Chemistry of Heterocyclic Compounds **2024**, *60*(7/8), 357–364

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

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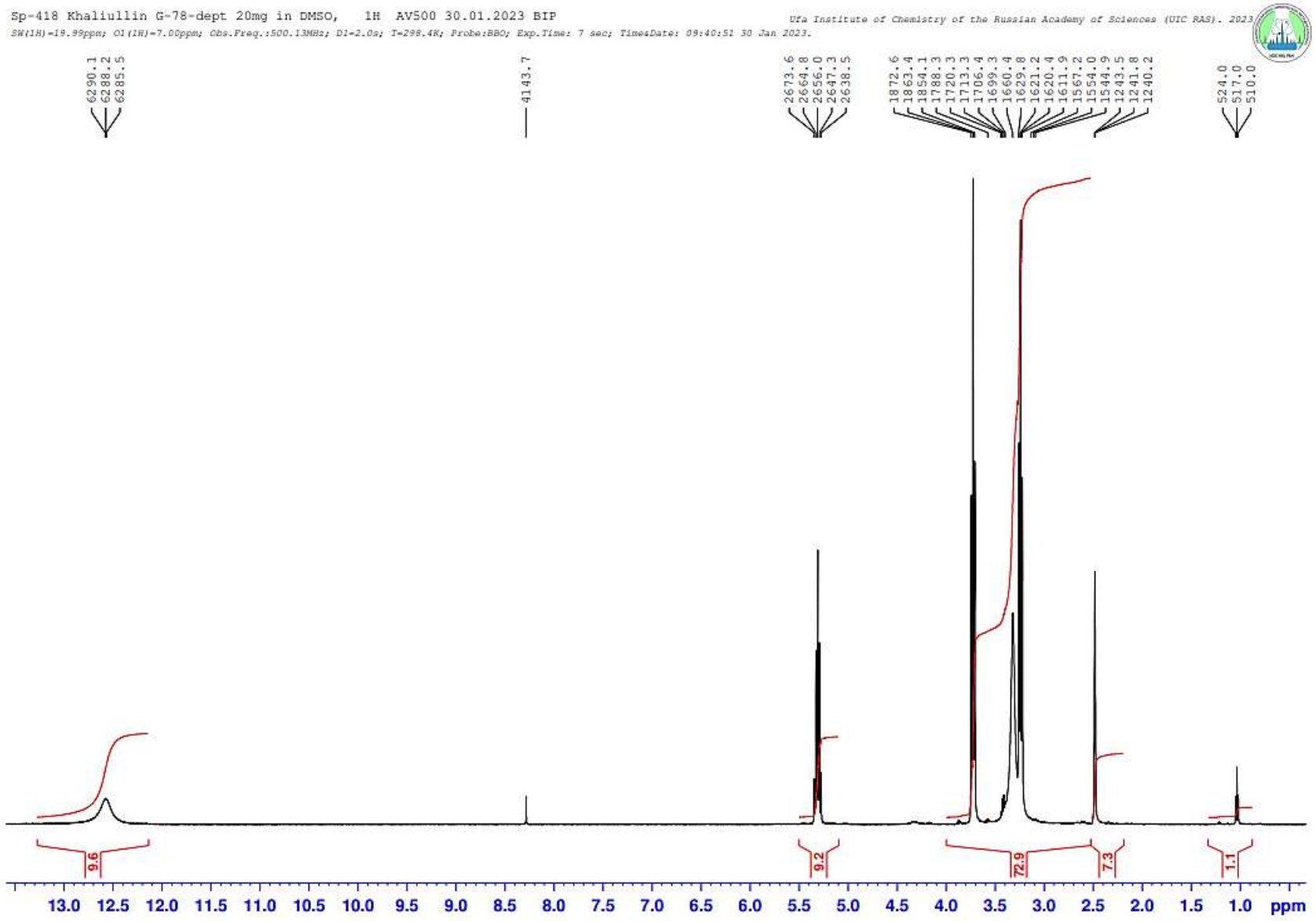
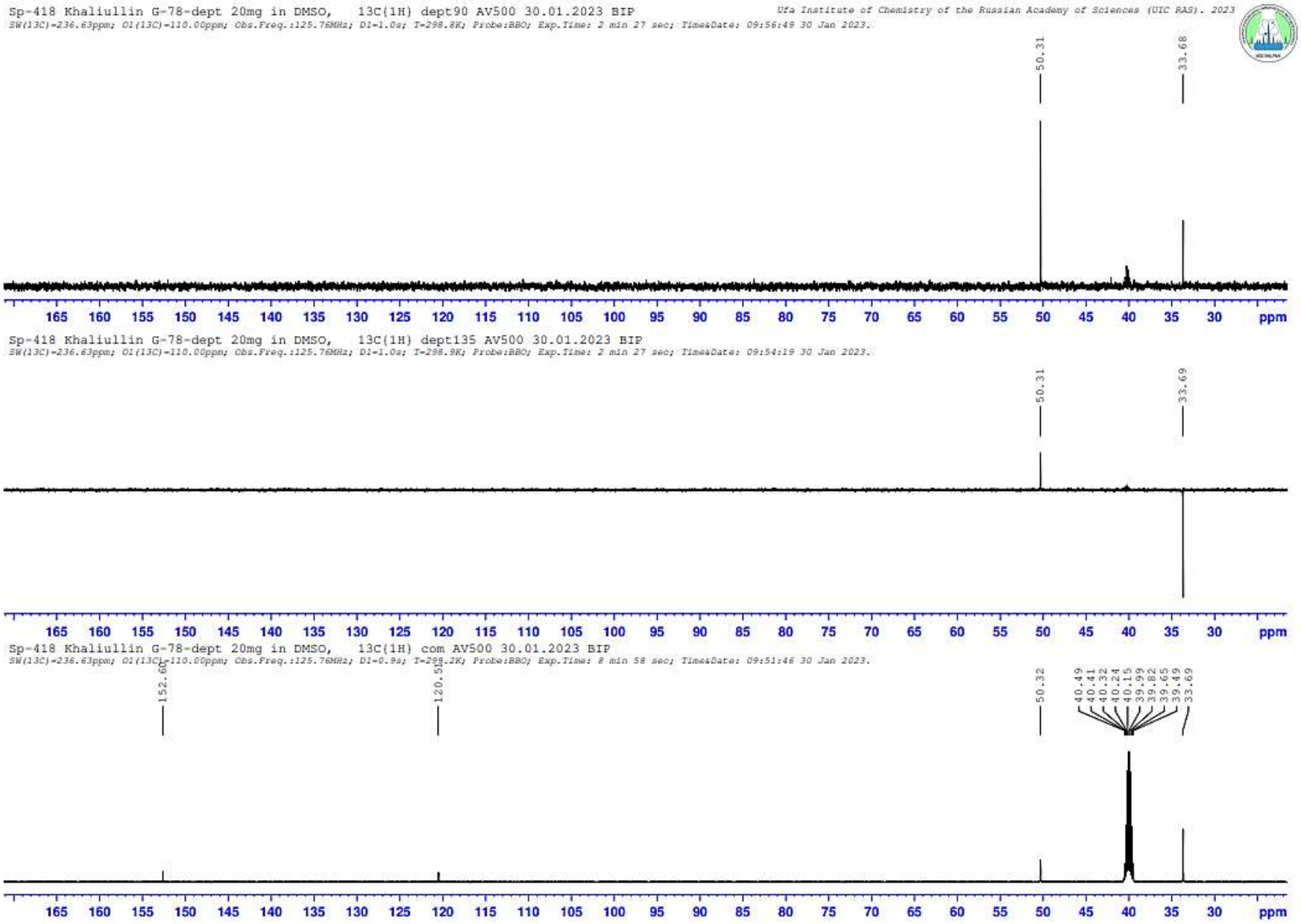
SUPPLEMENTARY INFORMATION

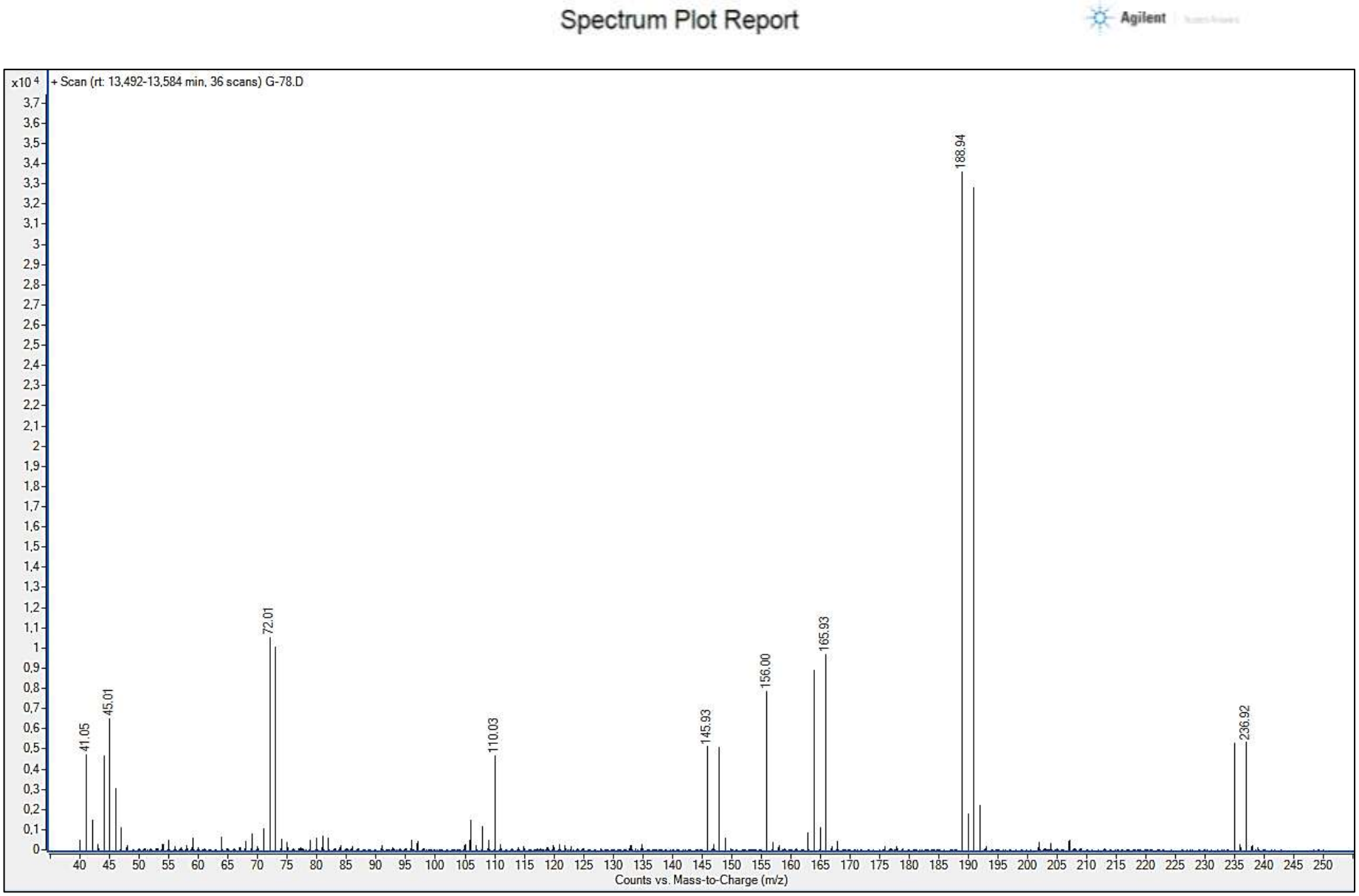
^{1}H NMR (300 MHz, DMSO-d_6) of 5-bromo-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2a**)



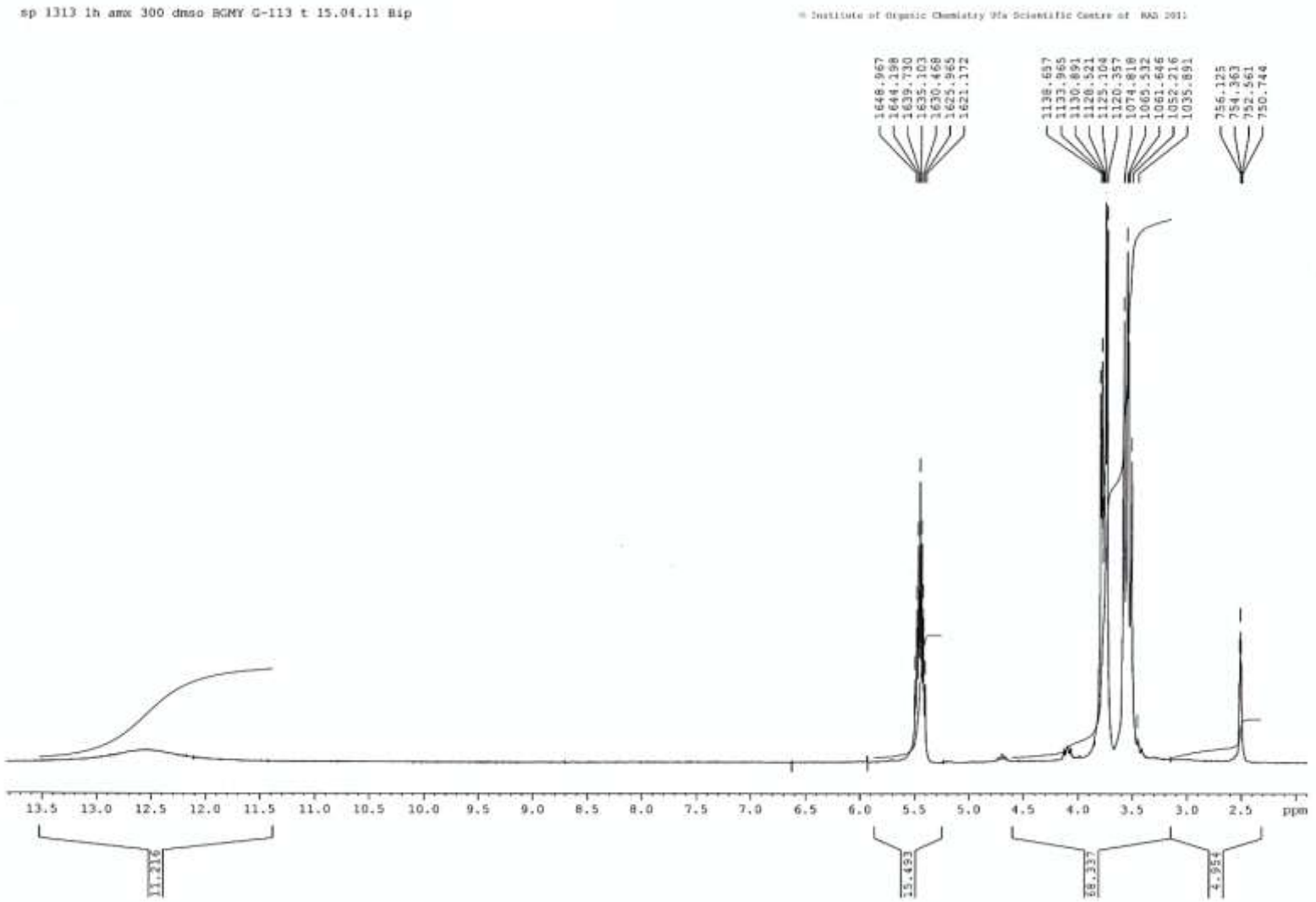
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2a**)



