

**Design, synthesis and molecular docking of novel bipyrazolyl thiazolone  
scaffold as a new class of antibacterial agents**

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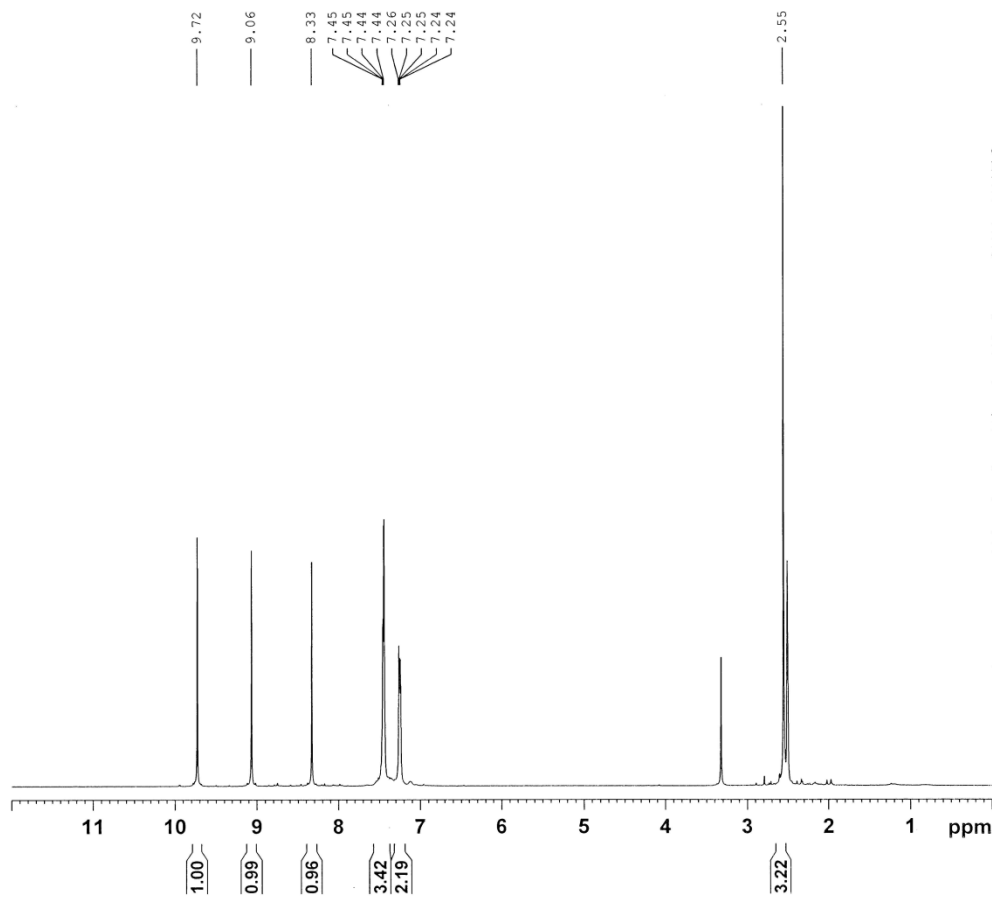
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Supplementary Information



