

**Reactions of thiiranes with NH-heterocycles:
III*. The synthesis of N^2/N^4 -mono- and N^2/N^4 -dithietane-containing
5-bromo-2,4-dihydro-1,2,4-triazol-3-ones
and their antidepressant activity**

**Elena E. Klen^{1*}, Irina L. Nikitina¹, Ferkat A. Khaliullin¹,
Galina A. Rozit¹, Ekaterina A. Nikitina¹, Gul'nara G. Gaisina¹,
Aleksandr V. Samorodov¹, Valentin N. Pavlov¹**

¹ *Bashkir State Medical University,
3 Lenina St., Ufa 450008, Russia; e-mail: klen_elena@yahoo.com*

SUPPLEMENTARY INFORMATION

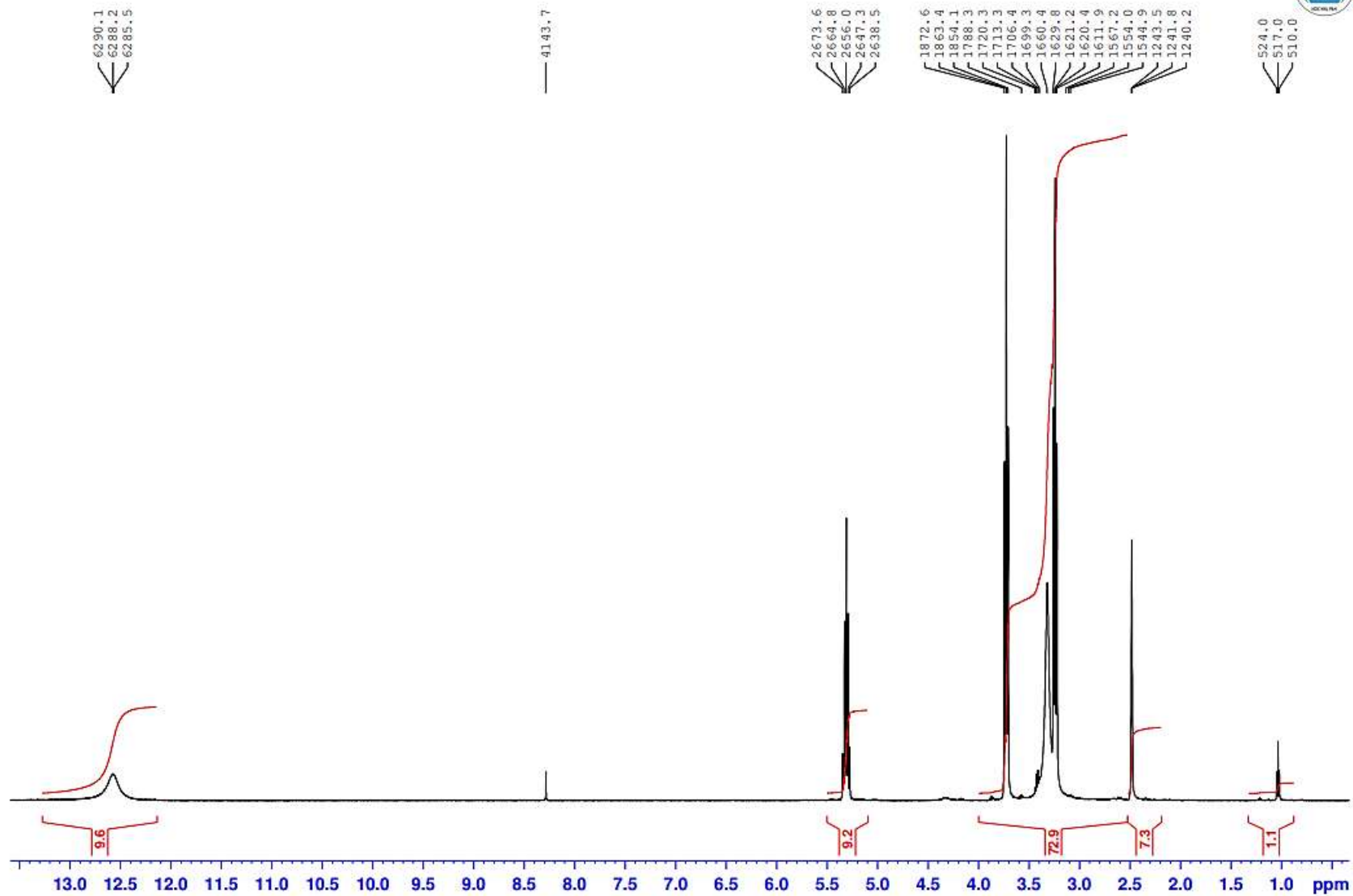
^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 5-bromo-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**2a**)

Sp-418 Khaliullin G-78-dept 20mg in DMSO, ^1H AV500 30.01.2023 BIP

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2023



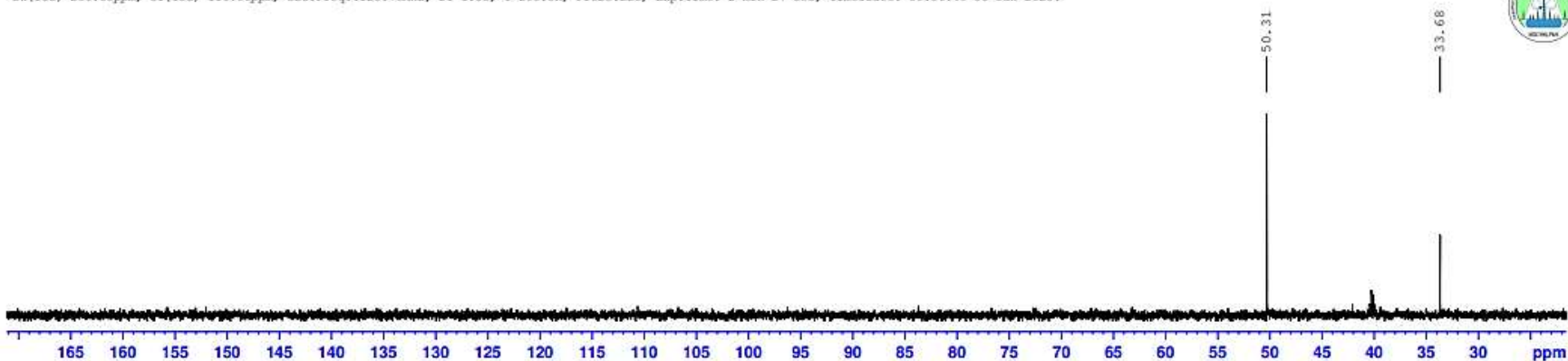
SW(^1H)=19.99ppm; O1(^1H)=7.00ppm; Obs.Freq.:500.13MHz; D1=2.0s; T=298.4K; Probe:BBO; Exp.Time: 7 sec; TimesDate: 09:40:51 30 Jan 2023.



^{13}C NMR (125 MHz, DMSO- d_6) of 5-bromo-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**2a**)

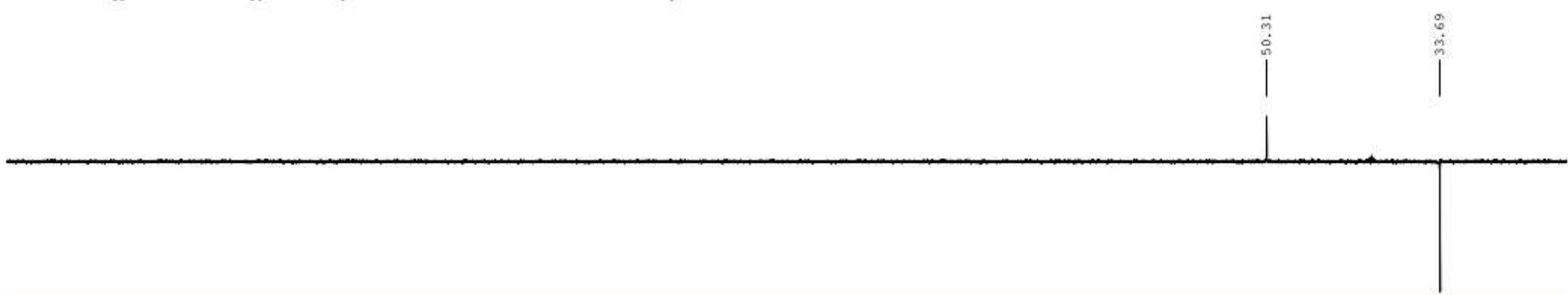
Sp-418 Khaliullin G-78-dept 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept90 AV500 30.01.2023 BIP
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=298.8K; Probe:BBO; Exp.Time: 2 min 27 sec; TimesDate: 09:56:49 30 Jan 2023.

Ufa Institute of Chemistry of the Russian Academy of Sciences (UIC RAS). 2023



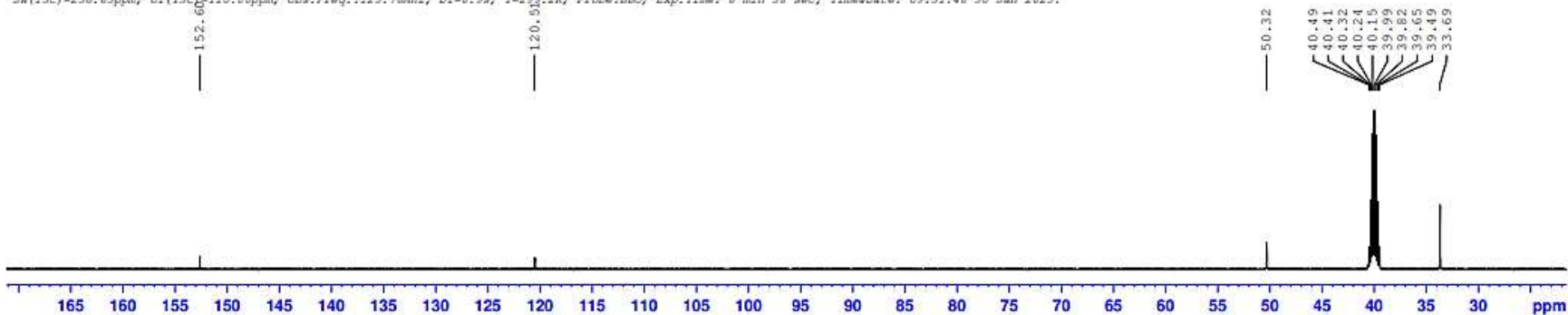
Sp-418 Khaliullin G-78-dept 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept135 AV500 30.01.2023 BIP

SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=298.9K; Probe:BBO; Exp.Time: 2 min 27 sec; TimesDate: 09:54:19 30 Jan 2023.



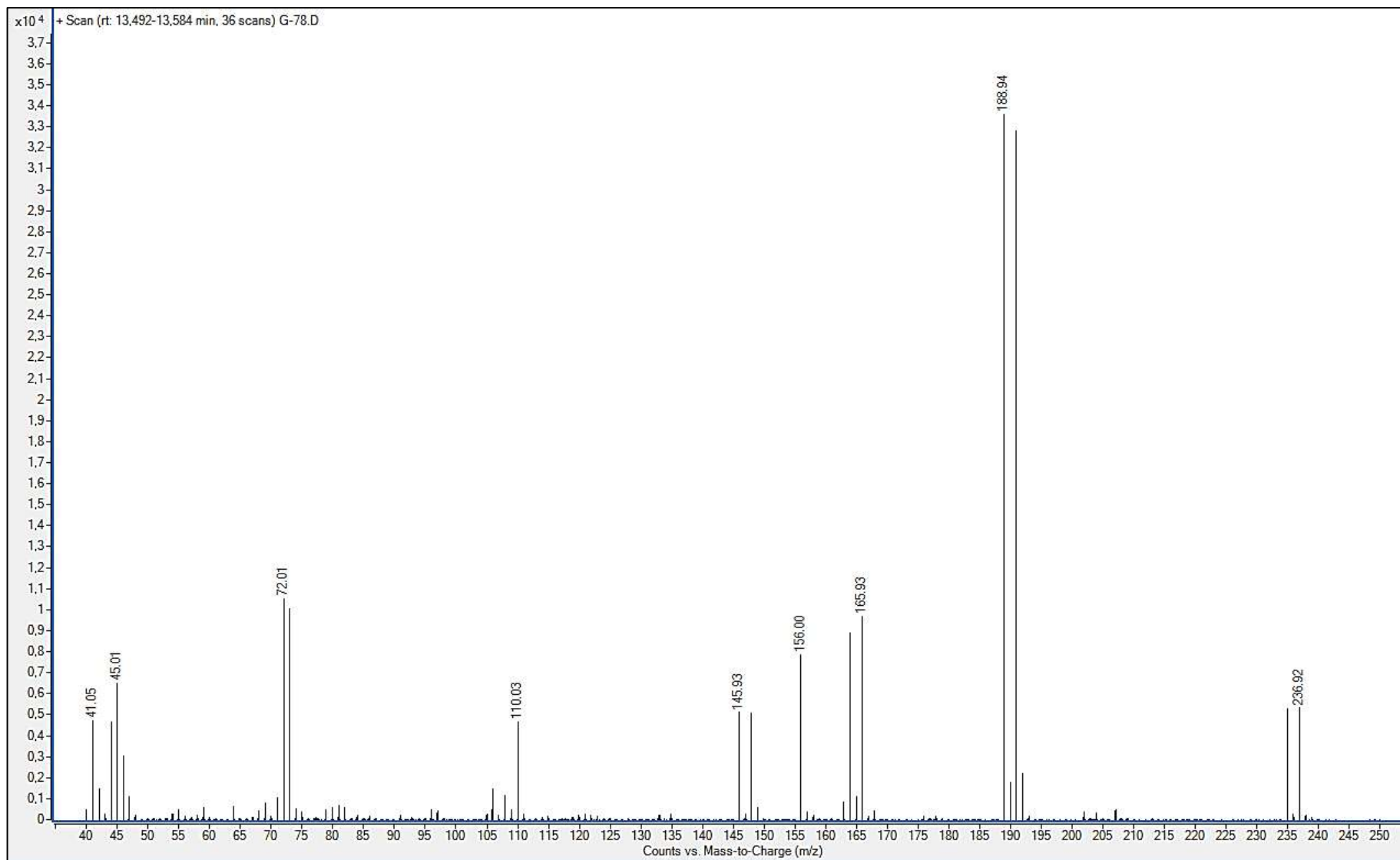
^{13}C NMR spectrum (bottom) showing chemical shifts in ppm from 165 to 30. The spectrum displays several signals: a sharp peak at 152.60 ppm, a smaller peak at 120.51 ppm, a sharp peak at 50.32 ppm, a cluster of peaks between 40 and 45 ppm (labeled 40.49, 40.41, 40.32, 40.24, 40.15, 39.99, 39.82, 39.65, 39.49), and a smaller peak at 33.69 ppm. The x-axis is labeled 'ppm' and ranges from 165 to 30.

Sp-418 Khaliullin G-78-dept 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ com AV500 30.01.2023 BIP
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=0.9s; T=298.2K; Probe:BBO; Exp.Time: 8 min 58 sec; TimesDate: 09:51:46 30 Jan 2023.

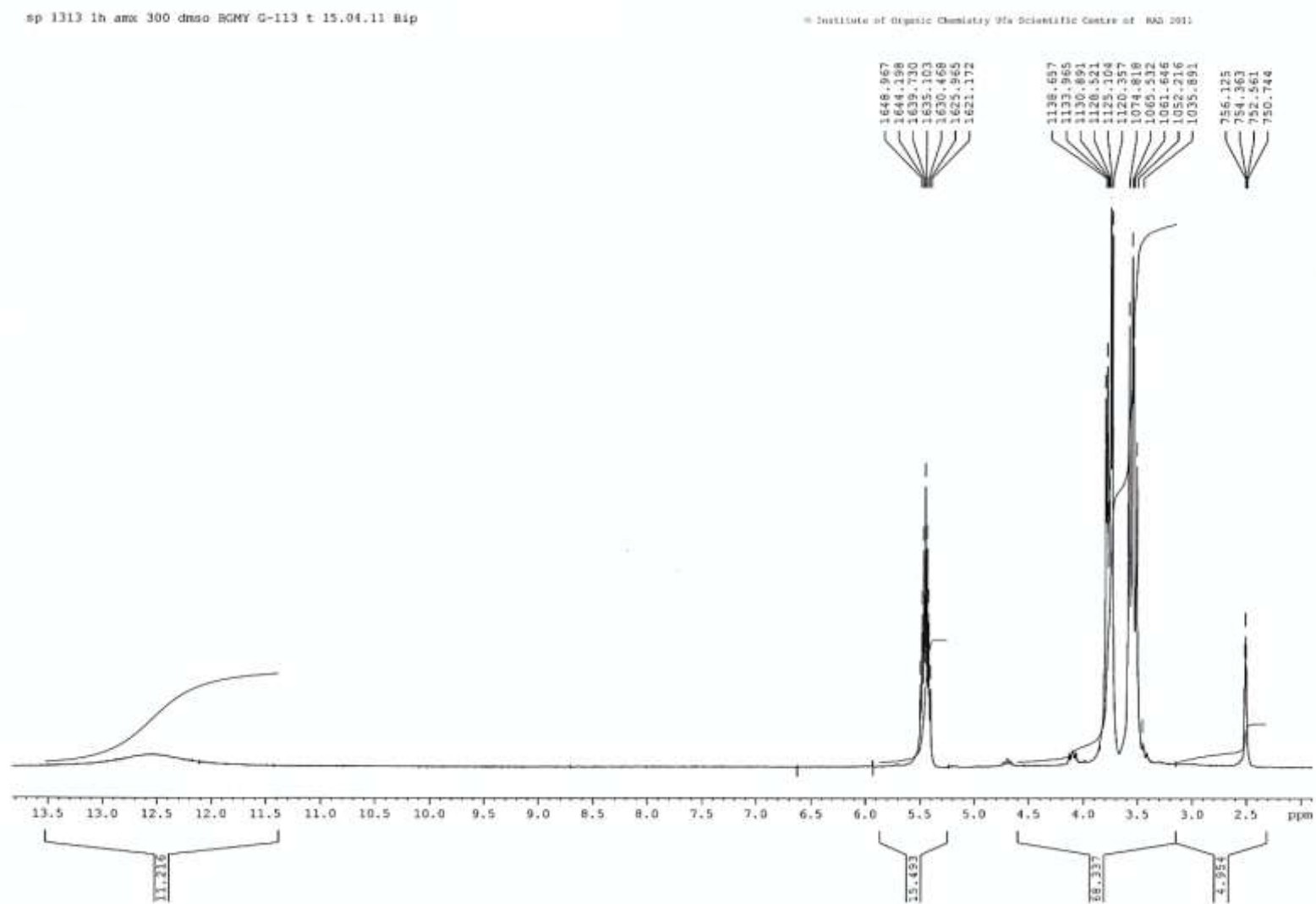


Mass spectrum (EI, 70 eV) of 5-bromo-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**2a**)

Spectrum Plot Report



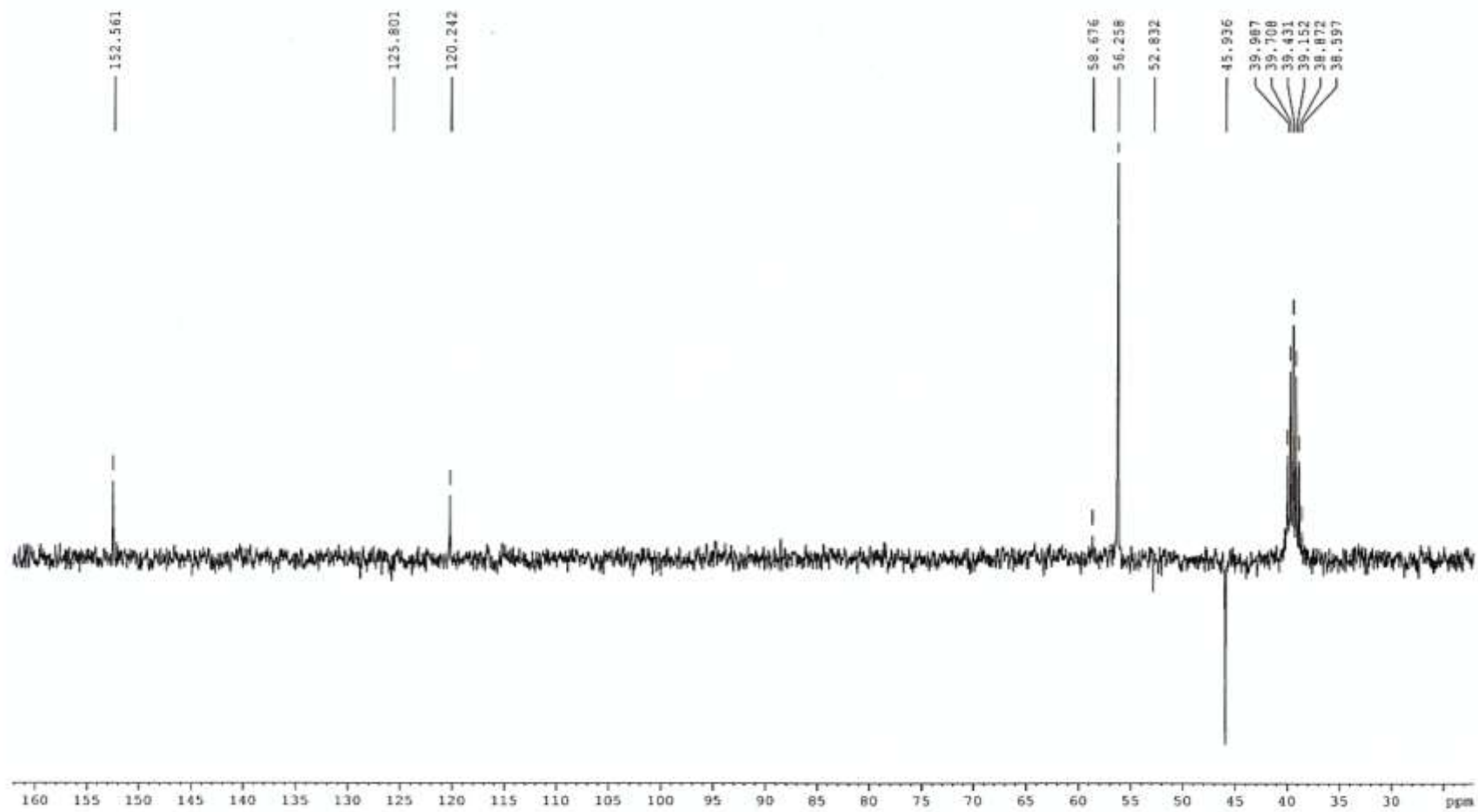
^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 5-bromo-2-(1-oxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2b**)



