

## **Reactions of thiiranes with NH-heterocycles**

### **1. An investigation of the reaction of 2-chloromethylthiirane with 3,5-dibromo-4-nitropyrazole**

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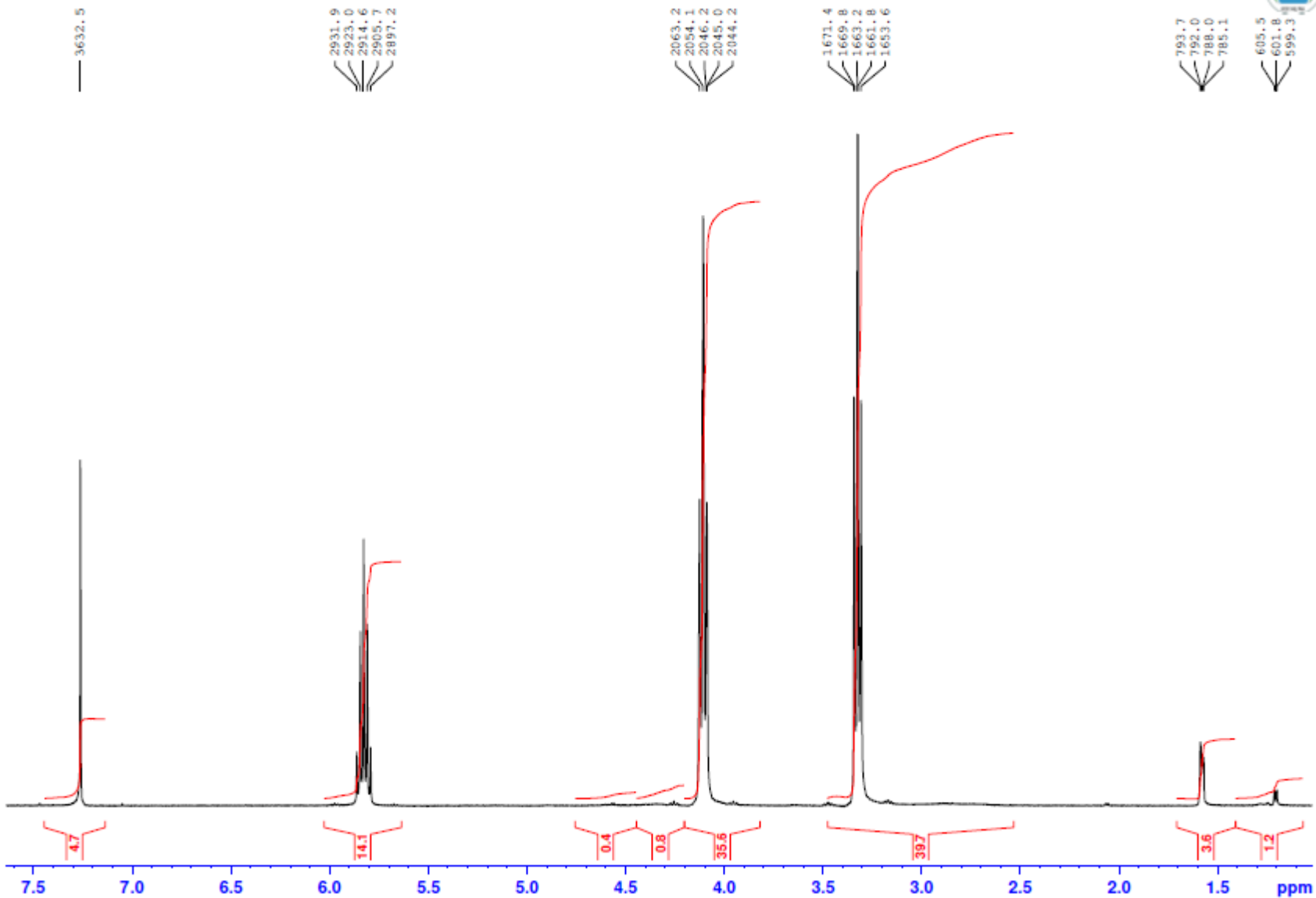
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**SUPPLEMENTARY INFORMATION**