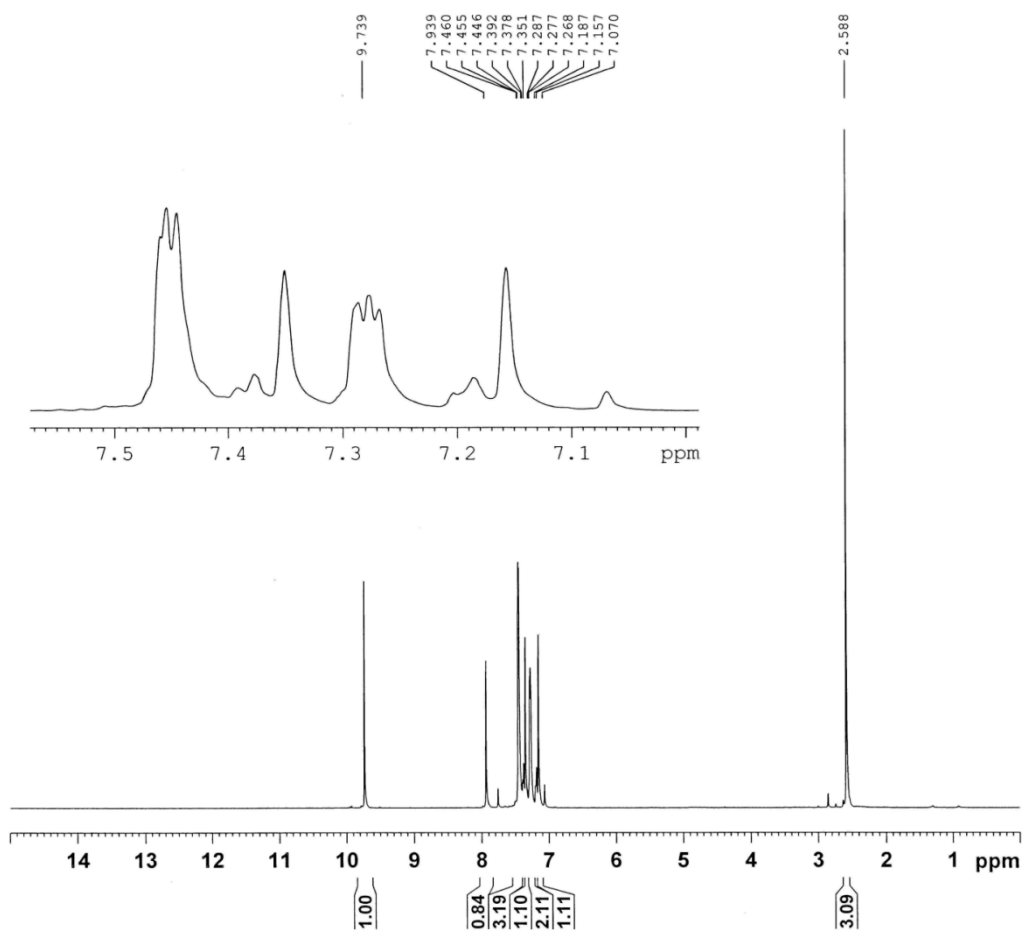
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 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
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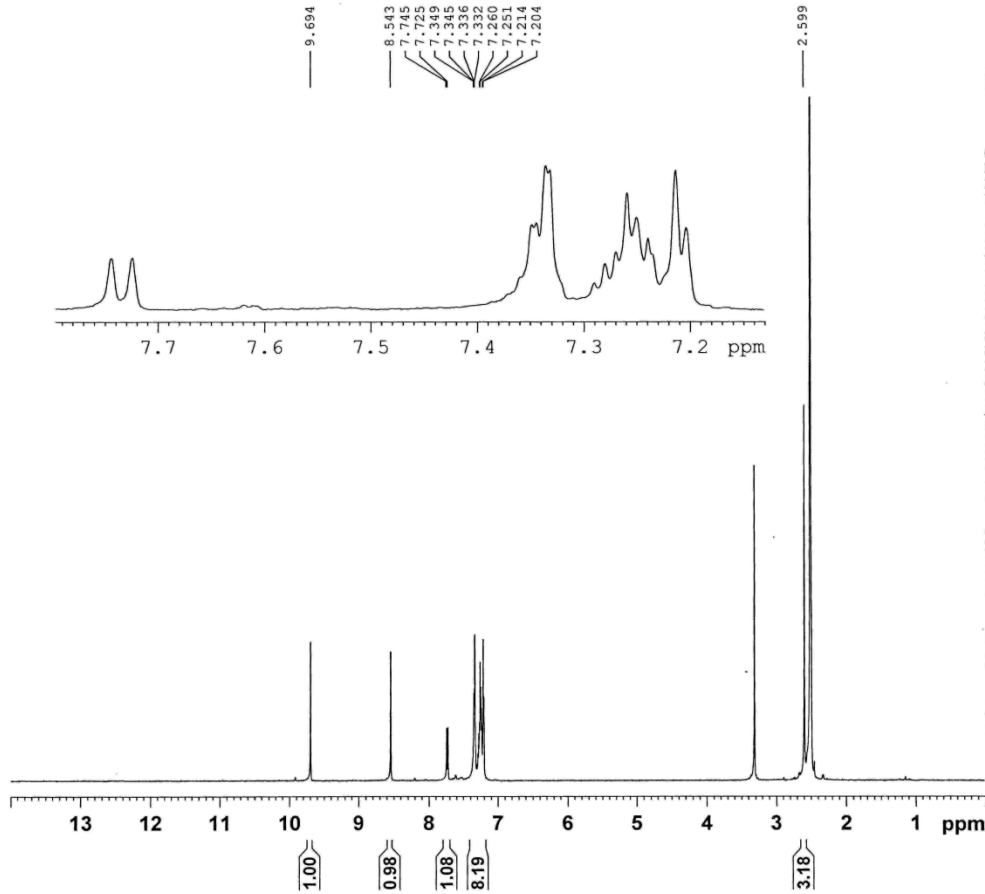
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<sup>1</sup>H NMR spectra of compound 3a



