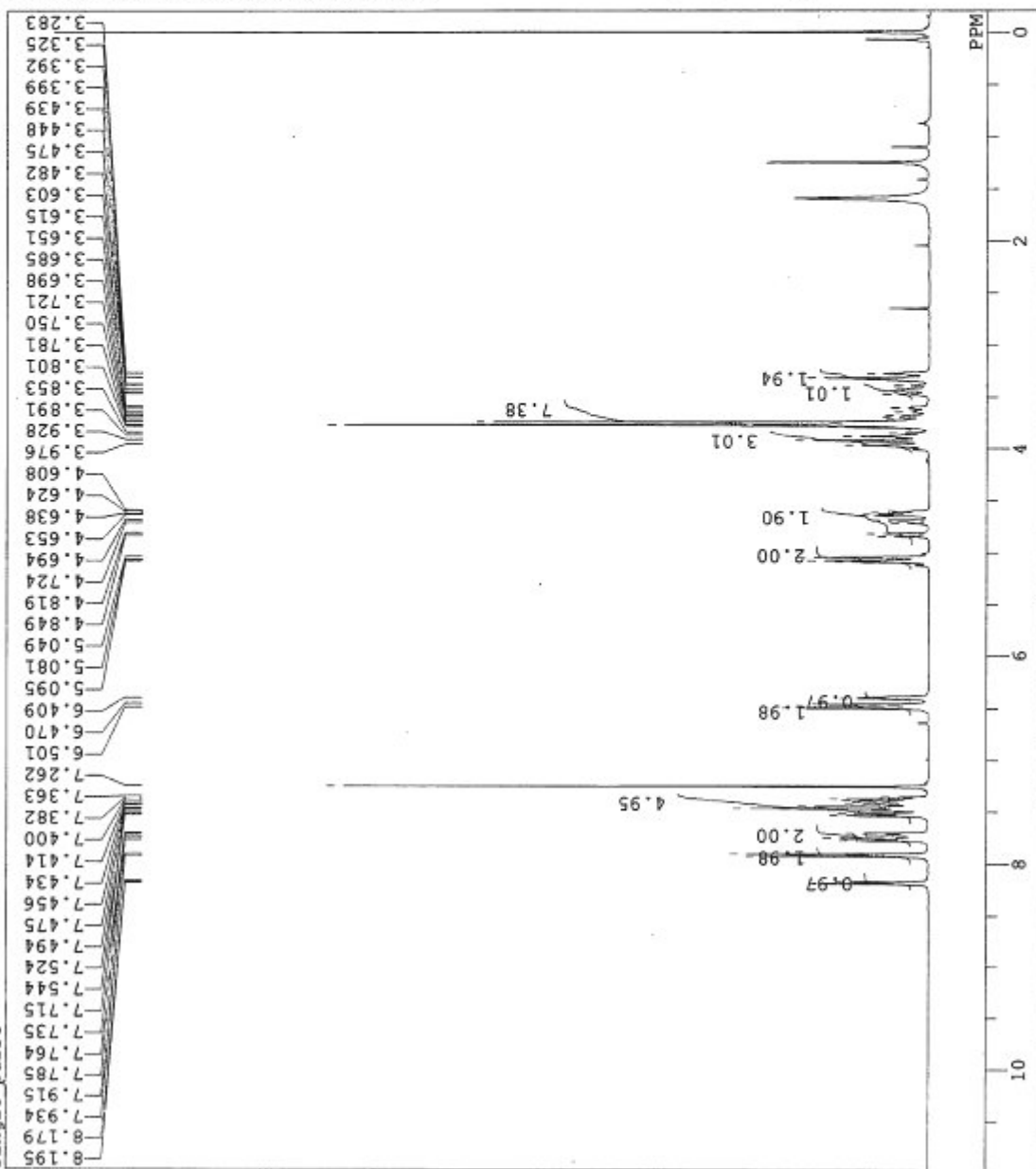


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SLVNT DMSO
EXREF 39.50 ppm
BF 0.12 Hz
RGAIN 25



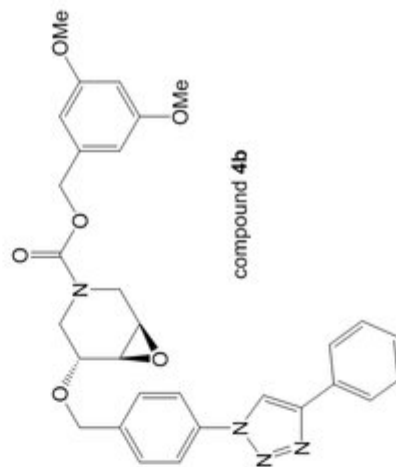
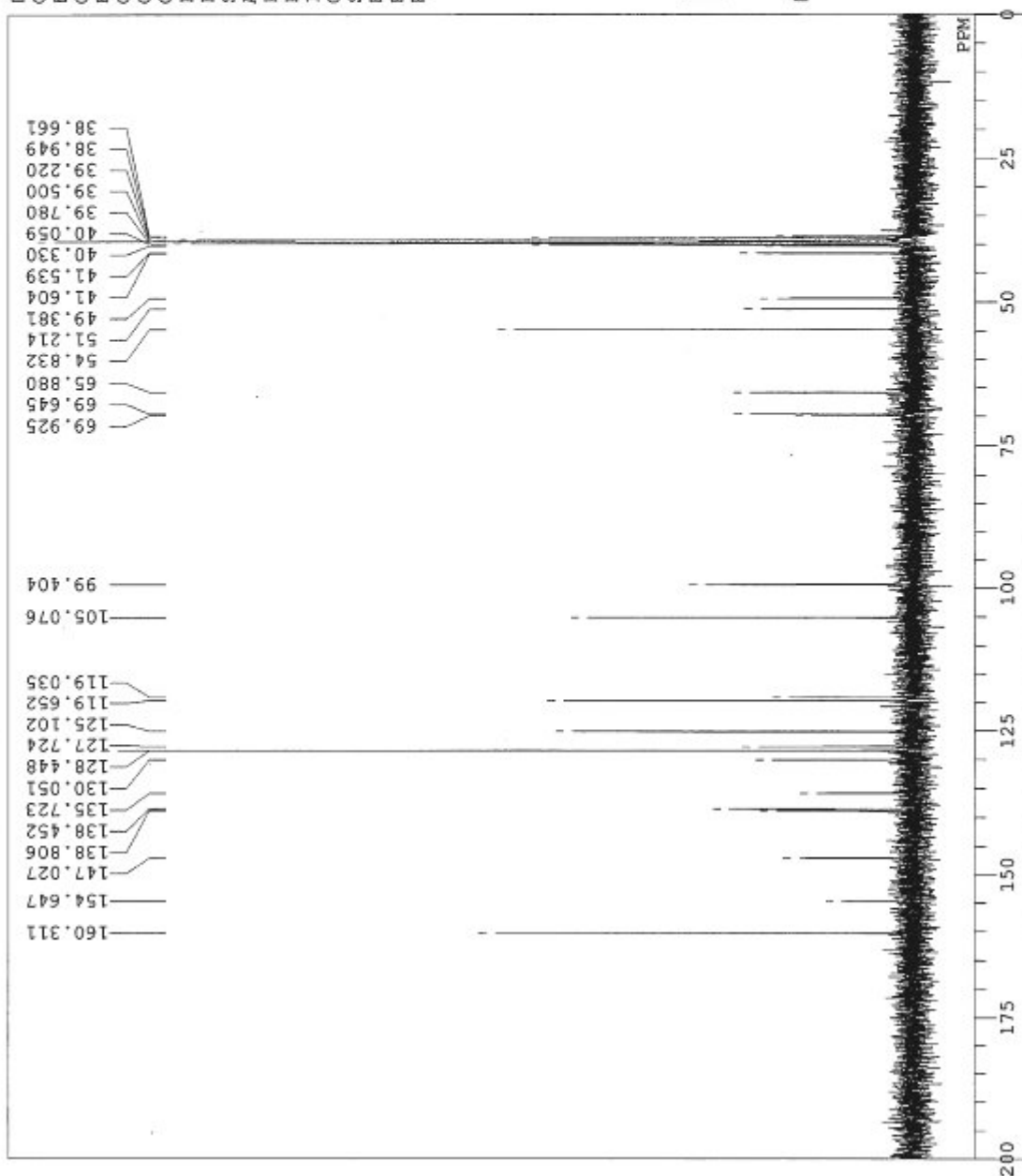
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 IRNUC 1H