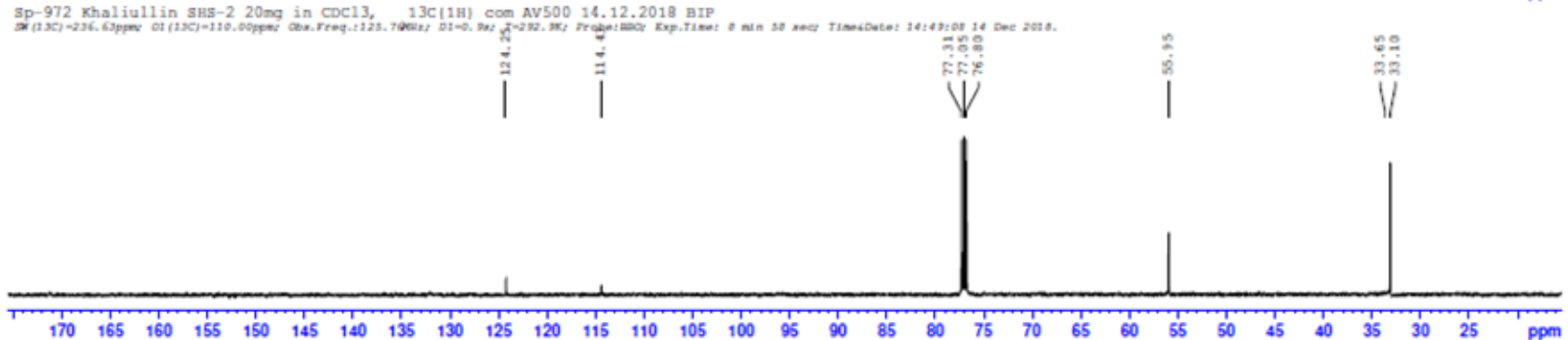
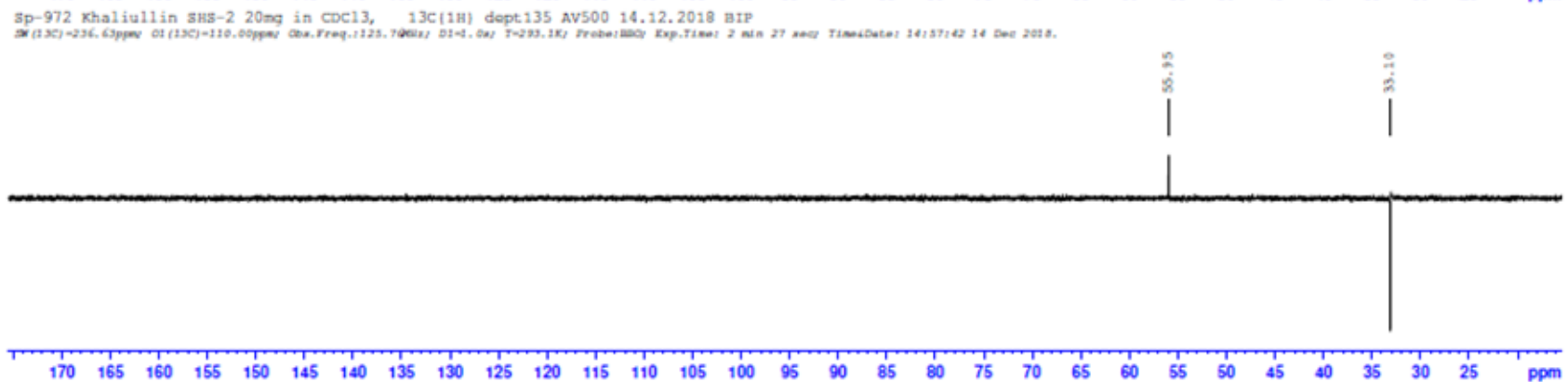
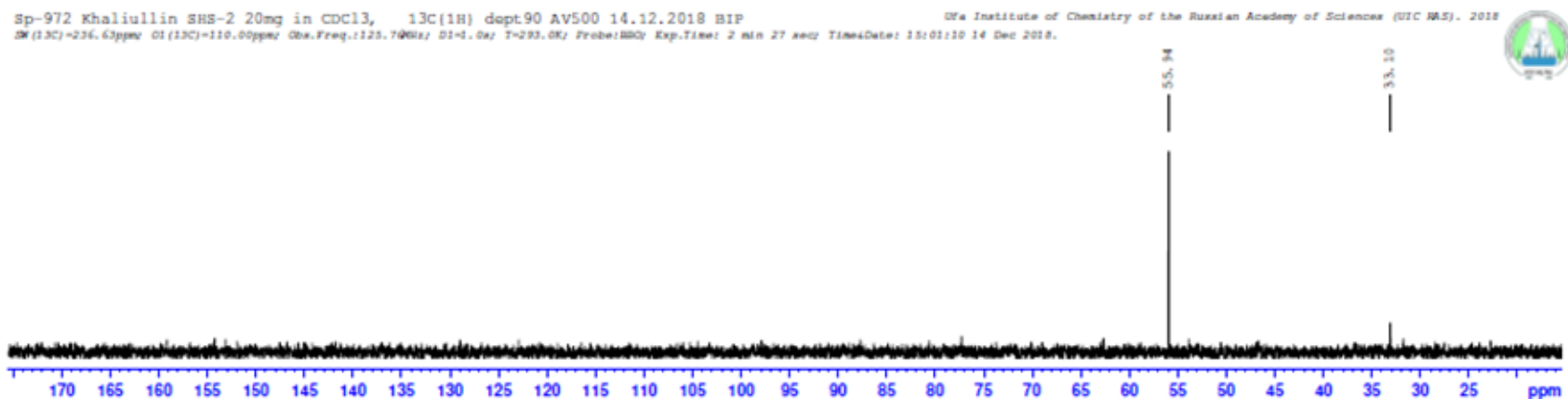
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of 3,5-dibromo-4-nitro-1-(thietan-3-yl)-1*H*-pyrazole (**3**)