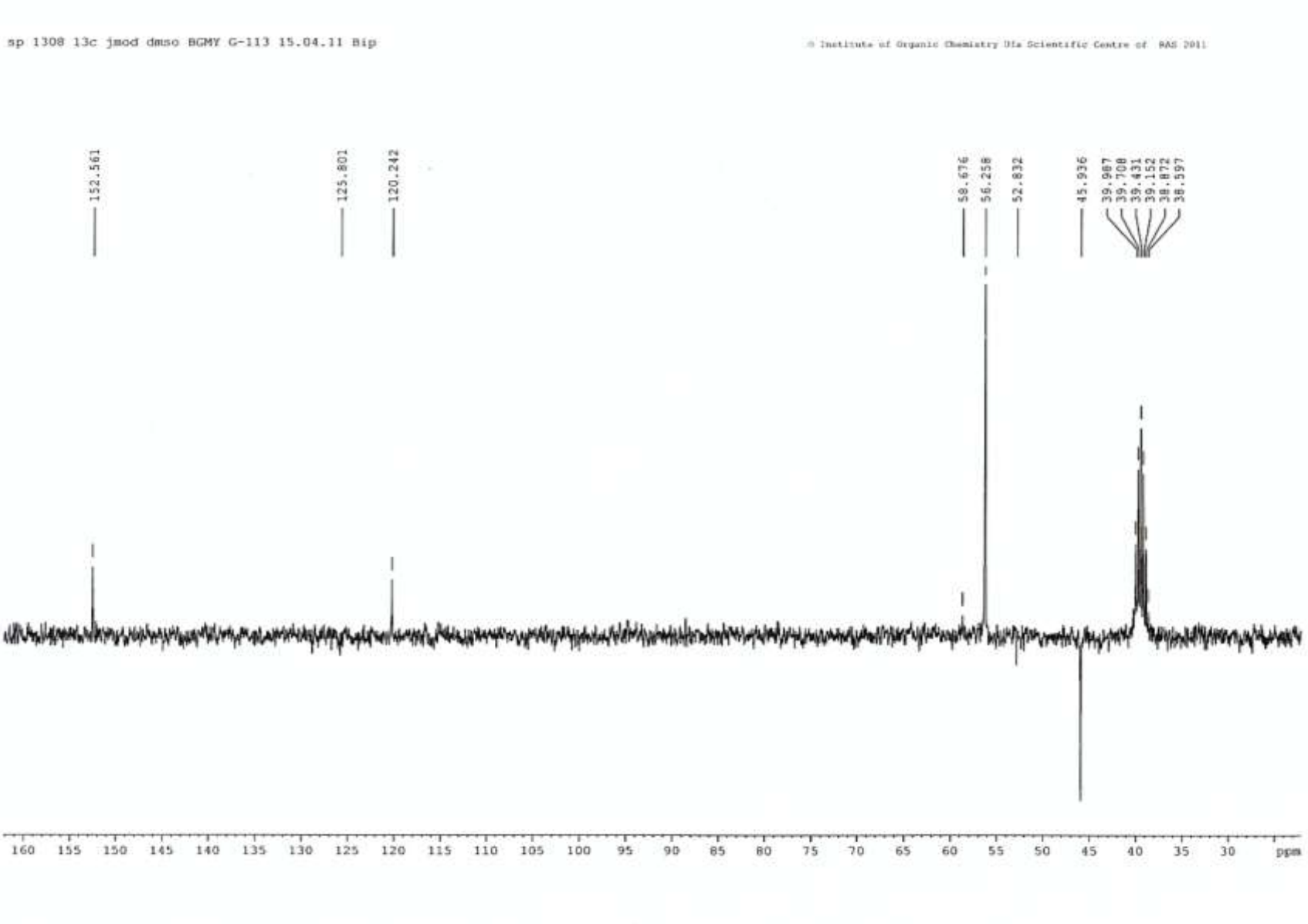
Mass spectrum (EI, 70 eV) of 5-bromo-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2a**)



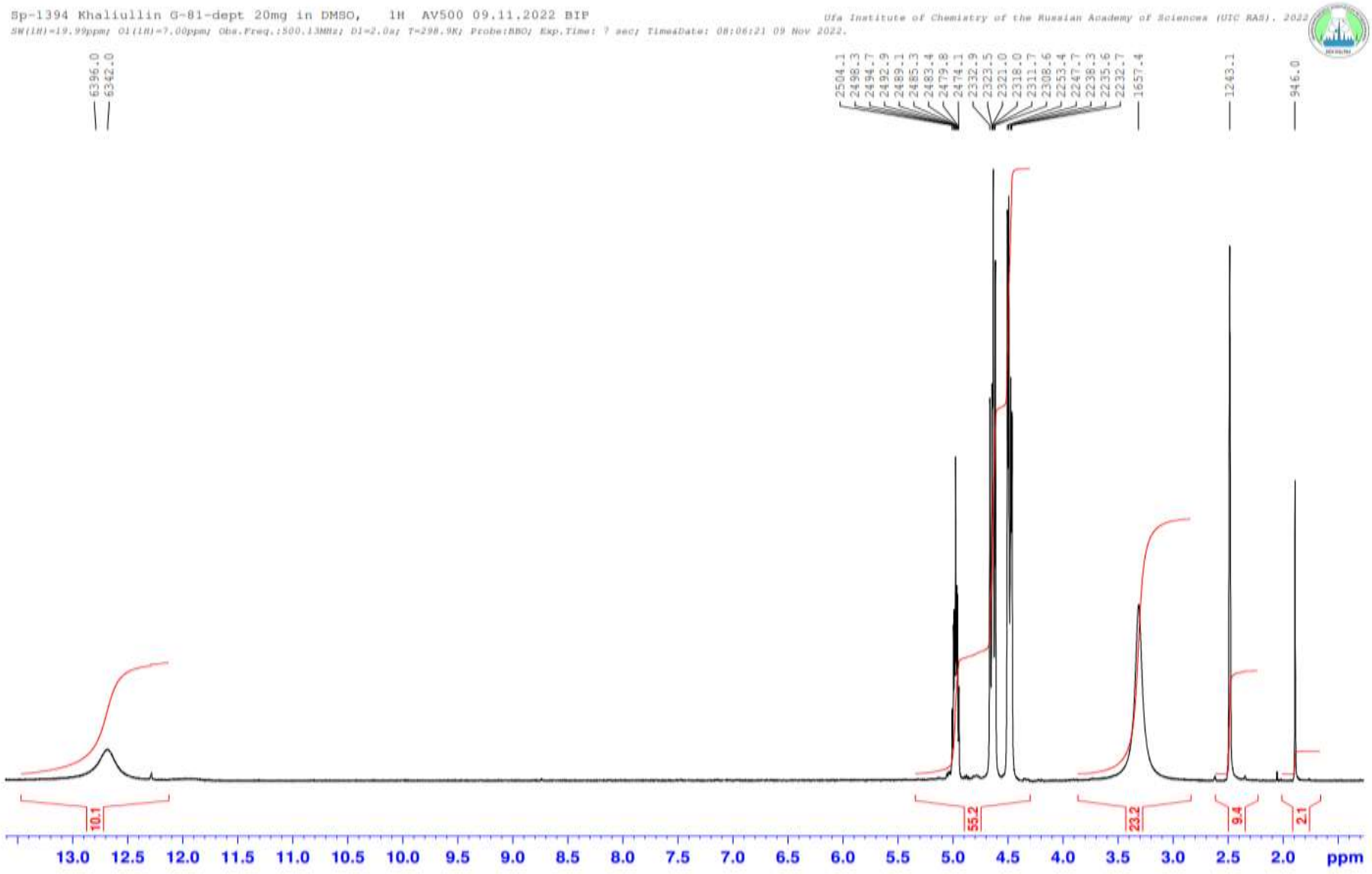
^{1}H NMR (300 MHz, DMSO-d_6) of 5-bromo-2-(1-oxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2b**)



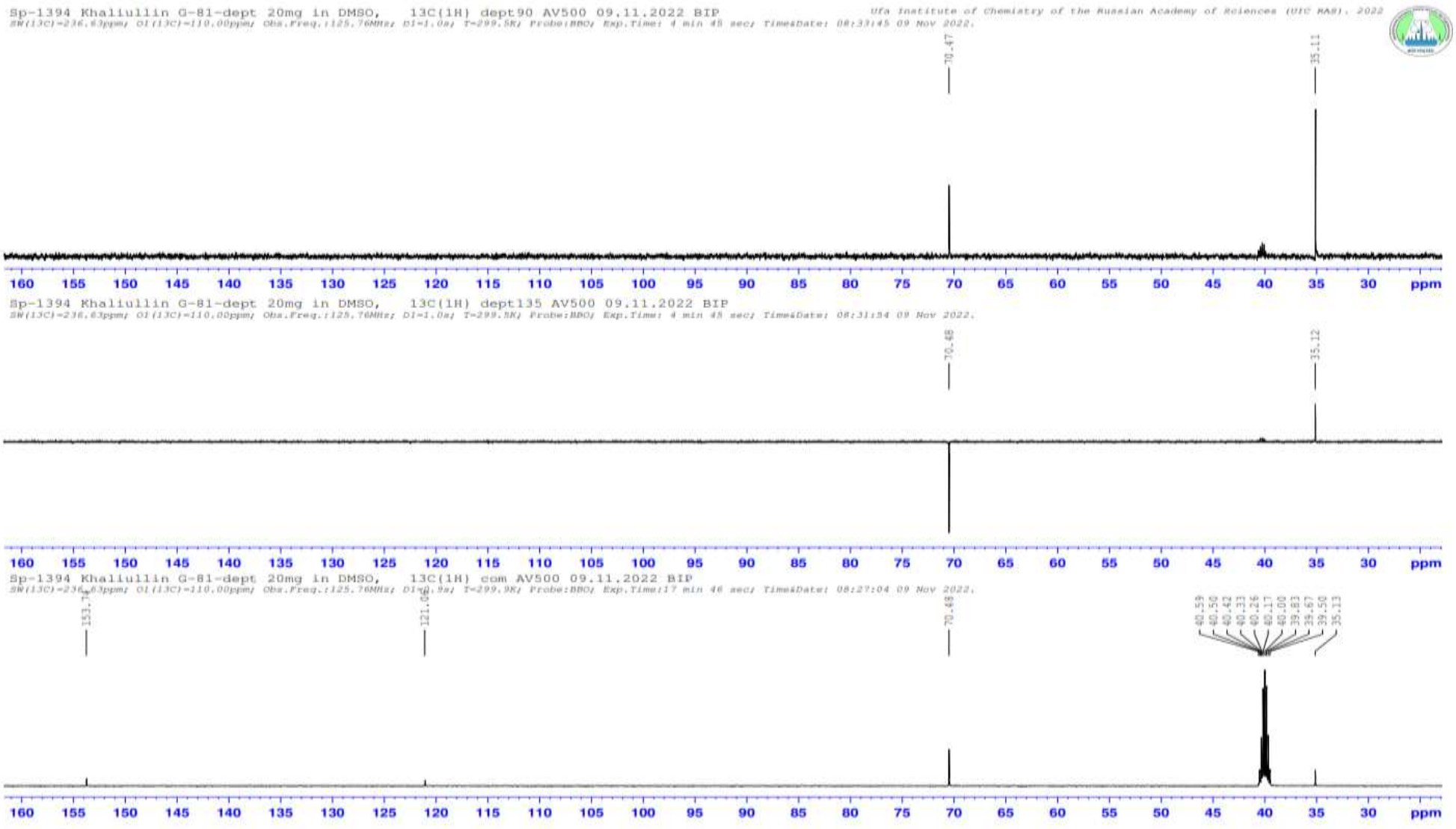
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2-(1-oxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2b**)



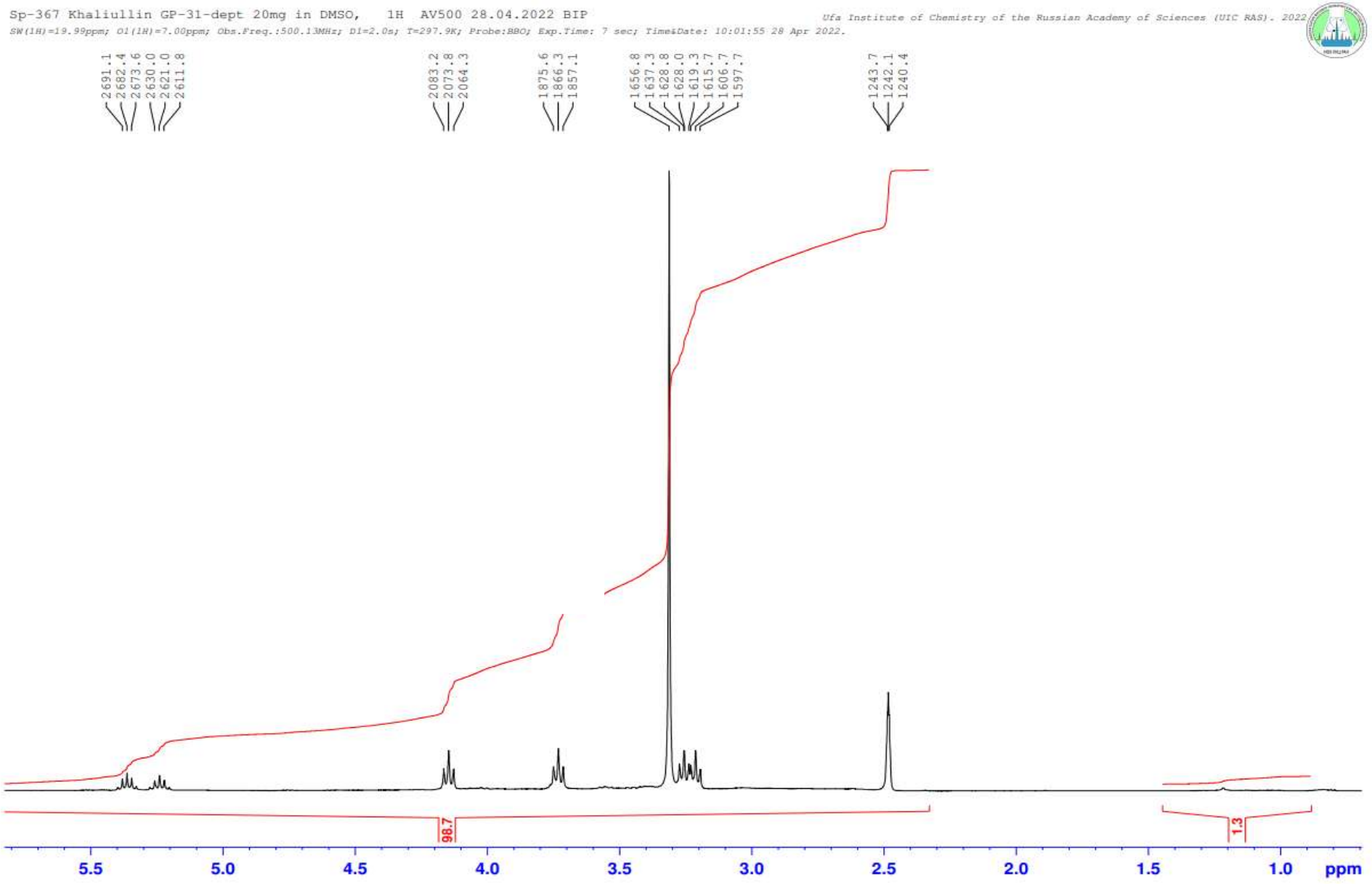
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2-(1,1-dioxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2c**)