 CTEMP 22.5 C
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 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 46



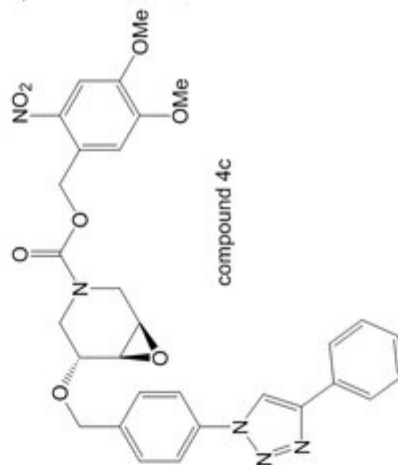
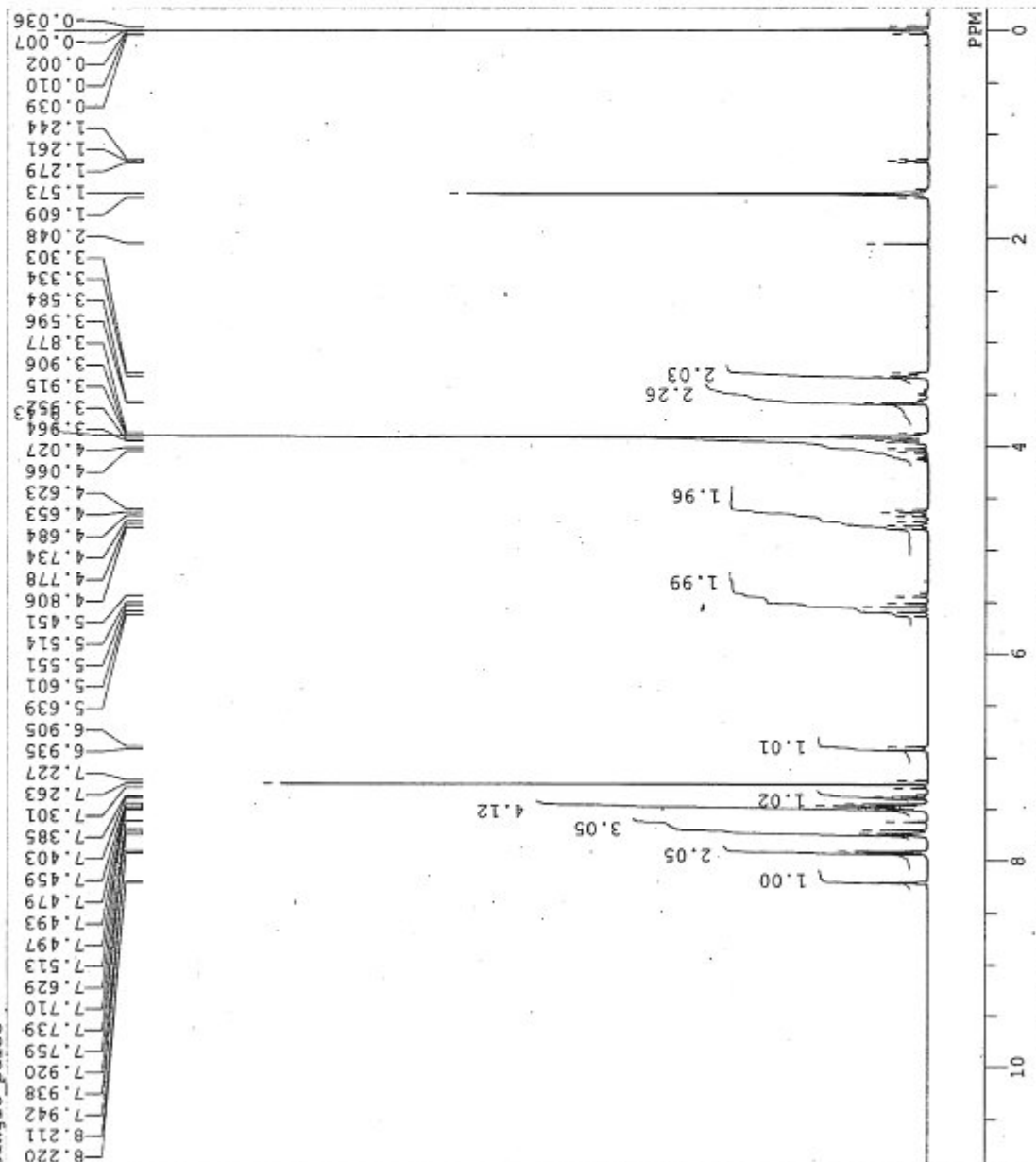