Sp-972 Khaliullin SHS-2 20mg in  $\text{CDCl}_3$ ,  $^1\text{H}$  AV500 14.12.2018 BIP

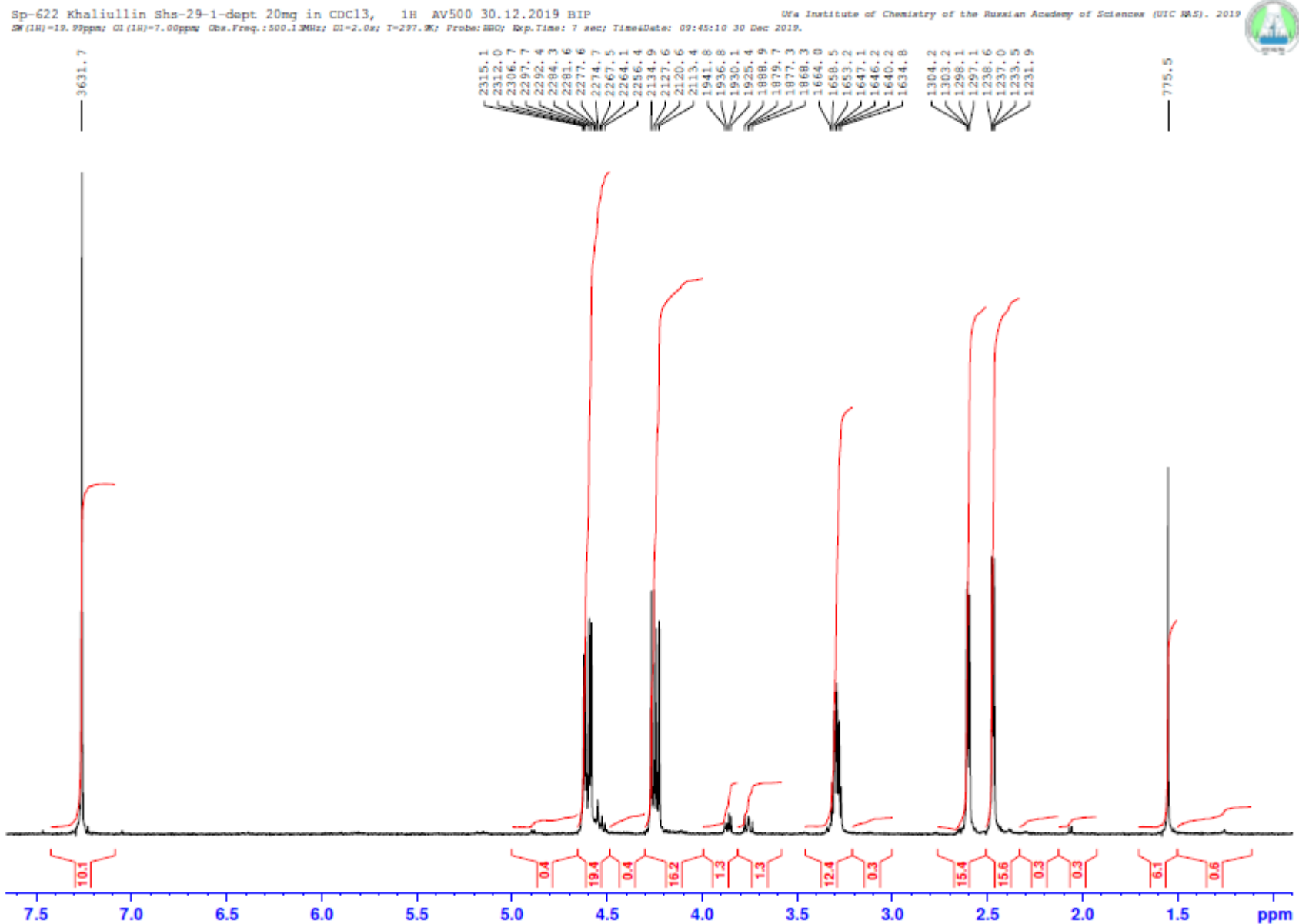
Ufa Institute of Chemistry of the Russian Academy of Sciences (IUC RAS), 2018