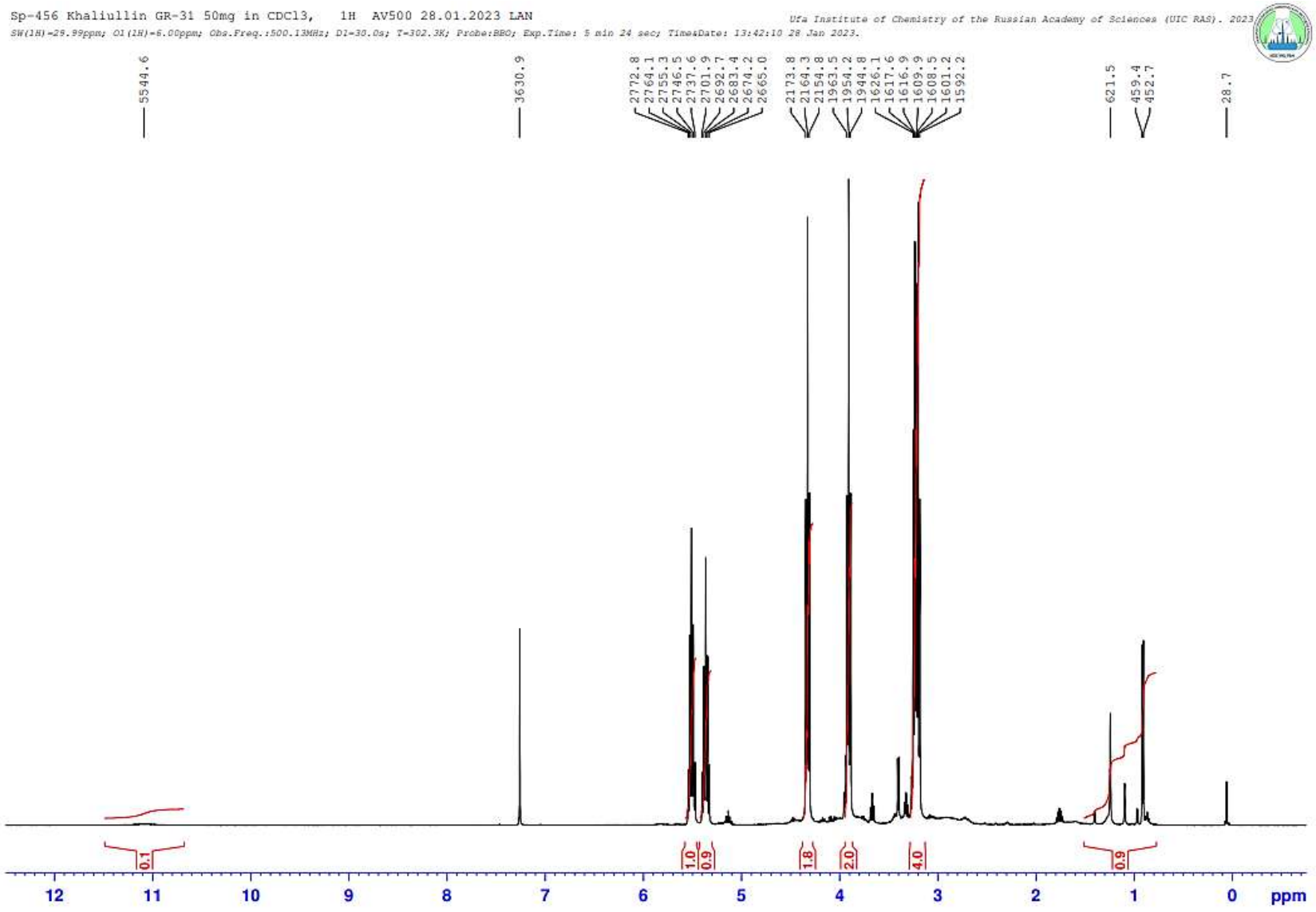
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2-(1,1-dioxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**2c**)



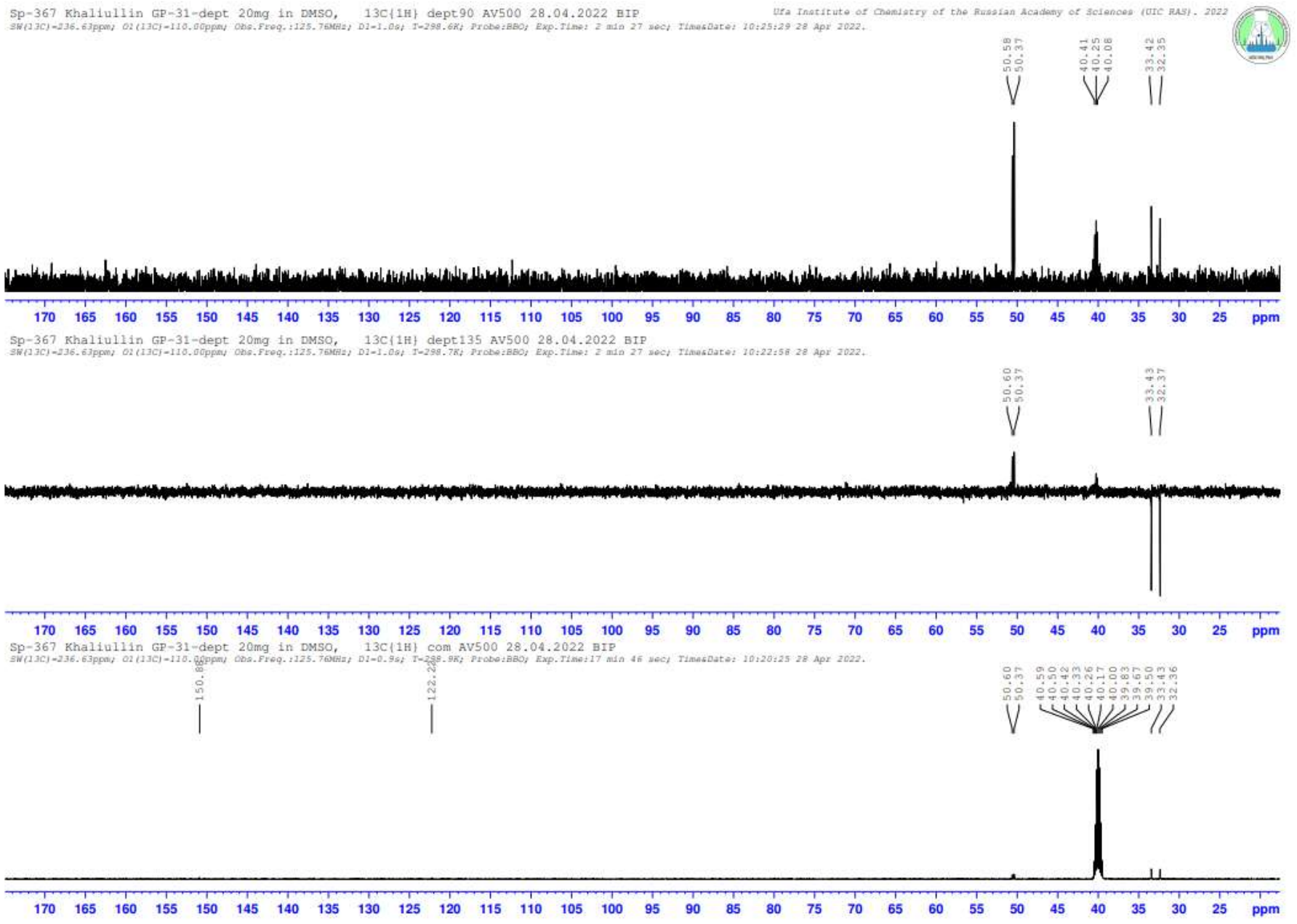
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



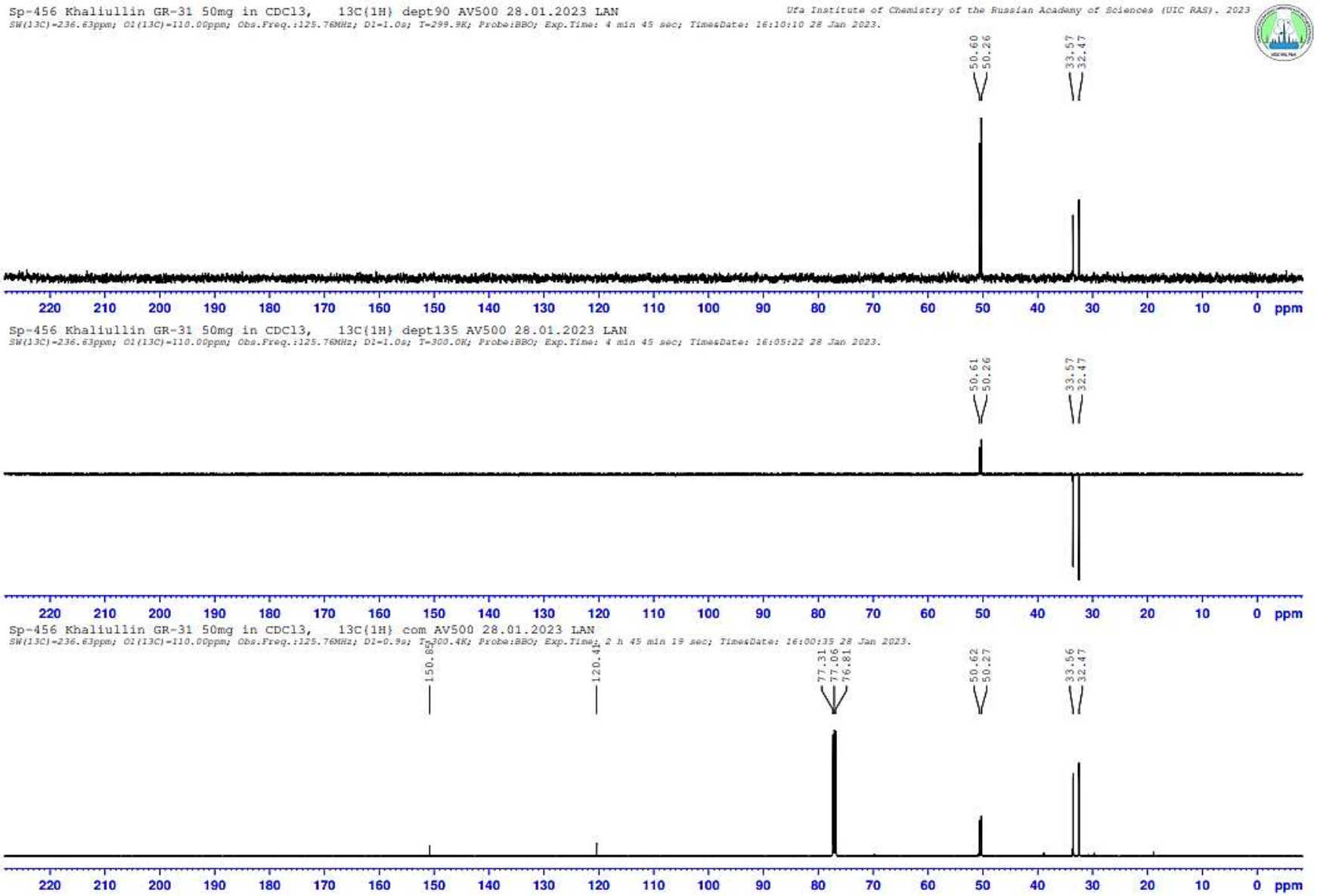
^{1}H NMR (500 MHz, $CDCl_3$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



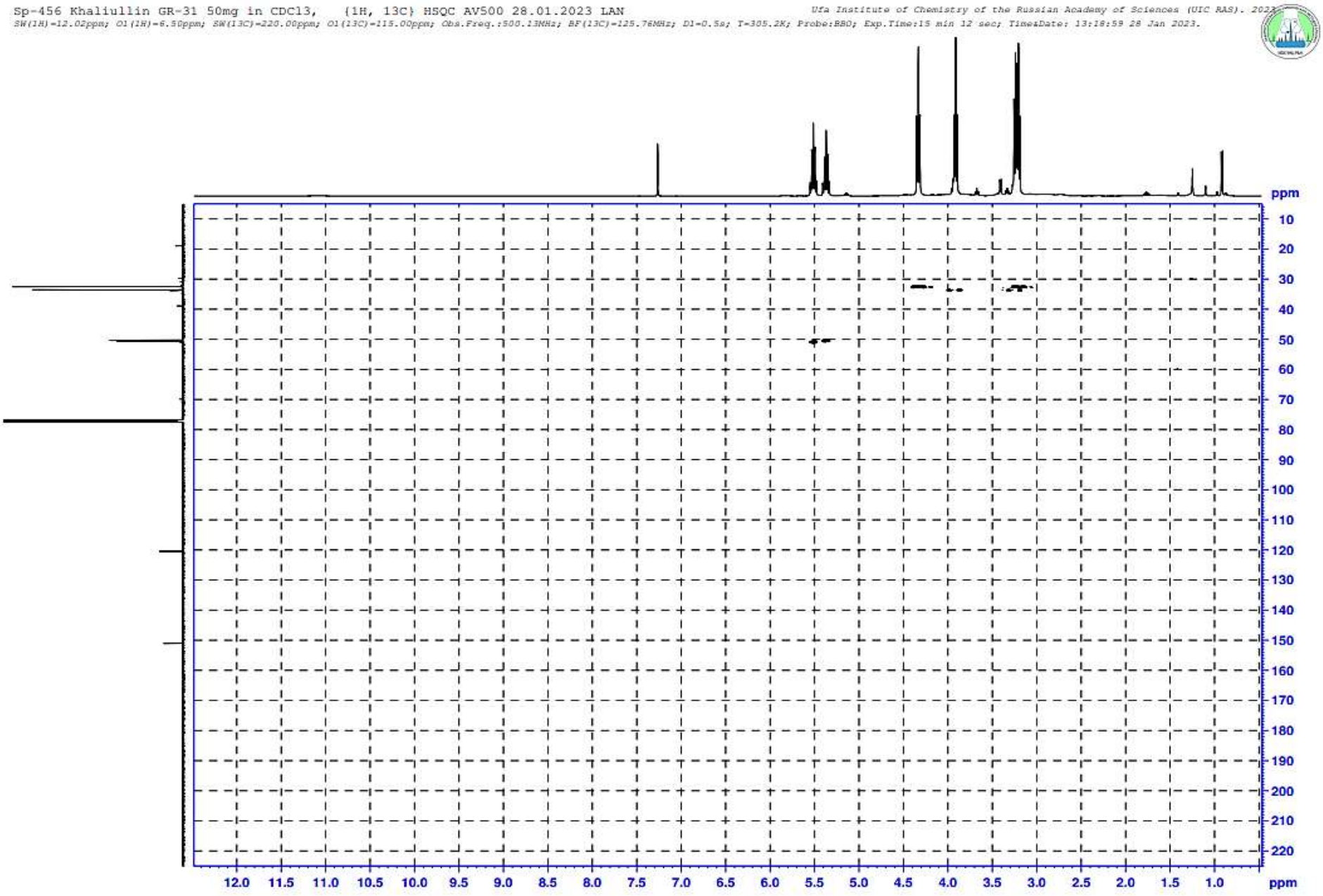
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



