

*Supplementary Information*

**Investigations of possible prodrug structures for 2-(2-mercaptophenyl)tetrahydropyrimidines:  
reductive conversion from anti-HIV agents with pyrimidobenzothiazine and isothiazolopyrimidine  
scaffolds**

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Hiroto Murayama,<sup>b</sup> Hiroaki Ohno,<sup>a</sup> Masao Matsuoka,<sup>b</sup> Nobutaka Fujii<sup>a\*</sup>

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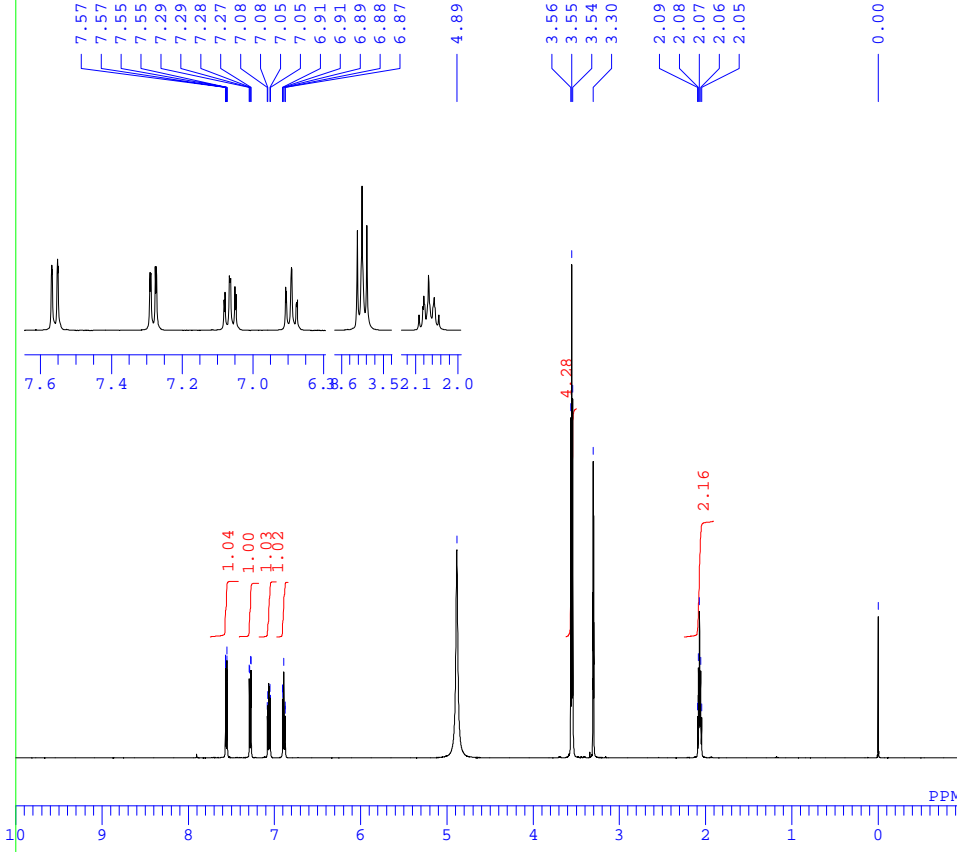
e-mail: soishi@pharm.kyoto-u.ac.jp (S.O.); nfujii@pharm.kyoto-u.ac.jp (N.F.)

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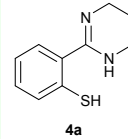
NMR spectra