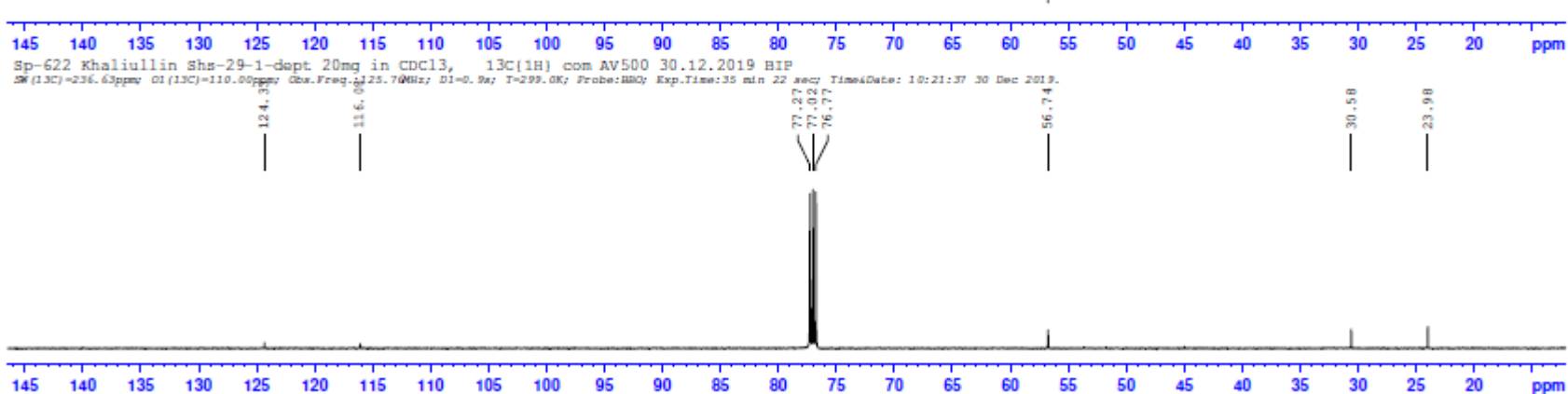
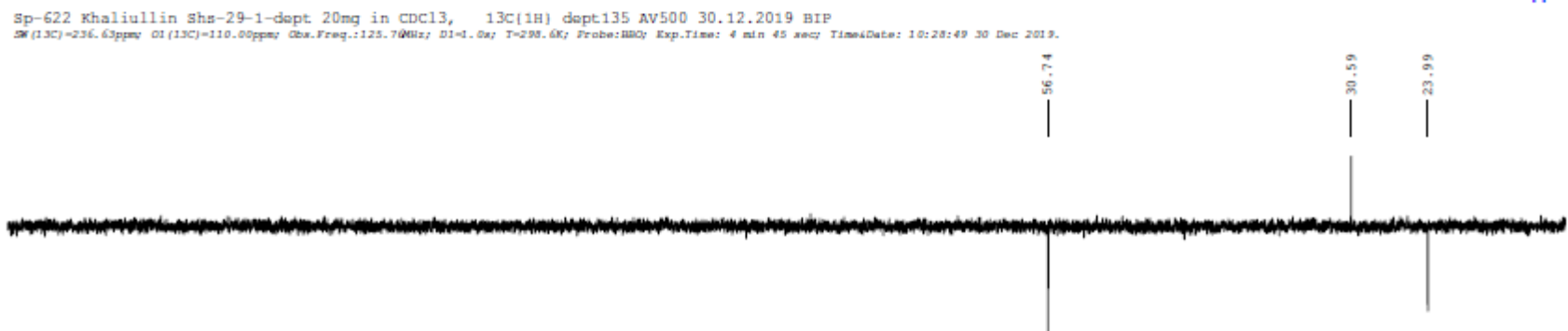
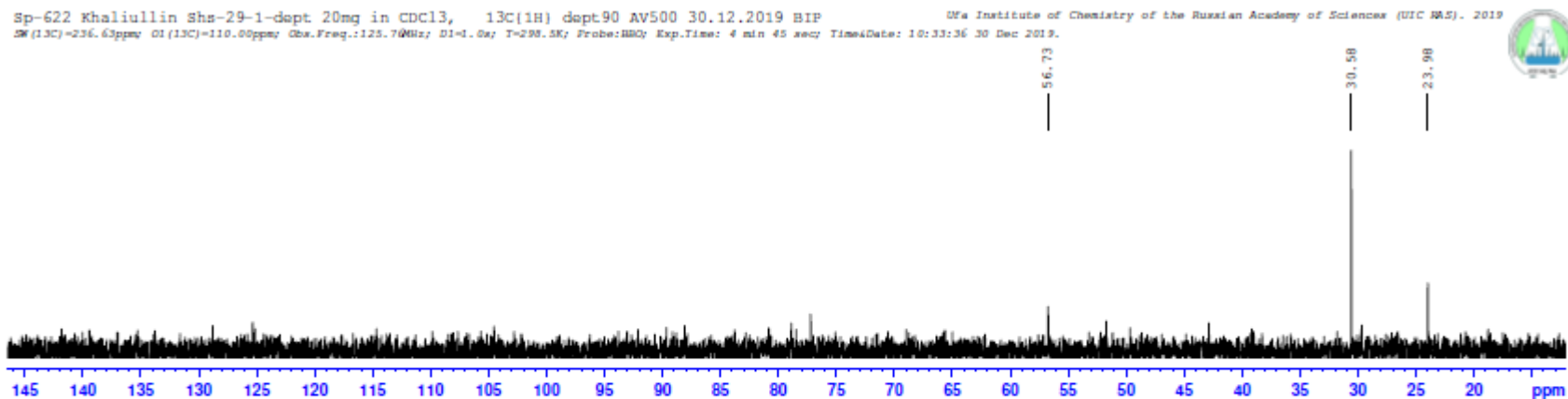
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of 3,5-dibromo-4-nitro-1-(thietan-3-yl)-1*H*-pyrazole (**3**)