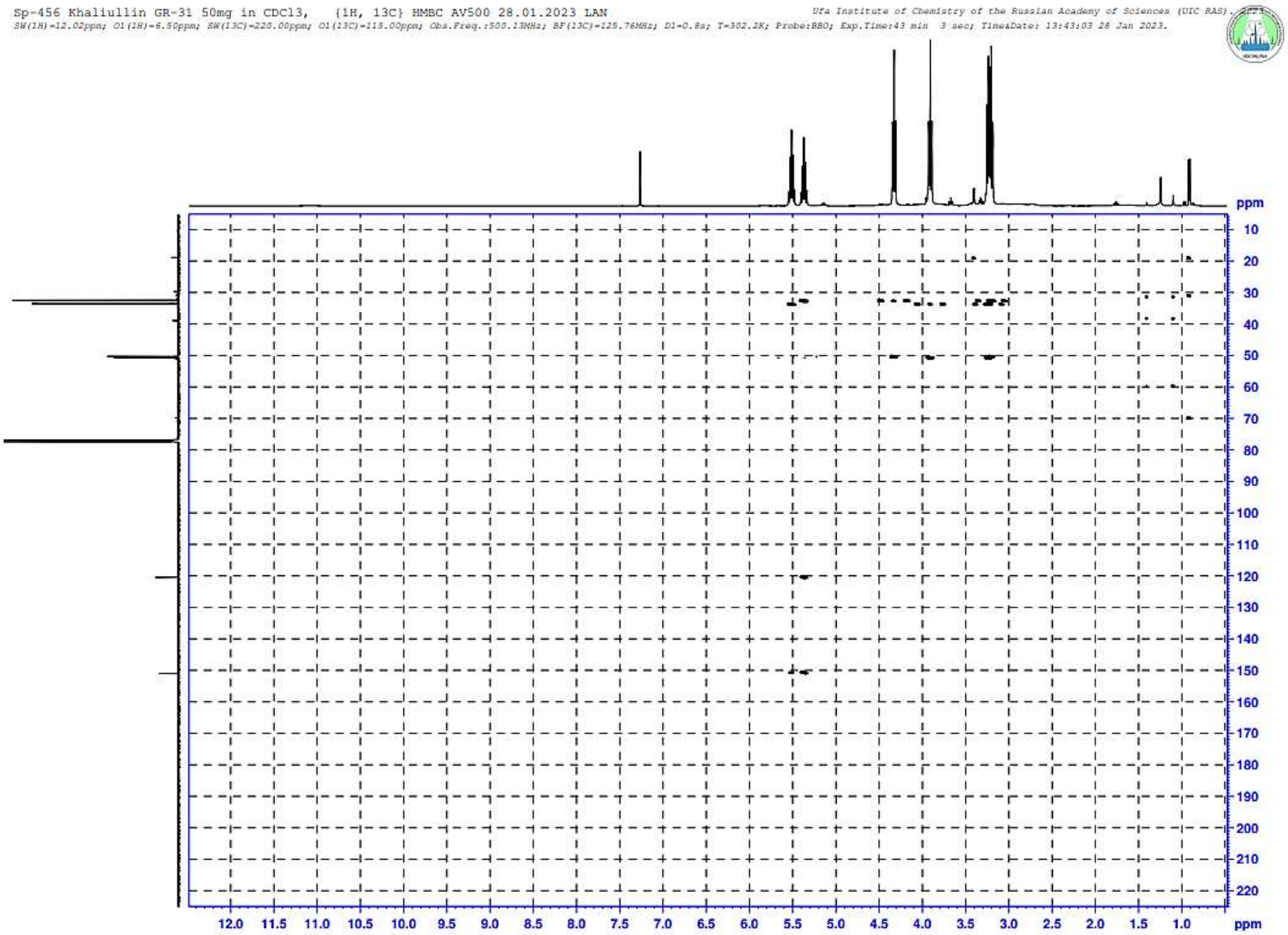
^{13}C NMR (125 MHz, $CDCl_3$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



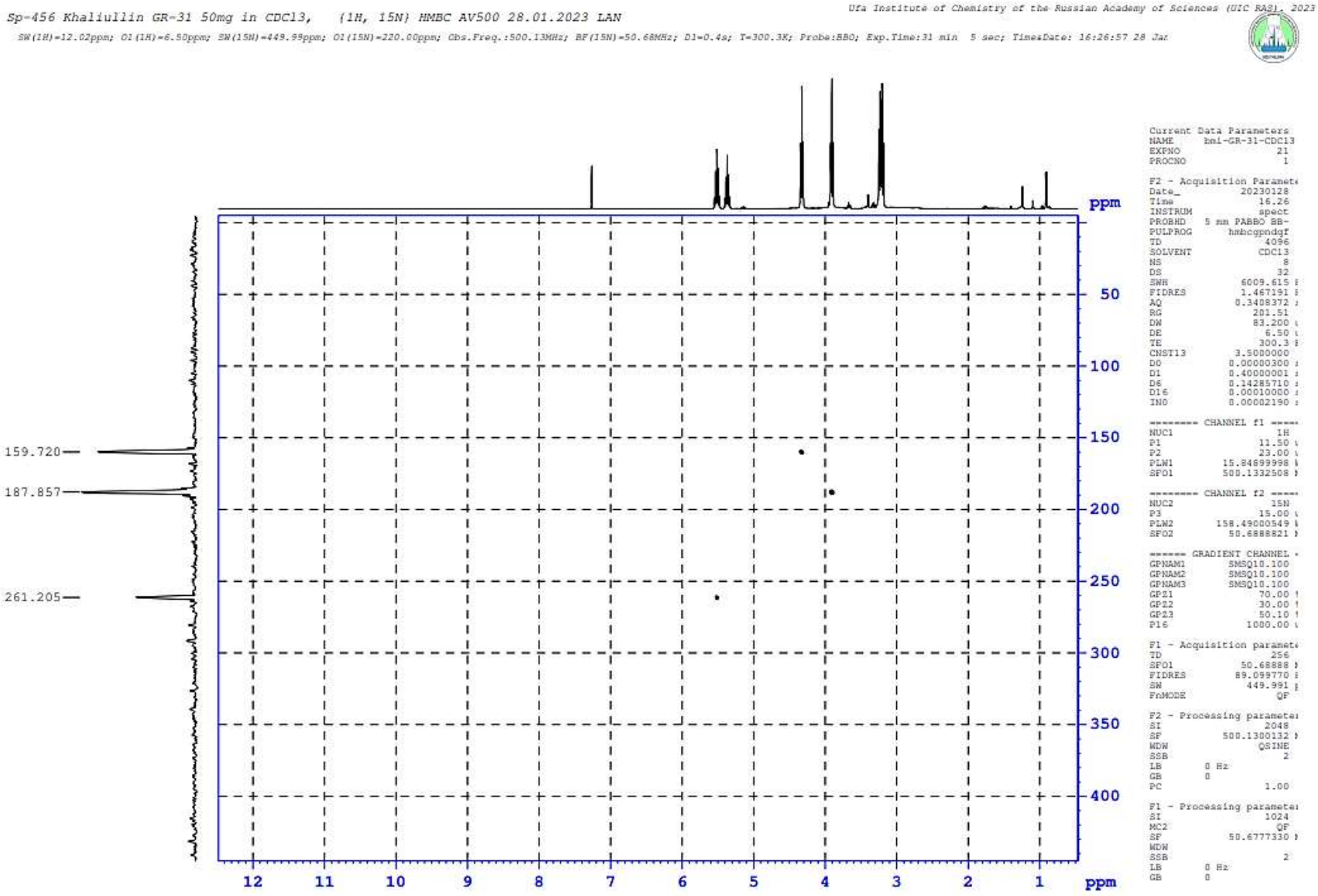
^{1}H-^{13}C HSQC ($CDCl_3$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



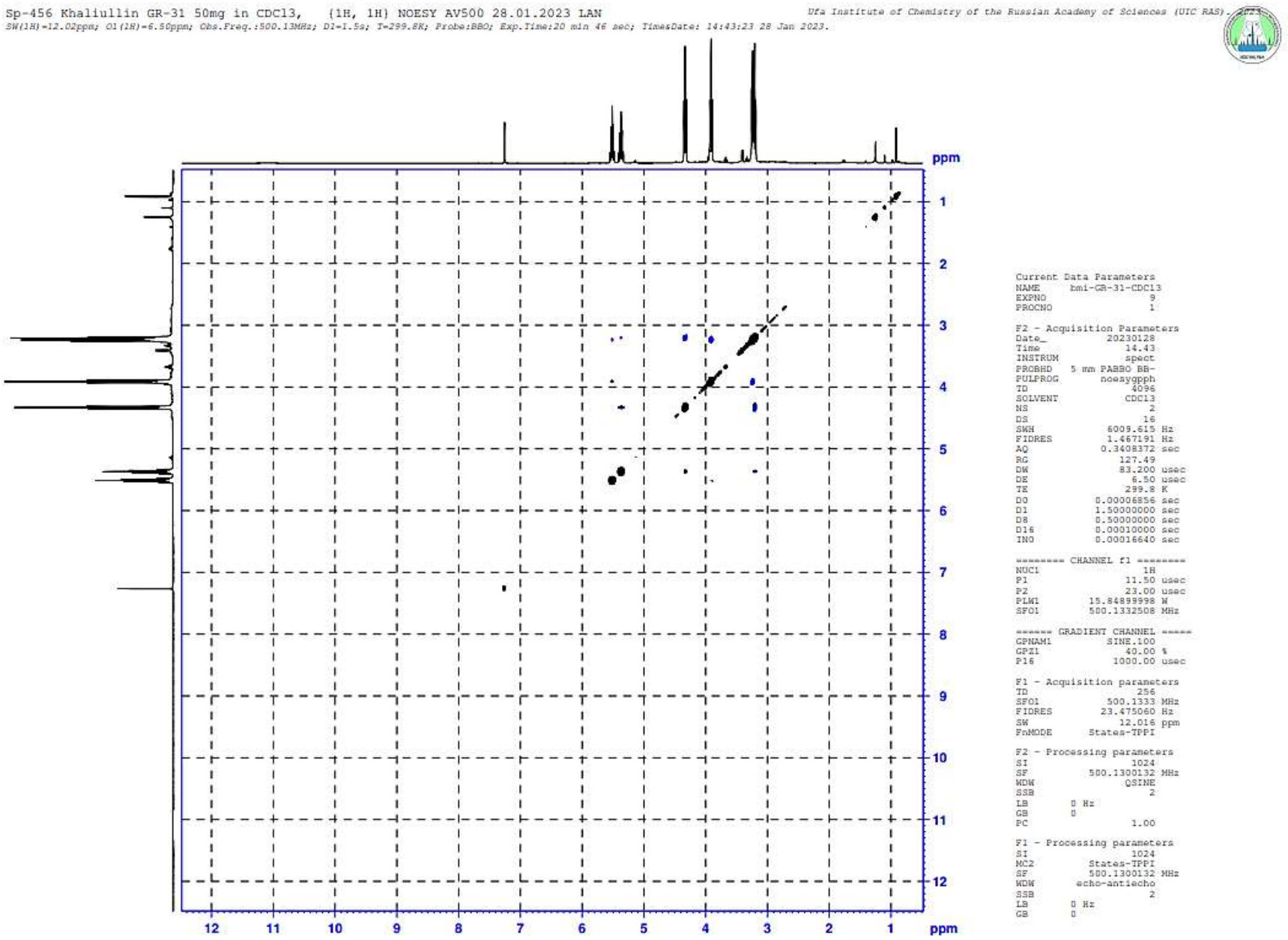
^{1}H-^{13}C HMBC ($CDCl_3$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



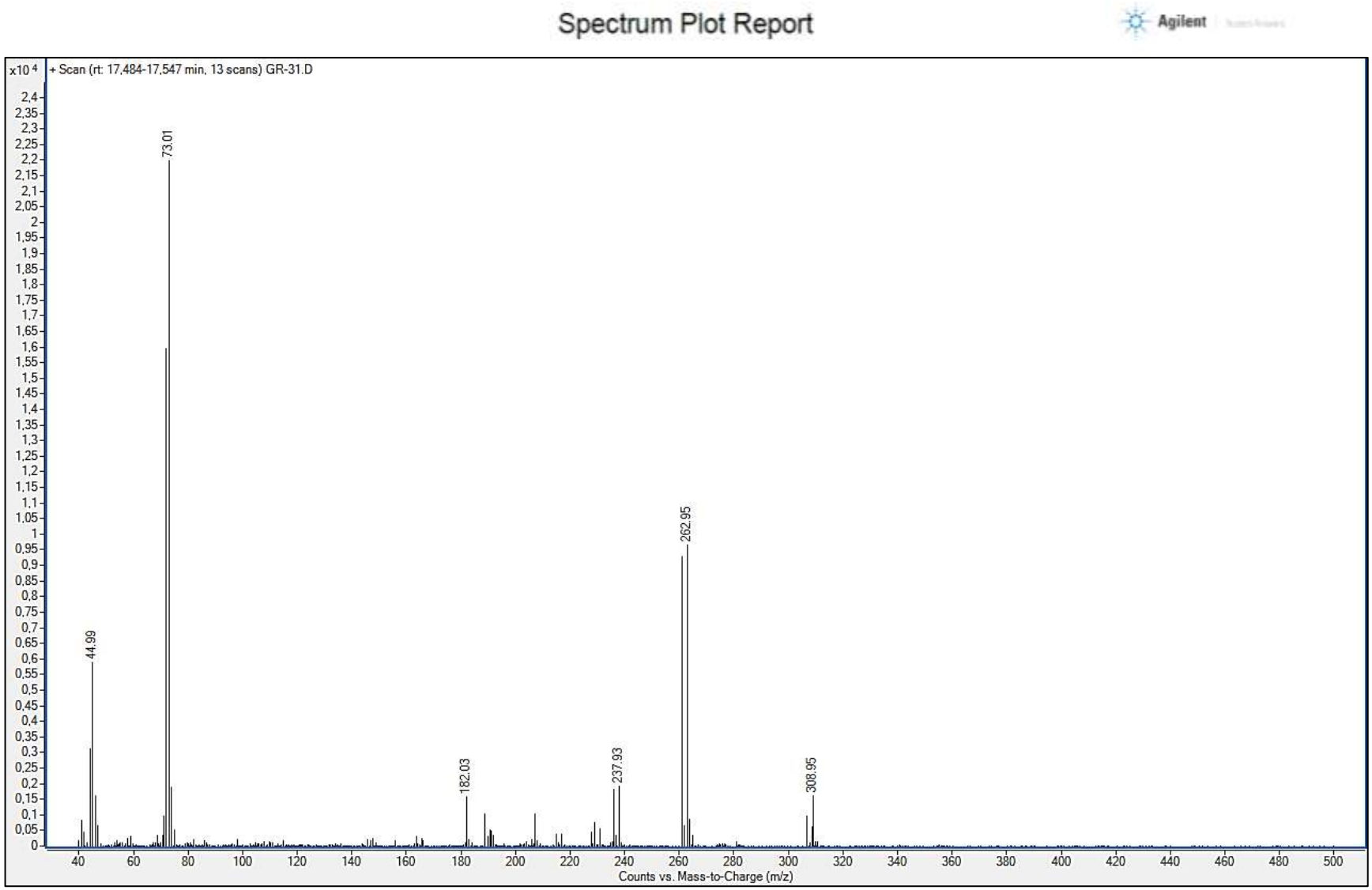
^{1}H-^{15}N HMBC ($CDCl_3$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