<sup>1</sup>H NMR spectra of compound **3b**



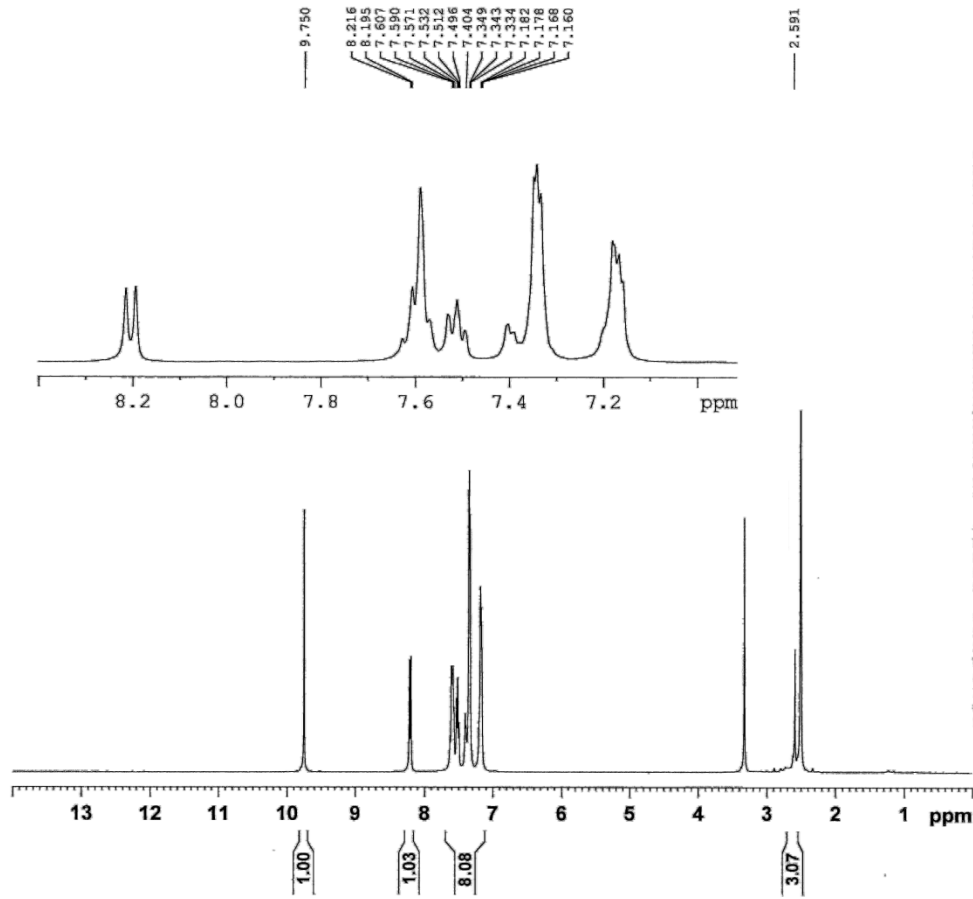
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 PULPROG zg30  
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 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
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<sup>1</sup>H NMR spectra of compound **3c**



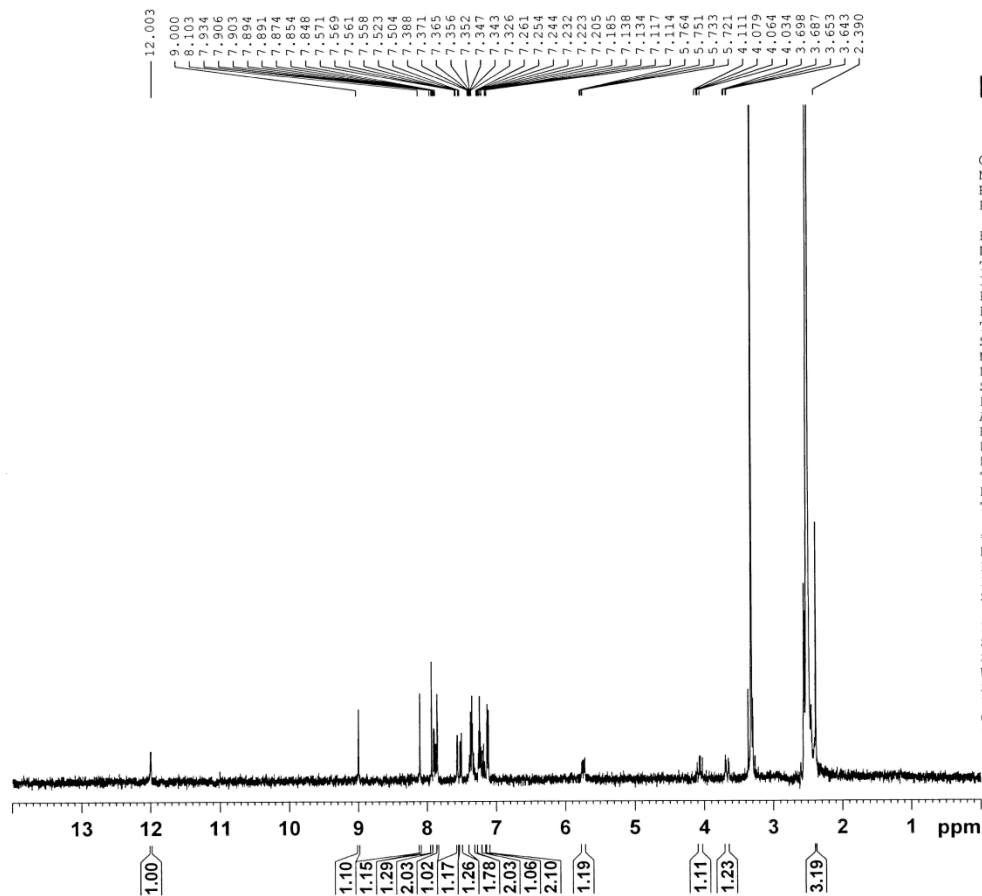
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 DS 2  
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 FIDRES 0.126314 Hz  
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 TE 298.1 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
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 P1 13.00 usec  
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F2 - Processing parameters  
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 GB 0  
 PC 1.00