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of 3,5-dibromo-4-nitro-1-(thiiran-2-ylmethyl)-1*H*-pyrazole (4)



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of 3,5-dibromo-4-nitro-1-(thiiran-2-ylmethyl)-1*H*-pyrazole (4)



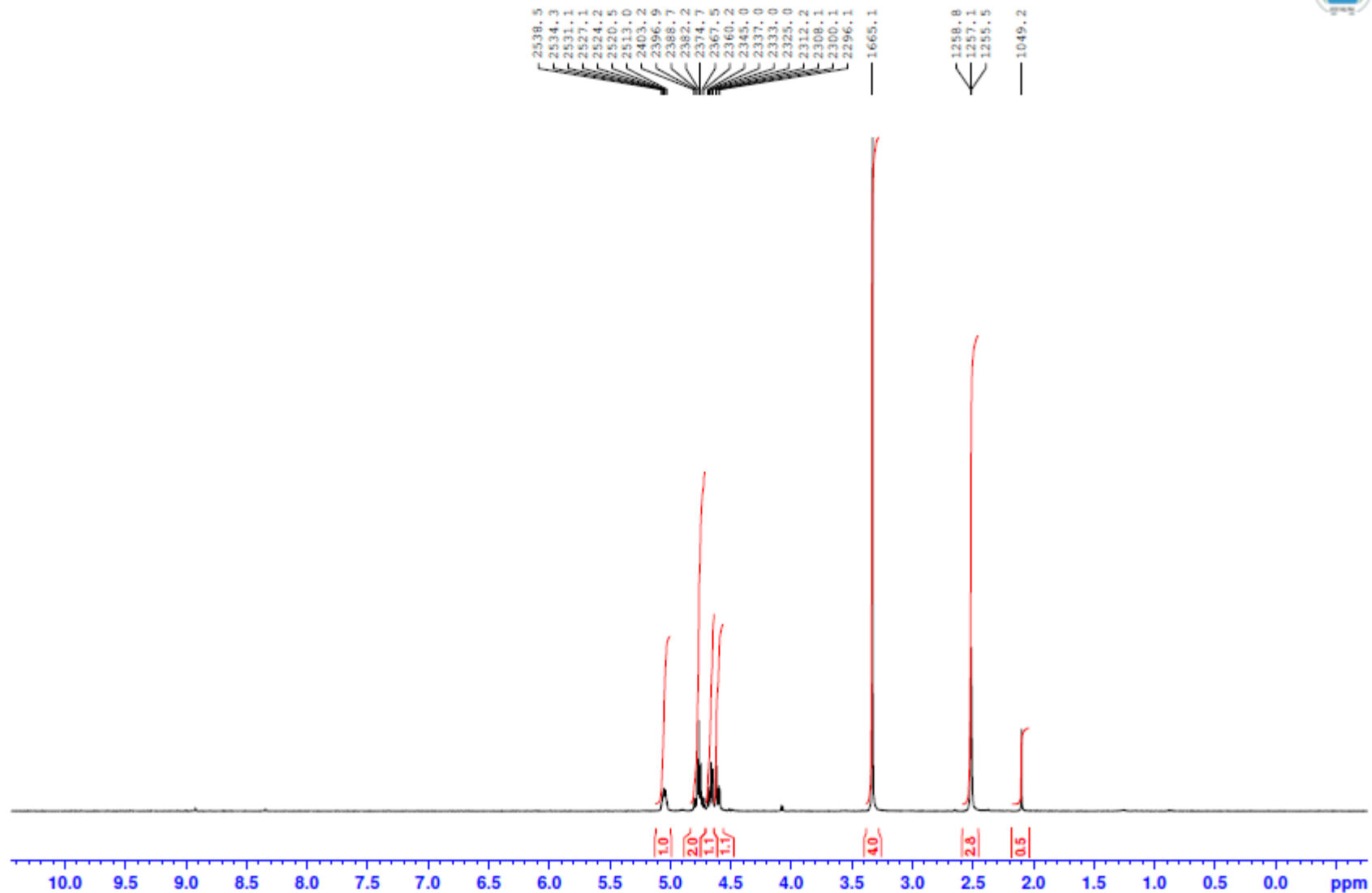
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) of 6-bromo-2-[(3,5-dibromo-4-nitro-1*H*-pyrazol-1-yl)methyl]-7-nitro-2,3-dihydropyrazolo[5,1-*b*]thiazole (5)