S2

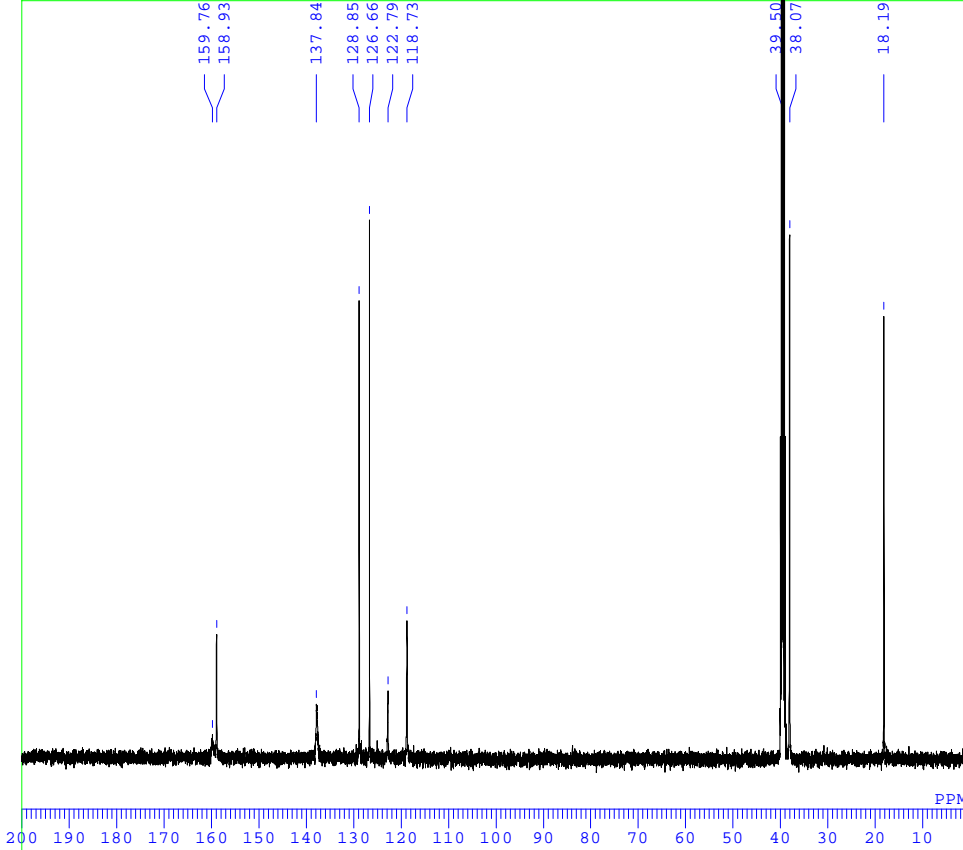
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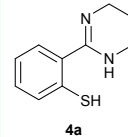
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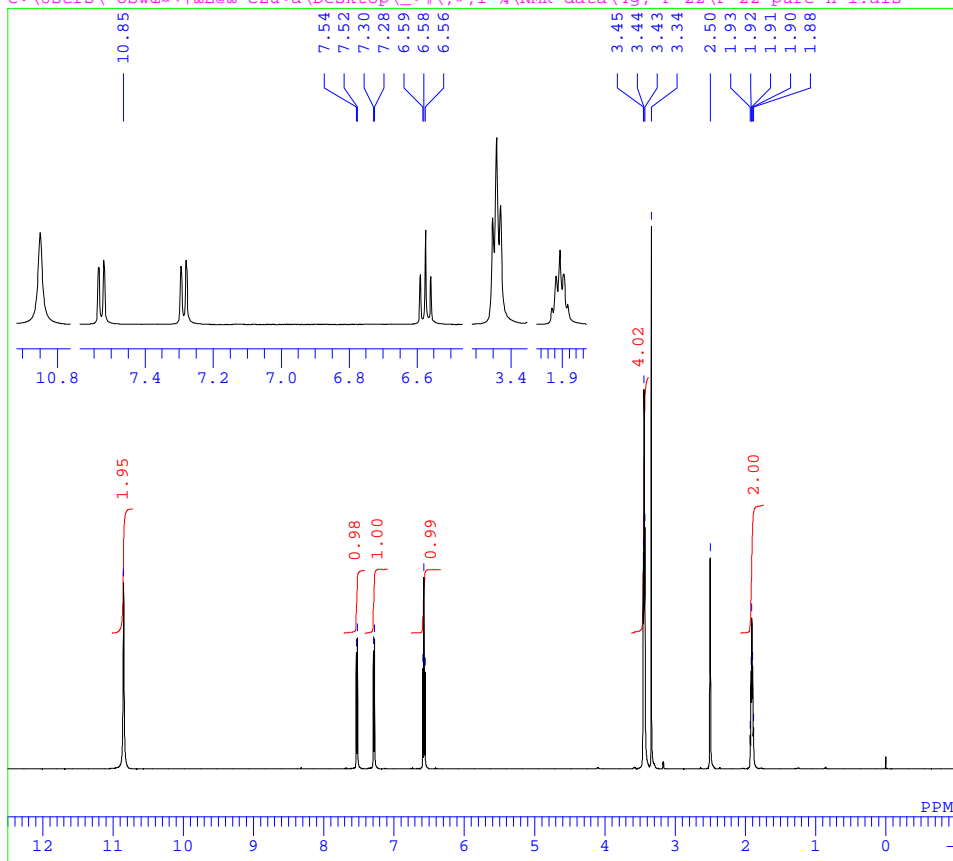
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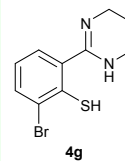
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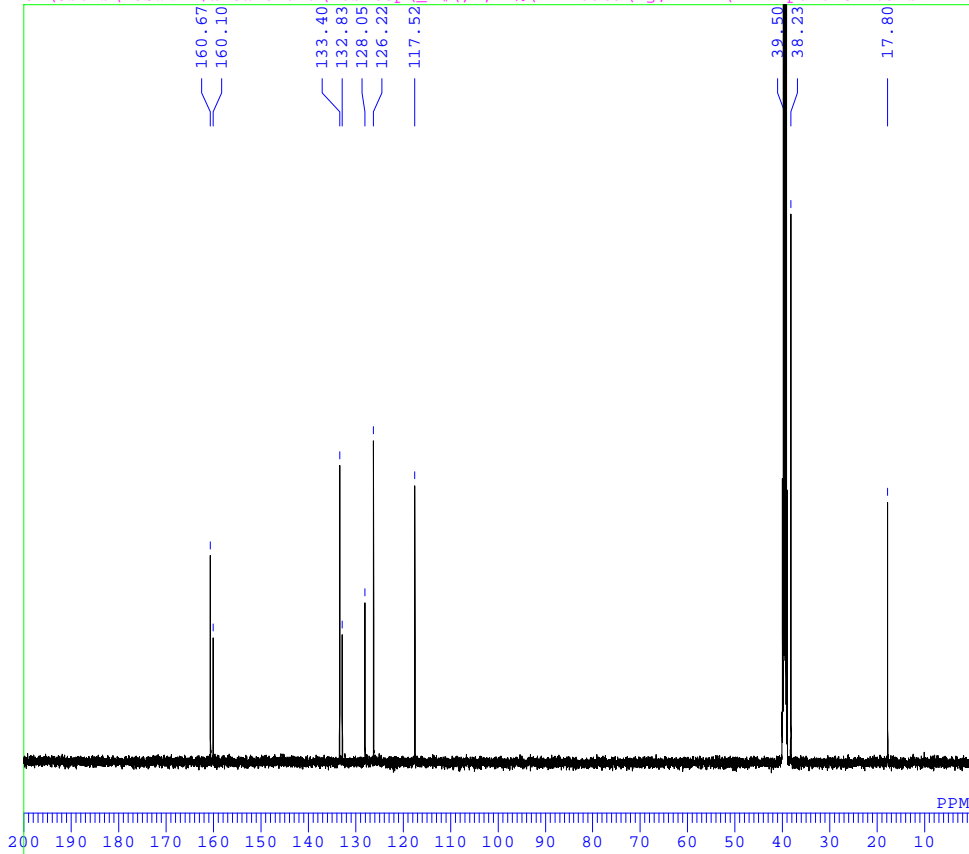
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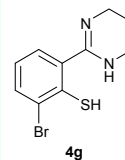
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 PD 5.0000 sec  
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 SLVNT DMSO  
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 BF 0.12 Hz  
 RGAIN 42