<sup>1</sup>H NMR spectra of compound **3d**



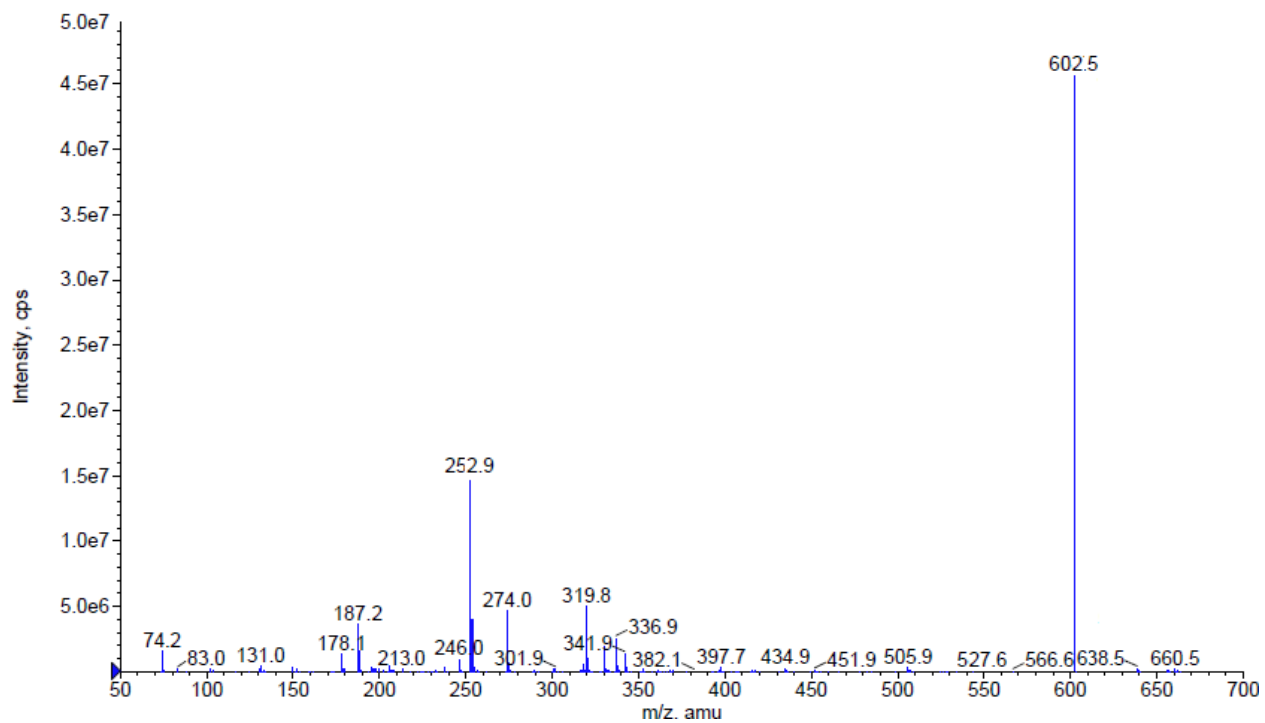
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DS 2  
SWH 8278.146 Hz  
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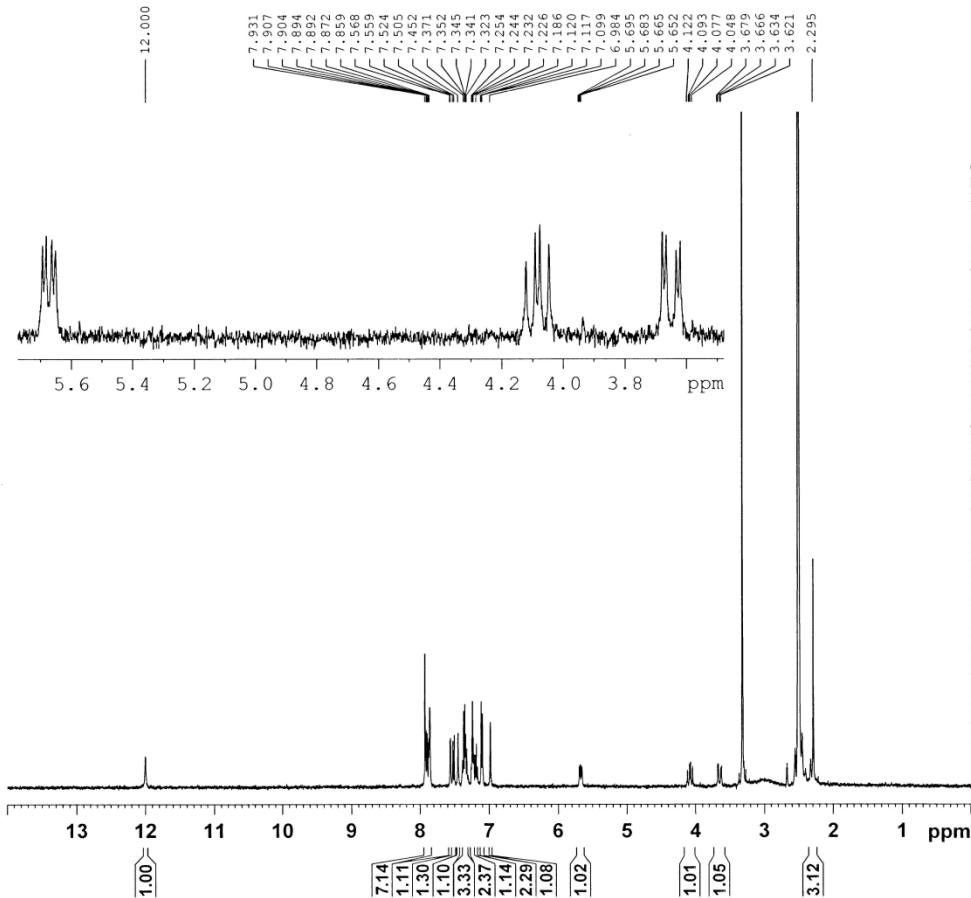
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GB 0  
PC 1.00