Sp-1073 Khaliullina Shs-29 10mg in DMSO, 1H AV500 20.02.2020 LAN

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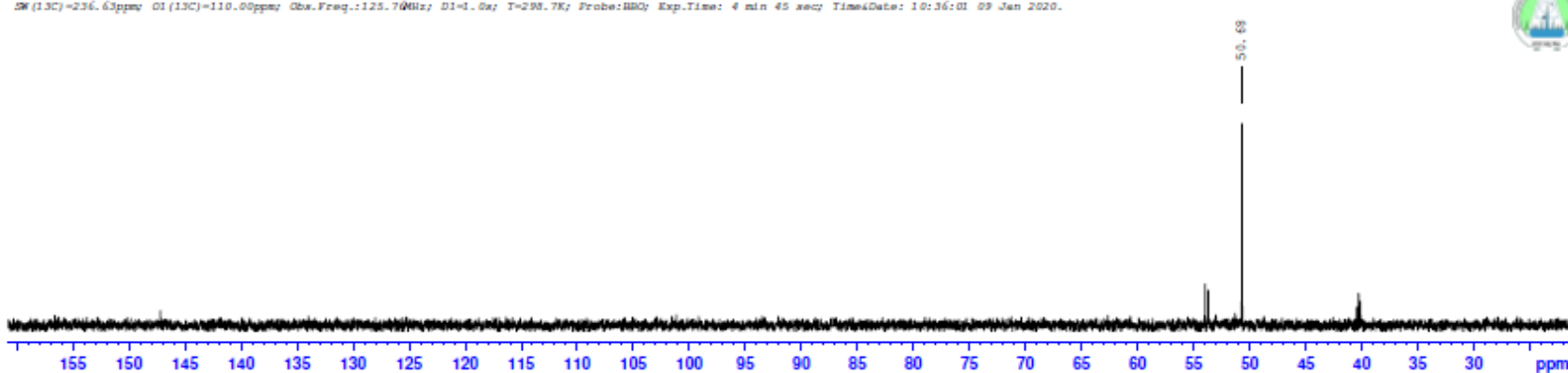
SW (1H)=19.99ppm; CI (1H)=7.00ppm Obs.Freq.:500.13MHz; D1=2.0s; T=298.0K; Probe:500; Exp.Time: 7 sec; TimeDate: 11:26:48 20 Feb 2020.