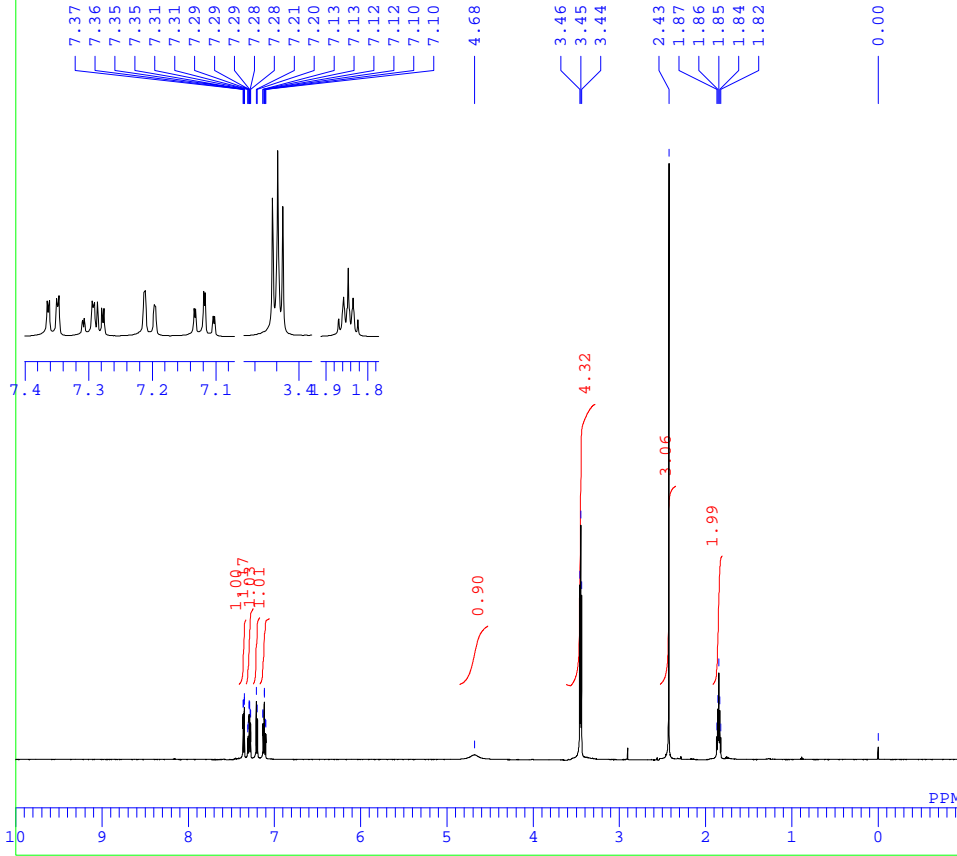
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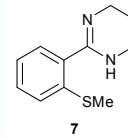
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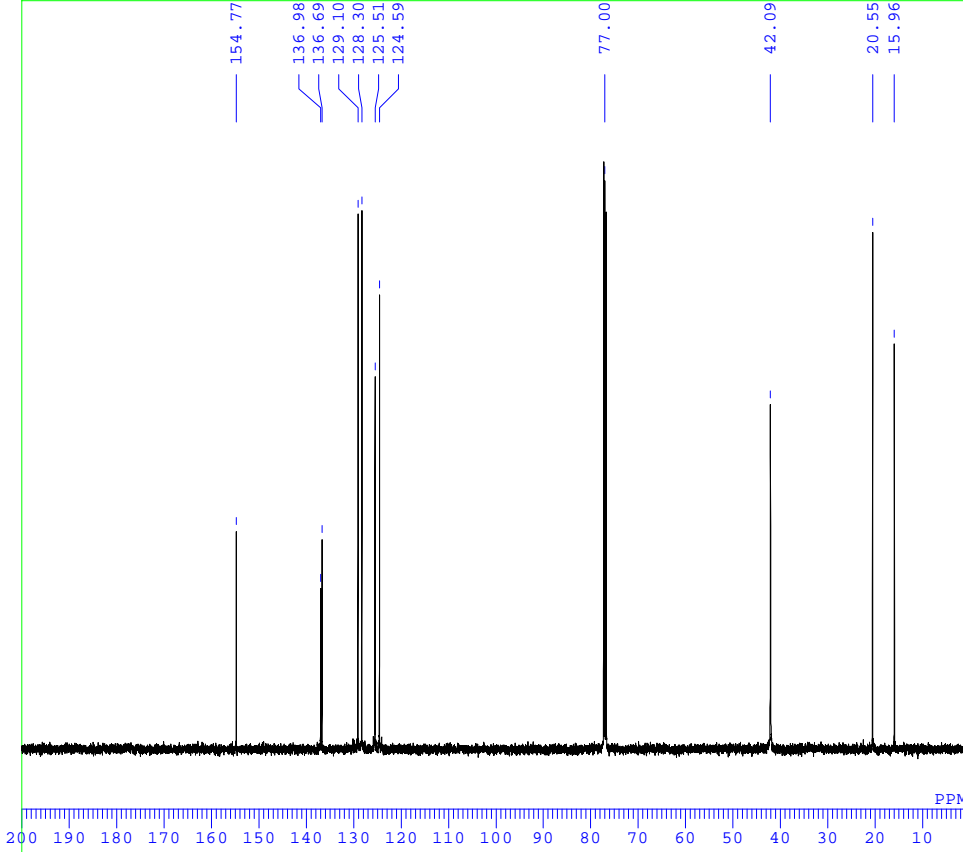
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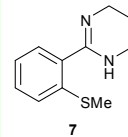
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 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.82 usec  
 IRNUC 1H  
 CTEMP 22.7 c  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF 0.12 Hz  
 RGAIN 38