$^1\text{H}$  NMR spectra of compound **10a**



Mass spectra of compound **10a**



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 EXPNO 27  
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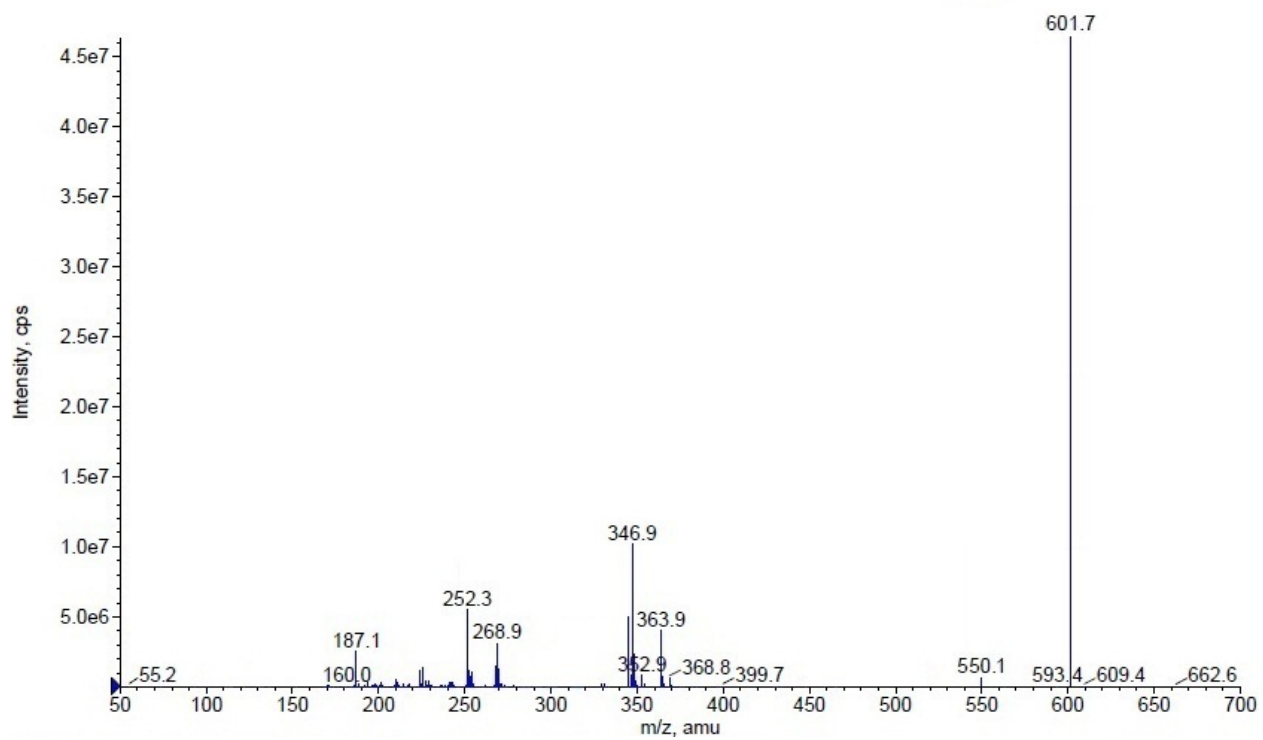
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 NS 16  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 1625.5  
 DW 60.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
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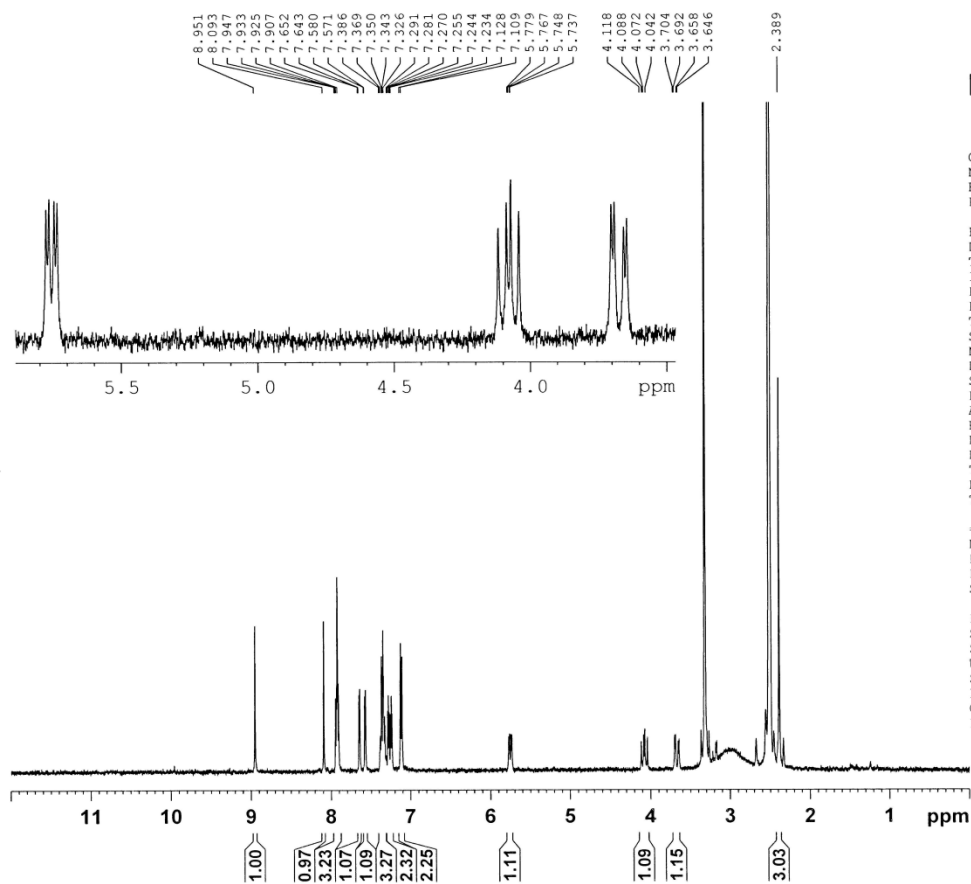
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<sup>1</sup>H NMR spectra of compound **10b**