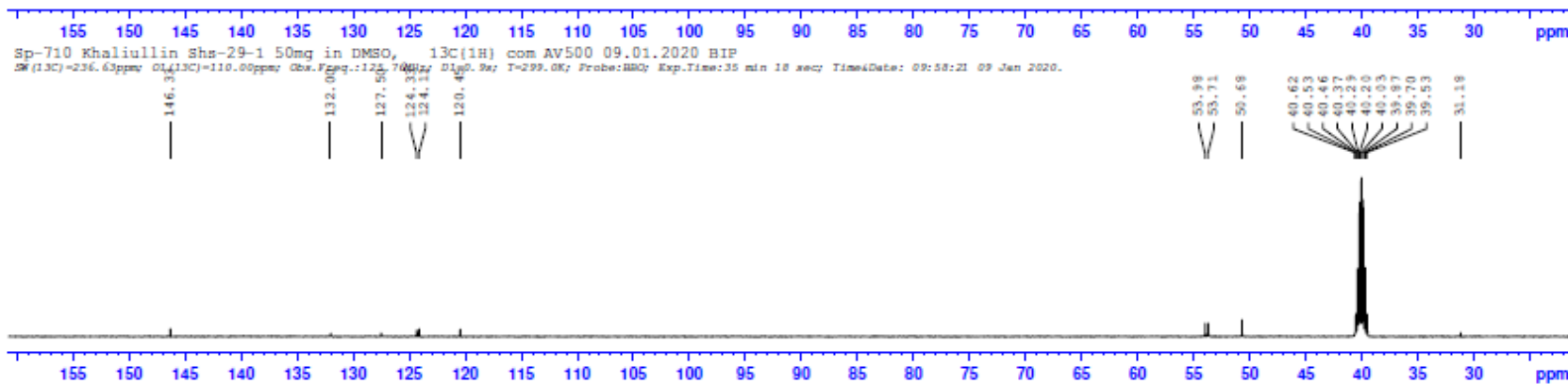
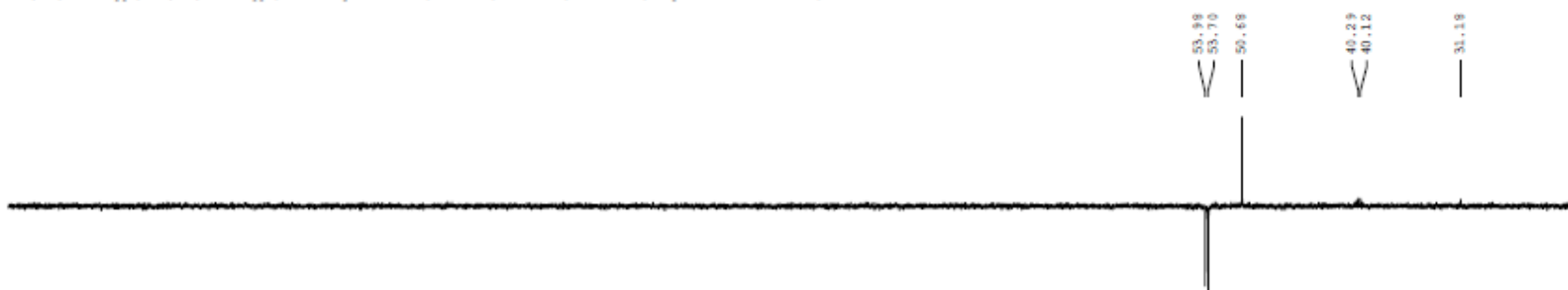
$^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) of 6-bromo-2-[(3,5-dibromo-4-nitro-1*H*-pyrazol-1-yl)methyl]-7-nitro-2,3-dihydropyrazolo[5,1-*b*]thiazole (5)

Sp-710 Khaliullin Shs-29-1 50mg in DMSO,  $^{13}\text{C}\{^1\text{H}\}$  dept90 AV500 09.01.2020 BIP