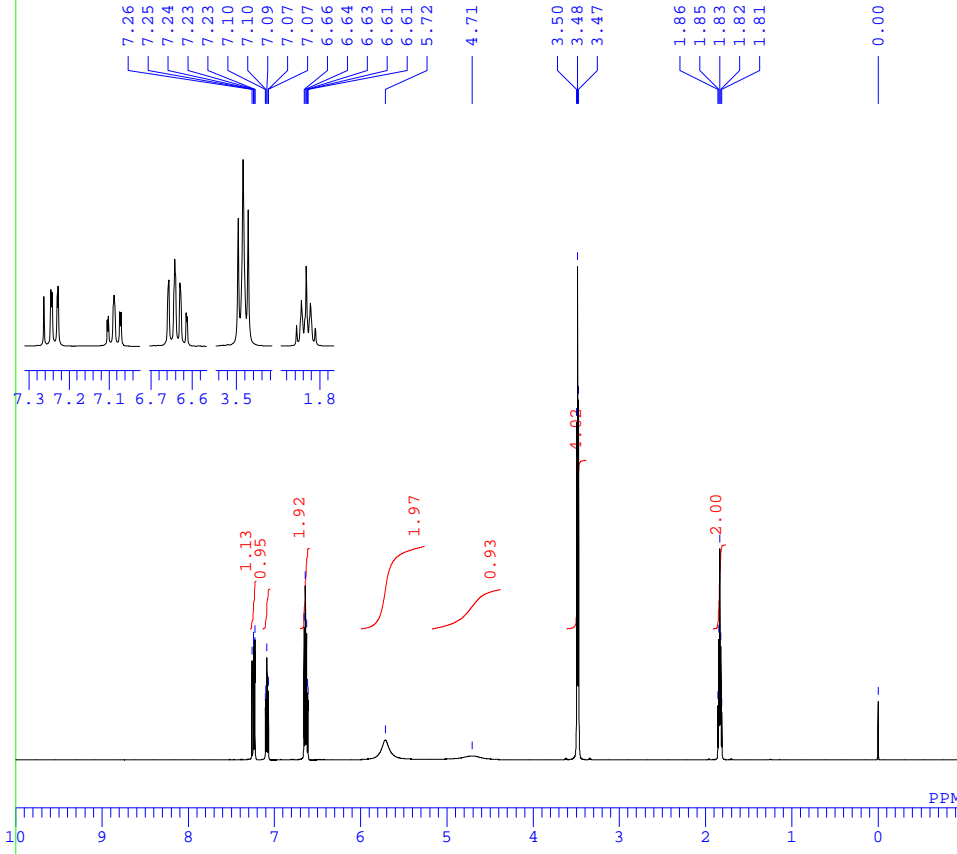
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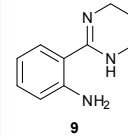
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 SCANS 1024  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
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 BF 1.20 Hz  
 RGAIN 52



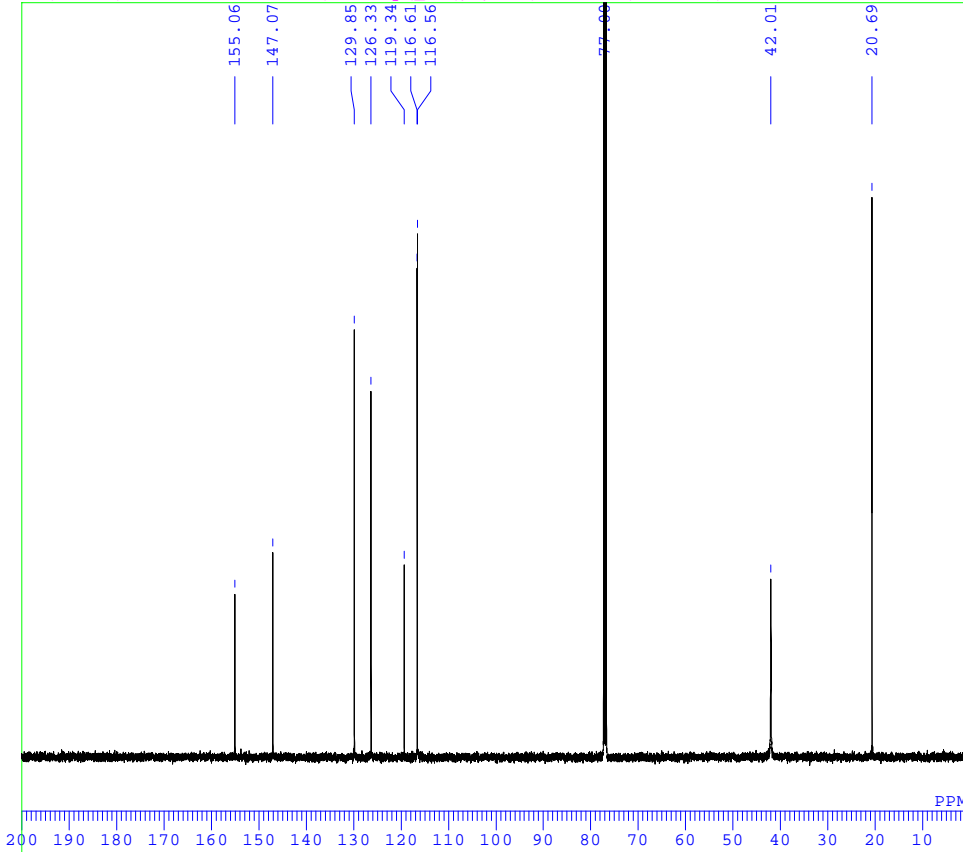
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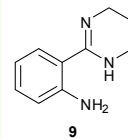
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 SCANS 8  
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 PD 5.0000 sec  
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 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF 0.12 Hz  
 RGAIN 38