Mass spectra of compound **10b**



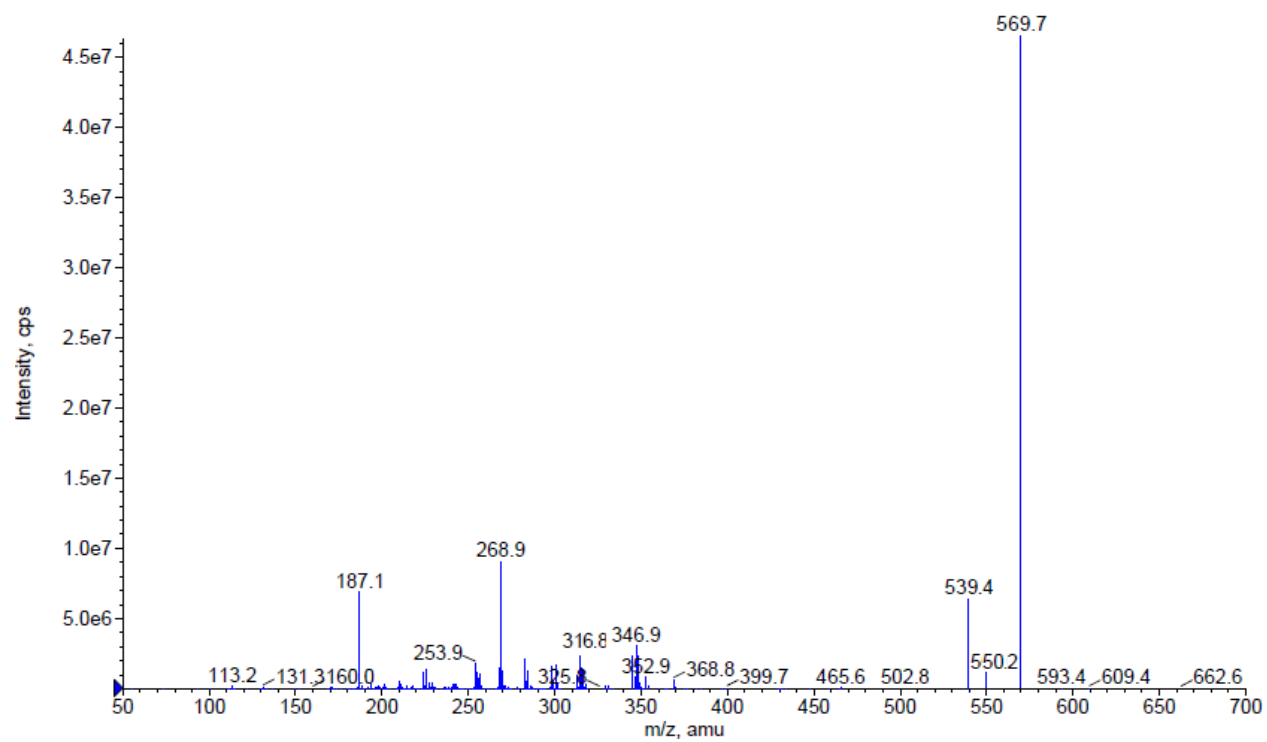
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 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
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 RG 1625.5  
 DW 60.400 usec  
 DE 6.00 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TDO 1