^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of 5-bromo-2-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**2b**)

sp 1308 13c jmod dms0 BGMV G-113 15.04.11 Big

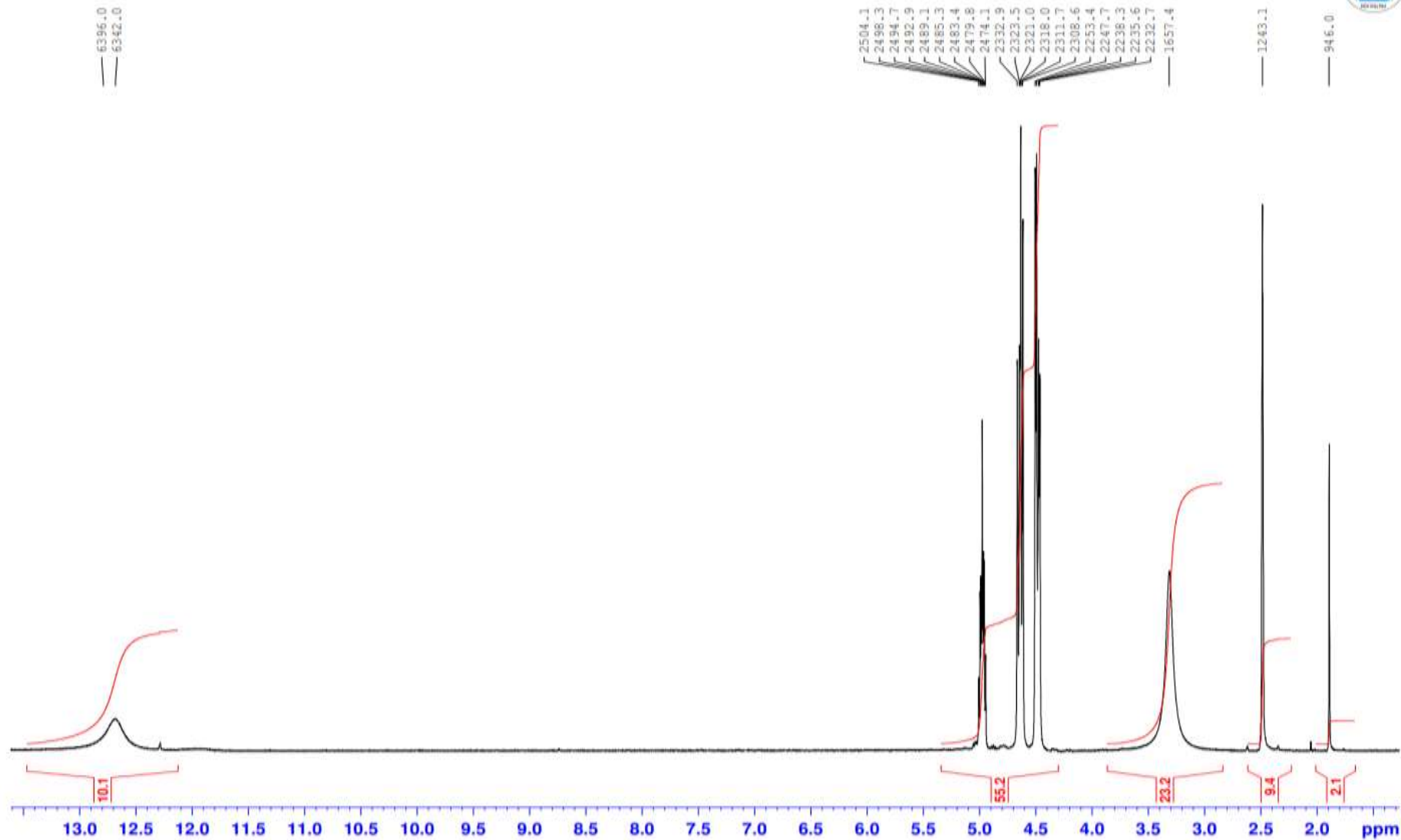
Institute of Organic Chemistry Ufa Scientific Centre of RAS 2011



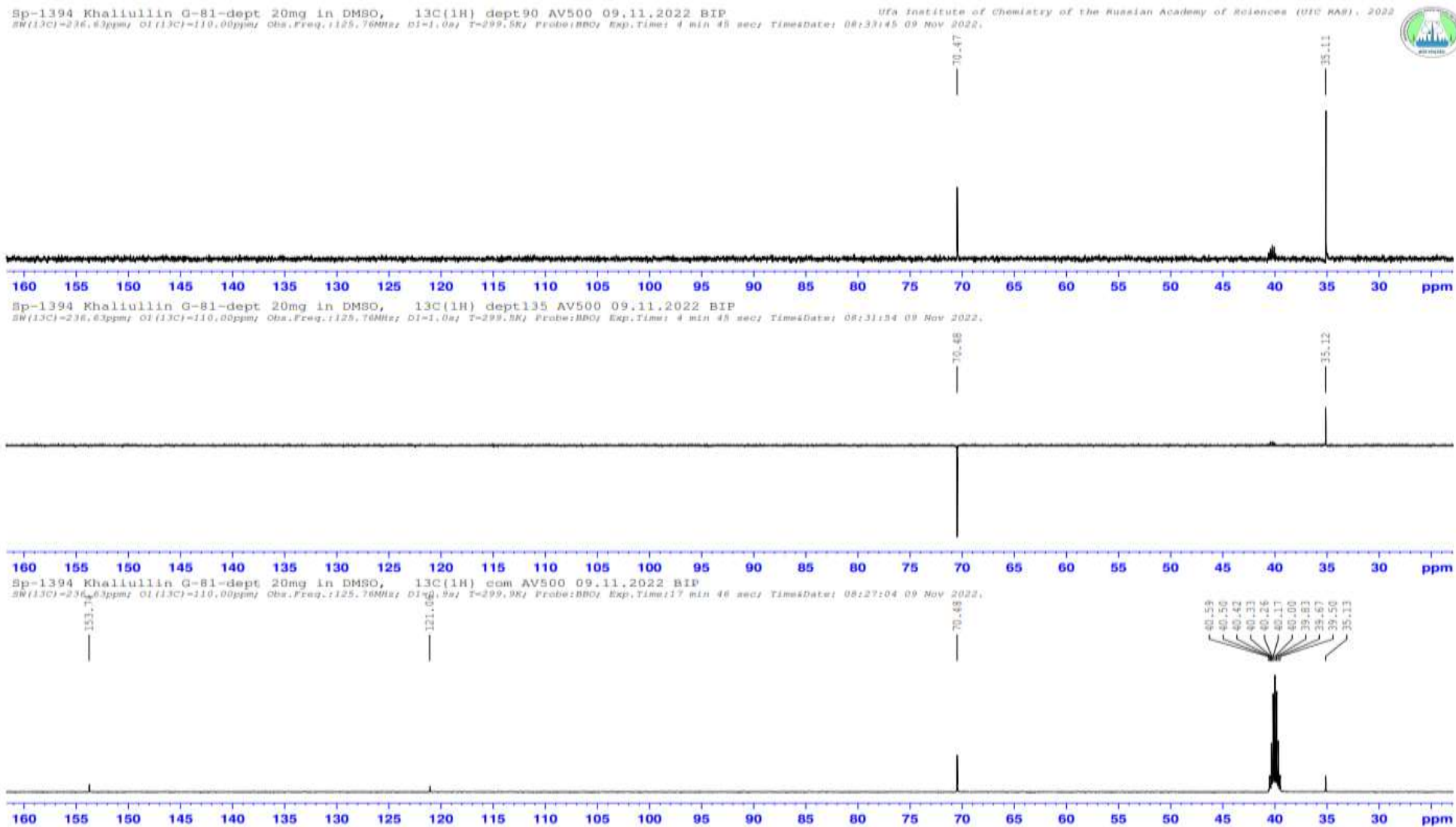
¹H NMR (500 MHz, DMSO-*d*₆) of 5-bromo-2-(1,1-dioxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2c**)

Sp-1394 Khaliullin G-81-dept 20mg in DMSO, 1H AV500 09.11.2022 BIP
SW(H)=19.99ppm; Q1(H)=7.00ppm; Obs.Freq.:500.13MHz; D1=2.0s; T=298.9K; Probe:BB0; Exp.Time: 7 sec; TimesDate: 08:06:21 09 Nov 2022.

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2022



^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of 5-bromo-2-(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**2c**)

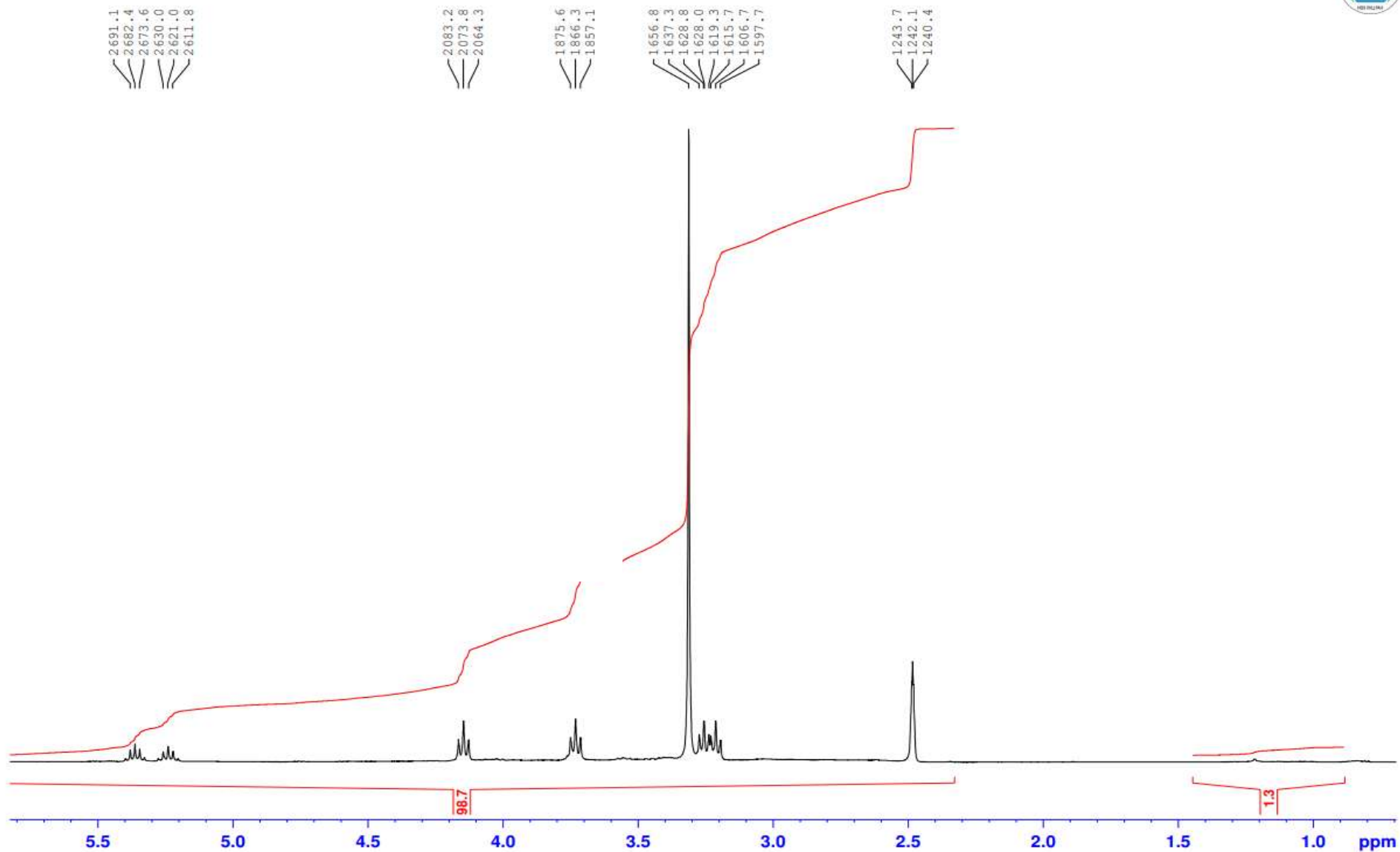


¹H NMR (500 MHz, DMSO-*d*₆) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)

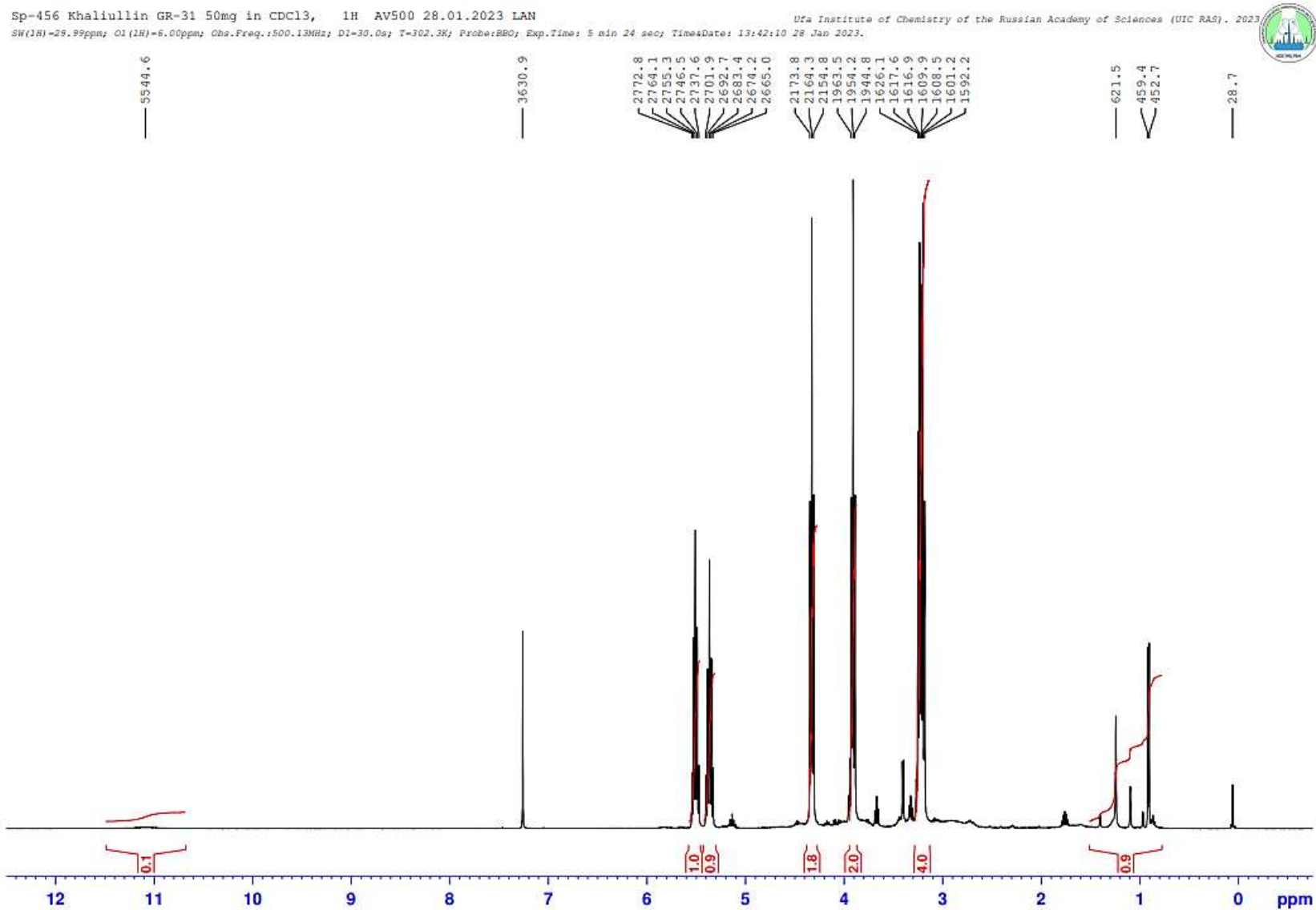
Sp-367 Khaliullin GP-31-dept 20mg in DMSO, 1H AV500 28.04.2022 BIP

Ufa Institute of Chemistry of the Russian Academy of Sciences (UIC RAS). 2022

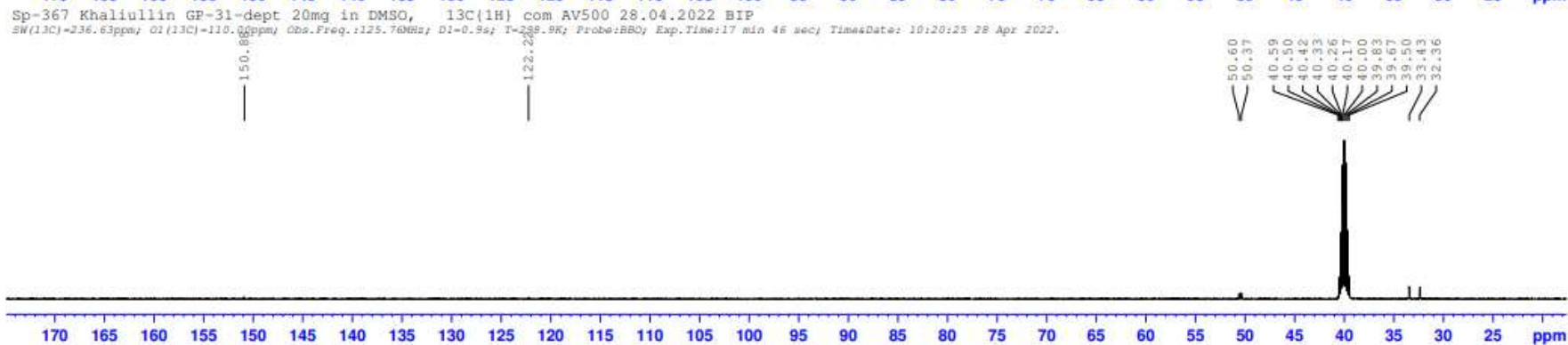
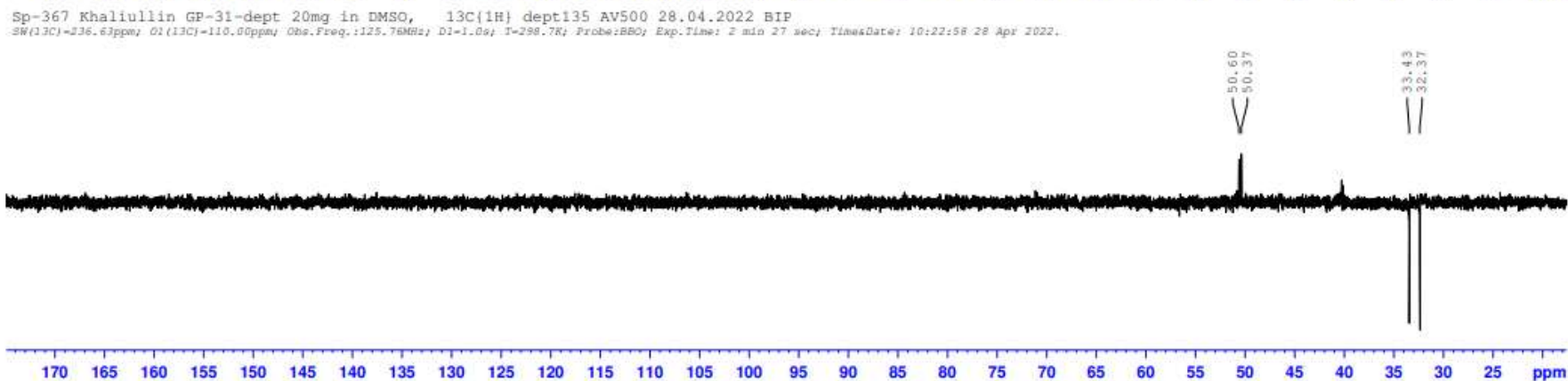
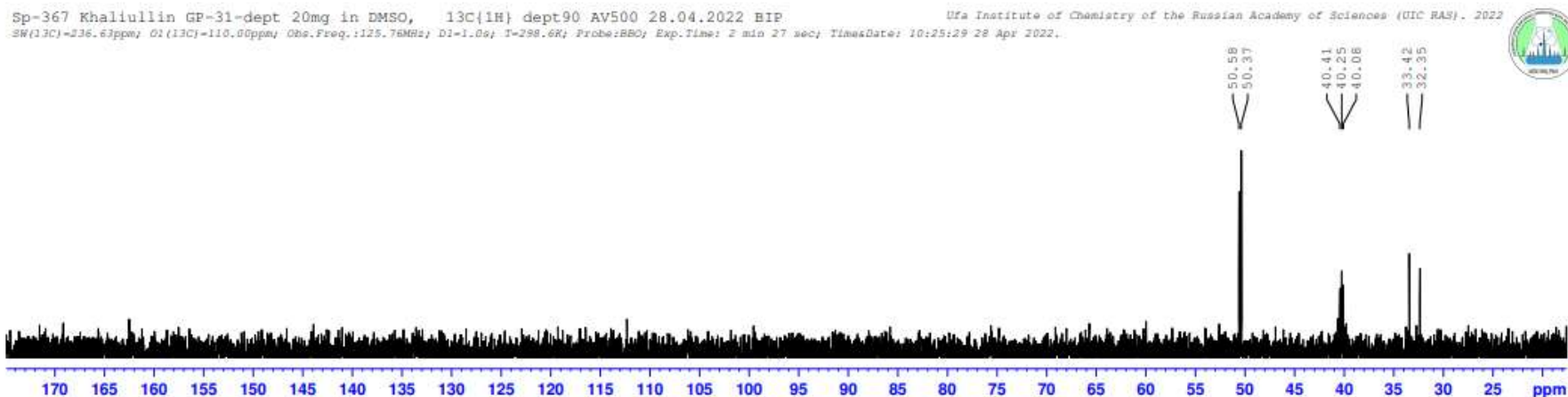
SW(1H)=19.99ppm; O1(1H)=7.00ppm; Obs.Freq.:500.13MHz; D1=2.0s; T=297.9K; Probe:BBO; Exp.Time: 7 sec; Time\$Date: 10:01:55 28 Apr 2022.