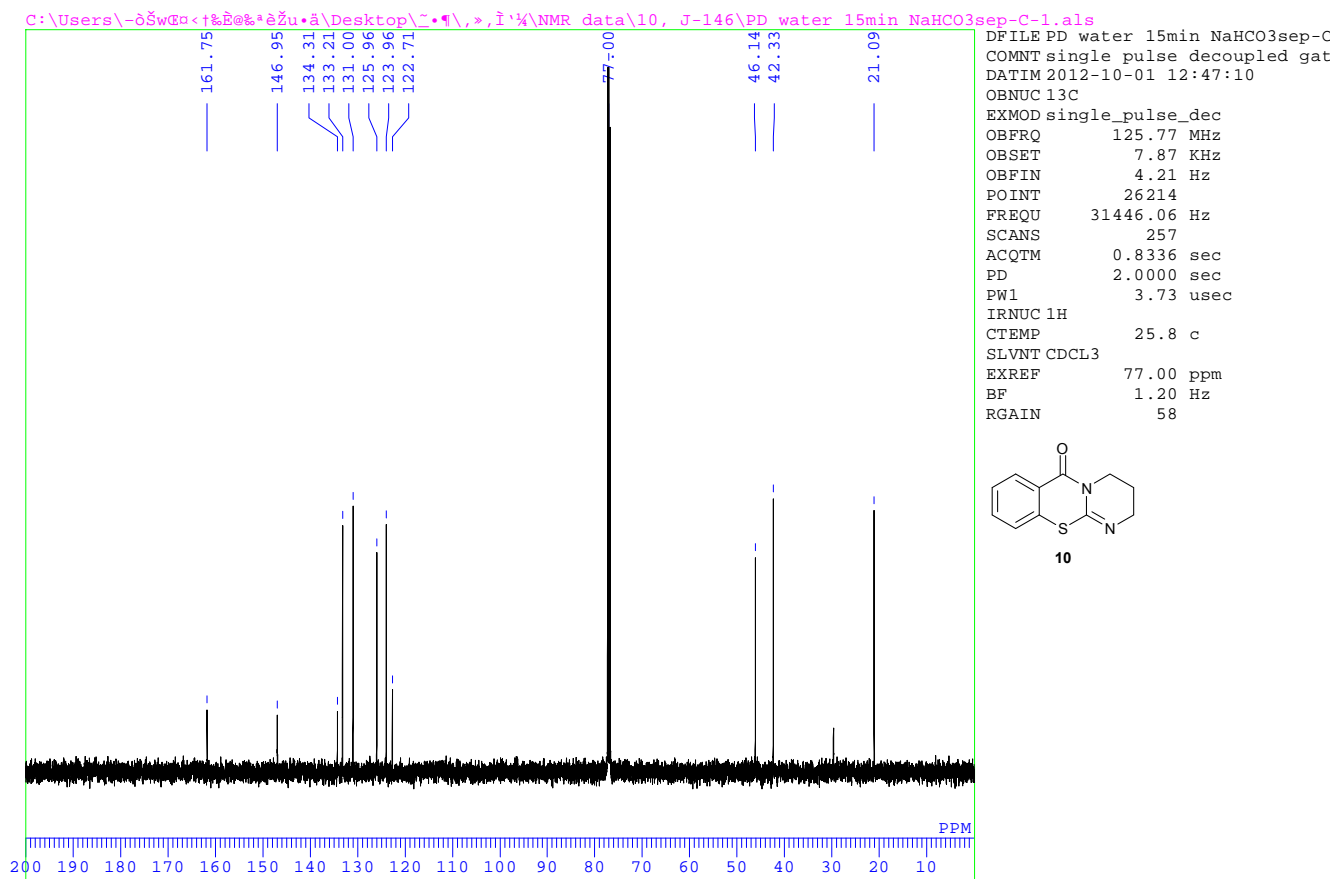
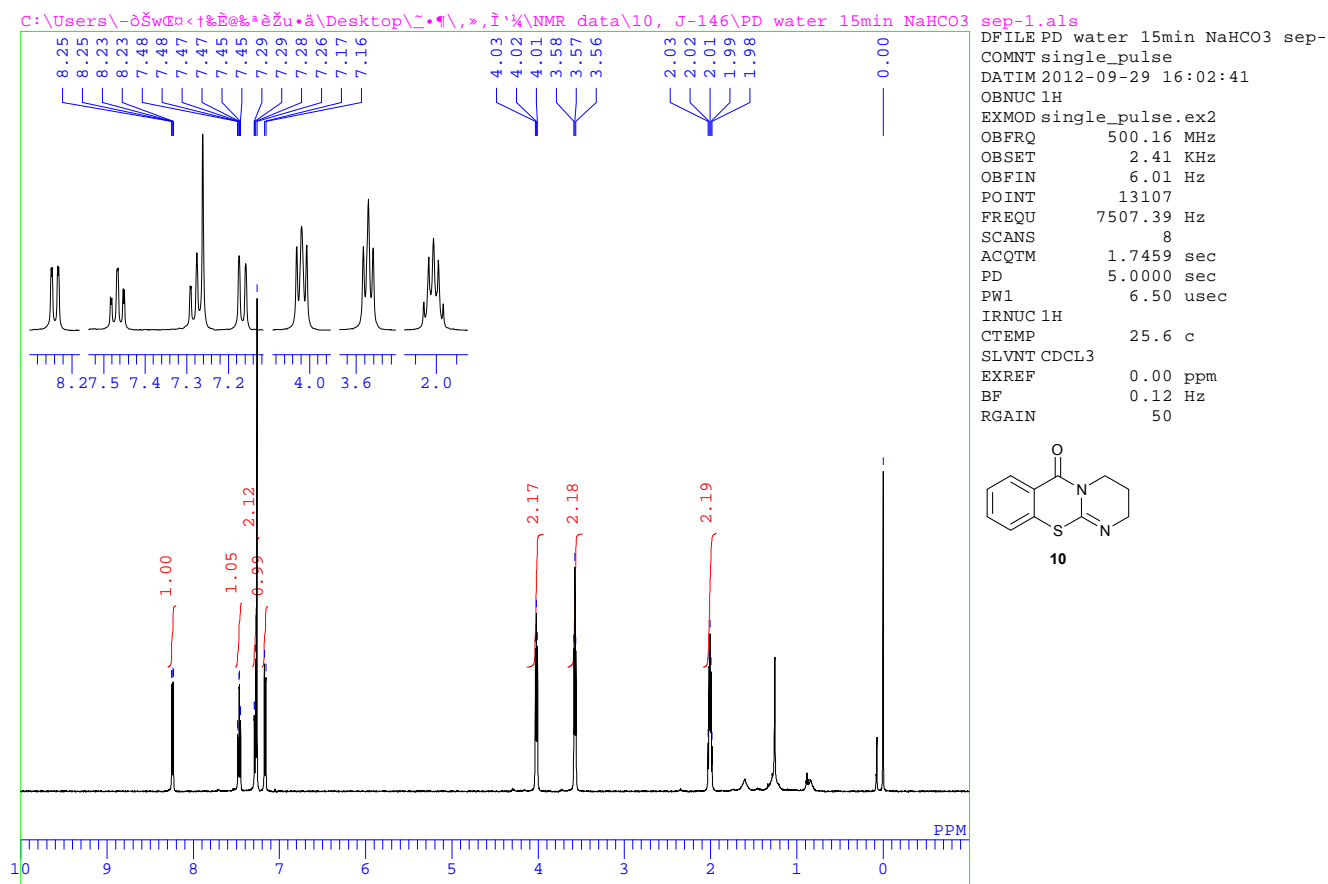