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BF 0.12 Hz
RGAIN 24

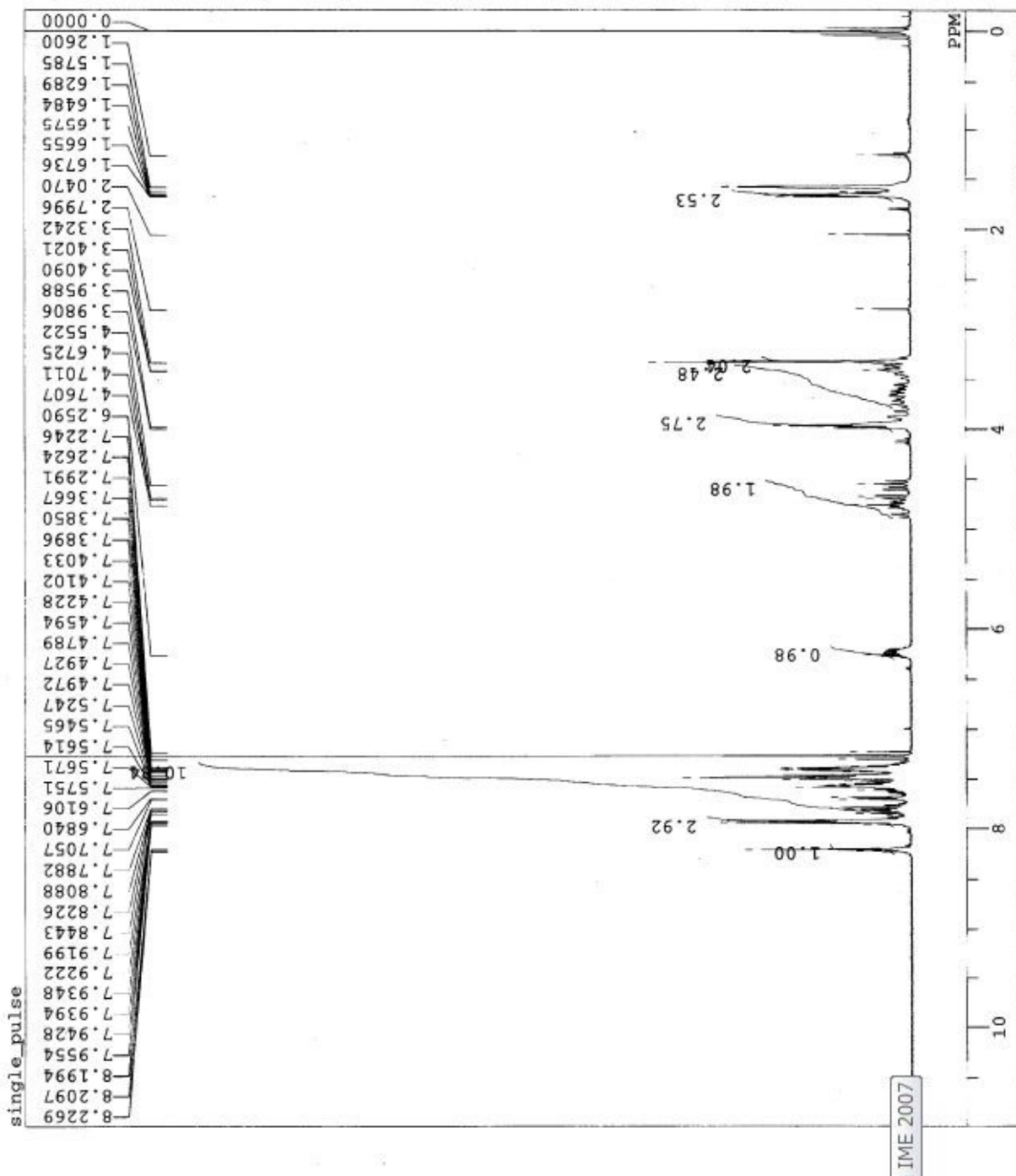
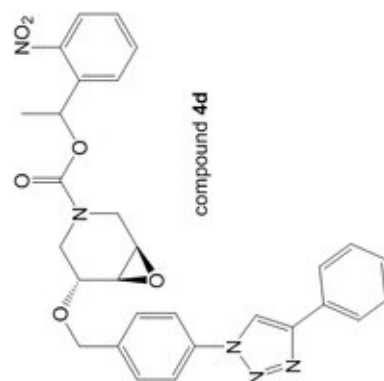


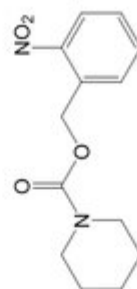
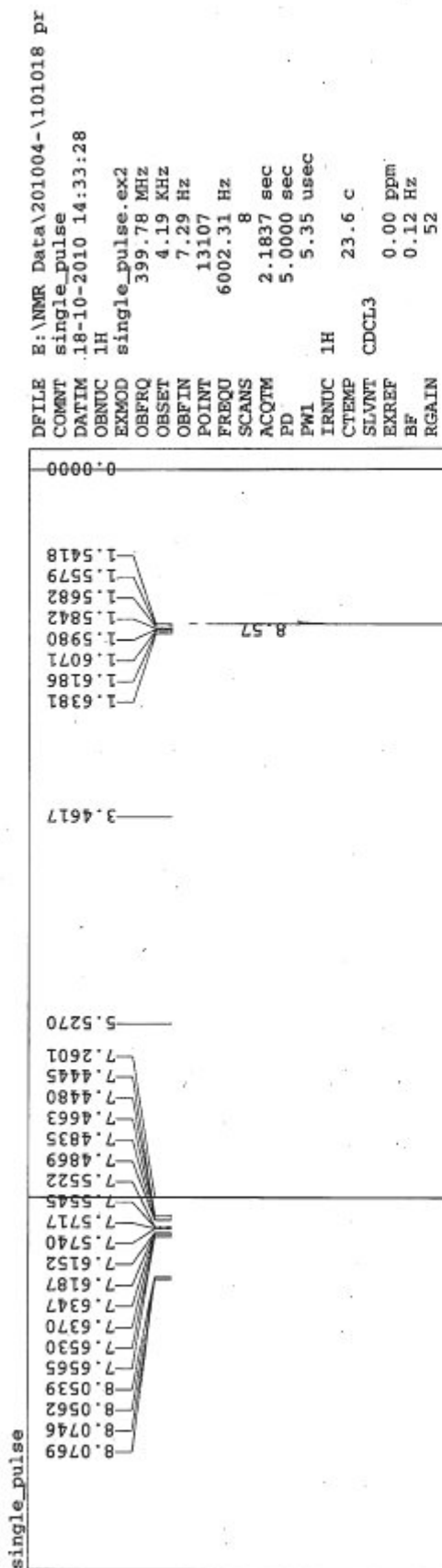
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 CTEMP 23.6 c