^1H NMR (500 MHz, CDCl_3) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)



^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)

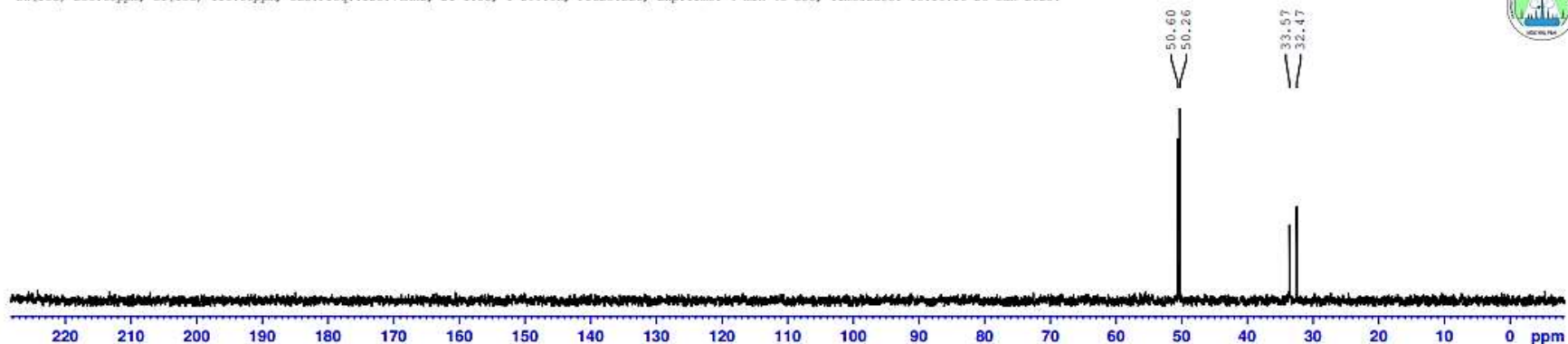


^{13}C NMR (125 MHz, CDCl_3) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)

Sp-456 Khaliullin GR-31 50mg in CDCl_3 , $^{13}\text{C}\{^1\text{H}\}$ dept90 AV500 28.01.2023 LAN

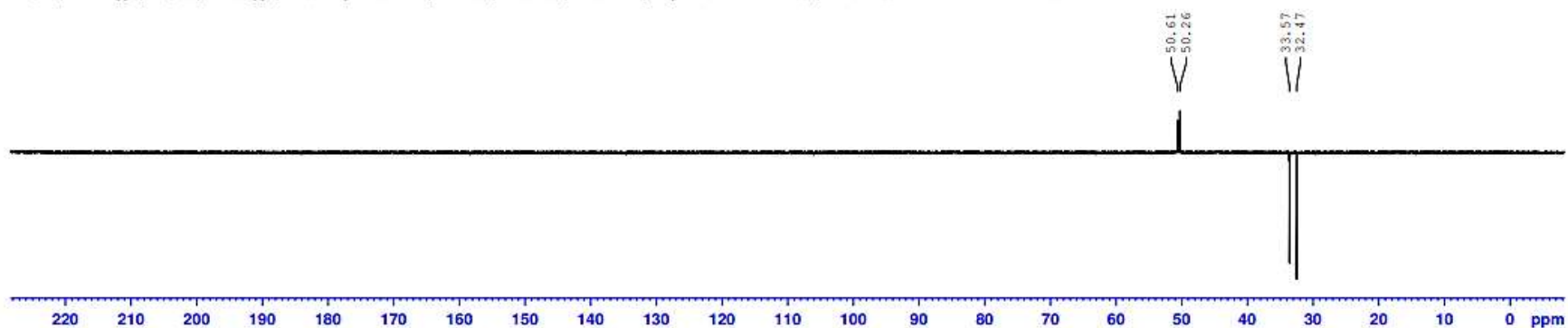
Ufa Institute of Chemistry of the Russian Academy of Sciences (UIC RAS). 2023

SW(^{13}C)=236.63ppm; O1(^{13}C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=299.9K; Probe:BB0; Exp.Time: 4 min 45 sec; TimesDate: 16:10:10 28 Jan 2023.



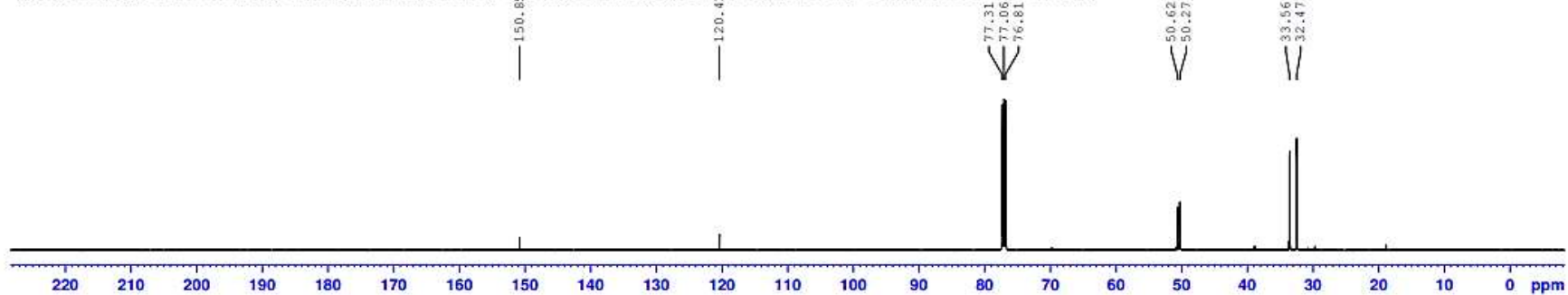
Sp-456 Khaliullin GR-31 50mg in CDCl_3 , $^{13}\text{C}\{^1\text{H}\}$ dept135 AV500 28.01.2023 LAN

SW(^{13}C)=236.63ppm; O1(^{13}C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=300.0K; Probe:BB0; Exp.Time: 4 min 45 sec; TimesDate: 16:05:22 28 Jan 2023.



Sp-456 Khaliullin GR-31 50mg in CDCl_3 , $^{13}\text{C}\{^1\text{H}\}$ com AV500 28.01.2023 LAN

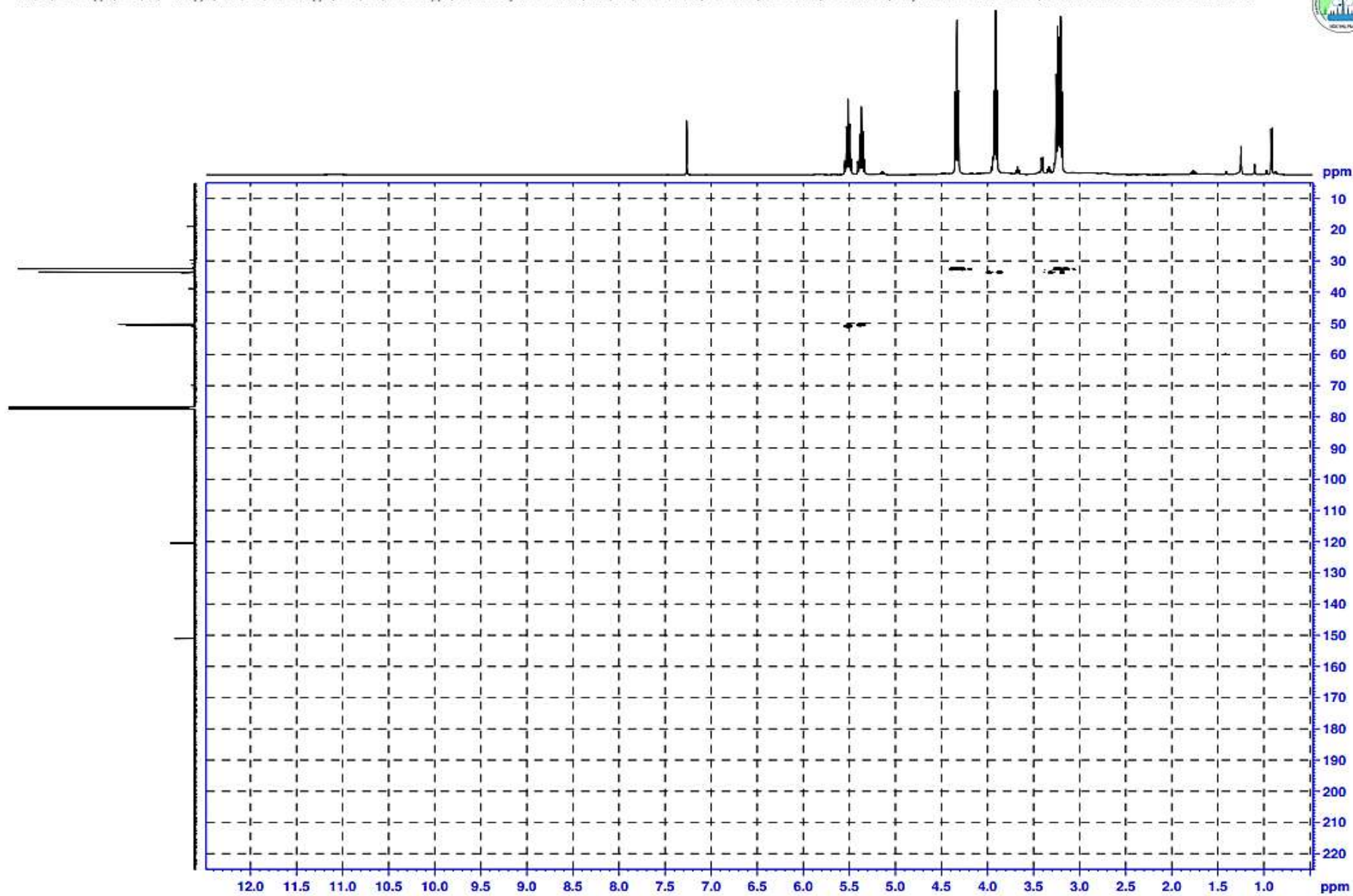
SW(^{13}C)=236.63ppm; O1(^{13}C)=110.00ppm; Obs.Freq.:125.76MHz; D1=0.9s; T=300.4K; Probe:BB0; Exp.Time: 2 h 45 min 19 sec; TimesDate: 16:00:35 28 Jan 2023.



^1H - ^{13}C HSQC (CDCl_3) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)

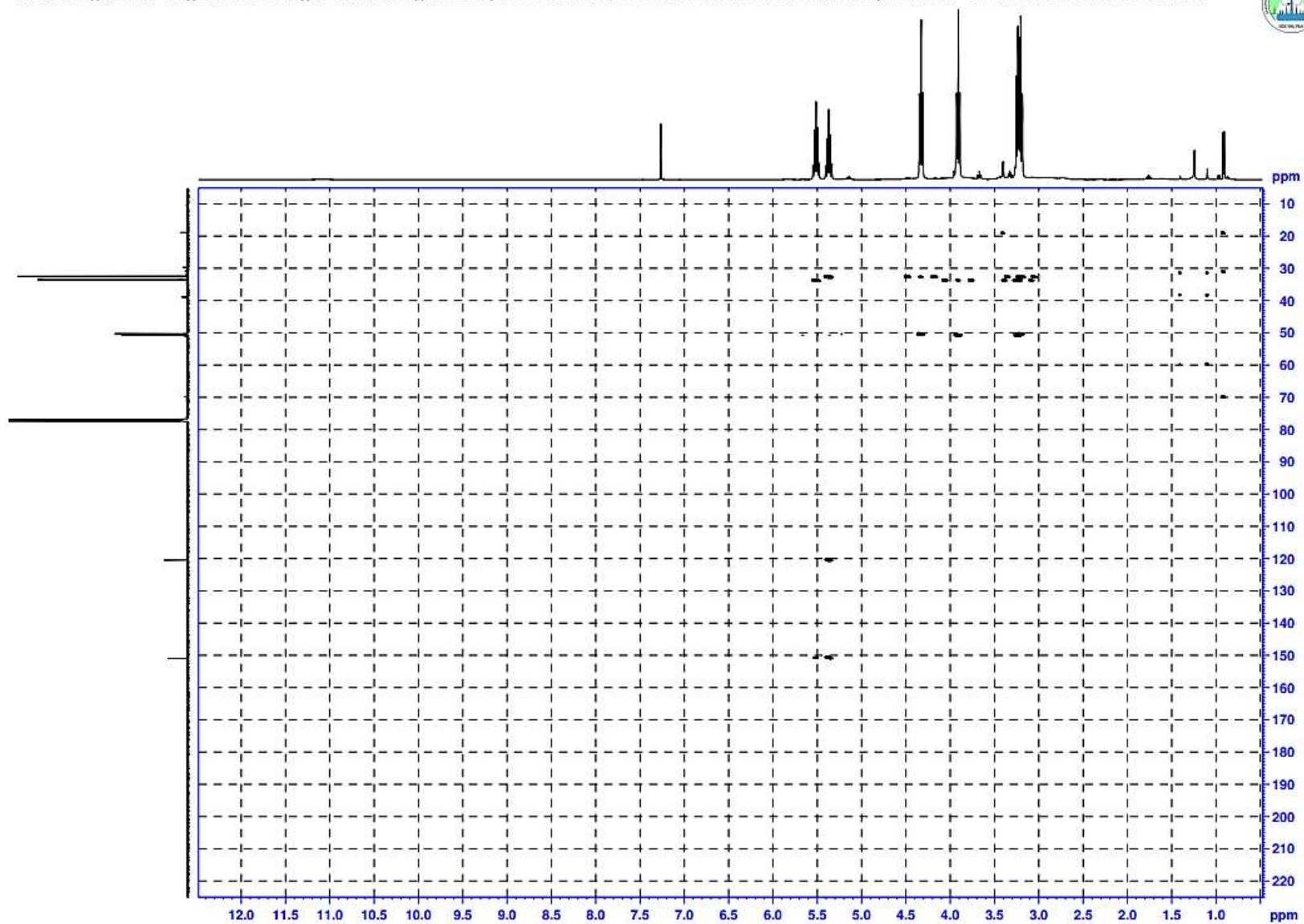
Sp-456 Khaliullin GR-31 50mg in CDCl_3 , (^1H , ^{13}C) HSQC AV500 28.01.2023 LAN
SW(^1H)=12.02ppm; O1(^1H)=6.50ppm; SW(^{13}C)=220.00ppm; O1(^{13}C)=115.00ppm; Obs.Freq.:500.13MHz; BF(^{13}C)=125.76MHz; D1=0.5s; T=305.2K; Probe:BB0; Exp.Time:15 min 12 sec; Time&Date: 13:18:59 28 Jan 2023.

Ufa Institute of Chemistry of the Russian Academy of Sciences (UIC RAS). 2023



^1H - ^{13}C HMBC (CDCl_3) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)

Sp-456 Khaliullin GR-31 50mg in CDCl_3 , $\{^1\text{H}, ^{13}\text{C}\}$ HMBC AV500 28.01.2023 LAN
SW(^1H)=12.02ppm; O1(^1H)=6.50ppm; SW(^{13}C)=220.00ppm; O1(^{13}C)=115.00ppm; Obs.Freq.=500.13MHz; BF(^{13}C)=125.76MHz; D1=0.8s; T=302.2K; Probe:BB0; Exp.Time:43 min 3 sec; TimeDate: 13:43:03 28 Jan 2023.

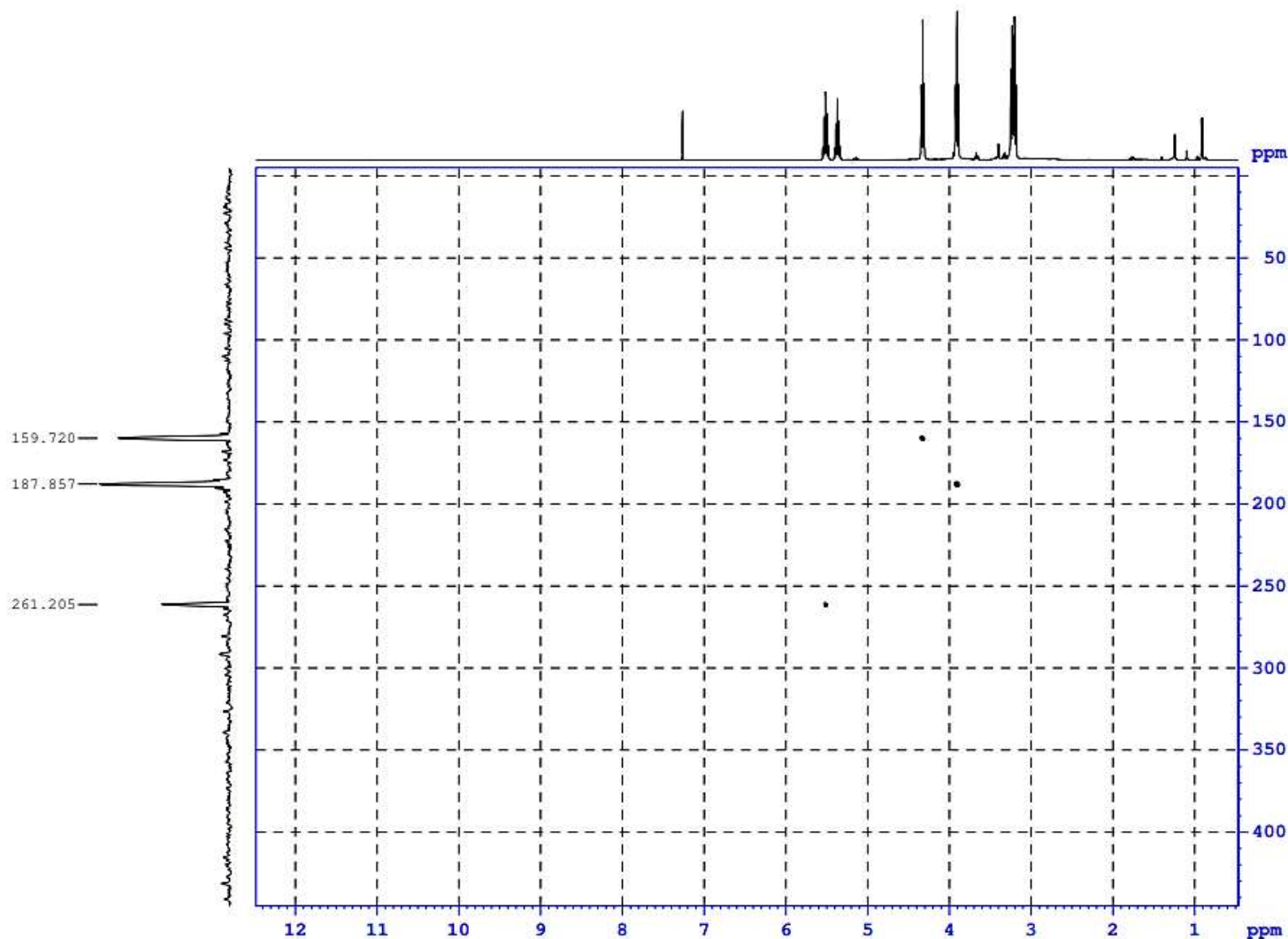


^1H - ^{15}N HMBC (CDCl₃) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)

Sp-456 Khaliullin GR-31 50mg in CDCl₃, $\{^1\text{H}, ^{15}\text{N}\}$ HMBC AV500 28.01.2023 LAN

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2023

SW(^1H)=12.02ppm; D1(^1H)=6.50ppm; SN(^{15}N)=449.99ppm; D1(^{15}N)=220.00ppm; Obs.Freq.=500.13MHz; RF(^{15}N)=50.68MHz; D1=0.4s; T=300.3K; Probe:BB0; Exp.Time:31 min 5 sec; TimesDate: 16:26:57 28 Jan



Current Data Parameters
NAME Imi-GR-31-CDCl3
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230128
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmqcpgndqf
TD 4096
SOLVENT CDCl3
NS 8
DS 32
SWH 6009.615 F
FIDRES 1.467191 F
AQ 0.3408372 s
RG 201.51
DM 83.200 s
DE 6.50 s
TE 300.3 K
CNST13 3.5000000
DD 0.00000300 s
D1 0.40000001 s
D6 0.14285710 s
D16 0.00010000 s
INO 0.00002190 s

----- CHANNEL f1 -----
NUC1 ^1H
P1 11.50 s
P2 23.00 s
PLN1 15.84899998 s
SF01 500.1332508 MHz

----- CHANNEL f2 -----
NUC2 ^{15}N
P3 15.00 s
PLN2 158.49000549 s
SF02 50.6888821 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GP21 70.00 s
GP22 30.00 s
GP23 50.10 s
P16 1000.00 s

F1 - Acquisition parameters
TD 256
SF01 50.68888 MHz
FIDRES 89.099770 F
SN 449.991 F
FhMODE QF

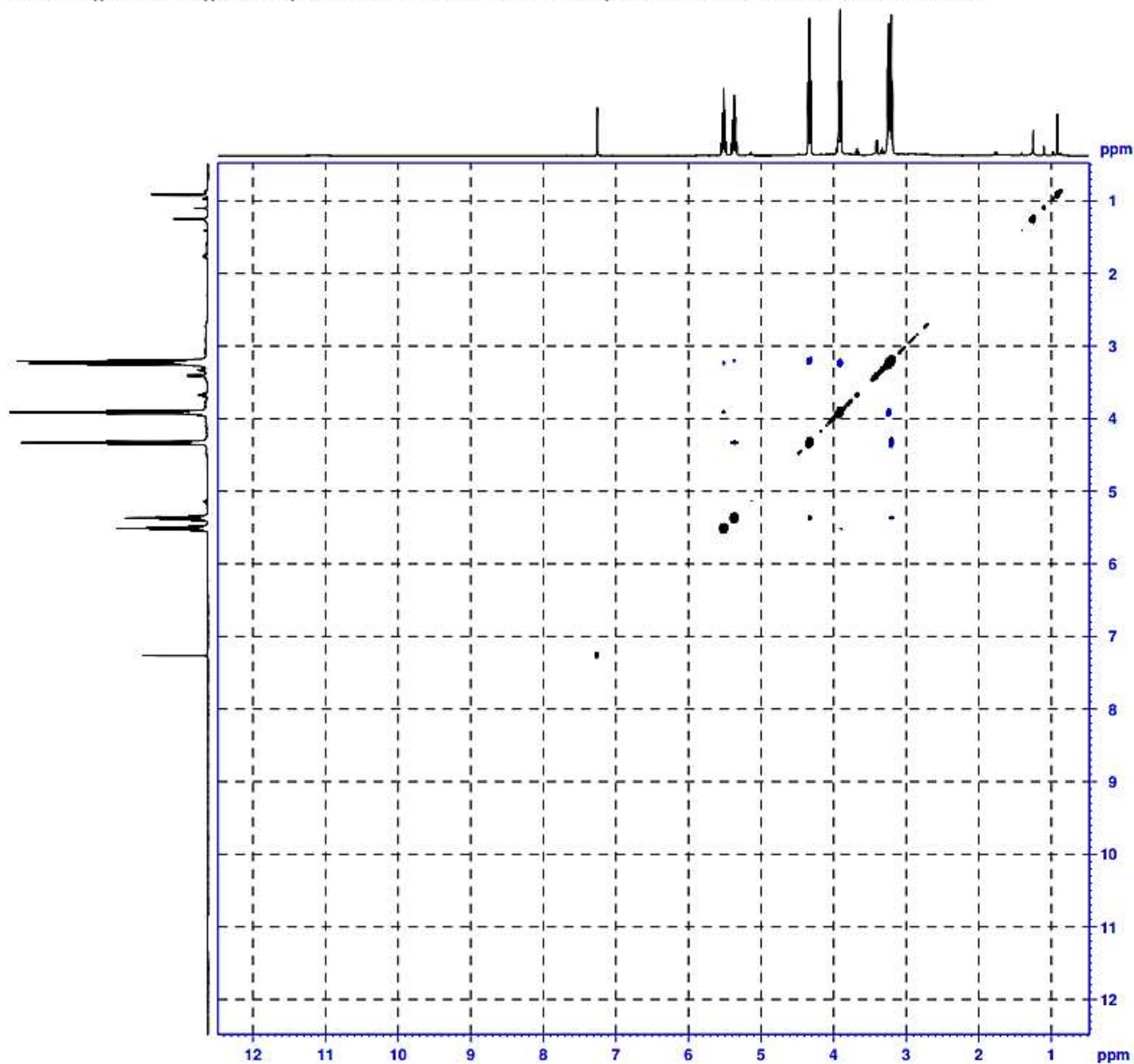
F2 - Processing parameters
SI 2048
SF 500.1300132 MHz
MDN QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 50.6777330 MHz
MDN
SSB 2
LB 0 Hz
GB 0

^1H - ^1H NOESY (CDCl_3) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)

Sp-456 Khaliullin GR-31 50mg in CDCl_3 , $\{^1\text{H}, ^1\text{H}\}$ NOESY AV500 28.01.2023 LAN
SW(^1H)=12.02ppm; O1(^1H)=6.50ppm; Obs.Freq.:500.13MHz; D1=1.5s; T=299.8K; Proba:BB0; Exp.Time:20 min 46 sec; TimesDate: 14:43:23 28 Jan 2023.