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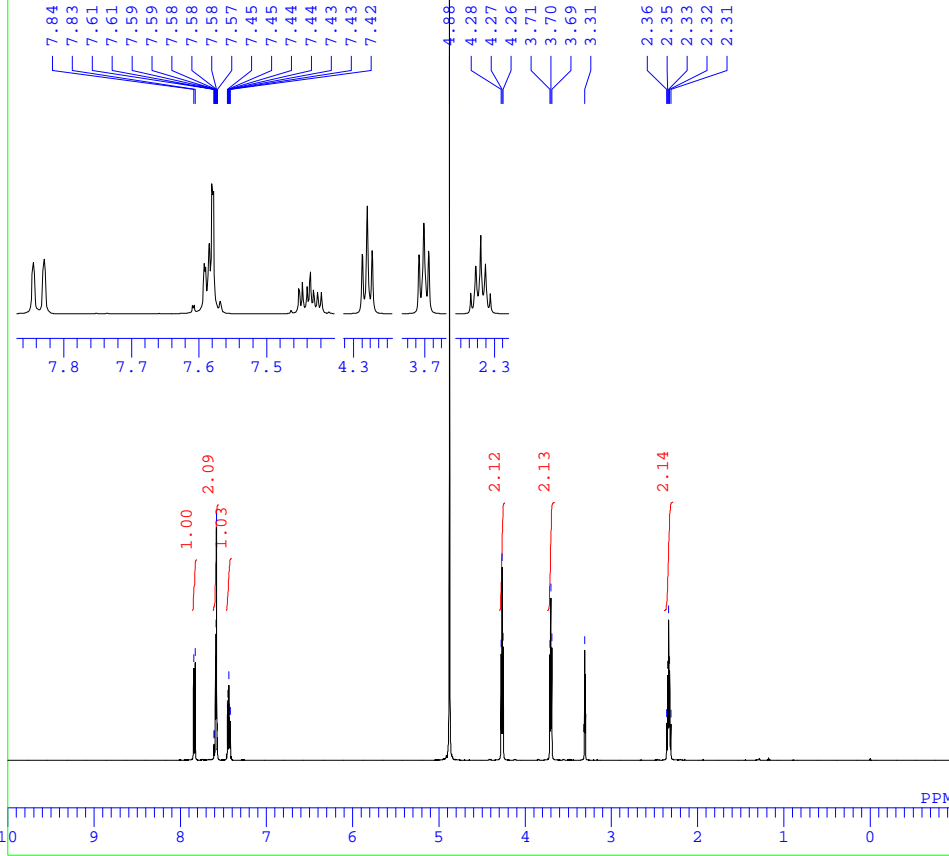


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 POINT 26214  
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 SCANS 1000  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
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 IRNUC 1H  
 CTEMP 21.8 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 1.20 Hz  
 RGAIN 54

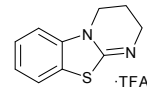




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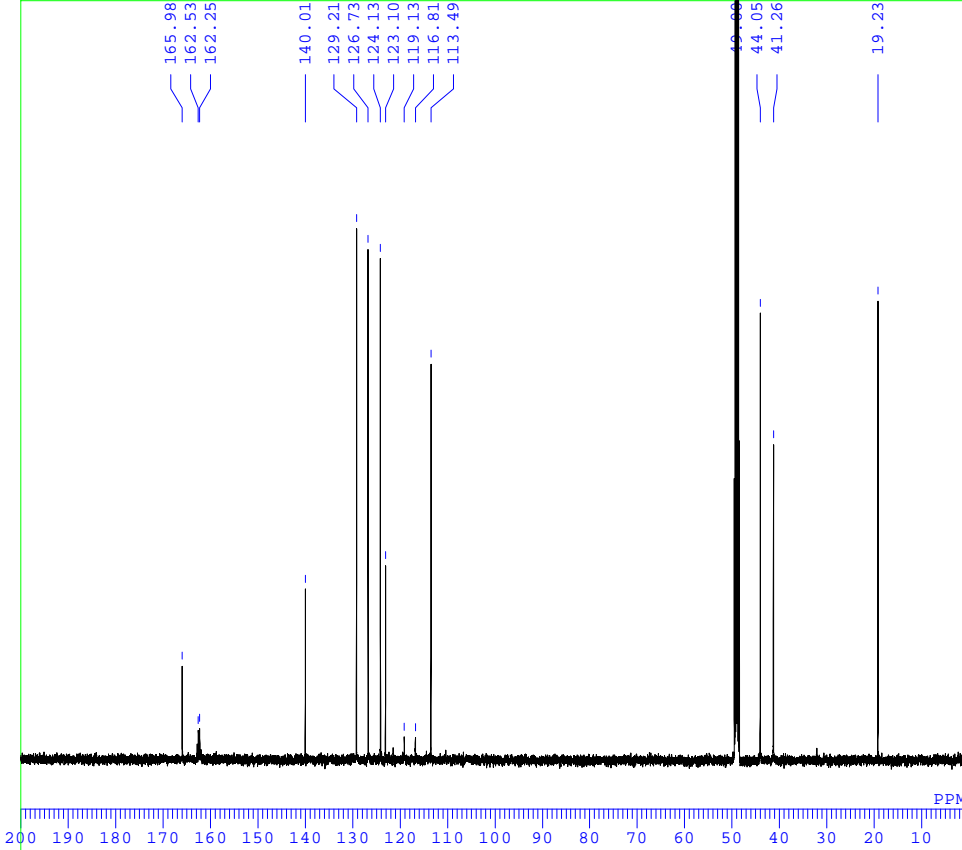