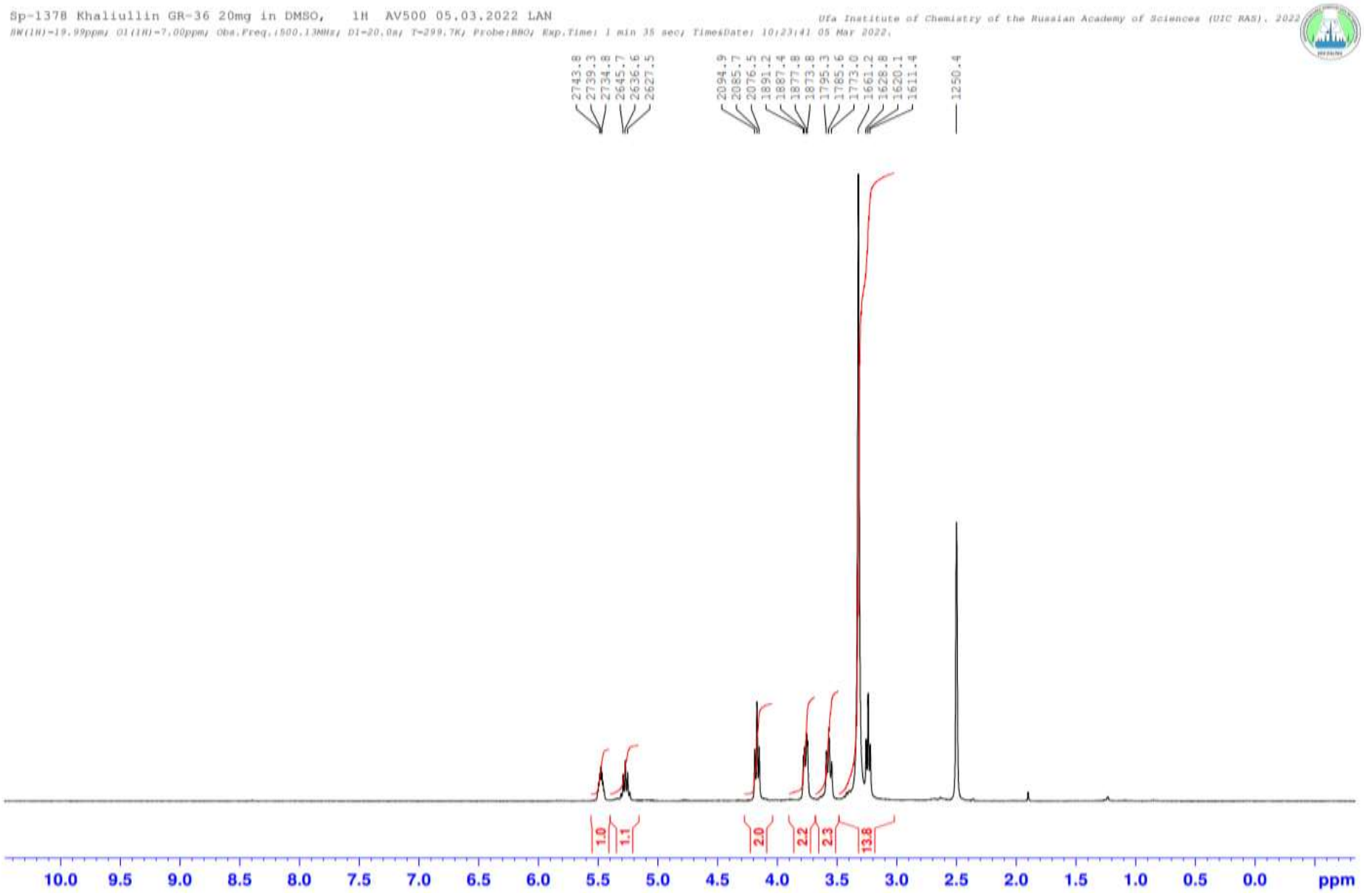
^{1}H-^{1}H NOESY ($CDCl_3$) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



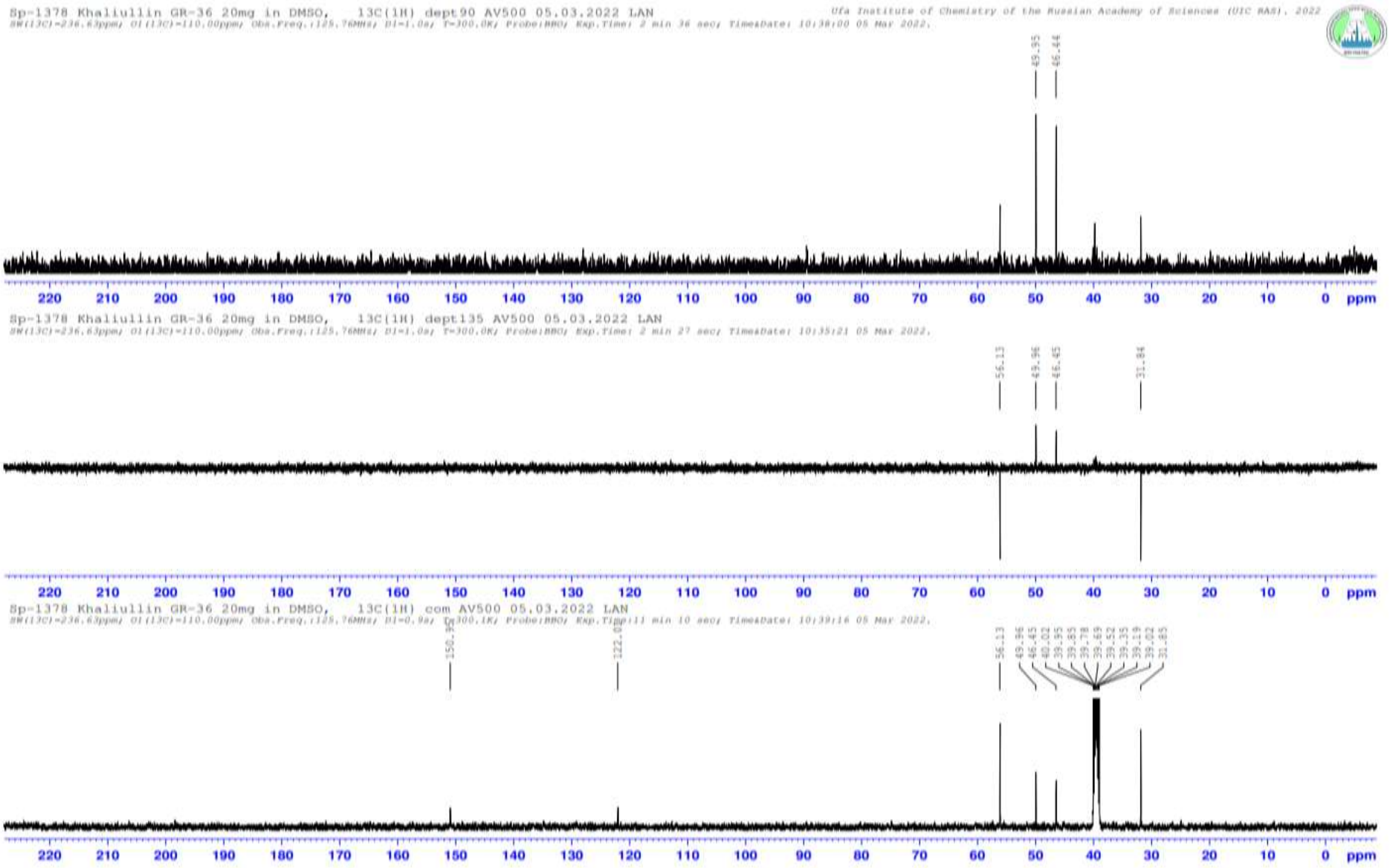
Mass spectrum (EI, 70 eV) of 5-bromo-2,4-di(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5a**)



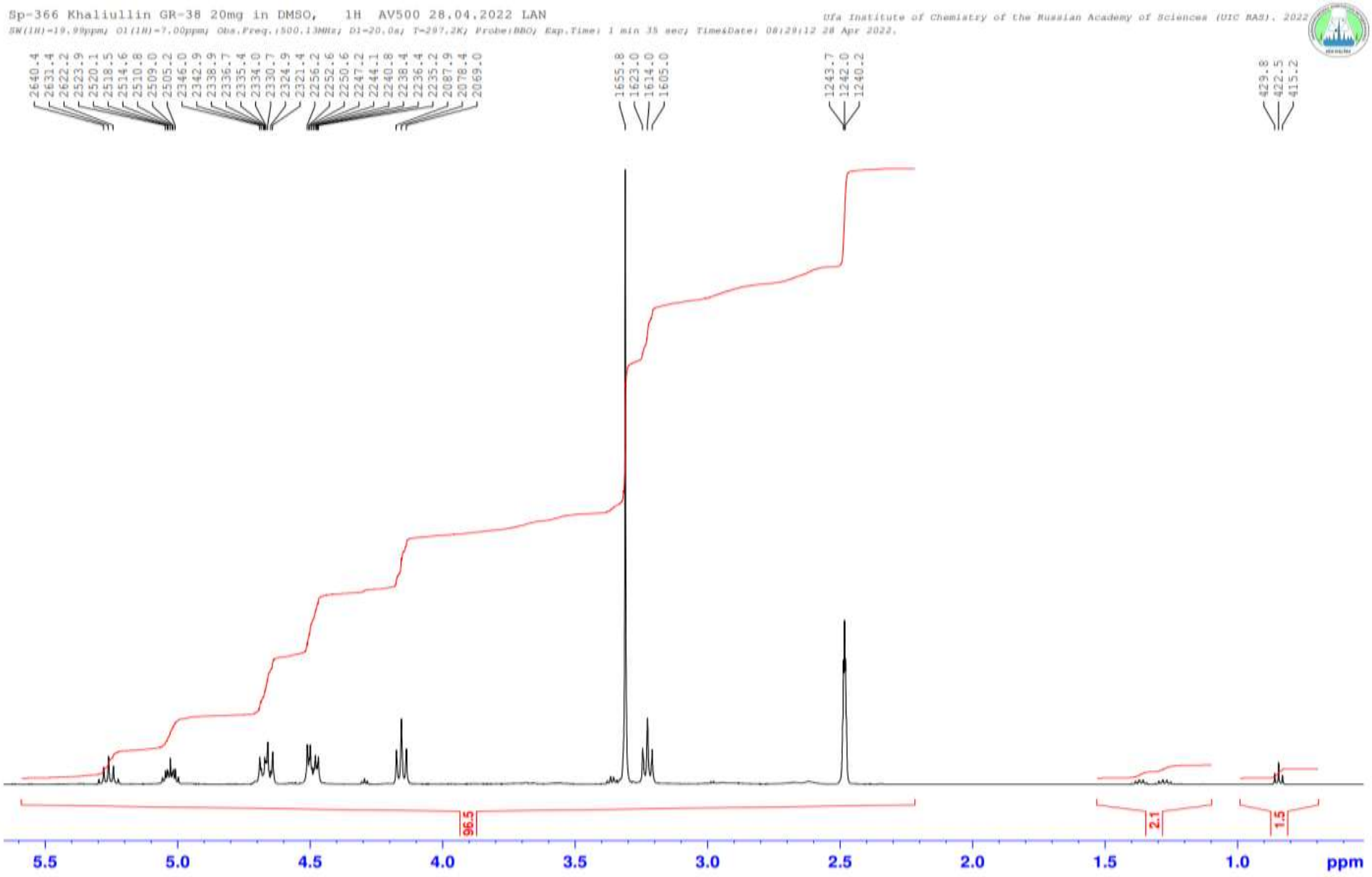
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2-(1-oxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5b**)



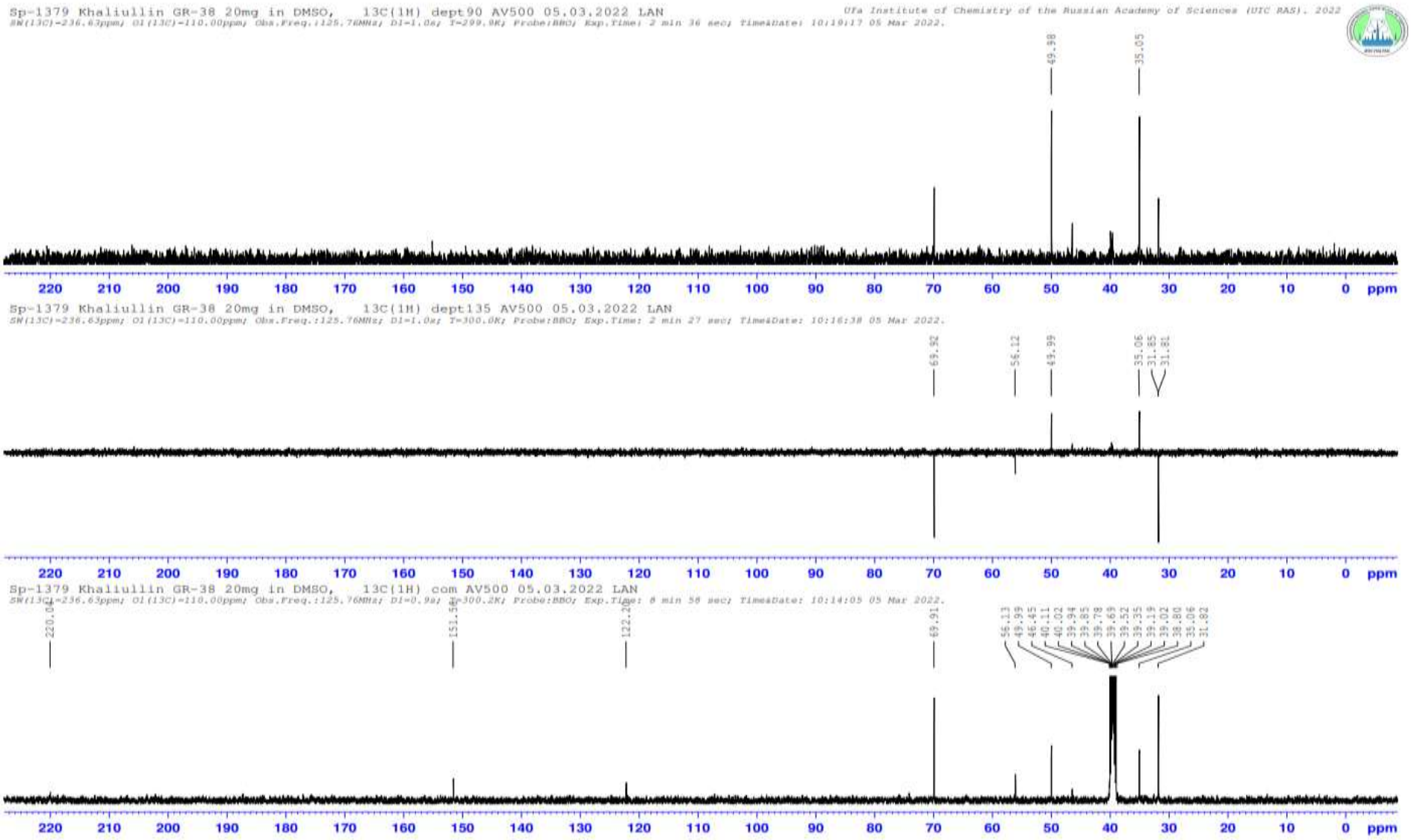
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2-(1-oxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5b**)



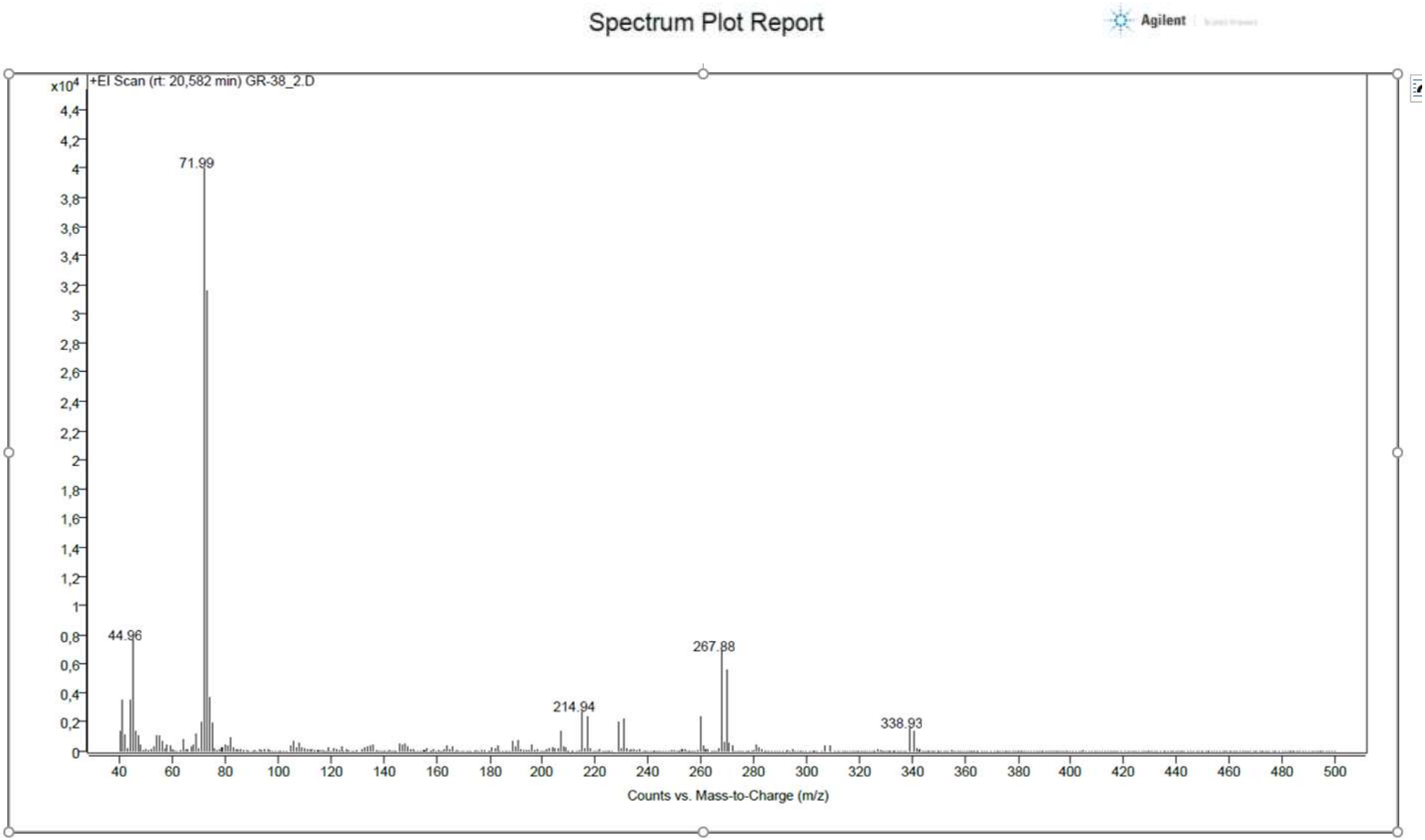
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5c**)