Ufa Institute of Chemistry of the Russian Academy of Sciences (UTC RAS)



Current Data Parameters
NAME hmi-GR-31-CDCl3
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230128
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
FULPROG noesygpph
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 1.467191 Hz
AQ 0.3408372 sec
RG 127.49
DW 83.200 usec
DE 6.50 usec
TE 299.8 K
DO 0.0006856 sec
D1 1.50000000 sec
D8 0.50000000 sec
D16 0.00010000 sec
INO 0.00016640 sec

----- CHANNEL f1 -----
NUC1 ^1H
P1 11.50 usec
P2 23.00 usec
PLW1 15.84899998 W
SFO1 500.132508 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
CPZ1 40.00 %
P16 1000.00 usec

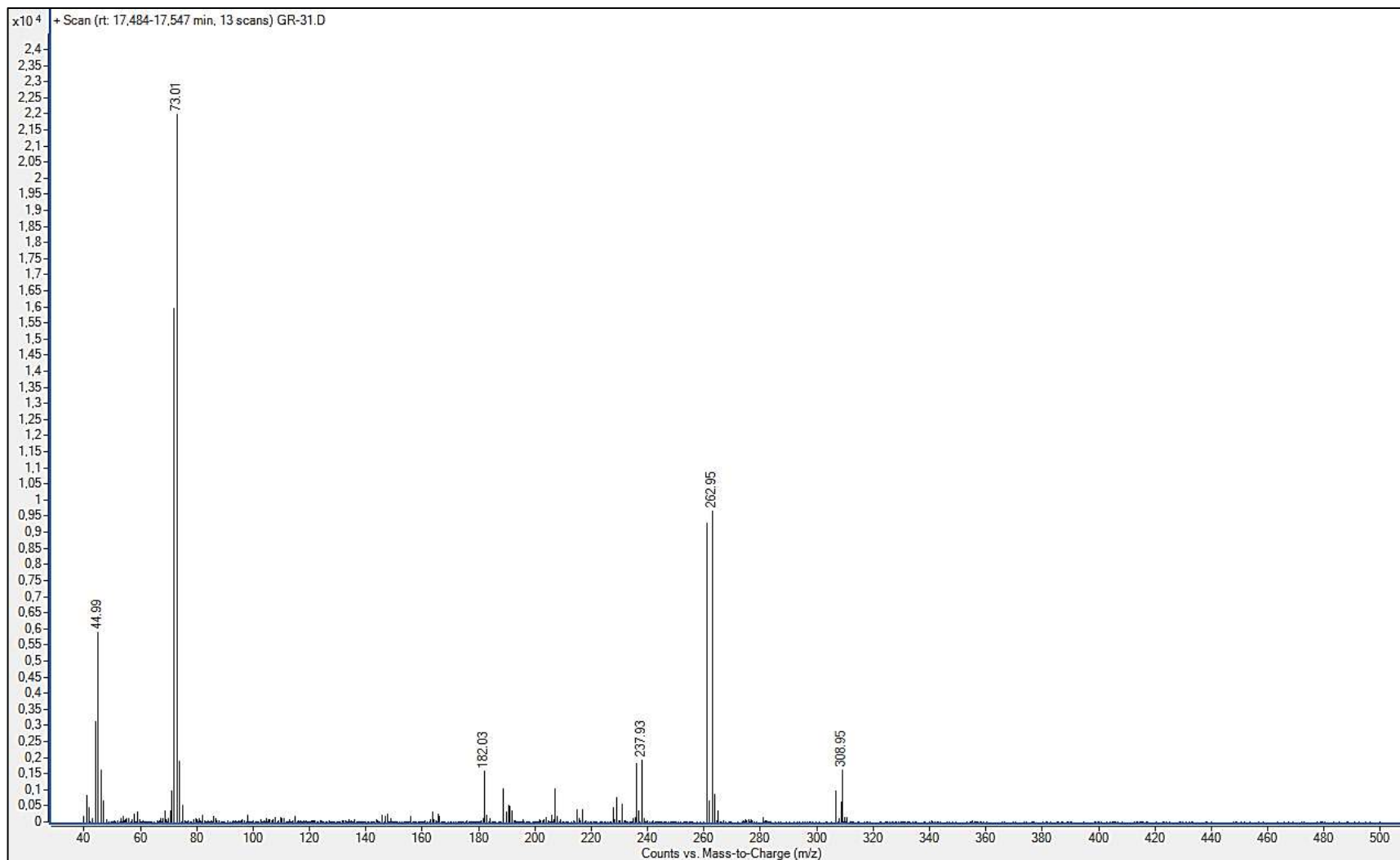
F1 - Acquisition parameters
TD 256
SFO1 500.1333 MHz
FIDRES 23.475060 Hz
SW 12.016 ppm
FwMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1300132 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 500.1300132 MHz
WDW echo-antlecho
SSB 2
LB 0 Hz
GB 0

Mass spectrum (EI, 70 eV) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5a**)

Spectrum Plot Report

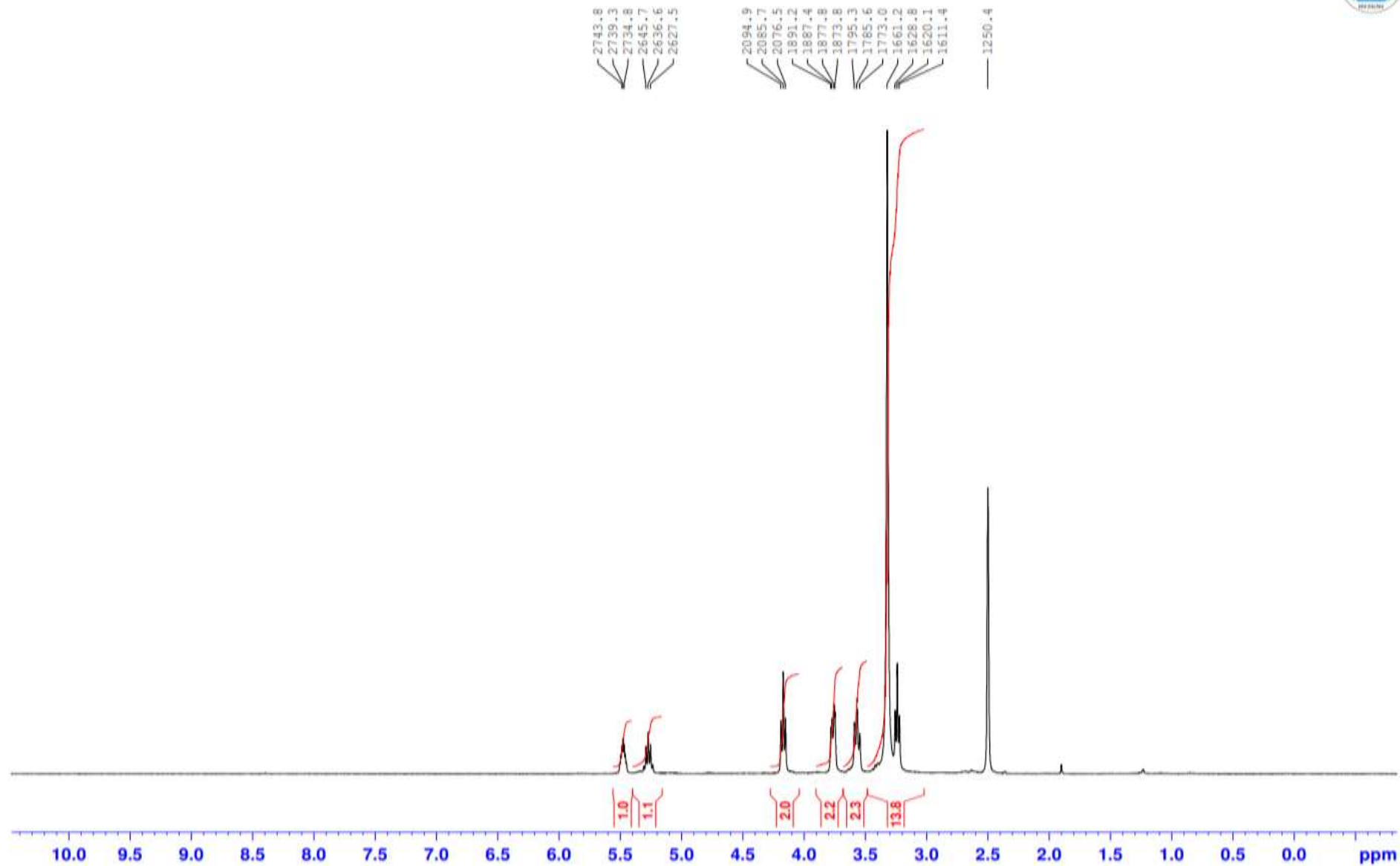


¹H NMR (500 MHz, DMSO-*d*₆) of 5-bromo-2-(1-oxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5b**)

Sp-1378 Khaliullin GR-36 20mg in DMSO, ¹H AV500 05.03.2022 LAN

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2022

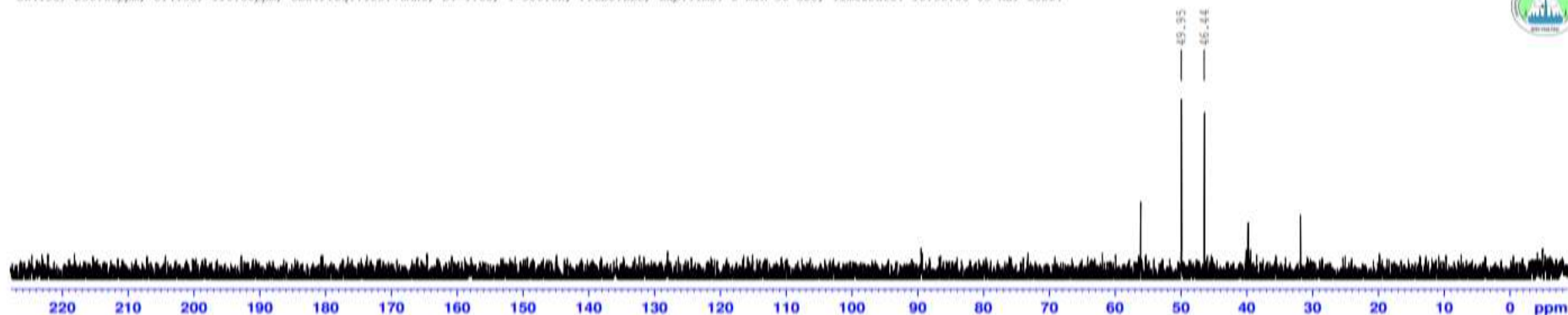
HN(1H)-19.99ppm; Q1(1H)=7.00ppm; Obs.Freq.:1500.13MHz; D1=20.0s; T=299.7K; Probe:BBQ; Exp.Time: 1 min 35 sec; TimesDate: 10:23:41 05 Mar 2022;



¹³C NMR (125 MHz, DMSO-*d*₆) of 5-bromo-2-(1-oxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5b**)

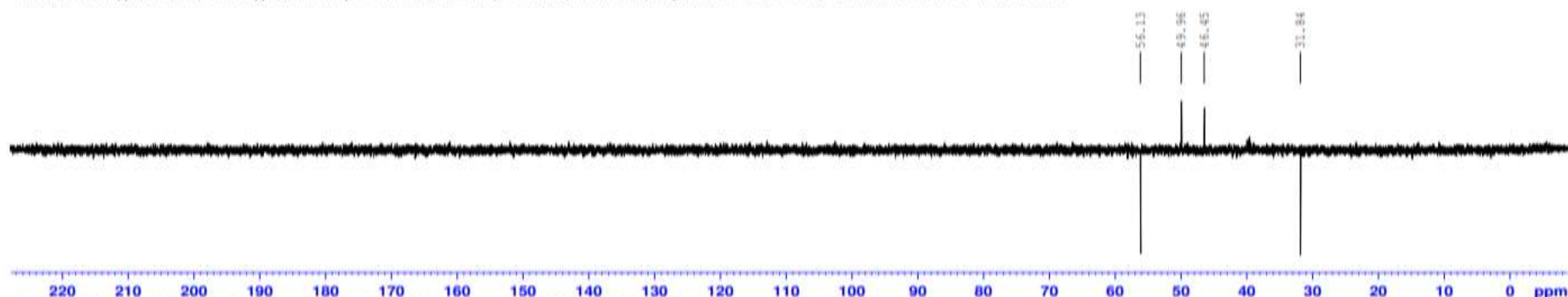
Sp-1378 Khaliullin GR-36 20mg in DMSO, ¹³C(1H) dept90 AV500 05.03.2022 LAN
BW(13C)=236.63ppm; D1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=300.0K; Probe:BB0; Exp.Time: 2 min 36 sec; TimeDate: 10:38:00 05 Mar 2022.

Ufa Institute of Chemistry of the Russian Academy of Sciences (UIC RAS), 2022



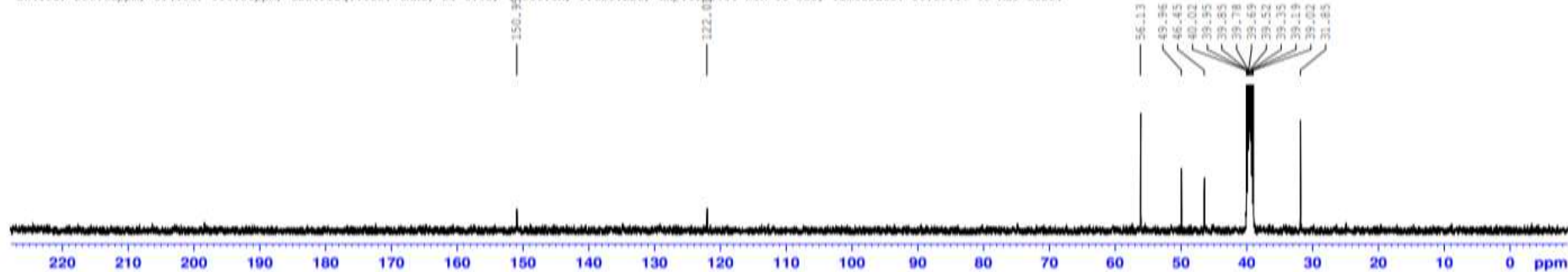
Sp-1378 Khaliullin GR-36 20mg in DMSO, ¹³C(1H) dept135 AV500 05.03.2022 LAN

BW(13C)=236.63ppm; D1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=300.0K; Probe:BB0; Exp.Time: 2 min 27 sec; TimeDate: 10:35:21 05 Mar 2022.



Sp-1378 Khaliullin GR-36 20mg in DMSO, ¹³C(1H) com AV500 05.03.2022 LAN

BW(13C)=236.63ppm; D1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=300.0K; Probe:BB0; Exp.Time: 11 min 10 sec; TimeDate: 10:39:16 05 Mar 2022.



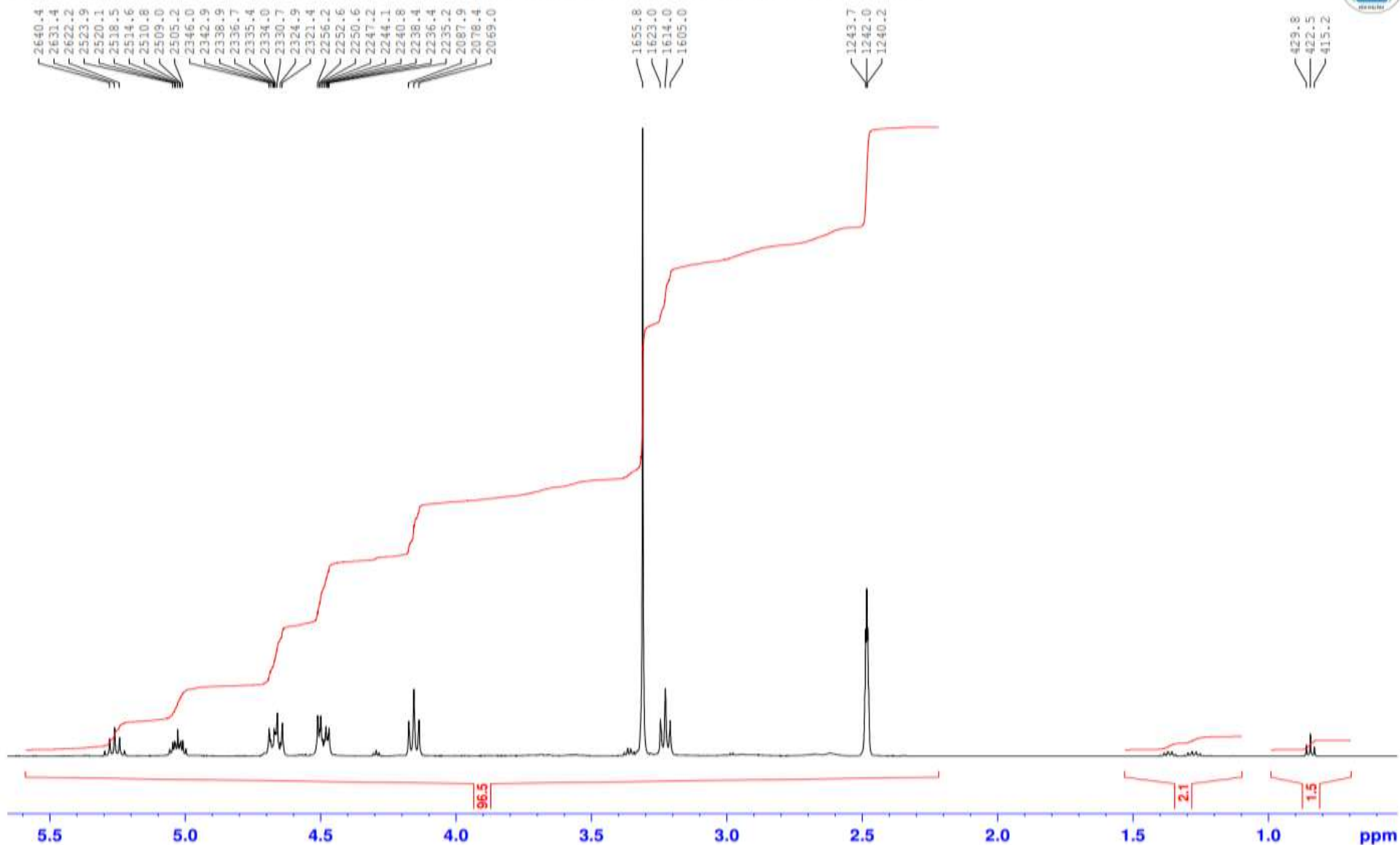
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5c**)

Sp-366 Khaliullin GR-38 20mg in DMSO, ^1H AV500 28.04.2022 LAN

Dfa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2022



$\text{BW}(1\text{H})=19.90\text{ppm}$ $\text{O1}(1\text{H})=7.00\text{ppm}$ Obs. Freq.: 500.13MHz; D1=20.0s; T=297.2K; Probe: BBO; Exp. Time: 1 min 35 sec; Time & Date: 08:29:12 28 Apr 2022.



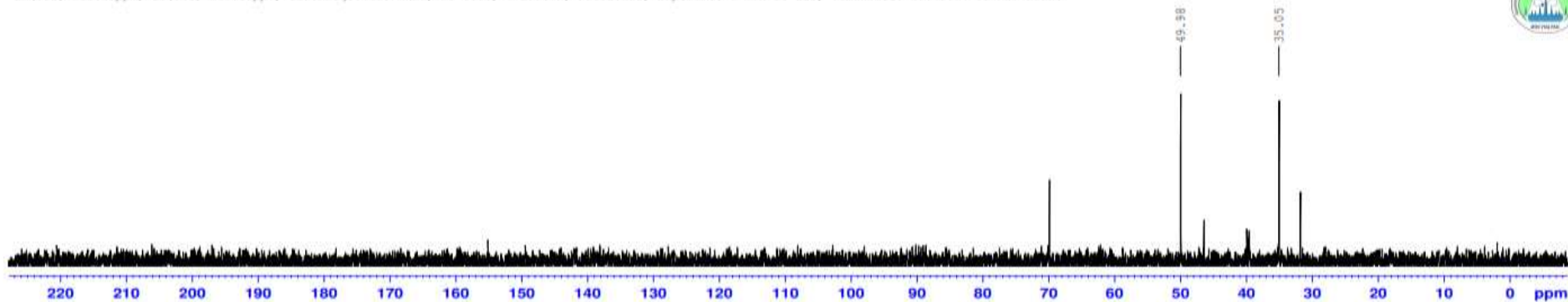
^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5c**)

Sp-1379 Khaliullin GR-38 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept90 AV500 05.03.2022 LAN

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2022

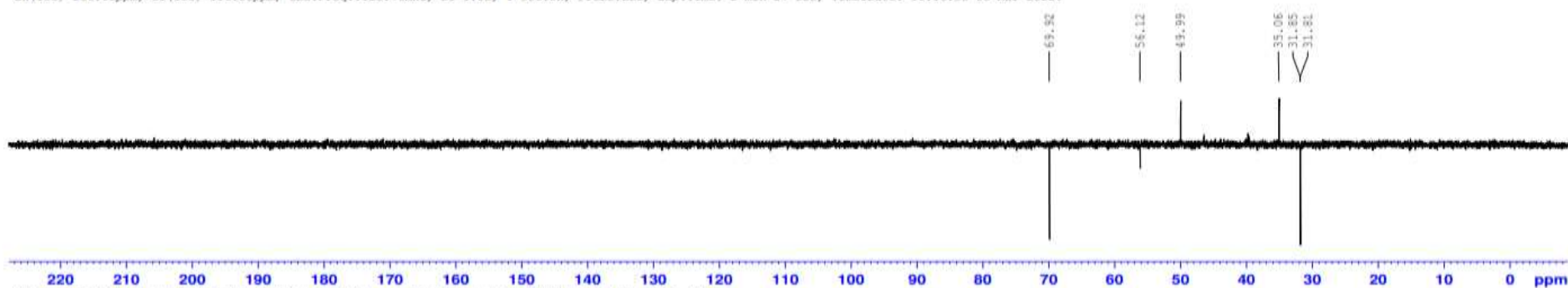


SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=299.9K; Probe:BBO; Exp.Time: 2 min 36 sec; TimeDate: 10:10:17 05 Mar 2022.