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 POINT 13107  
 FREQU 7507.39 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
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 IRNUC 1H  
 CTEMP 24.8 c  
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 BF 0.12 Hz  
 RGAIN 40

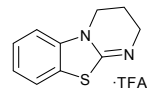


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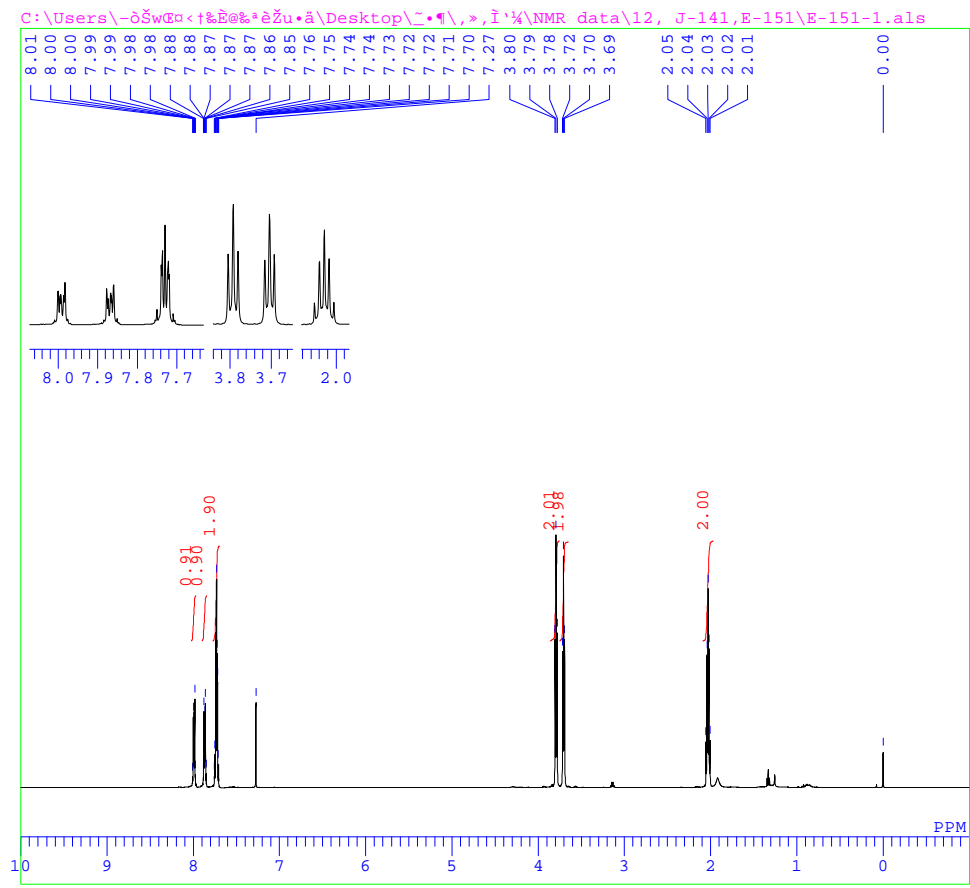
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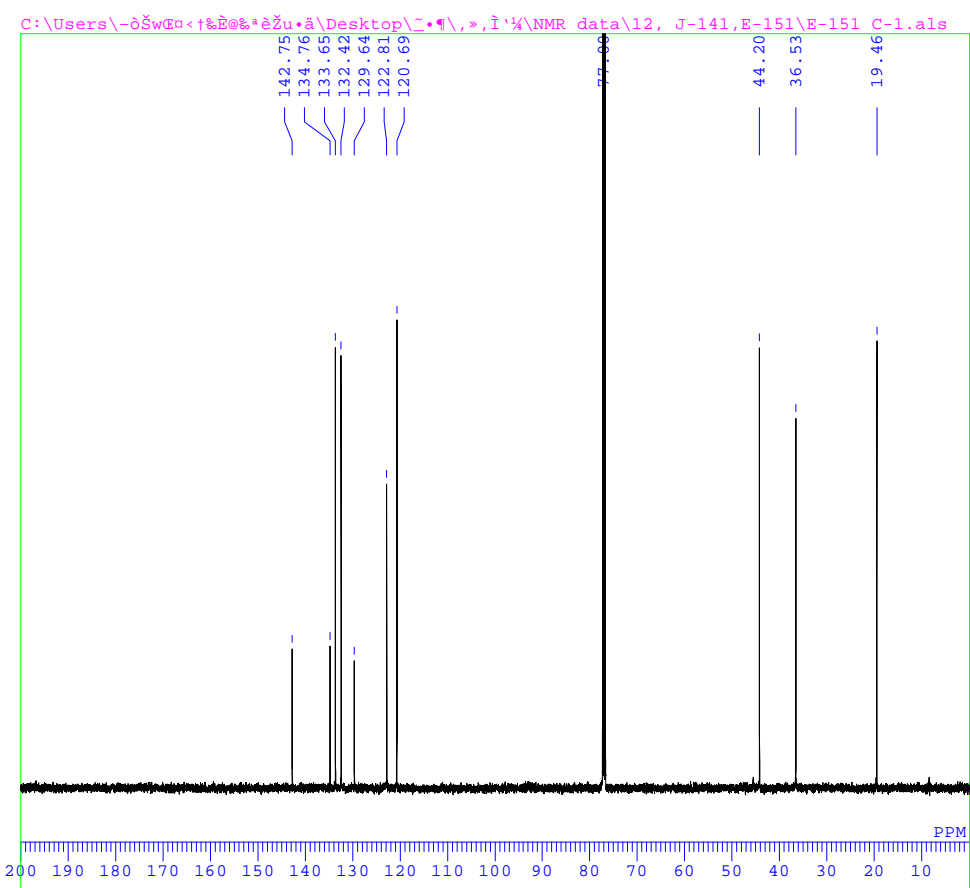
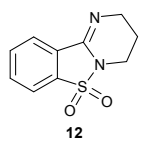
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 OBSSET 7.87 KHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.06 Hz  
 SCANS 1000  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.73 usec  
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 RGAIN 58