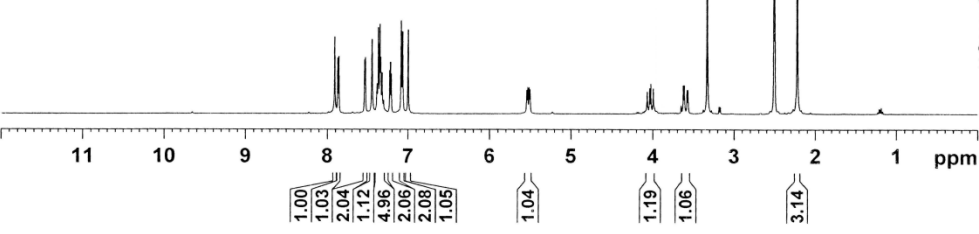
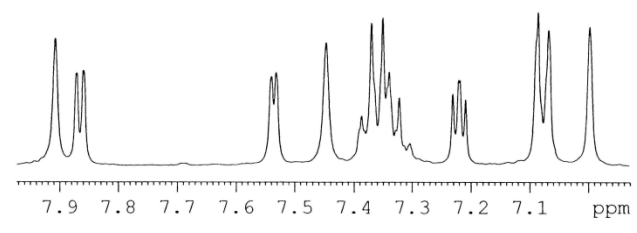
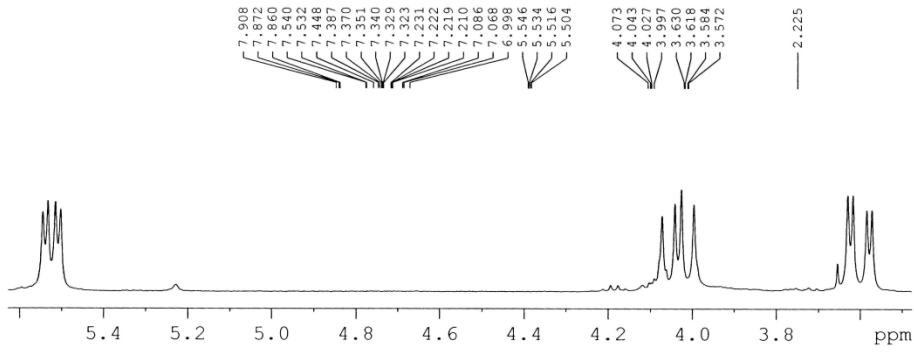
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 SF 400.1300000 MHz  
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 GB 0  
 PC 1.00

<sup>1</sup>H NMR spectra of compound **11a**



Mass spectra of compound **11a**



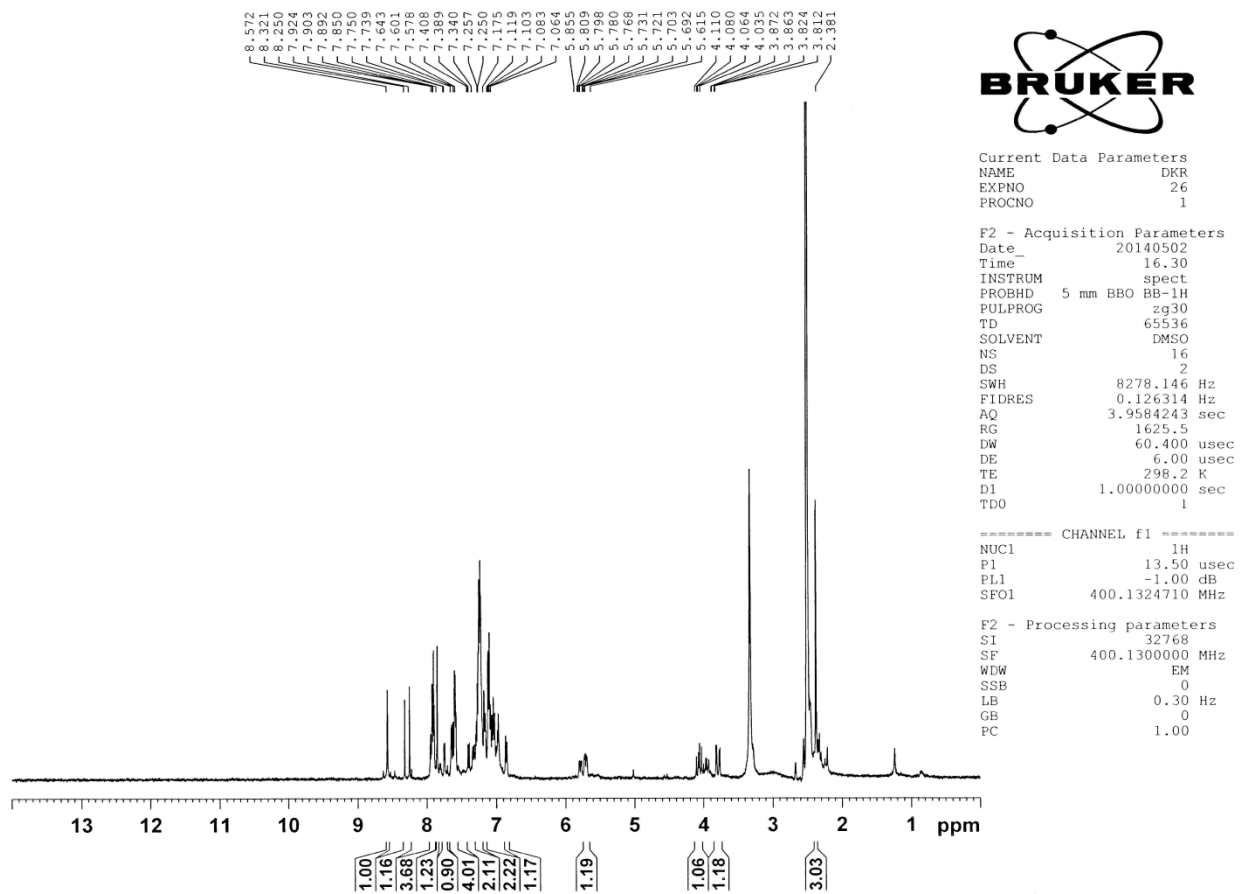
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 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
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 FIDRES 0.126314 Hz  
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 TD0 1