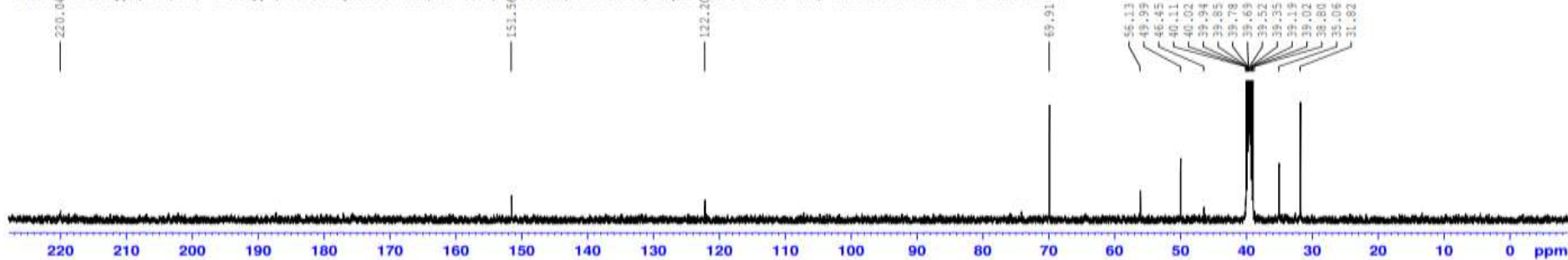
Sp-1379 Khaliullin GR-38 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept135 AV500 05.03.2022 LAN

SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=300.0K; Probe:BBO; Exp.Time: 2 min 27 sec; TimeDate: 10:16:38 05 Mar 2022.



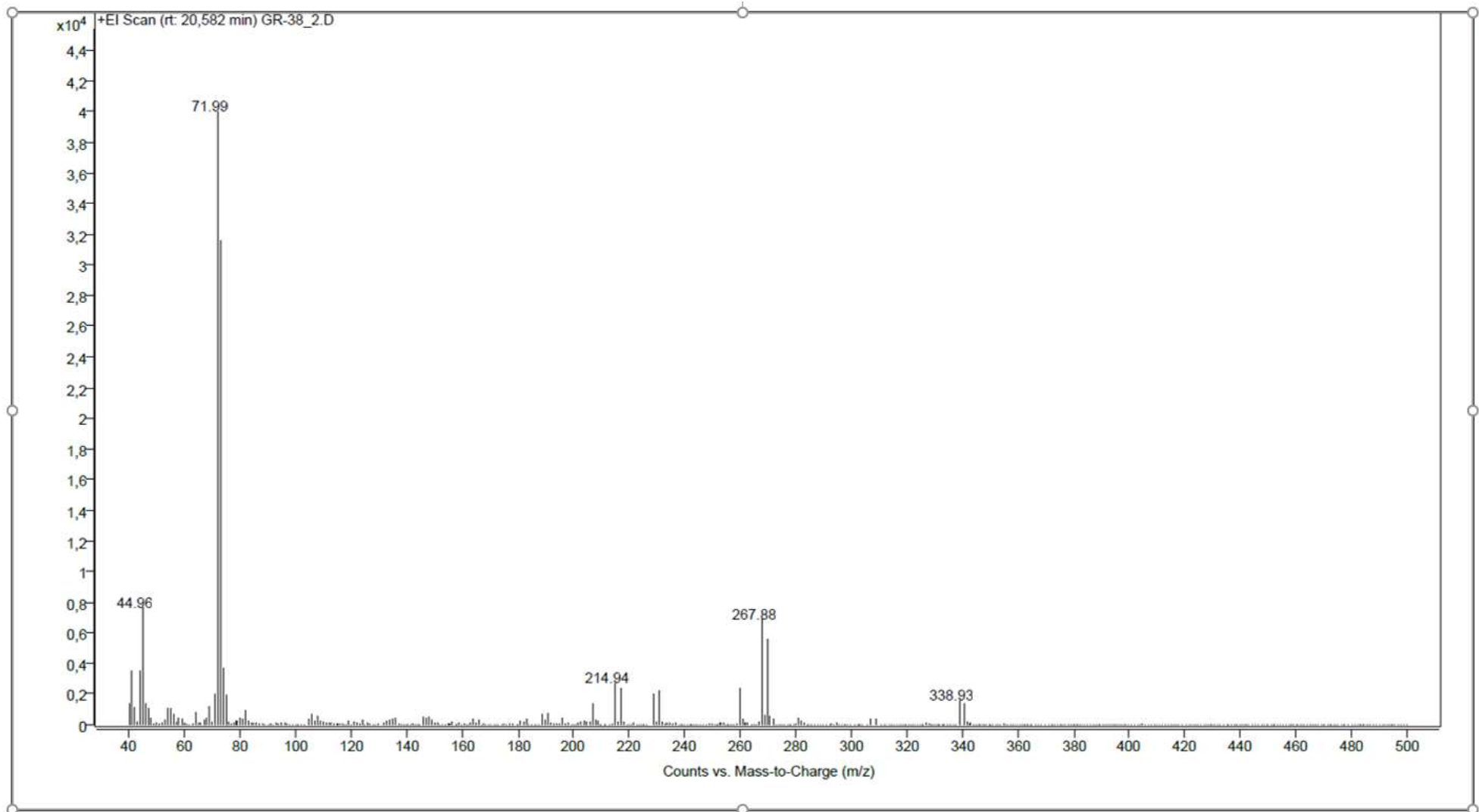
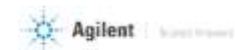
Sp-1379 Khaliullin GR-38 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ com AV500 05.03.2022 LAN

SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=0.9s; T=300.2K; Probe:BBO; Exp.Time: 8 min 58 sec; TimeDate: 10:14:05 05 Mar 2022.



Mass spectrum (EI, 70 eV) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**5c**)

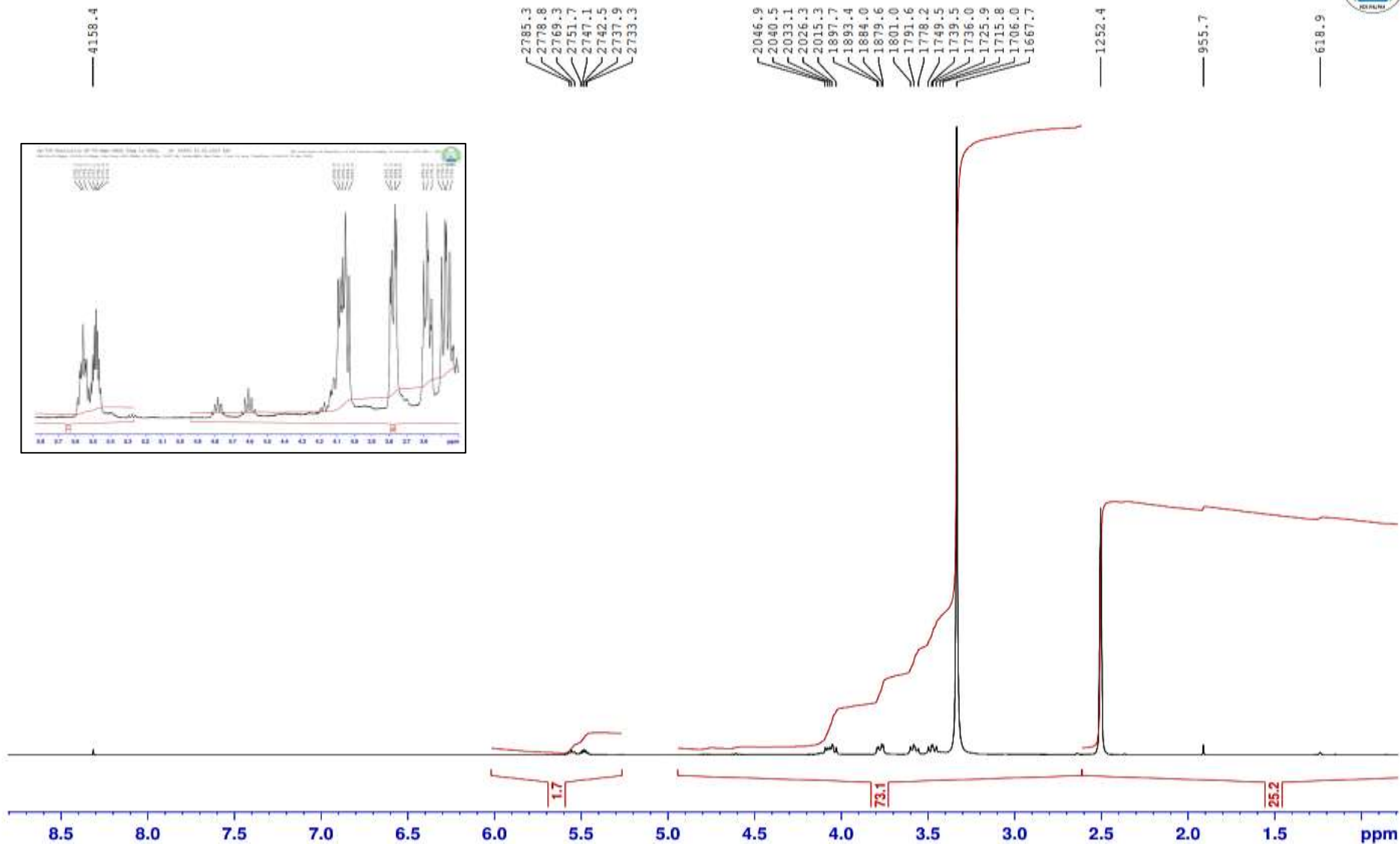
Spectrum Plot Report



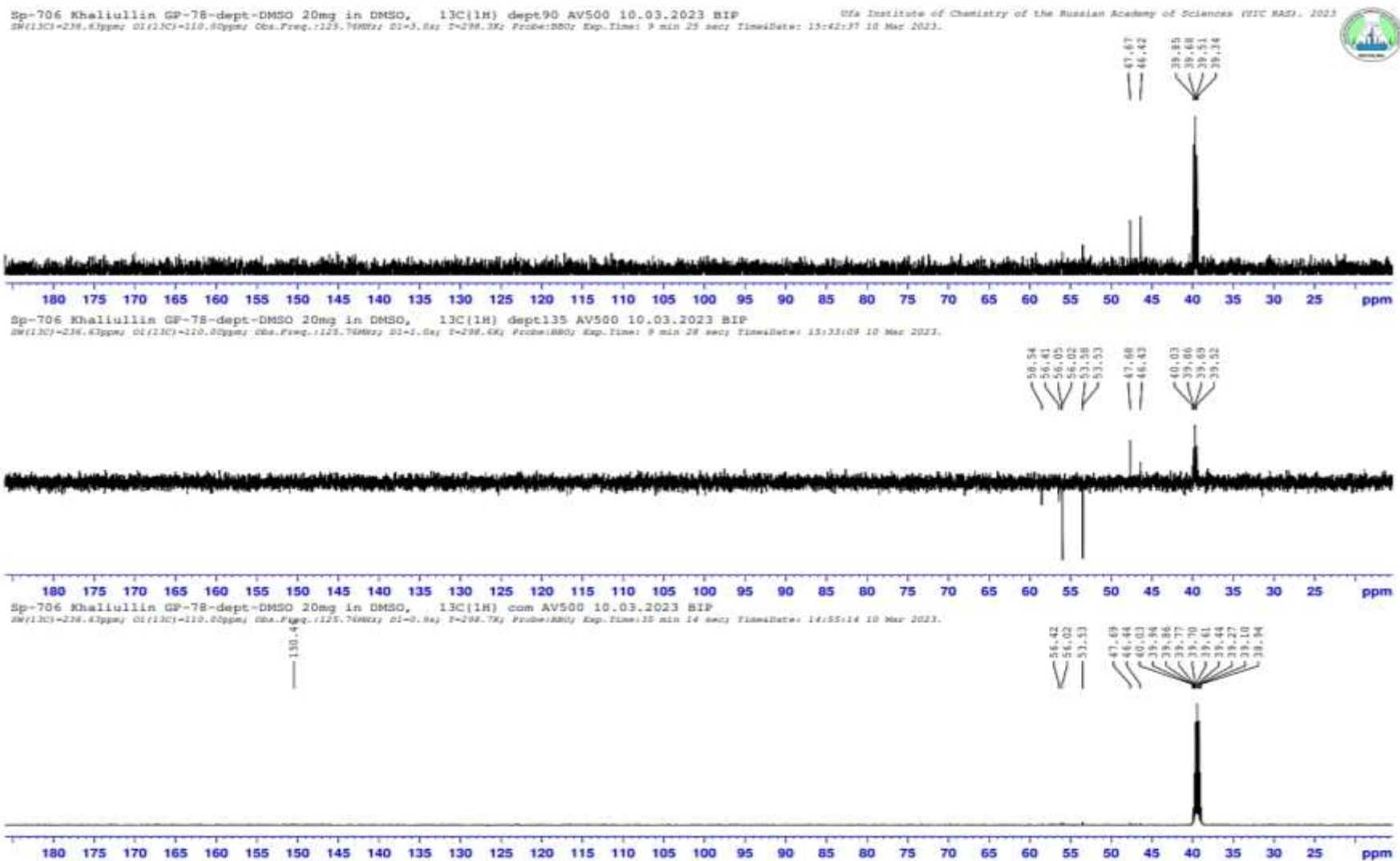
^1H NMR (500 MHz, $\text{DMSO}-d_6$) of 5-bromo-2,4-bis(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**6a**)

Sp-706 Khaliullin GP-78-dept-DMSO 20mg in DMSO, ^1H AV500 10.03.2023 BIP
SW(^1H)=29.99ppm; CI(^1H)=6.00ppm; Obs.Freq.:500.13MHz; D1=30.0s; T=297.9K; Probe:BBQ; Exp.Time: 5 min 24 sec; TimeDate: 14:48:12 10 Mar 2023.

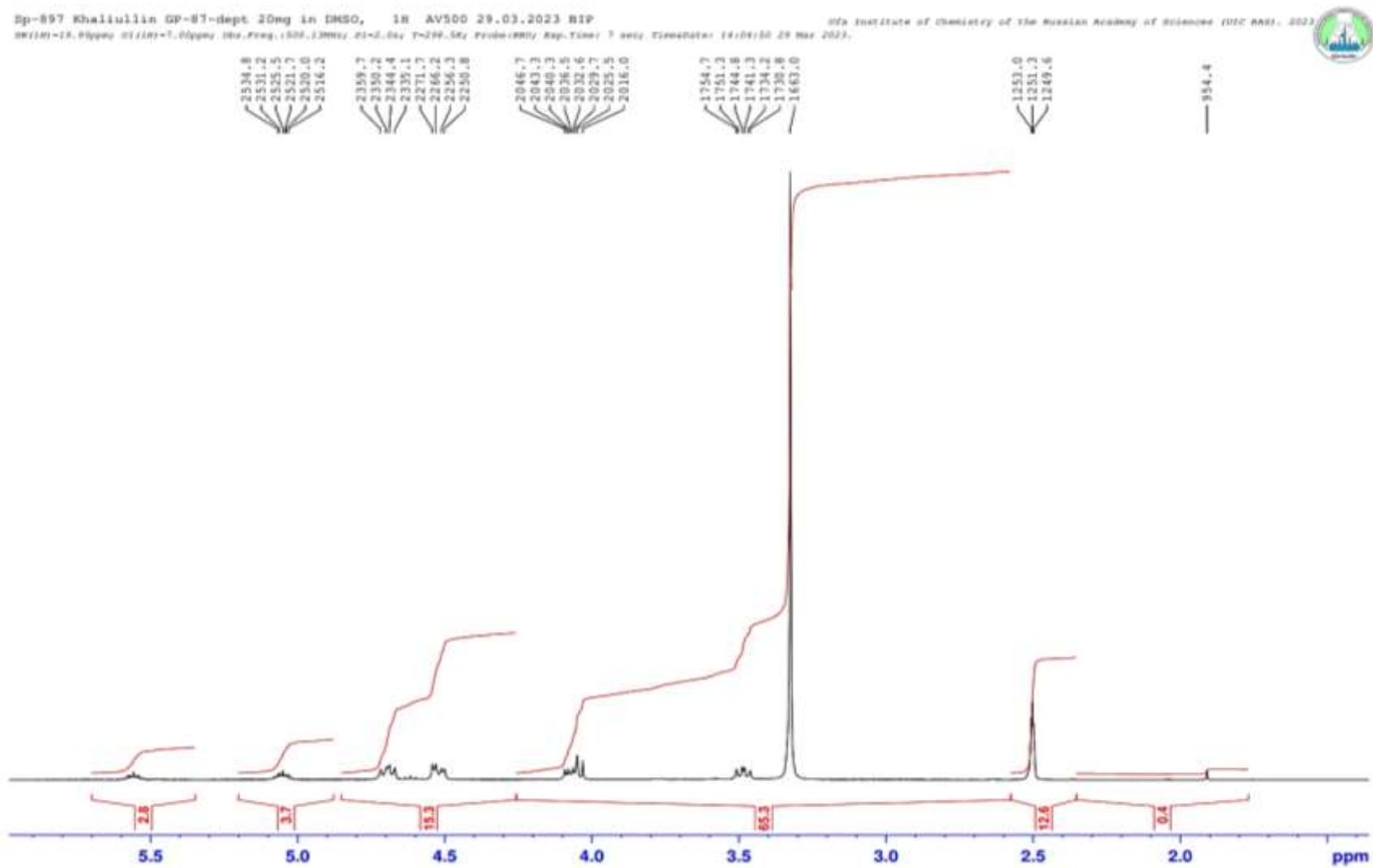
Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2023



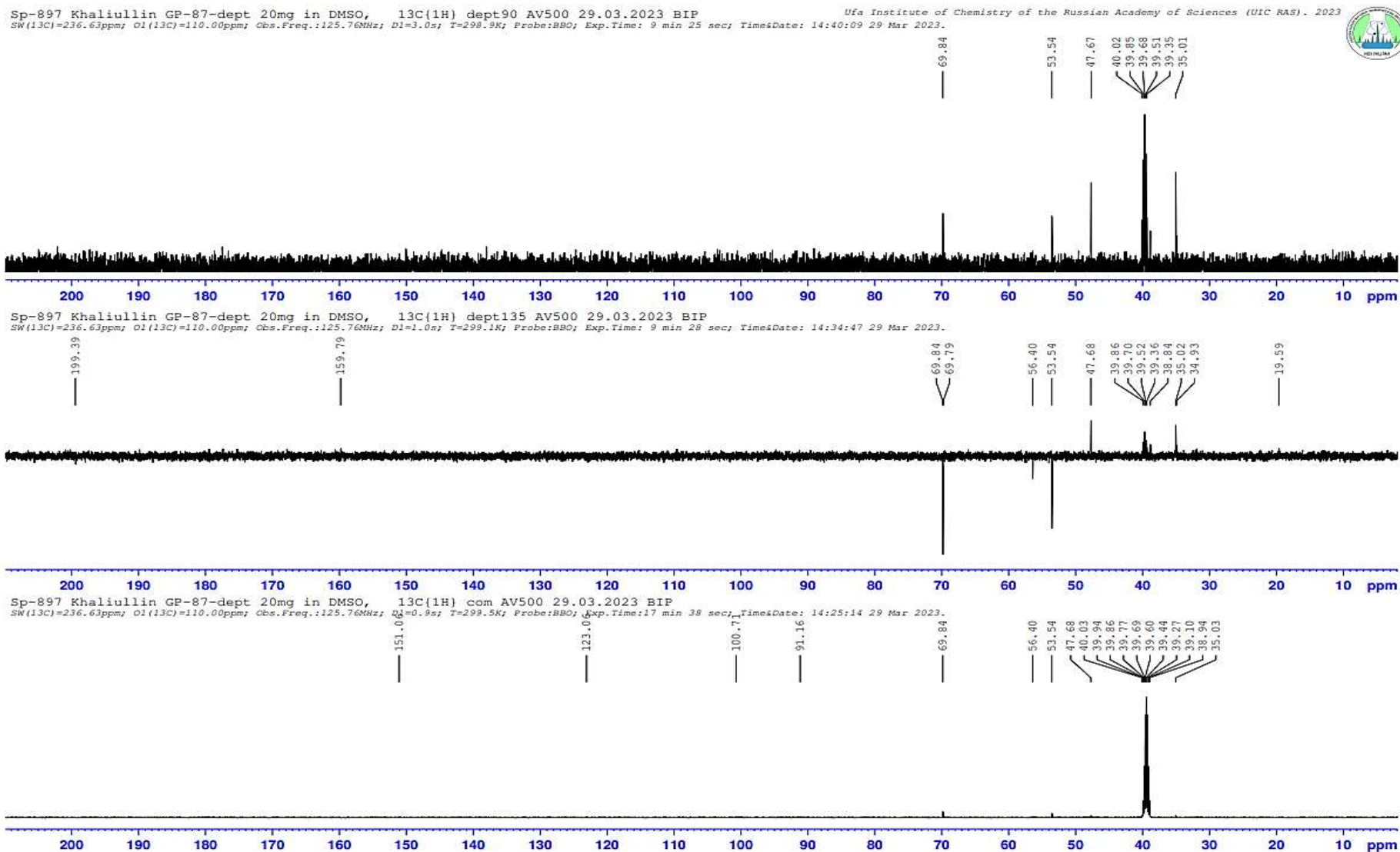
^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) of 5-bromo-2,4-bis(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**6a**)



^1H NMR (500 MHz, $\text{DMSO}-d_6$) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**6b**)



^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**6b**)