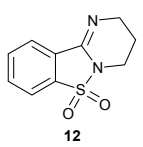
11



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 EXMOD single\_pulse.ex2  
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 OBSSET 2.41 KHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.39 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.82 usec  
 IRNUC 1H  
 CTEMP 24.4 c  
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 EXREF 0.00 ppm  
 BF 0.12 Hz  
 RGAIN 42

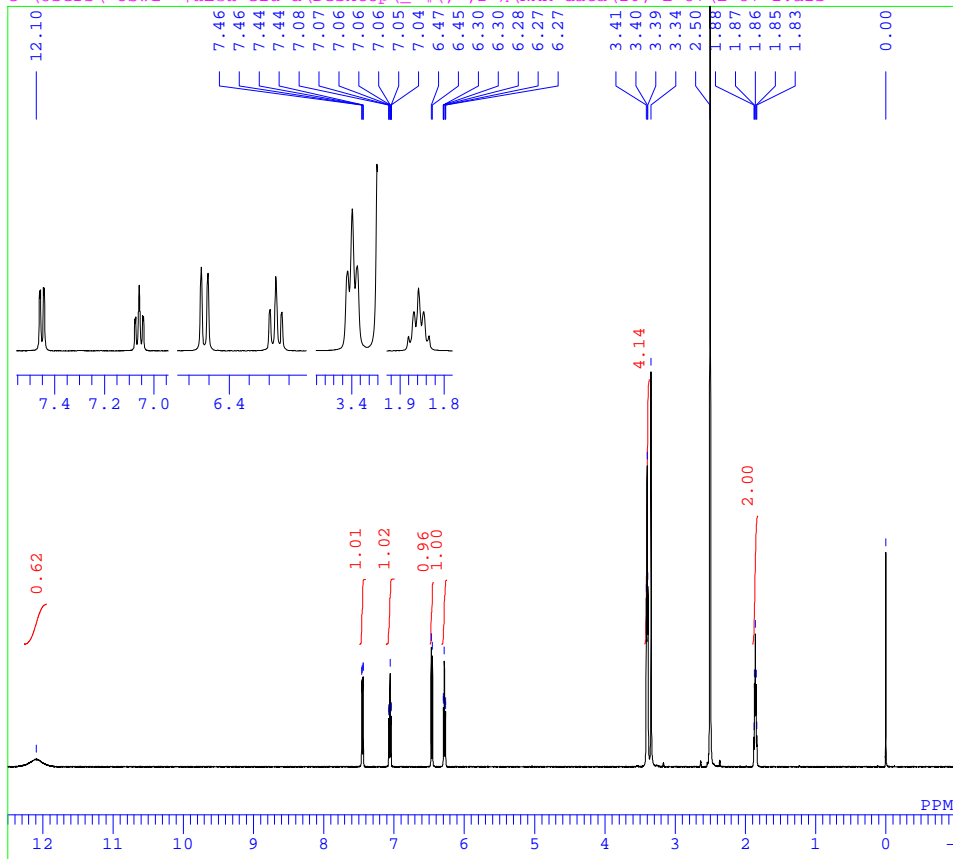


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 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.06 Hz  
 SCANS 1000  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
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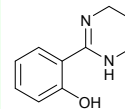




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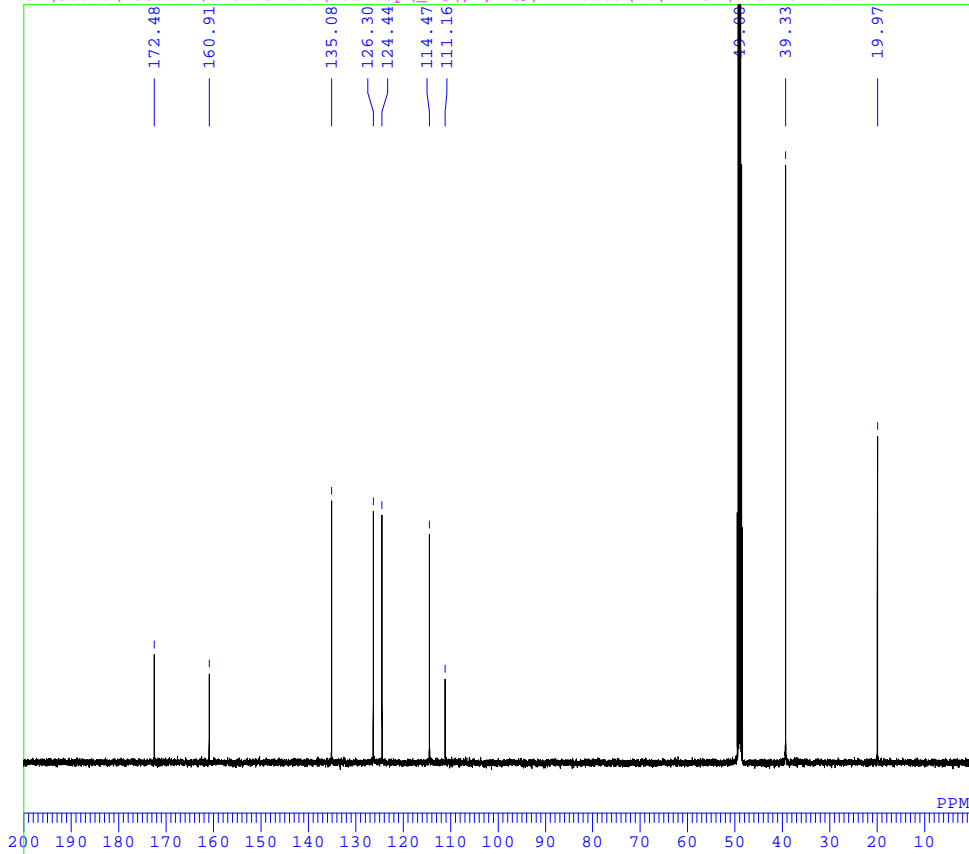


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 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
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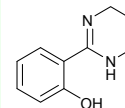


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 PD 2.0000 sec  
 PW1 3.50 usec  
 IRNUC 1H  
 CTEMP 20.1 c  
 SLVNT CD3OD  
 EXREF 49.00 ppm  
 BF 1.20 Hz  
 RGAIN 54



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