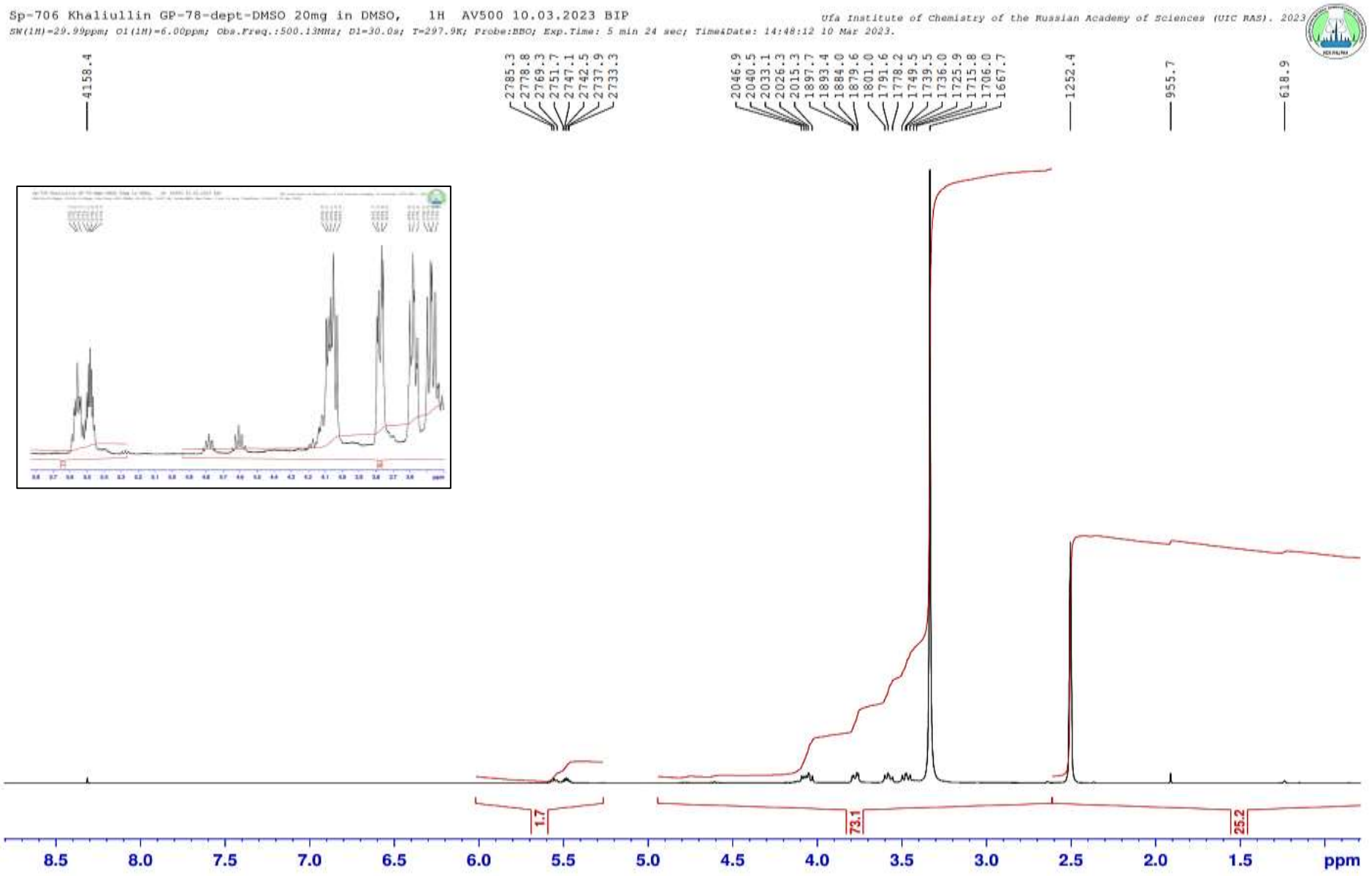
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5c**)



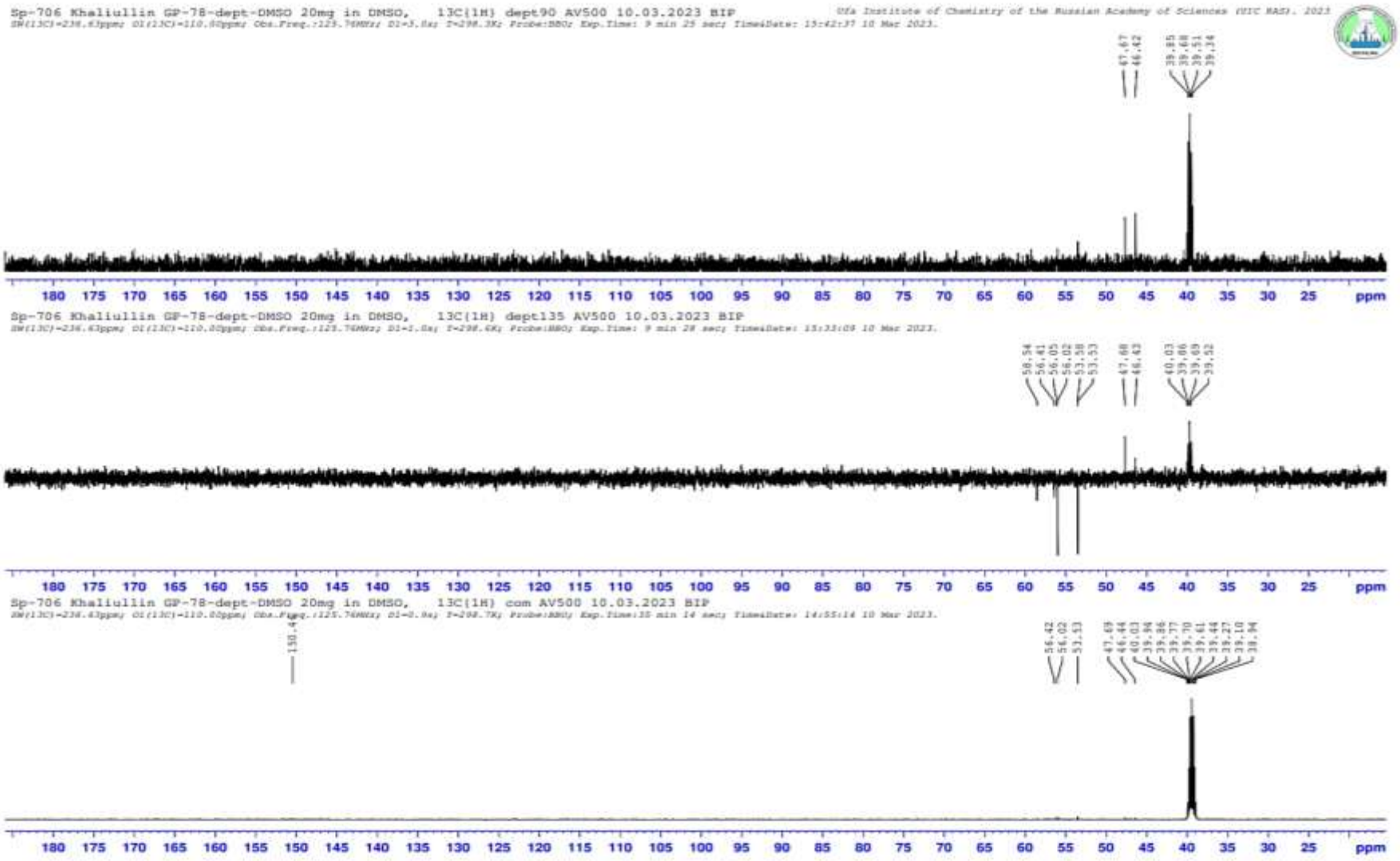
Mass spectrum (EI, 70 eV) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**5c**)



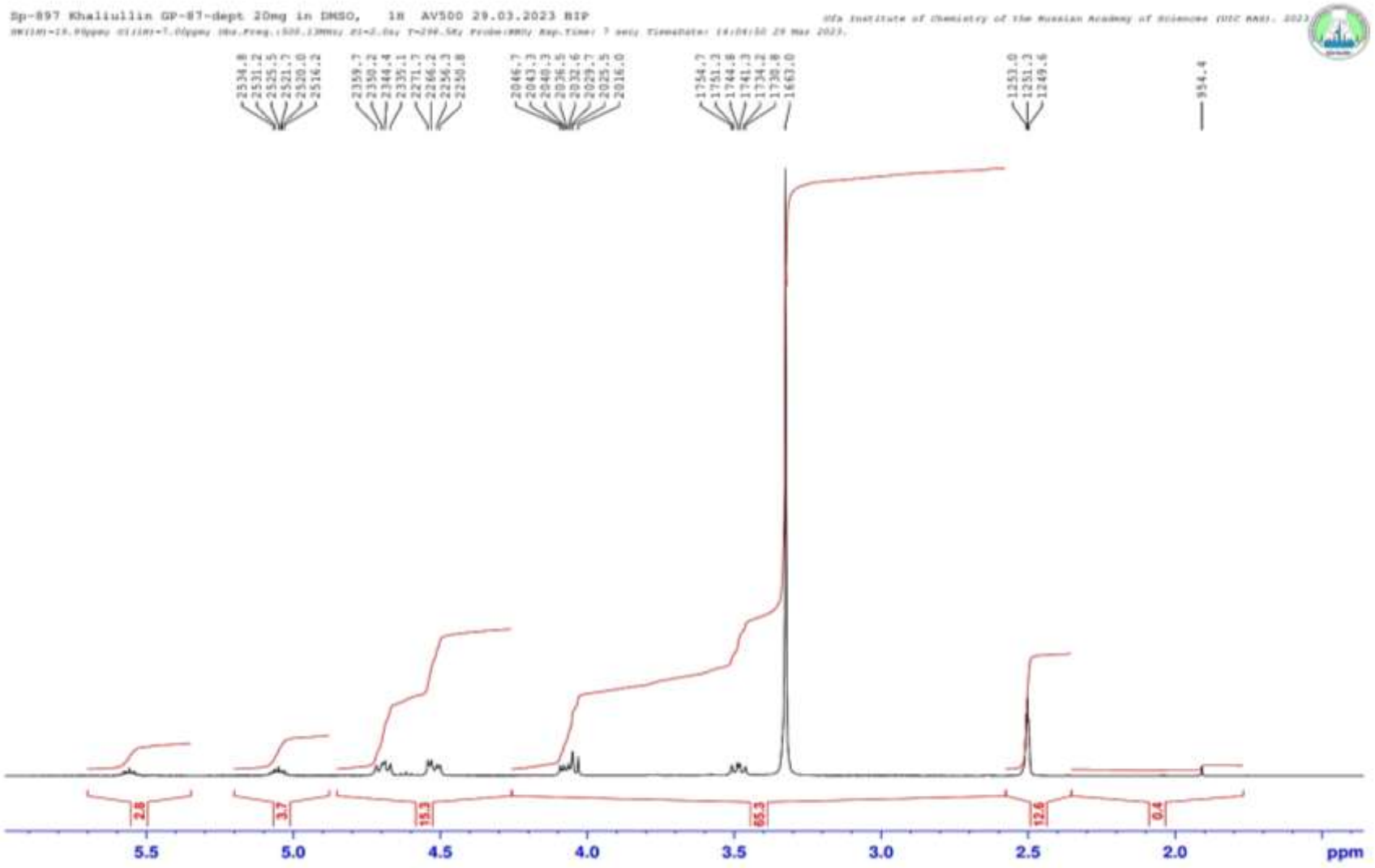
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2,4-bis(1-oxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**6a**)



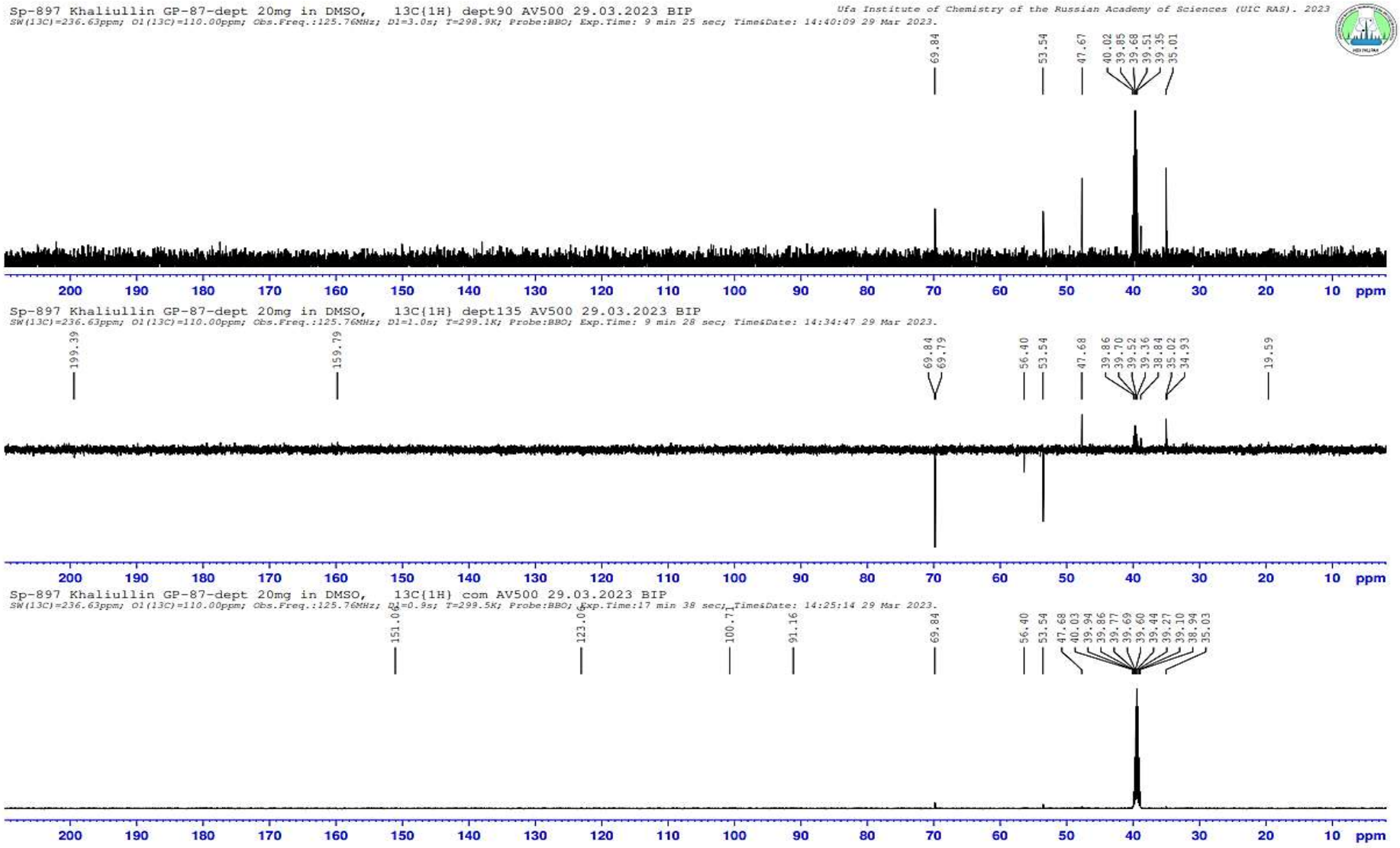
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-2,4-bis(1-oxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one **(6a)**