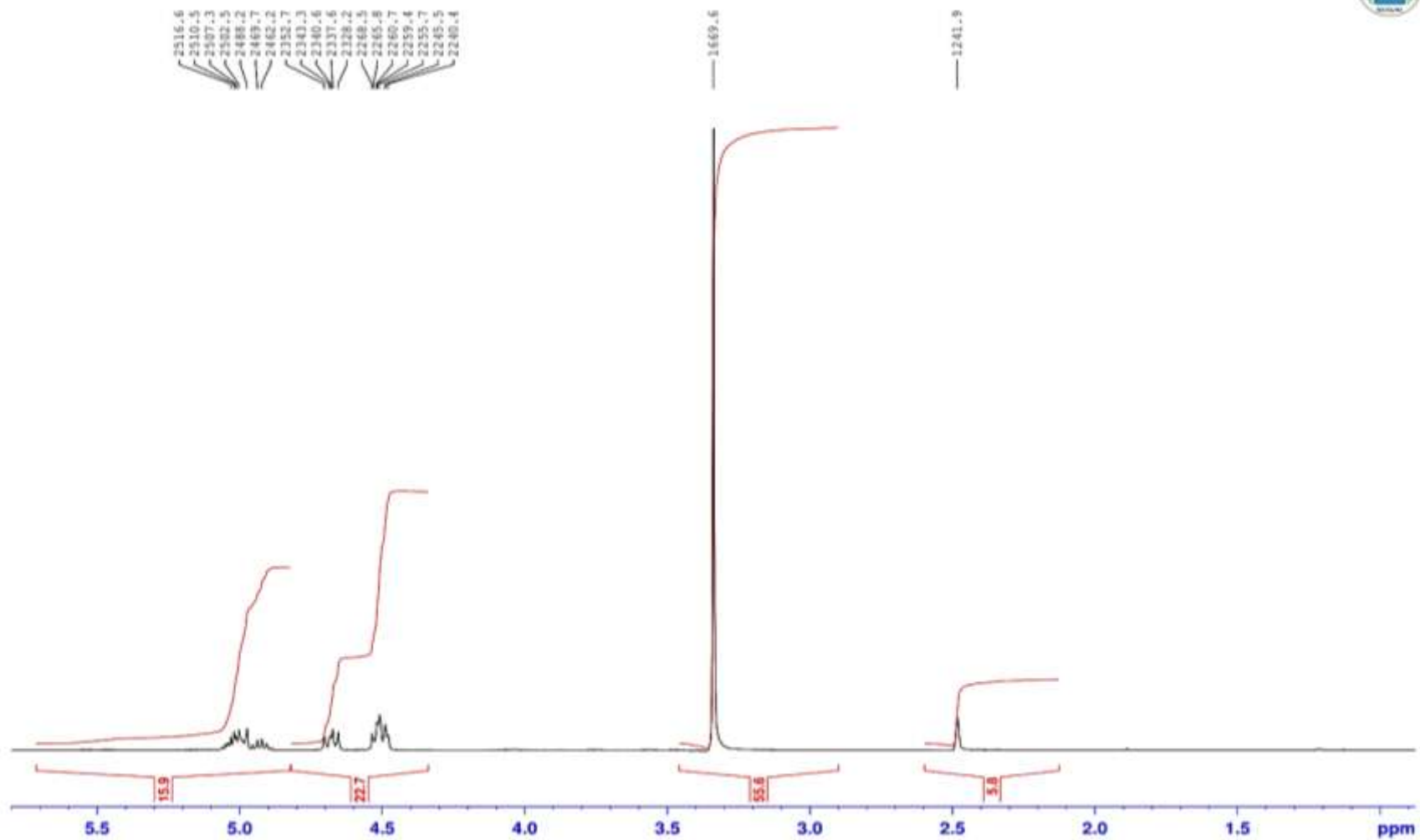


^1H NMR (500 MHz, $\text{DMSO-}d_6$) of 5-bromo-2,4-bis(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**6c**)

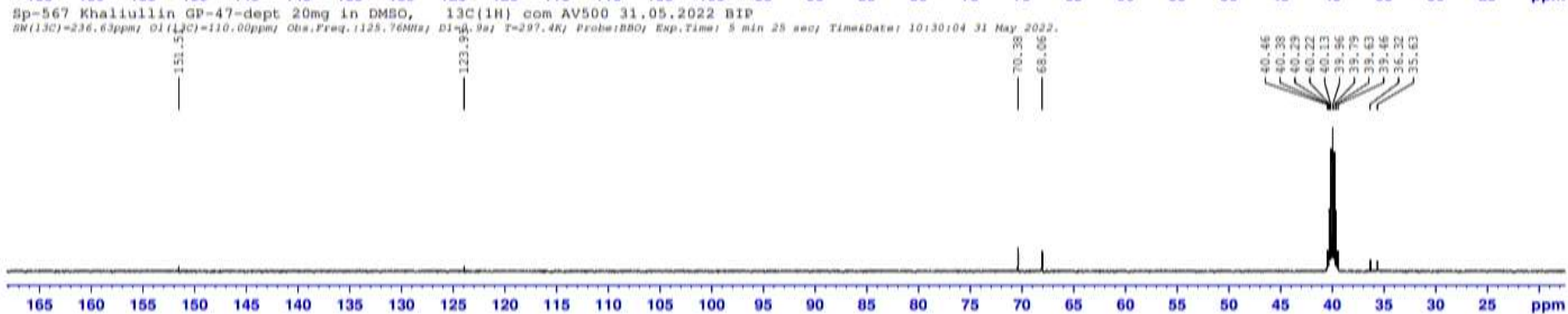
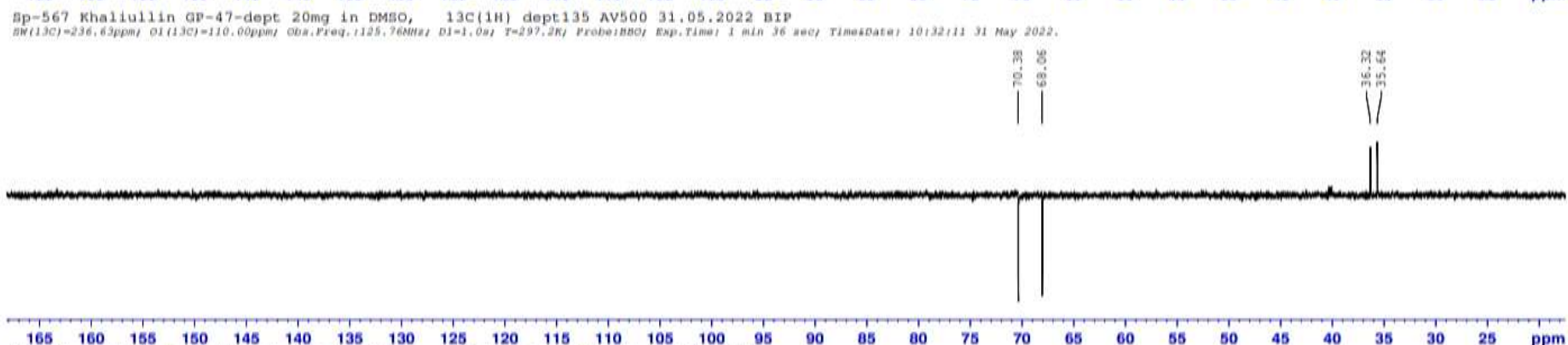
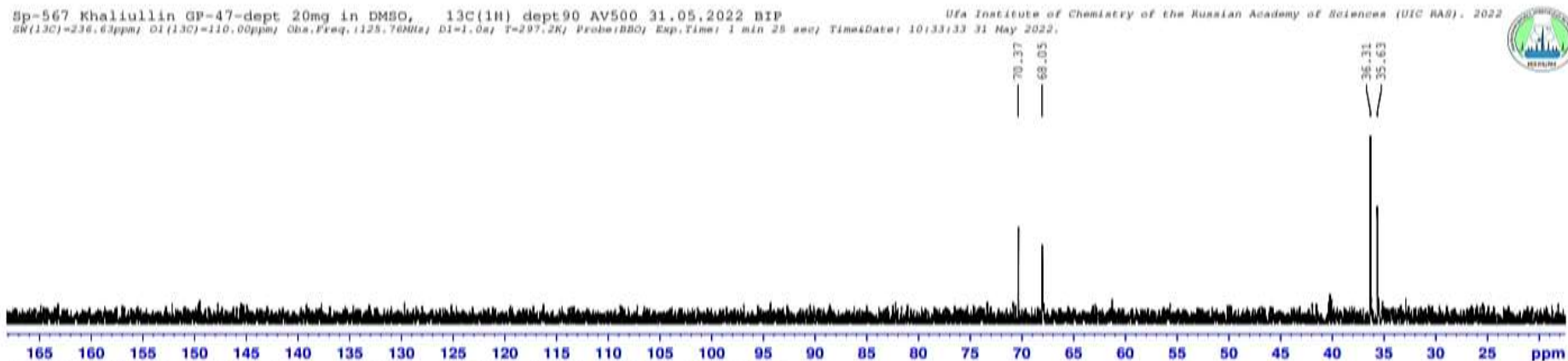
Sp-567 Khaliullin GP-47-dept 20mg in DMSO, 1H AV500 31.05.2022 BIP

Ufa Institute of Chemistry of the Russian Academy of Sciences (IUC RAS), 2022

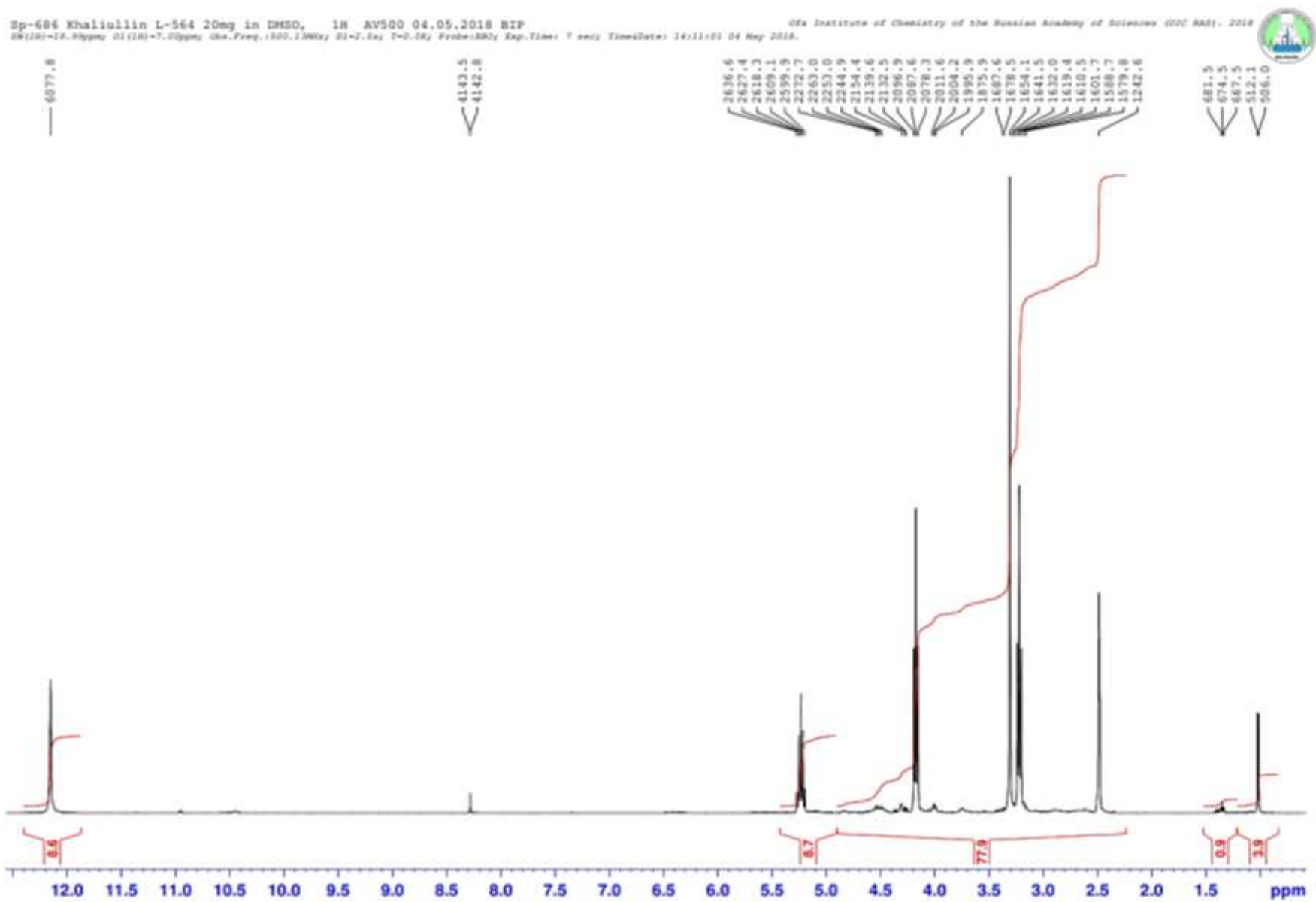
SWH=12.80ppm SI=10 T=300.13MHz SI=2.0s T=206.7K Probe=BB04 Exp.Time: 7 sec TimeDate: 10:25:08 31 May 2022.



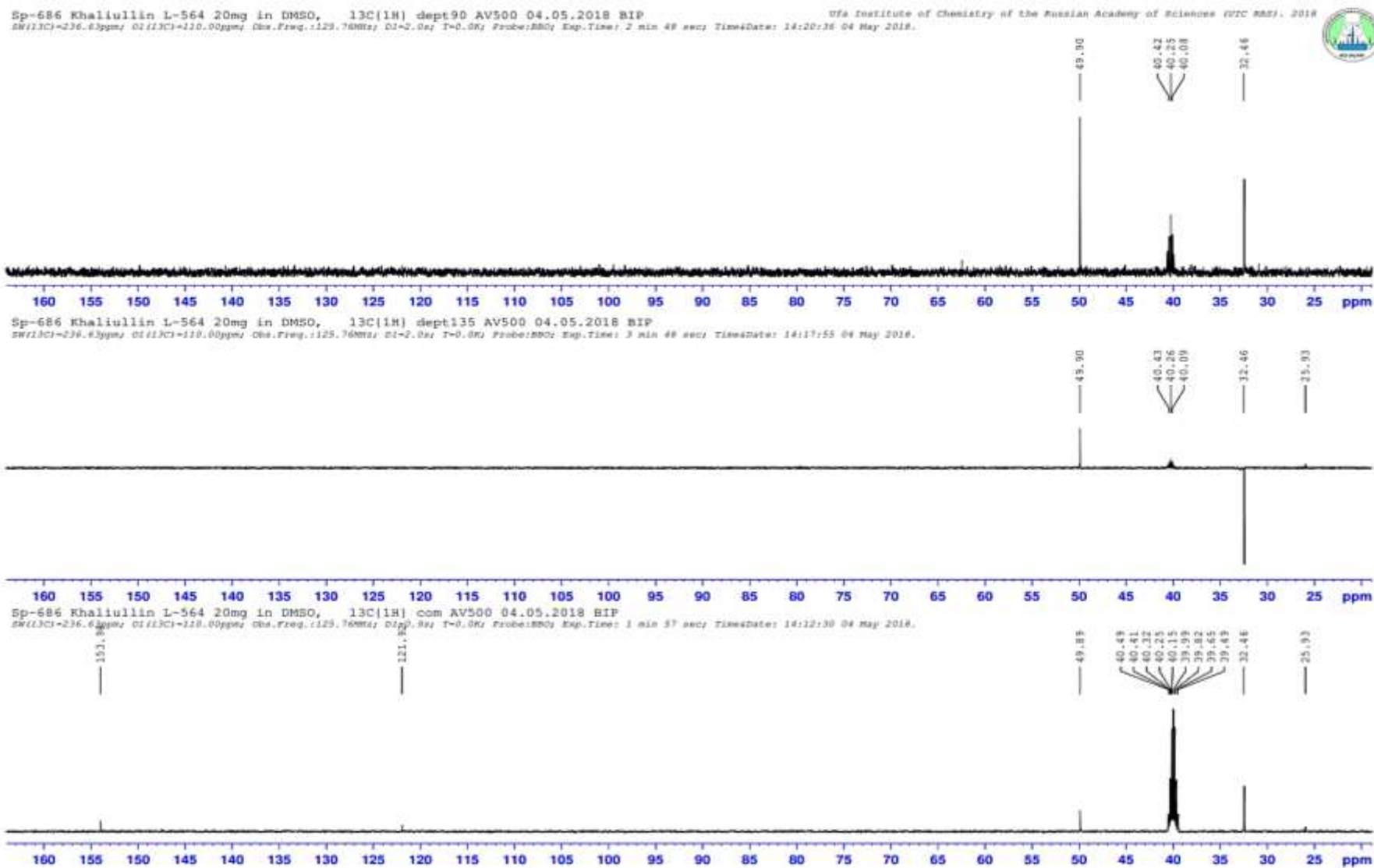
^{13}C NMR (125 MHz, DMSO- d_6) of 5-bromo-2,4-bis(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**6c**)



^1H NMR (300 MHz, $\text{DMSO}-d_6$) of 5-bromo-4-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7a**)

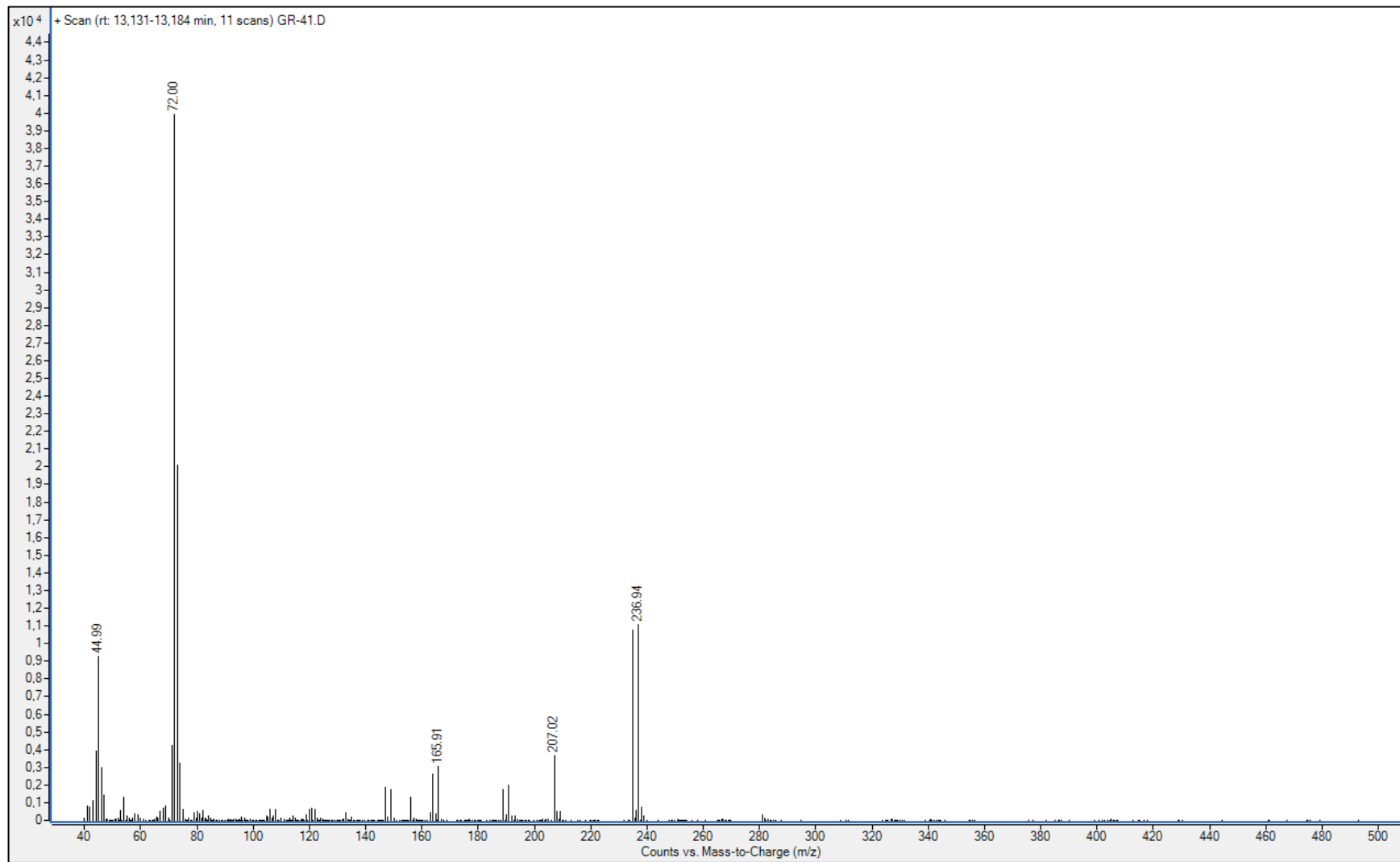
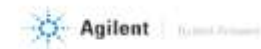


^{13}C NMR (125 MHz, DMSO- d_6) of 5-bromo-4-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7a**)



Mass spectrum (EI, 70 eV) of 5-bromo-4-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7a**)

Spectrum Plot Report

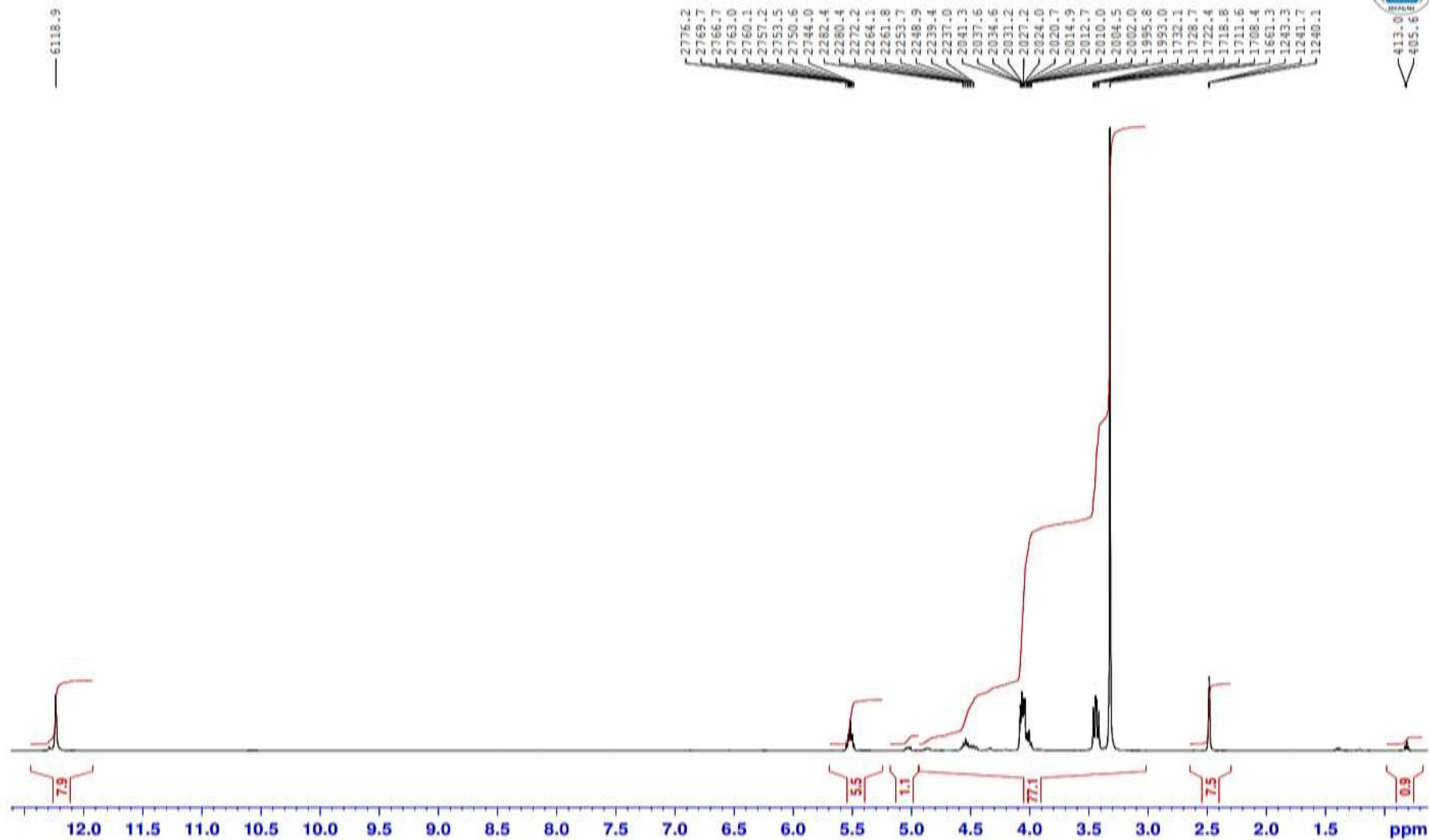


^1H NMR (300 MHz, $\text{DMSO}-d_6$) of 5-bromo-4-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7b**)