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 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 50



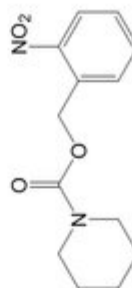
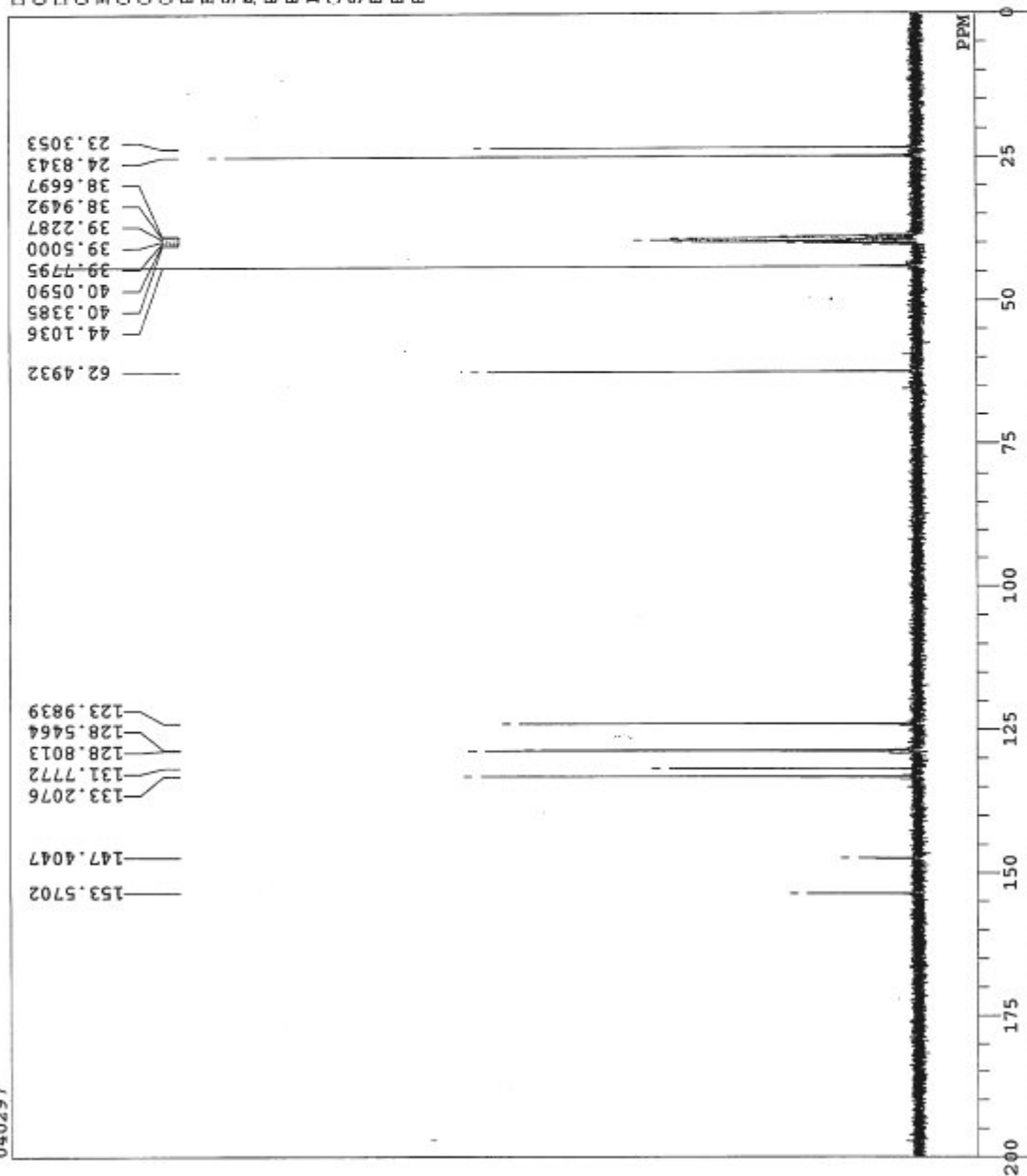
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 BF 0.12 Hz