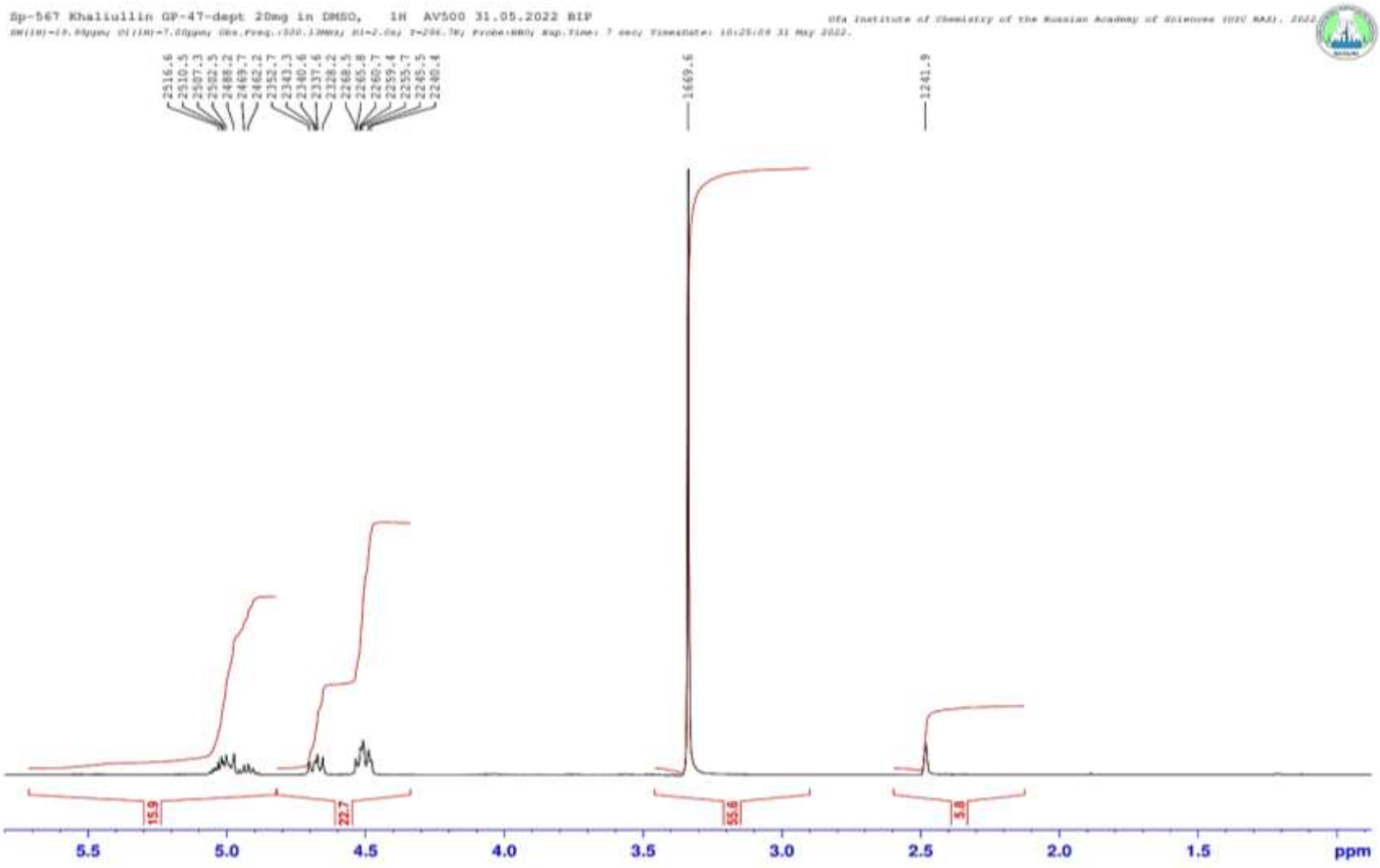
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2-(1,1-dioxothietanyl-3)-4-(1-oxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**6b**)



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



^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-2,4-bis(1,1-dioxothietanyl-3)-2,4-dihydro-3*H*-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 (UIC RAS), 2022
2516.6
2510.5
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55.6
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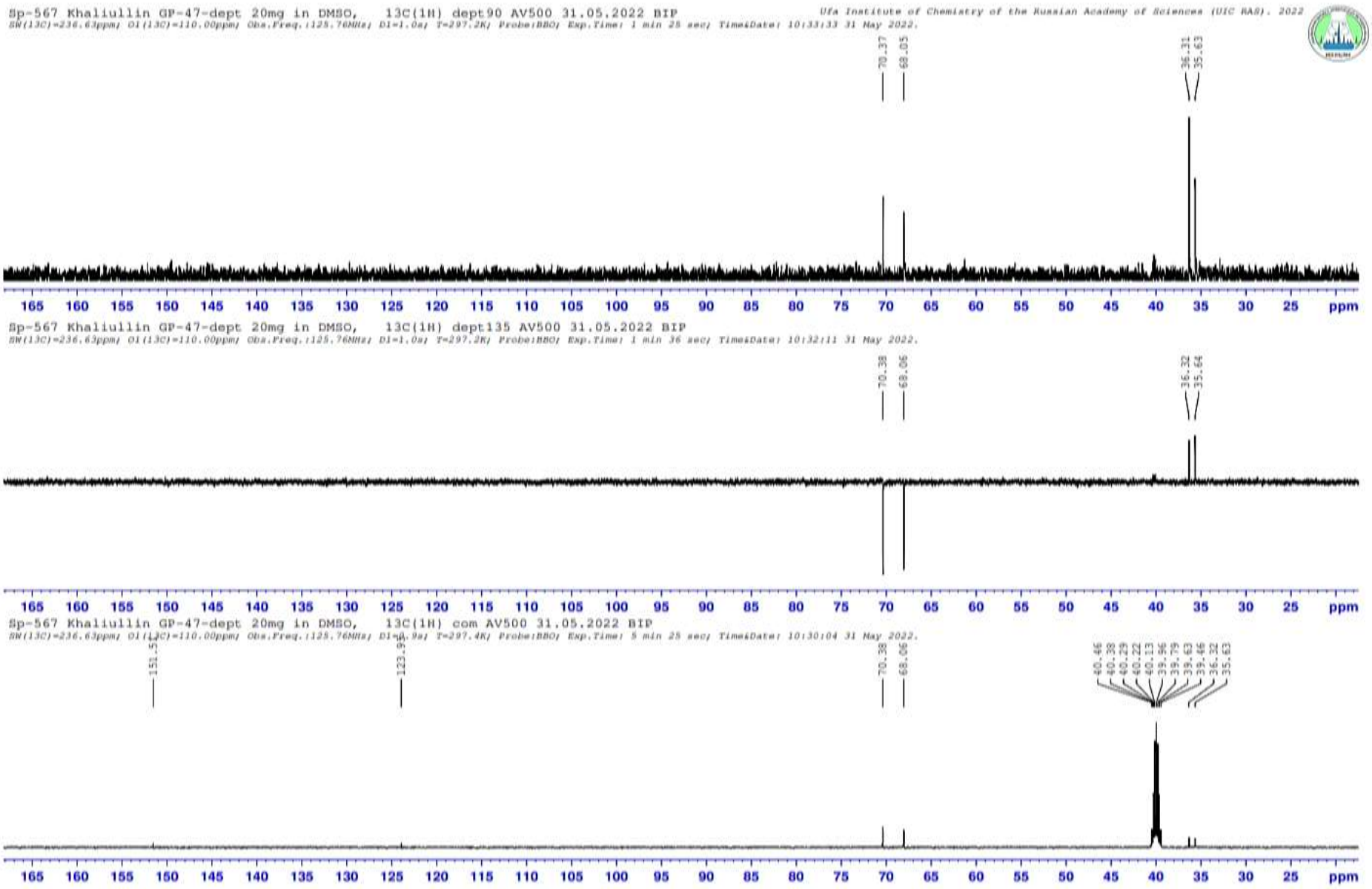
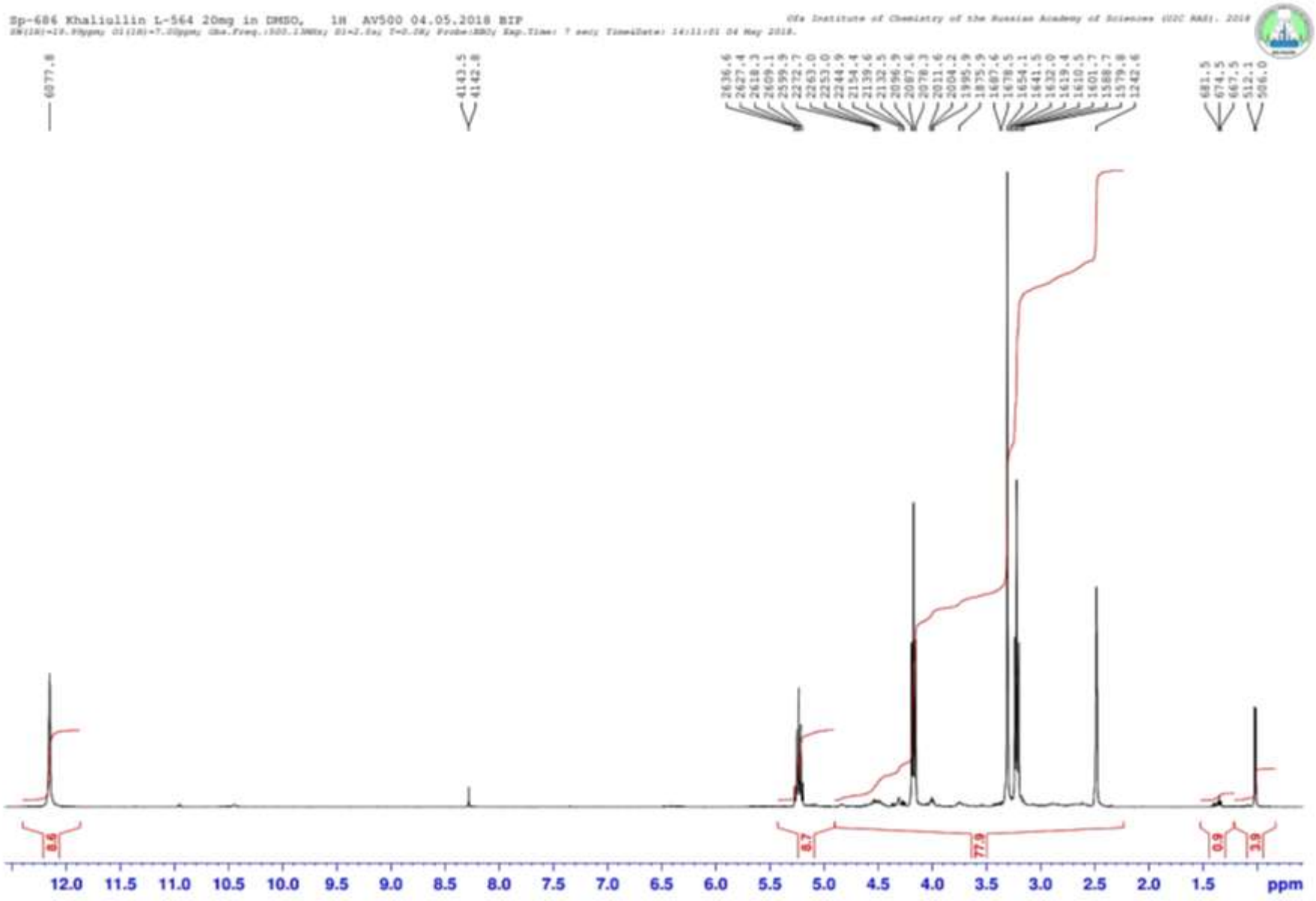
ppm