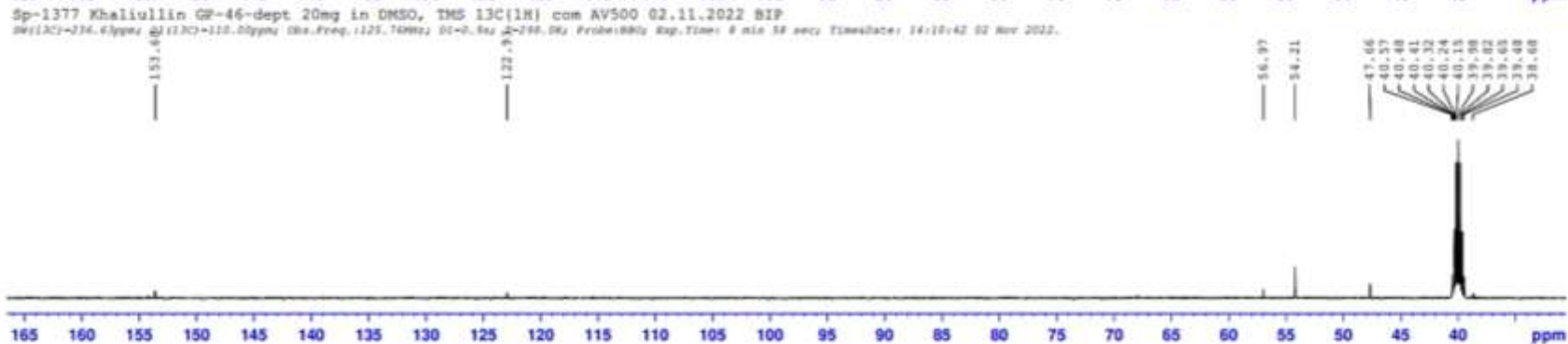
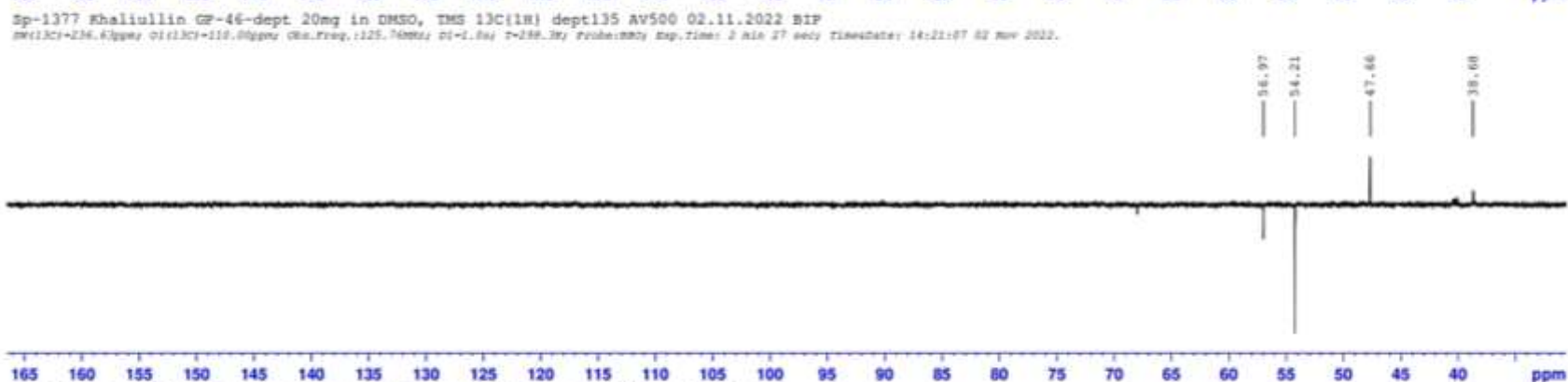
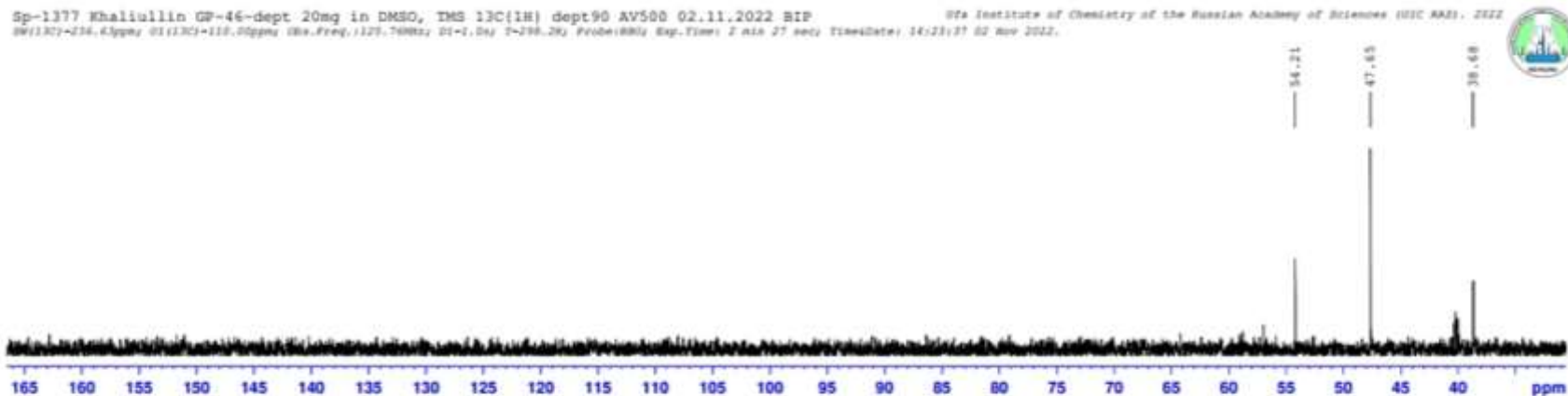
Sp-1377 Khaliullin GP-46-dept 20mg in DMSO, TMS 1H AV500 02.11.2022 BIP

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS), 2022

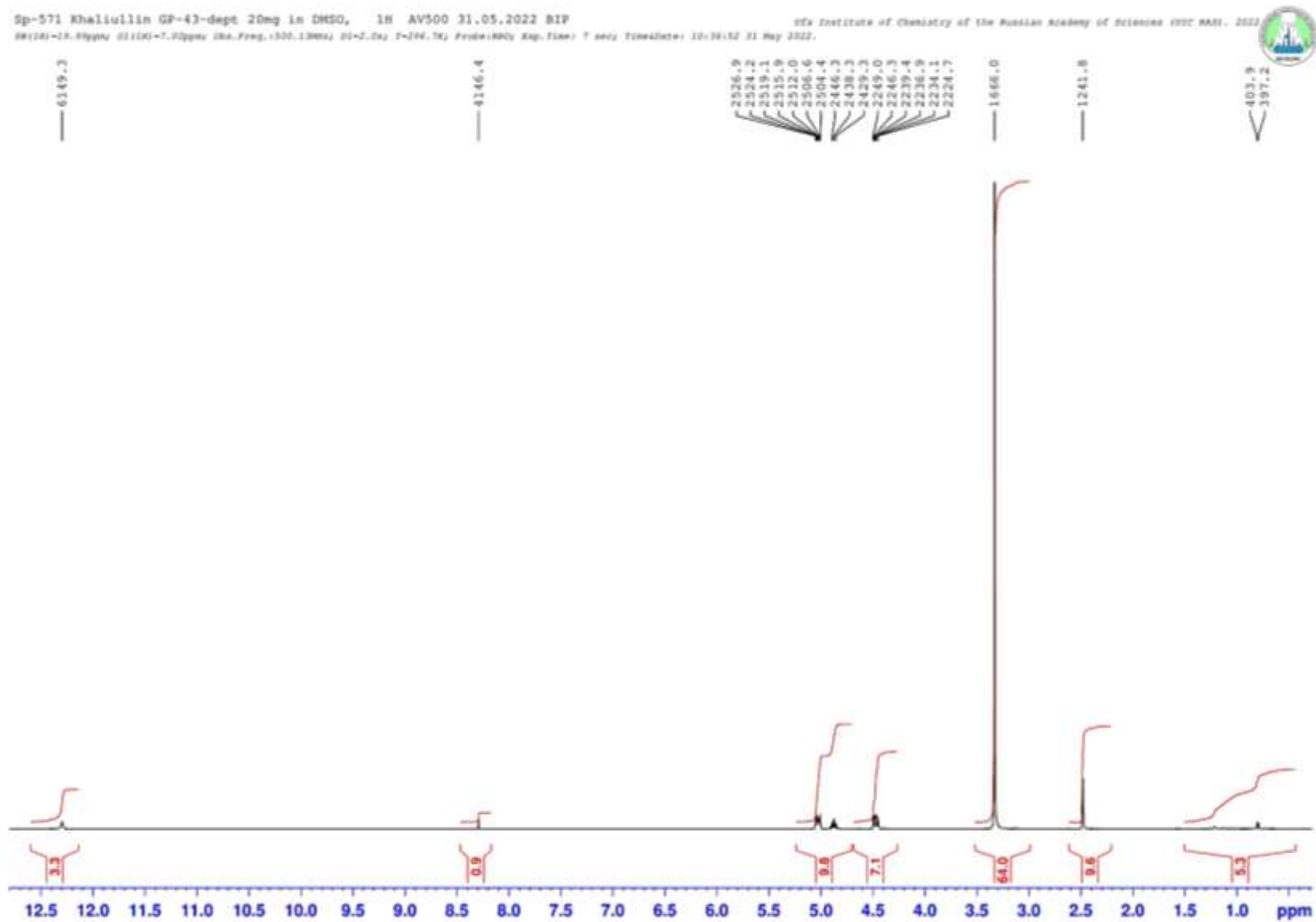
SWH=19.99ppm; Q1(1H)=7.00ppm; Obs.Freq.:500.13MHz; D1=2.0s; T=297.7K; Probe:BB0; Exp.Time: 7 sec; TimeDate: 14:07:55 02 Nov 2022.



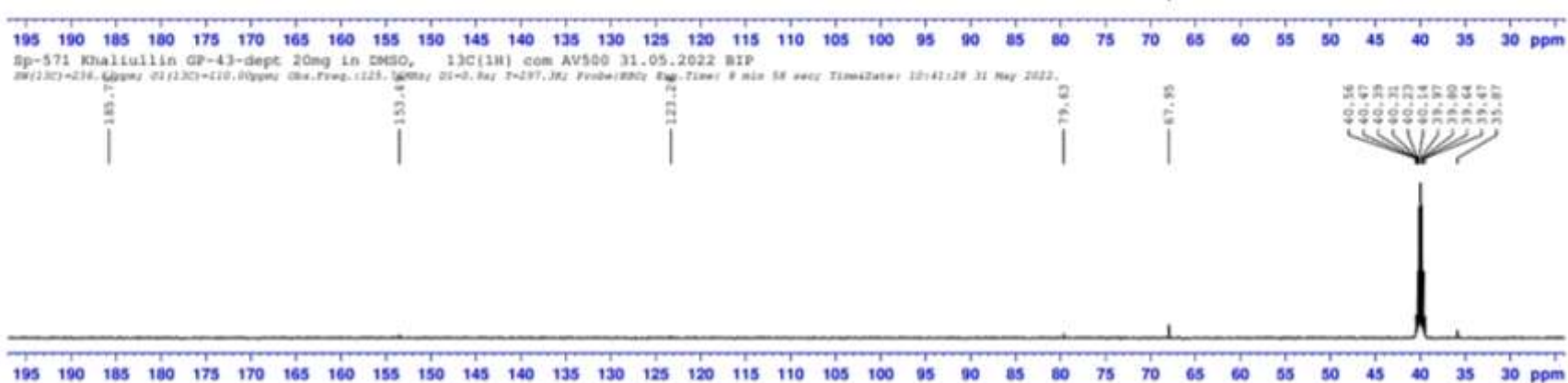
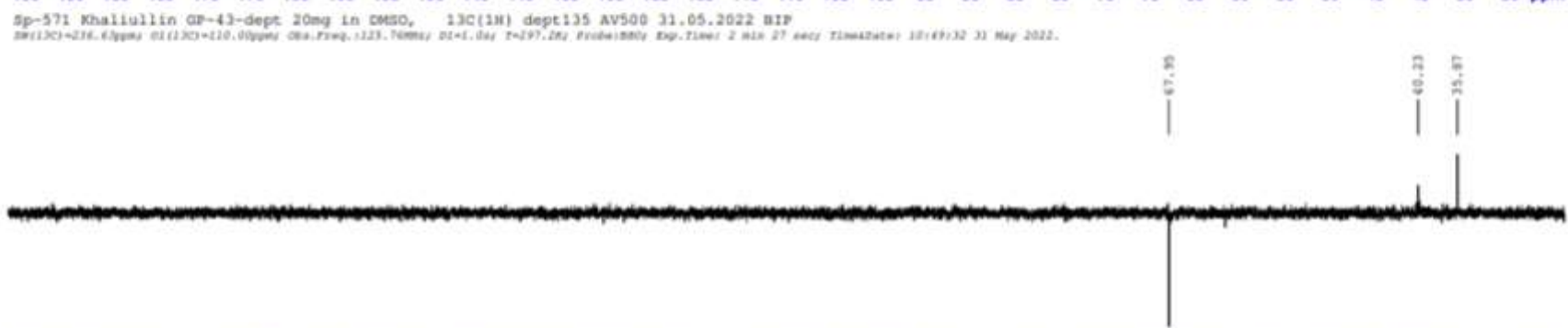
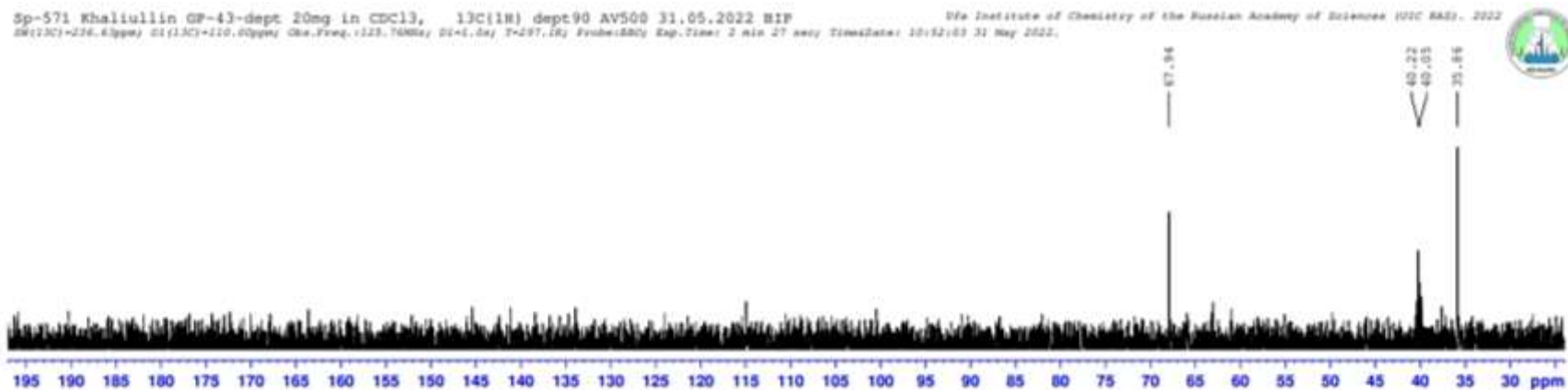
^{13}C NMR (125 MHz, DMSO- d_6) of 5-bromo-4-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7b**)



^1H NMR (500 MHz, $\text{DMSO}-d_6$) of 5-bromo-4-(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7c**)

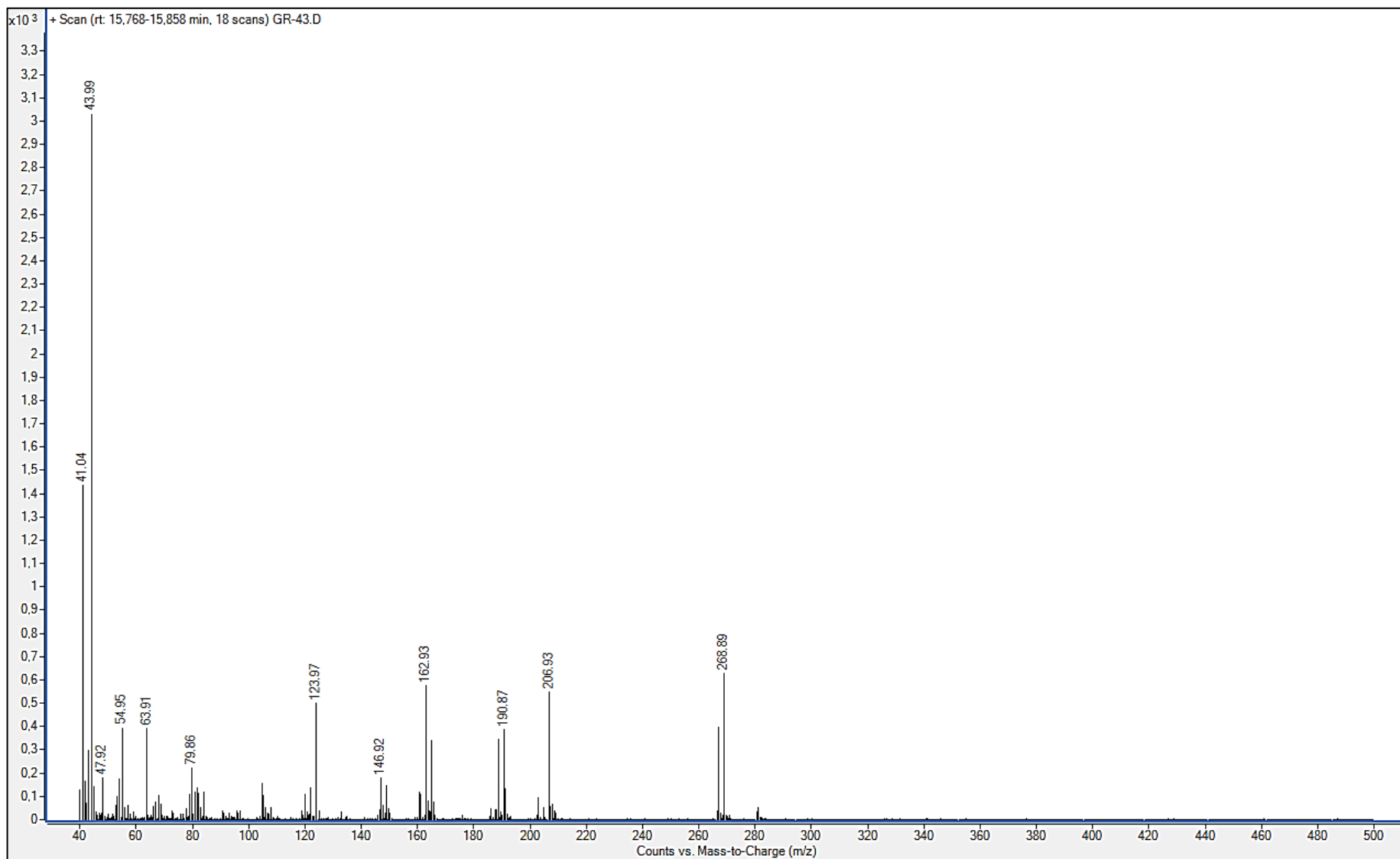


^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) of 5-bromo-4-(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7c**)



Mass spectrum (EI, 70 eV) of 5-bromo-4-(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7c**)

Spectrum Plot Report

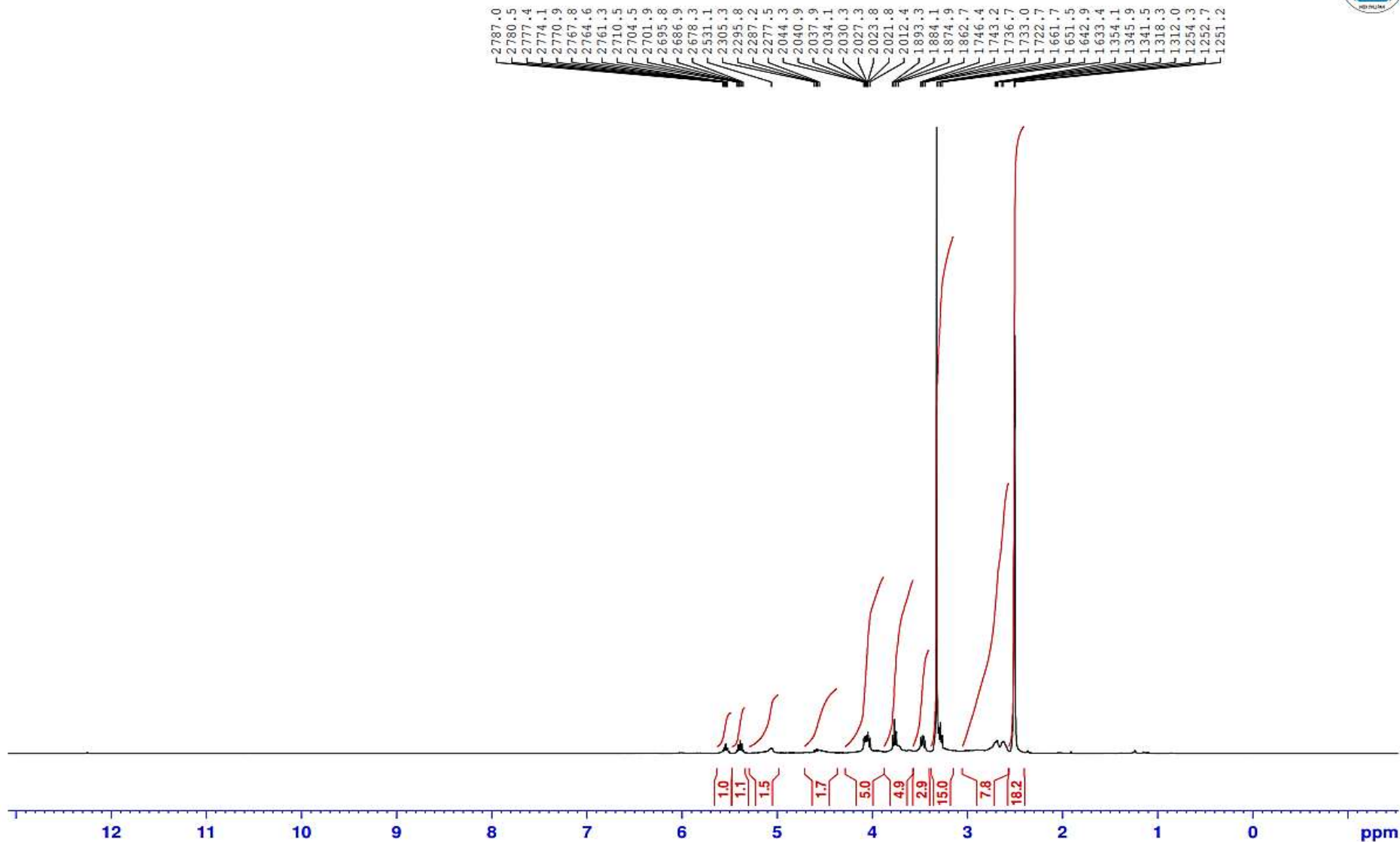


^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 5-bromo-4-(1-oxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**8a**)

Sp-1183 Khaliullin GR-80 20mg in DMSO, ^1H AV500 27.04.2023 LAN

Ufa Institute of Chemistry of the Russian Academy of Sciences (UIC RAS), 2023

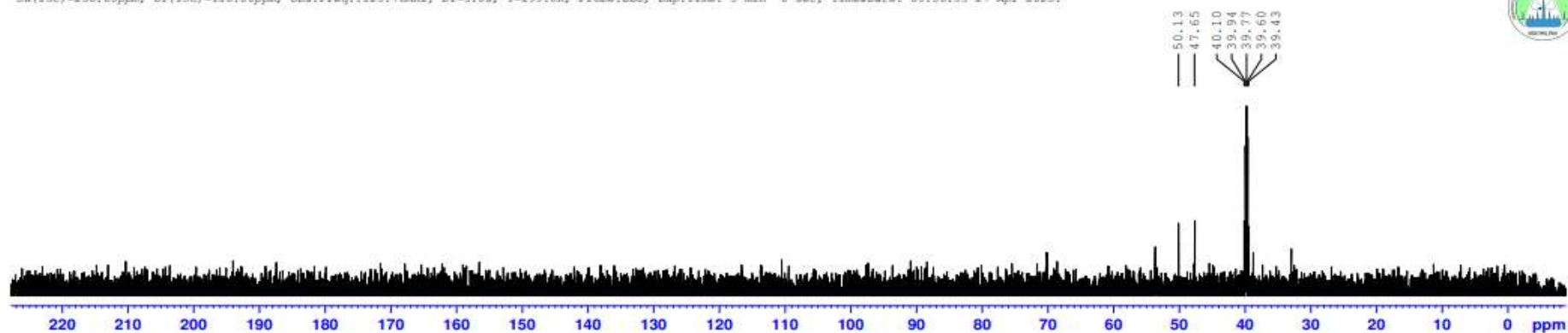
SW(^1H)=29.99ppm; O1(^1H)=6.00ppm; Obs.Freq.:500.13MHz; D1=30.0s; T=298.6K; Probe:BBO; Exp.Time: 5 min 24 sec; TimesDate: 09:27:36 27 Apr 2023.