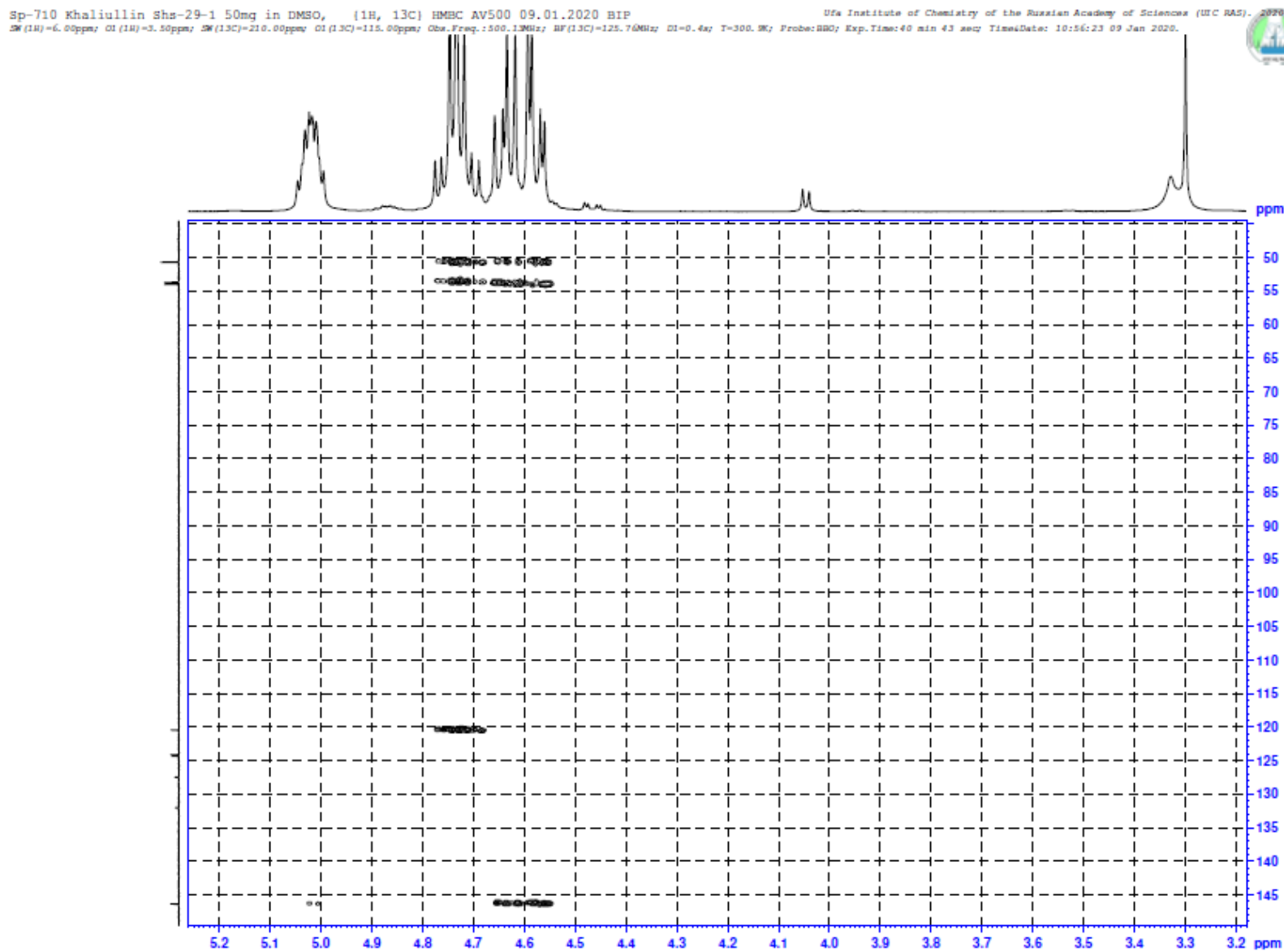
Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS). 2020



Sp-710 Khaliullin Shs-29-1 50mg in DMSO,  $^{13}\text{C}\{^1\text{H}\}$  dept135 AV500 09.01.2020 BIP



$^1\text{H}$  -  $^{13}\text{C}$  NMR HMBC (DMSO- $d_6$ ) of 6-bromo-2-[(3,5-dibromo-4-nitro-1*H*-pyrazol-1-yl)methyl]-7-nitro-2,3-dihydropyrazolo[5,1-*b*]thiazole (**5**)





$^1\text{H} - ^{15}\text{N}$  NMR HMBC (DMSO- $d_6$ ) of 6-bromo-2-[(3,5-dibromo-4-nitro-1*H*-pyrazol-1-yl)methyl]-7-nitro-2,3-dihydropyrazolo[5,1-*b*]thiazole (**5**)

Sp-710 Khaliullin Shs-29-1 50mg in DMSO, (1H, 15N) HMBC AV500 09.01.2020 BIP

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS). 2019

SW(1H)=6.00ppm; Q1(1H)=3.50ppm; SW(15N)=399.98ppm; Q1(15N)=200.00ppm; Obs.Freq.:500.13MHz; RF(15N)=50.68MHz; Q1=0.4s; T=298.0K; Probe:BBQ; Exp.Time: 1 h 3 min 45 sec; TimeDate: 12:45:51 09 Jan 2020.