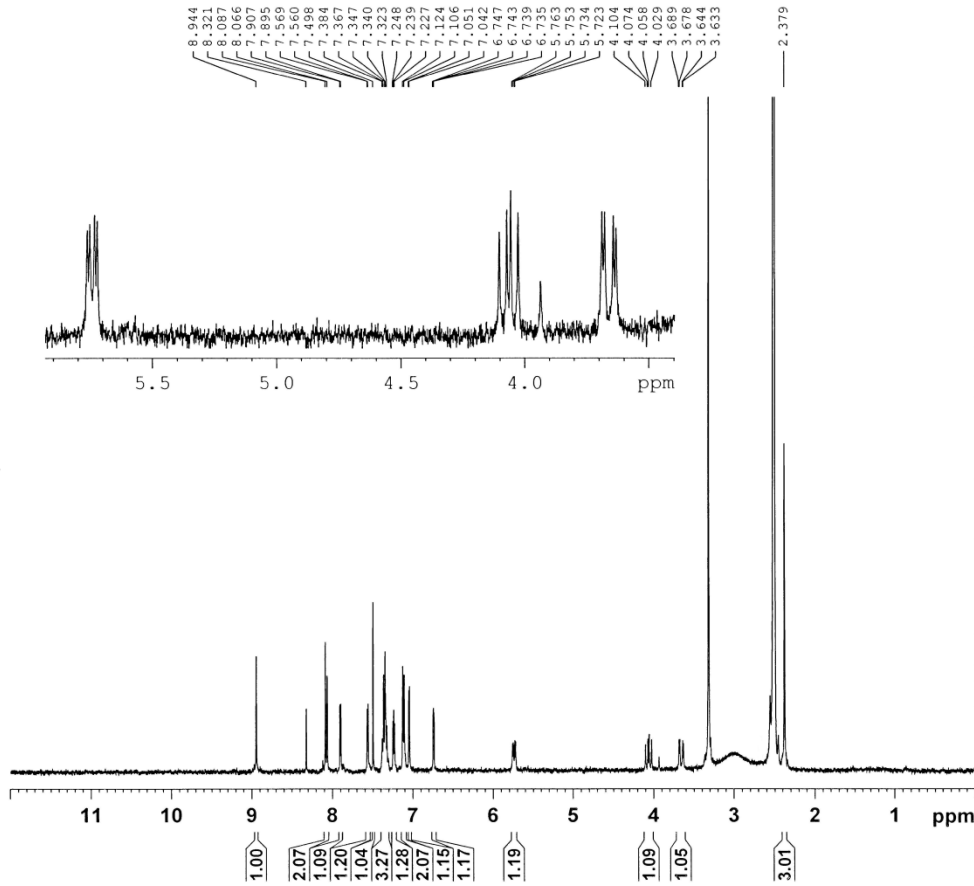
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 PC 1.00

<sup>1</sup>H NMR spectra of compound **11b**



<sup>1</sup>H NMR spectra of compound 11c



Current Data Parameters  
 NAME DKR  
 EXPNO 18  
 PROCNO 1

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 NS 16  
 DS 2  
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 RG 2048  
 DW 60.400 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.0000000 sec  
 TD0 1

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 PL1 -1.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
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 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR spectra of compound **12a**