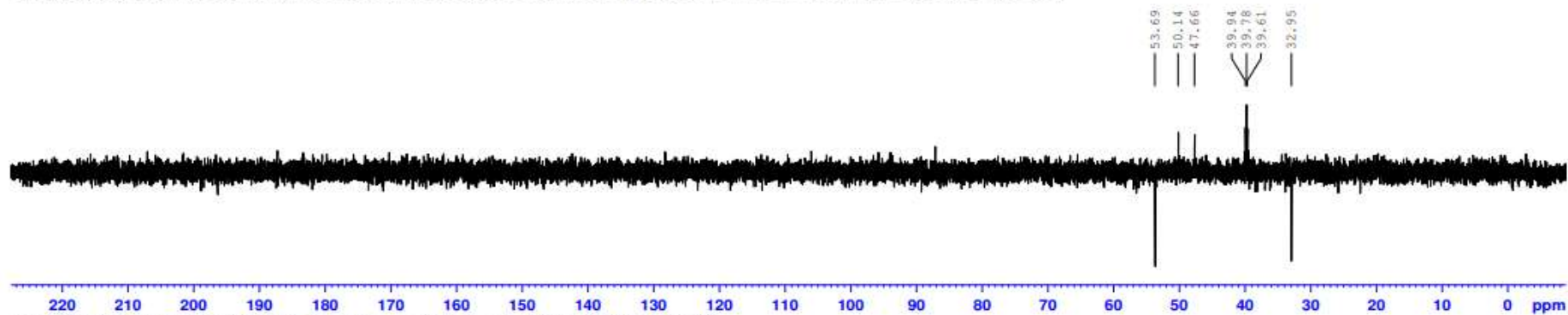
^{13}C NMR (125 MHz, DMSO- d_6) of 5-bromo-4-(1-oxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**8a**)

Sp-1183 Khaliullin GR-80 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept90 AV500 27.04.2023 LAN
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=3.0s; T=299.0K; Probe:BB0; Exp.Time: 5 min 0 sec; TimesDate: 09:56:33 27 Apr 2023.

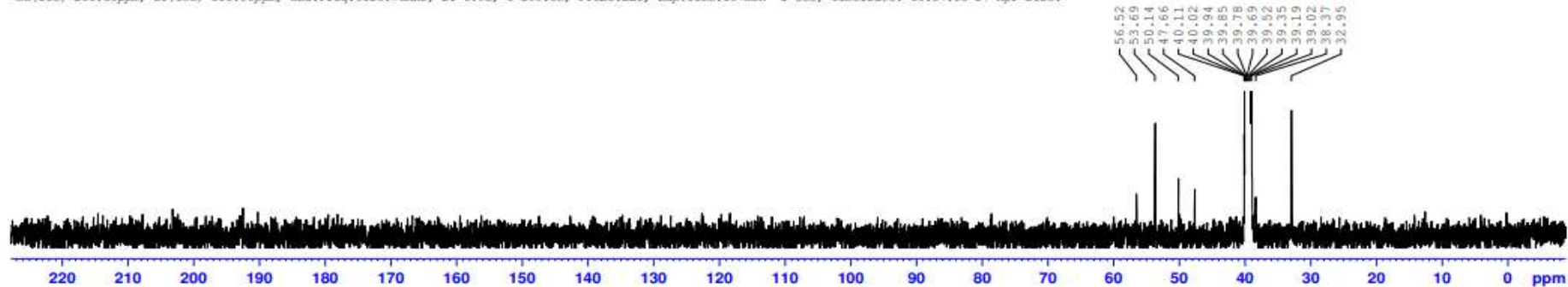
Ufa Institute of Chemistry of the Russian Academy of Sciences (UTC RAS), 2023



Sp-1183 Khaliullin GR-80 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept135 AV500 27.04.2023 LAN
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=299.2K; Probe:BB0; Exp.Time: 4 min 53 sec; TimesDate: 09:53:43 27 Apr 2023.



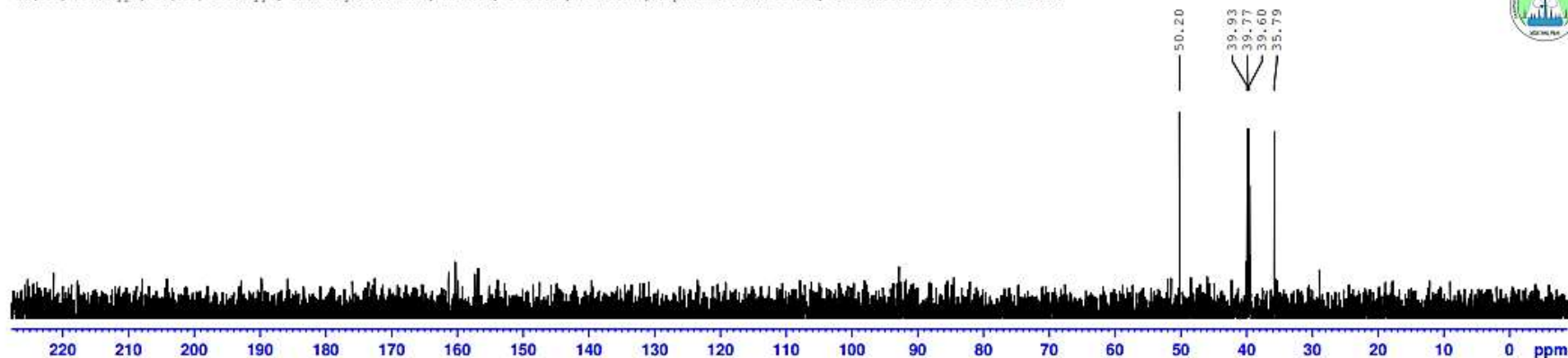
Sp-1183 Khaliullin GR-80 20mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ com AV500 27.04.2023 LAN
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=0.5s; T=299.0K; Probe:BB0; Exp.Time:18 min 1 sec; TimesDate: 09:57:03 27 Apr 2023.



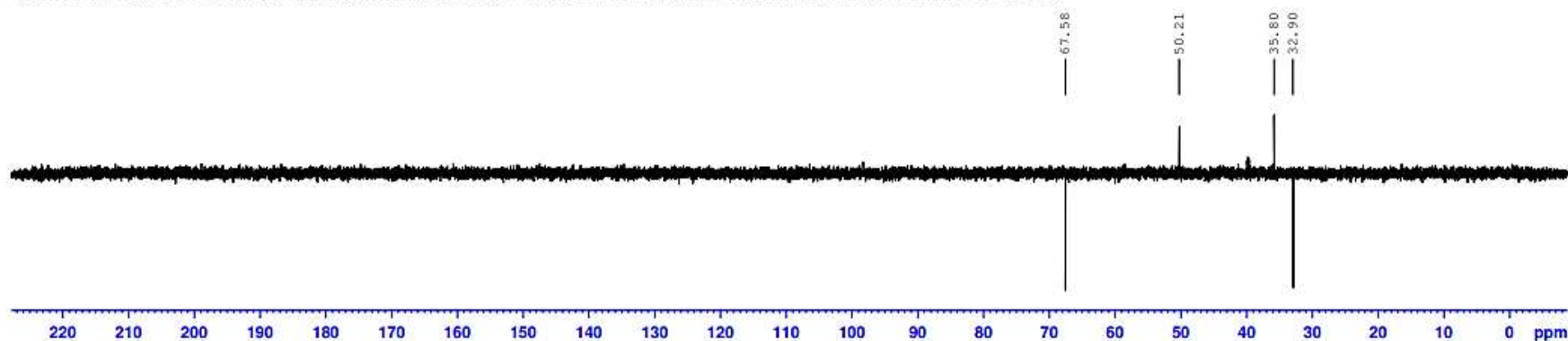
^{13}C NMR (125 MHz, DMSO- d_6) of 5-bromo-4-(1,1-dioxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**8b**)

Sp-910 Khaliullin GR-73 10mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept90 AV500 12.07.2022 LAN
SW(13C)=236.63ppm; O1(13C)=-110.00ppm; Obs.Freq.:125.76MHz; D1=3.0s; T=300.0K; Probe:BBO; Exp.Time: 2 min 31 sec; TimesDate: 09:30:56 12 Jul 2022.

Ufa Institute of Chemistry of the Russian Academy of Sciences (IIC RAS). 2022

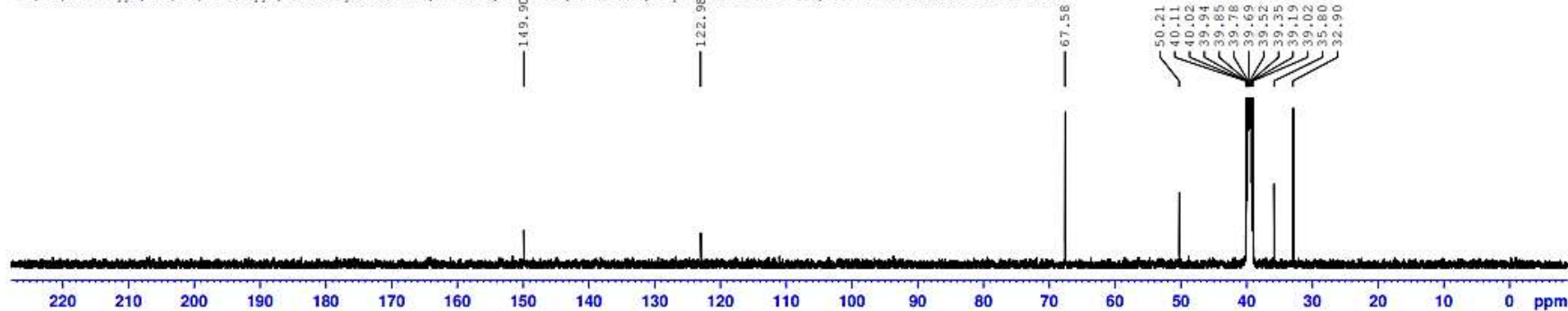


Sp-910 Khaliullin GR-73 10mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ dept135 AV500 12.07.2022 LAN
SW(13C)=236.63ppm; O1(13C)=-110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=300.2K; Probe:BBO; Exp.Time: 2 min 27 sec; TimesDate: 09:28:23 12 Jul 2022.



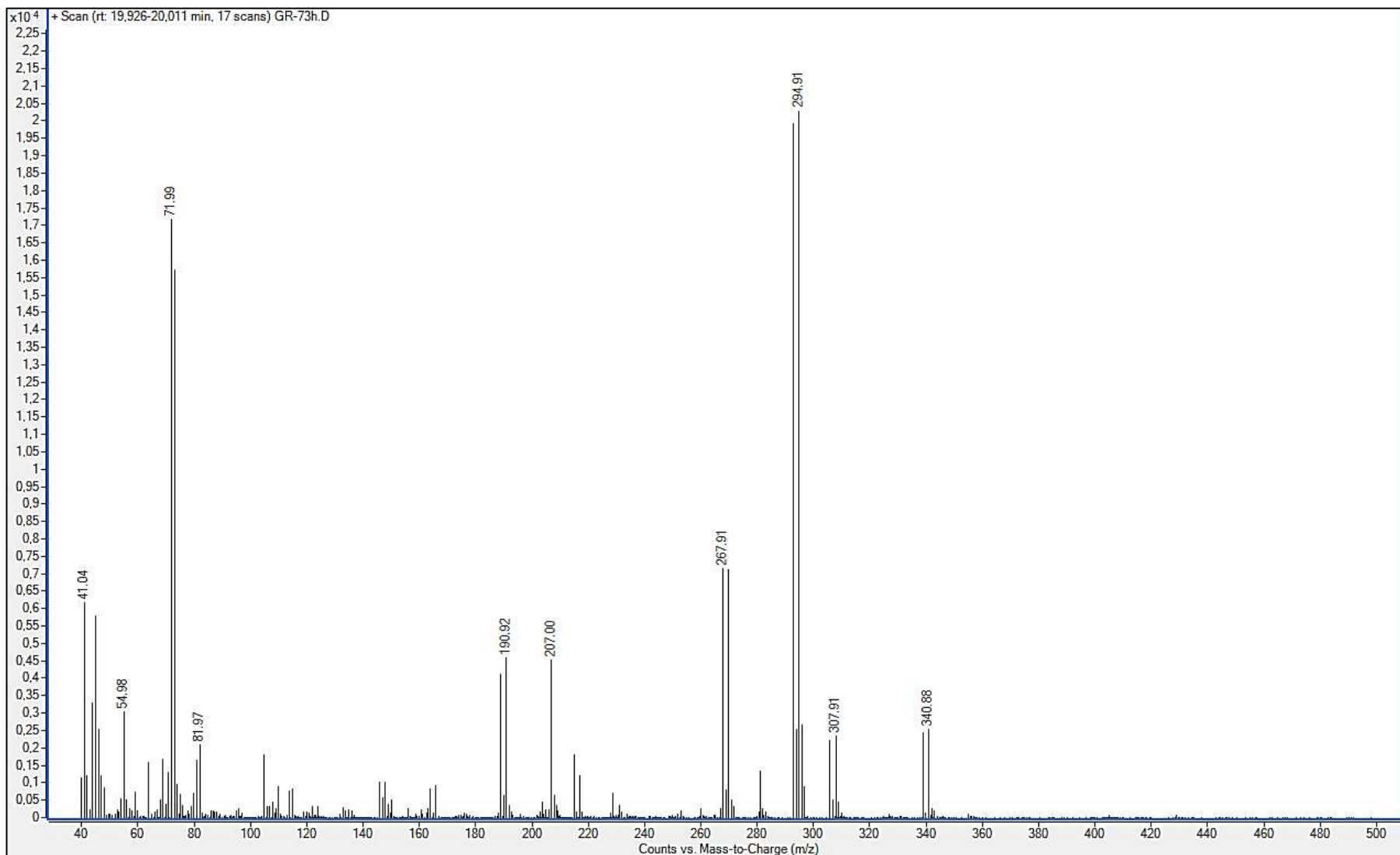
Sp-910 Khaliullin GR-73 10mg in DMSO, $^{13}\text{C}\{^1\text{H}\}$ com AV500 12.07.2022 LAN

SW(13C)=236.63ppm; O1(13C)=-110.00ppm; Obs.Freq.:125.76MHz; D1=0.9s; T=300.3K; Probe:BBO; Exp.Time: 21 min 29 sec; TimesDate: 09:32:31 12 Jul 2022.



Mass spectrum (EI, 70 eV) of 5-bromo-4-(1,1-dioxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**8b**)

Spectrum Plot Report



^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 5-bromo-4-(1,1-dioxothietanyl-3)-2-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**8c**)

Sp-1184 Khaliullin GP-88-com 20mg in DMSO, ^1H AV500 05.05.2023 BIP

Ufa Institute of Chemistry of the Russian Academy of Sciences (UTC RAS), 2023

SW(^1H)=19.99ppm; O1(^1H)=7.00ppm; Obs.Freq.:500.13MHz; D1=2.0s; T=297.8K; Probe:BB0; Exp.Time: 7 sec; TimesDate: 14:48:06 05.May.2023.

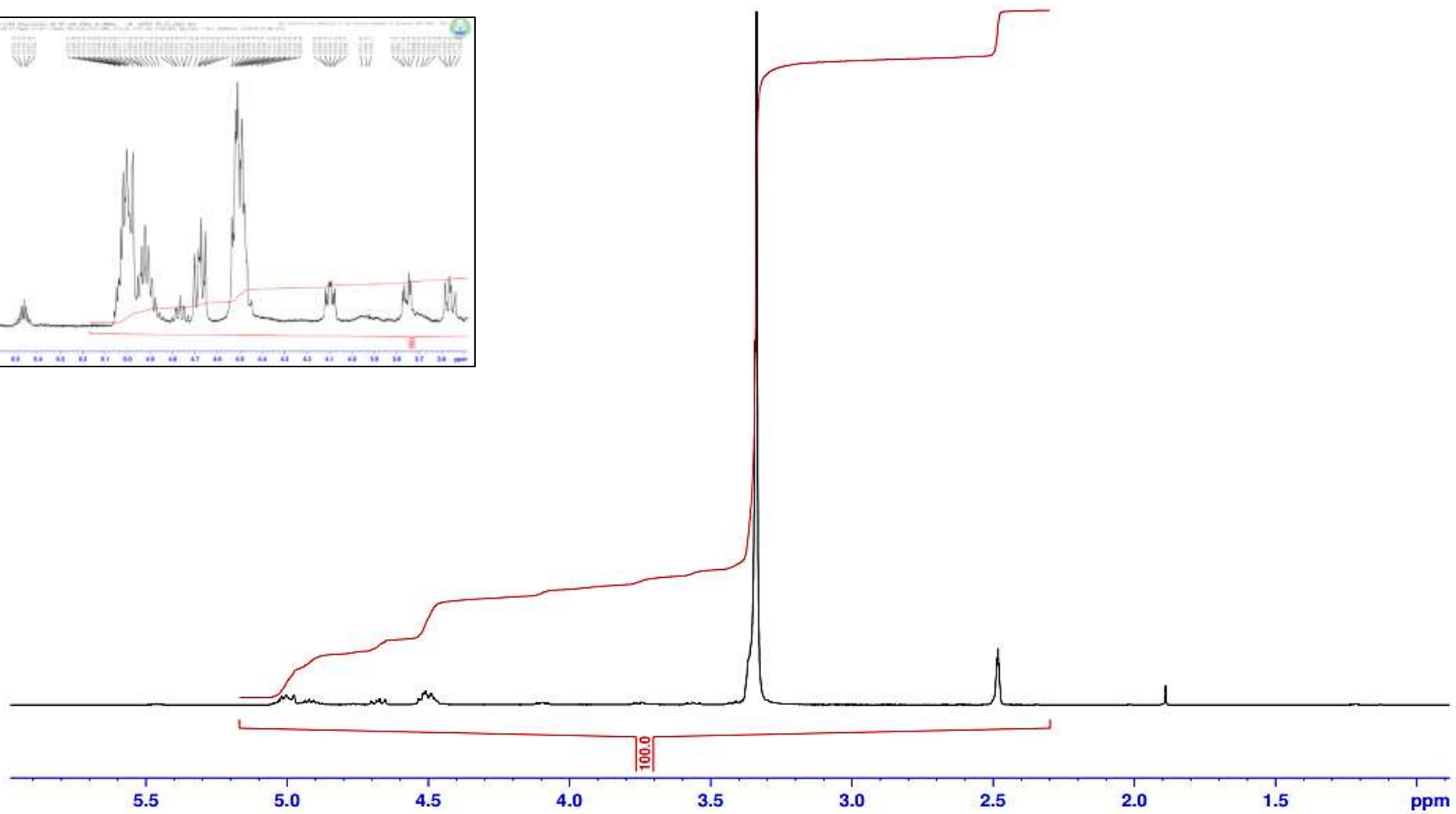
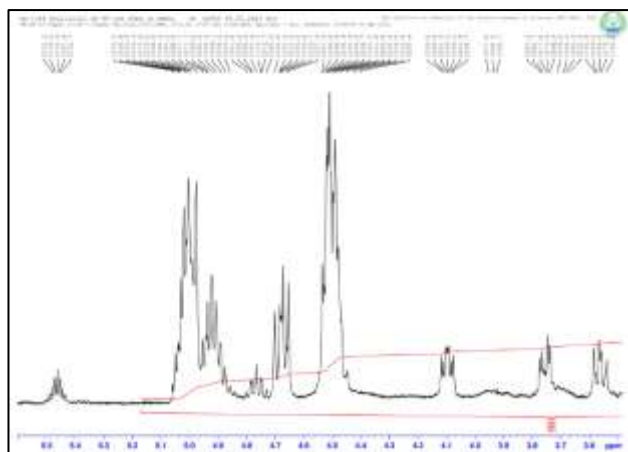


2.515.5
2.510.2
2.506.0
2.502.6
2.497.2
2.488.5
2.461.6
2.336.8
2.327.5
2.267.9
2.265.0
2.260.8
2.258.4
2.255.4
2.253.2
2.248.7
2.245.6
2.241.0
2.240.0

1.671.8
1.669.3

1.243.4
1.241.7
1.240.1

0.944.5



^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of 5-bromo-4-(1,1-dioxothietanyl-3)-2-(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**8c**)