 RGAIN 48



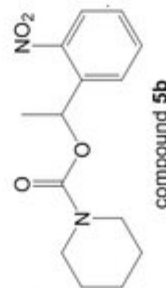
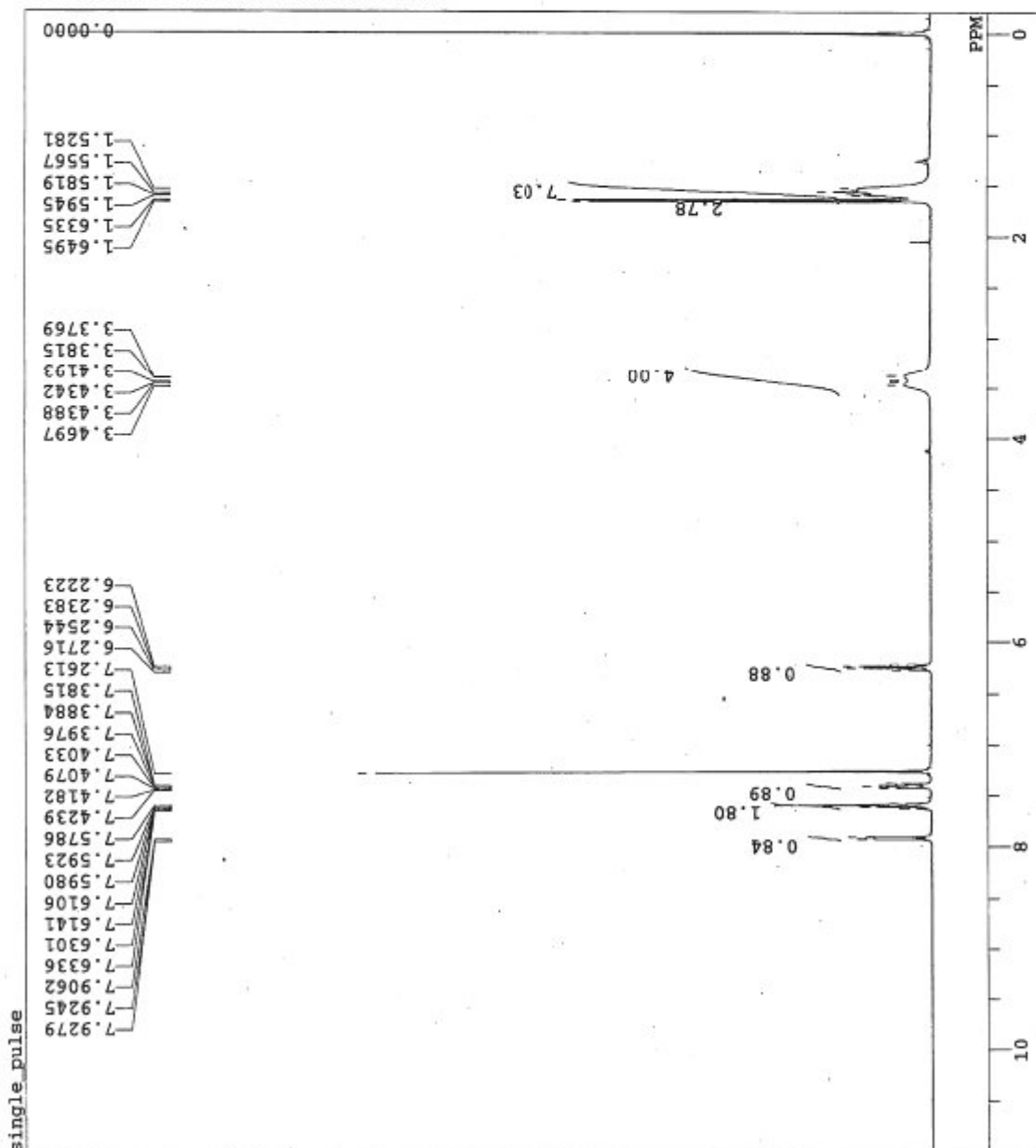


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FREQU 20356.23 Hz
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PD 1.3900 sec
PWL 4.50 usec
IRNUC 1H
CTEMP 79.9 c
SLVNT DMSO
EXREF 39.50 ppm
BF 0.12 Hz
RGAIN 27



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PD 5.0000 sec
PWL 5.35 usec
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CTEMP 23.6 c
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EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50



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040297

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PW1 4.50 usec
IRNUC 1H
CTEMP 79.9 C
SLVNT DMSO
EXREF 39.50 ppm
BF 0.12 Hz
RGAIN 27