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



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



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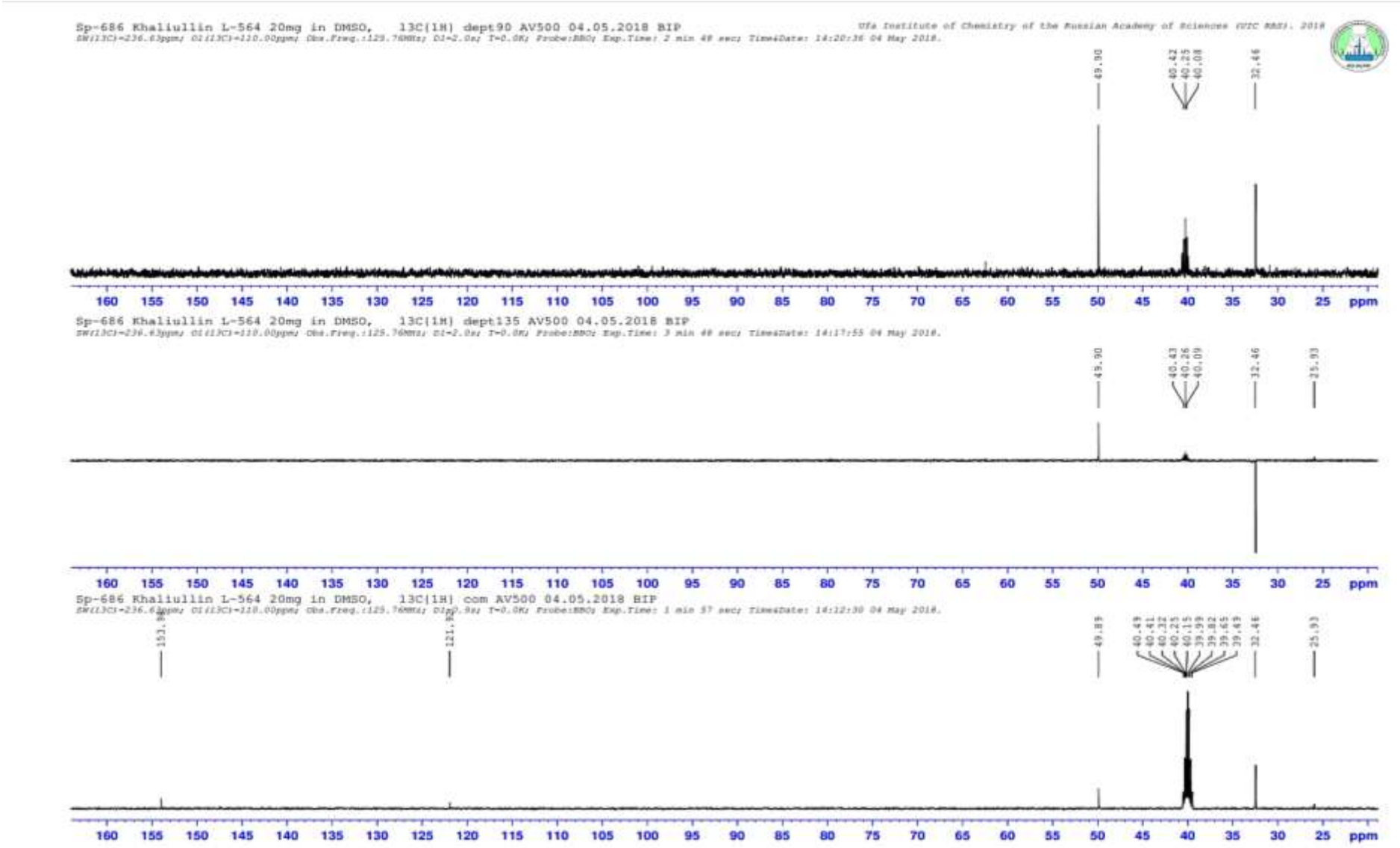
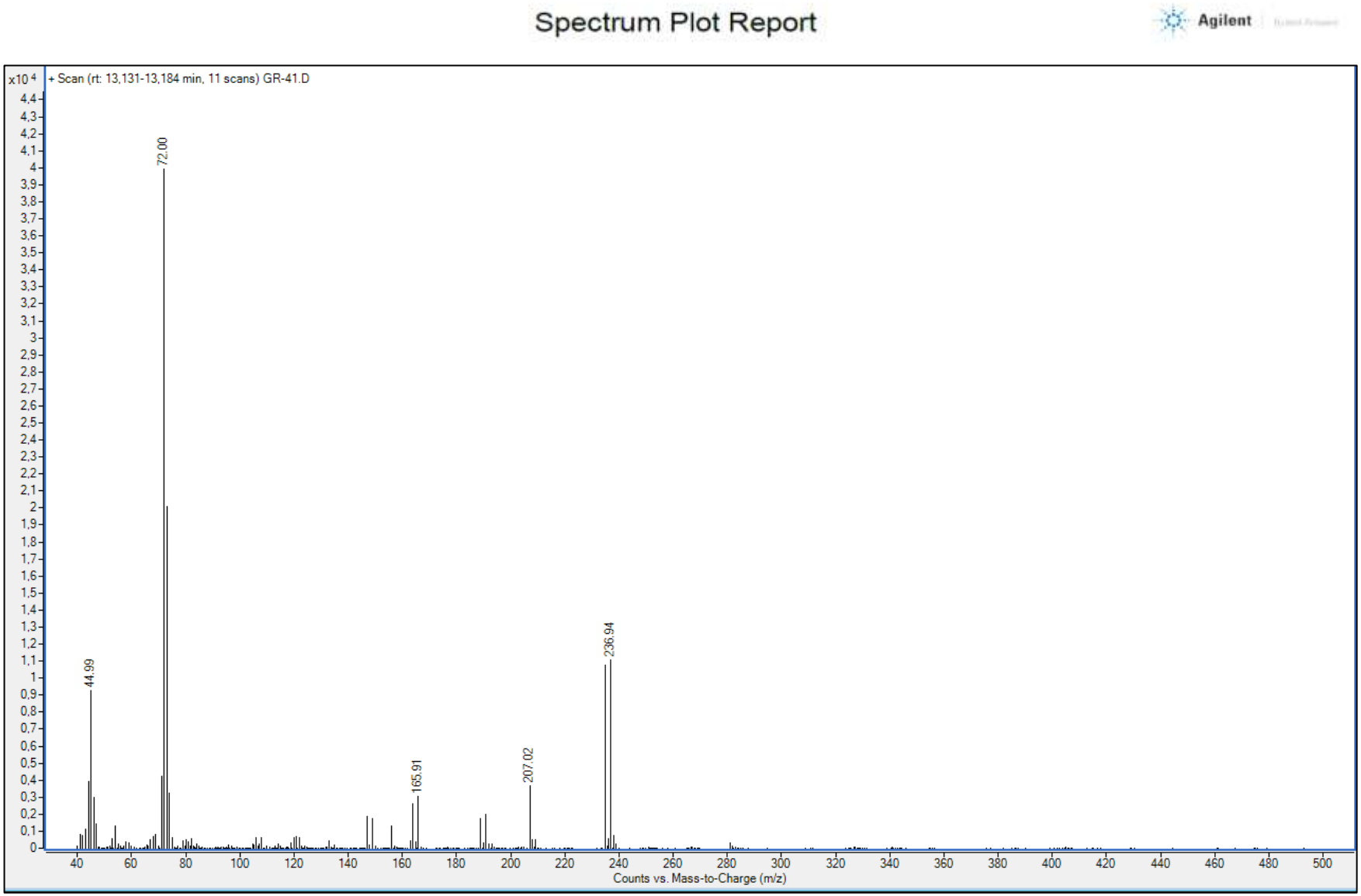
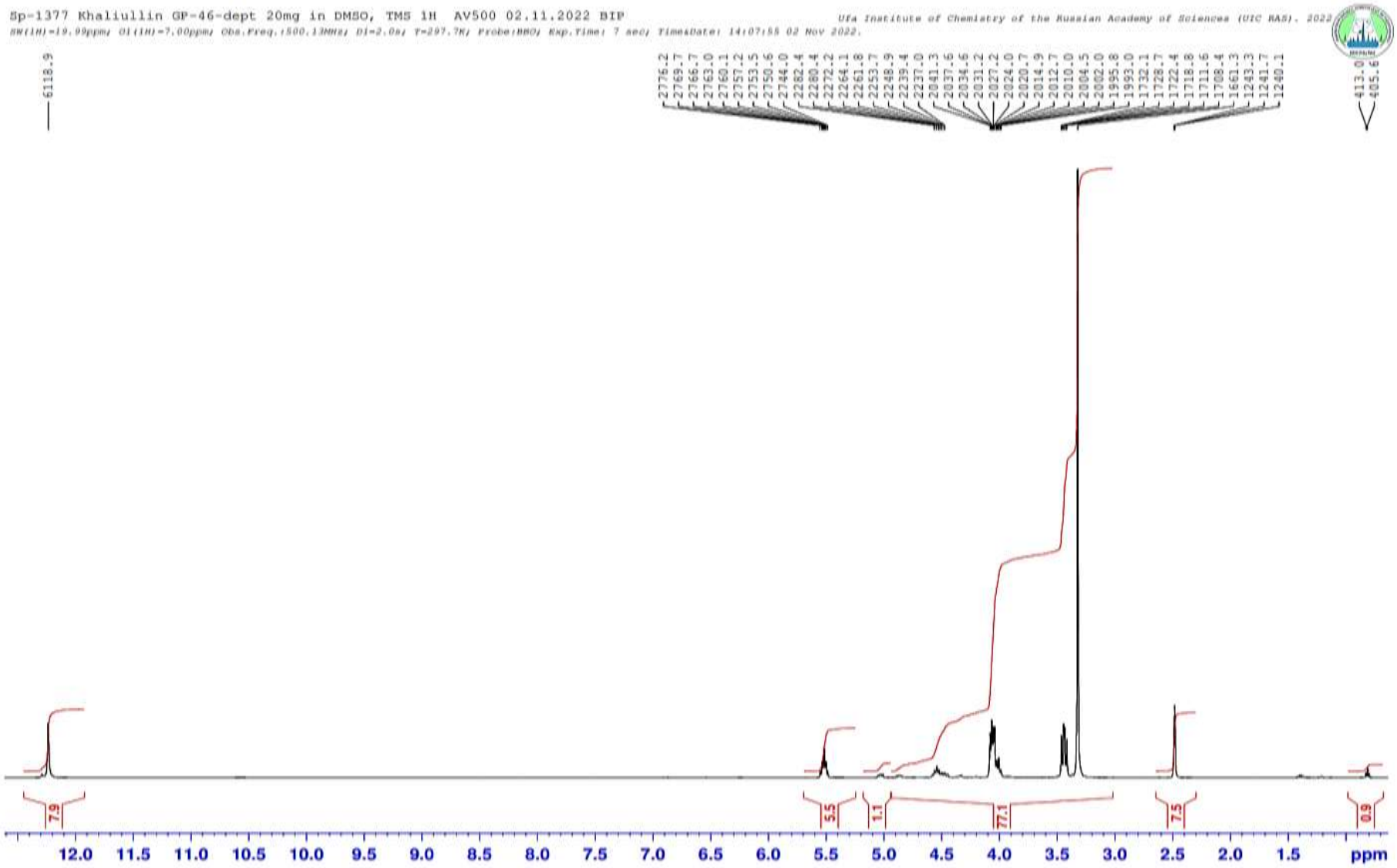


Mass spectrum (EI, 70 eV) of 5-bromo-4-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**7a**)



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



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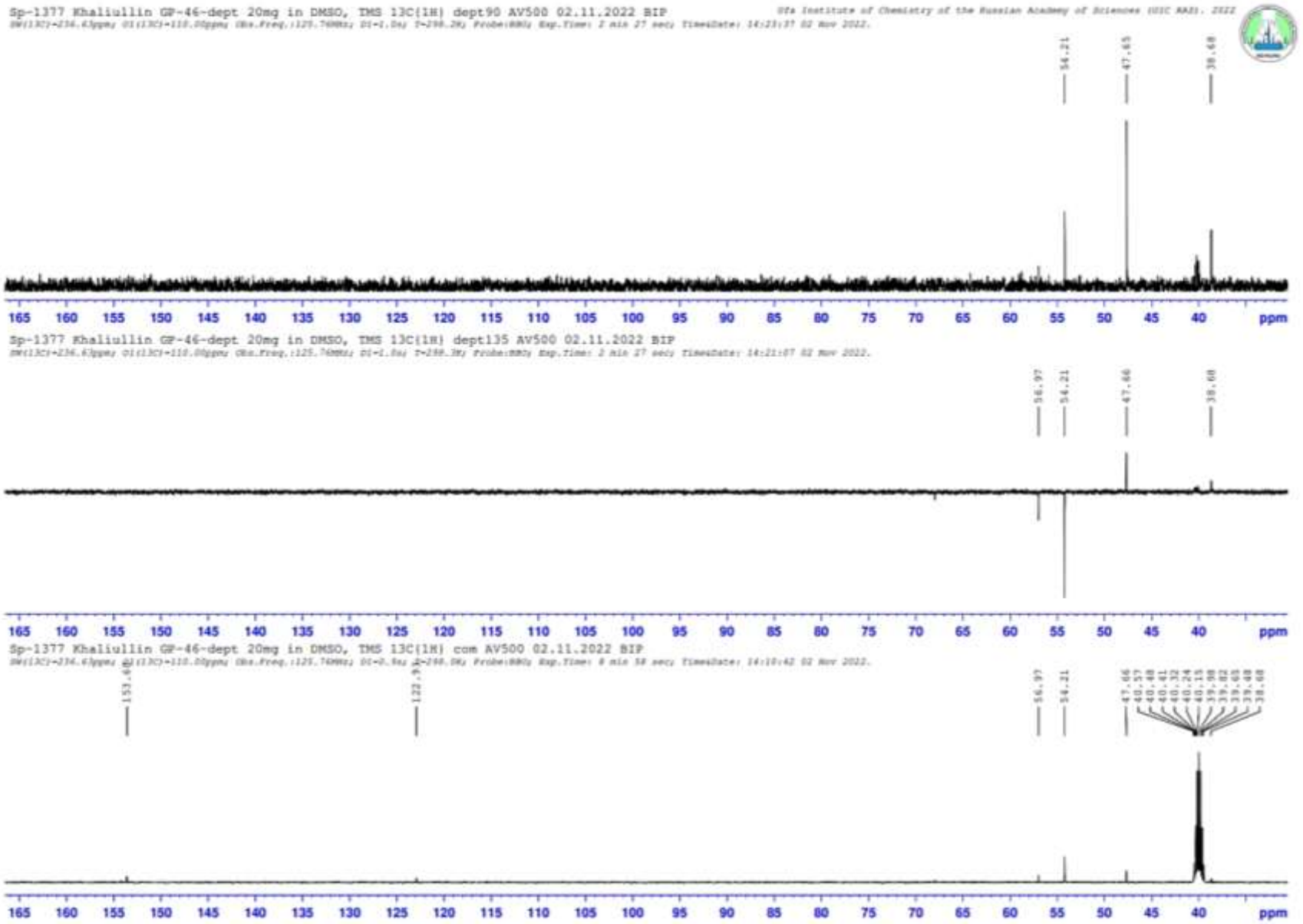
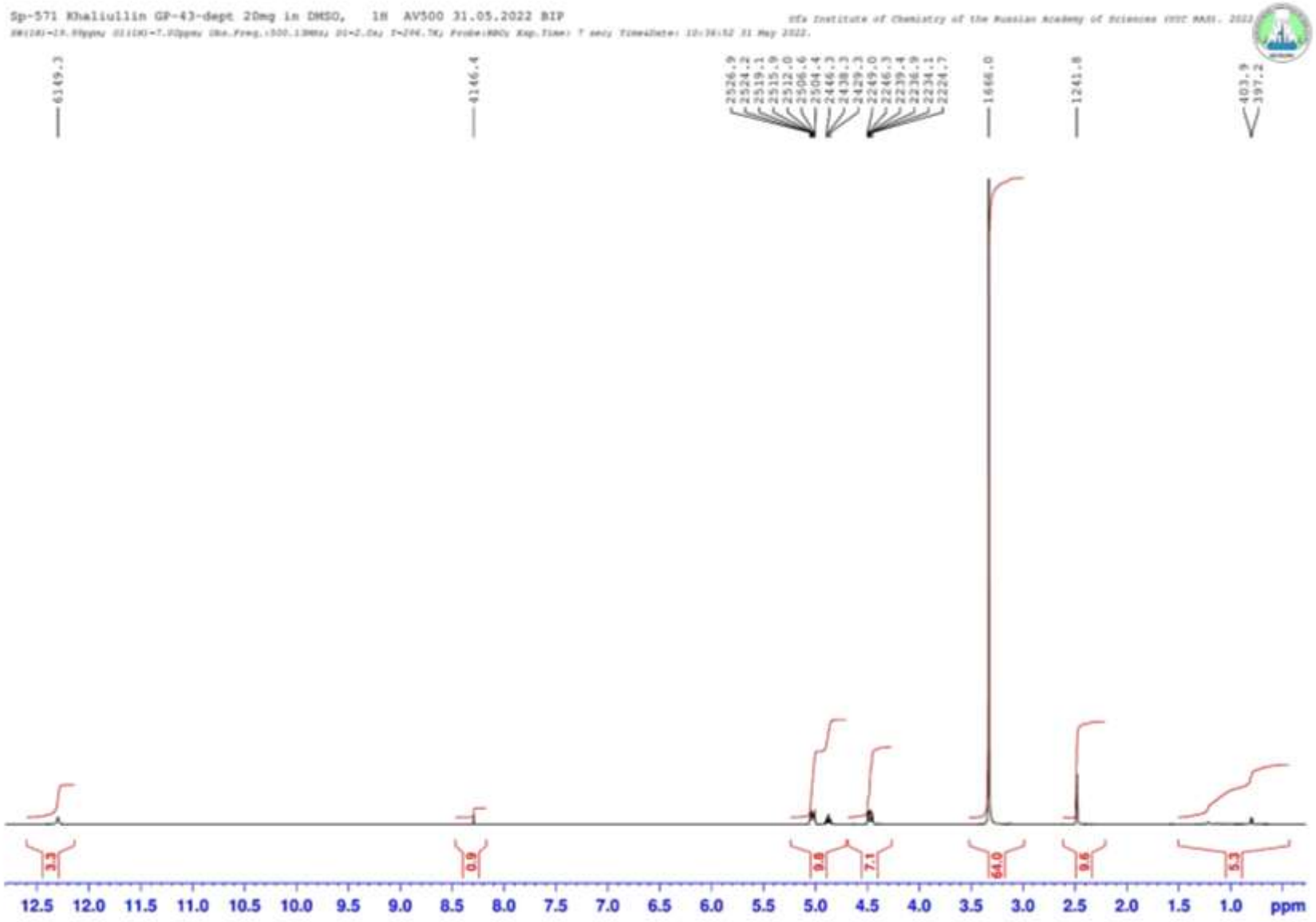
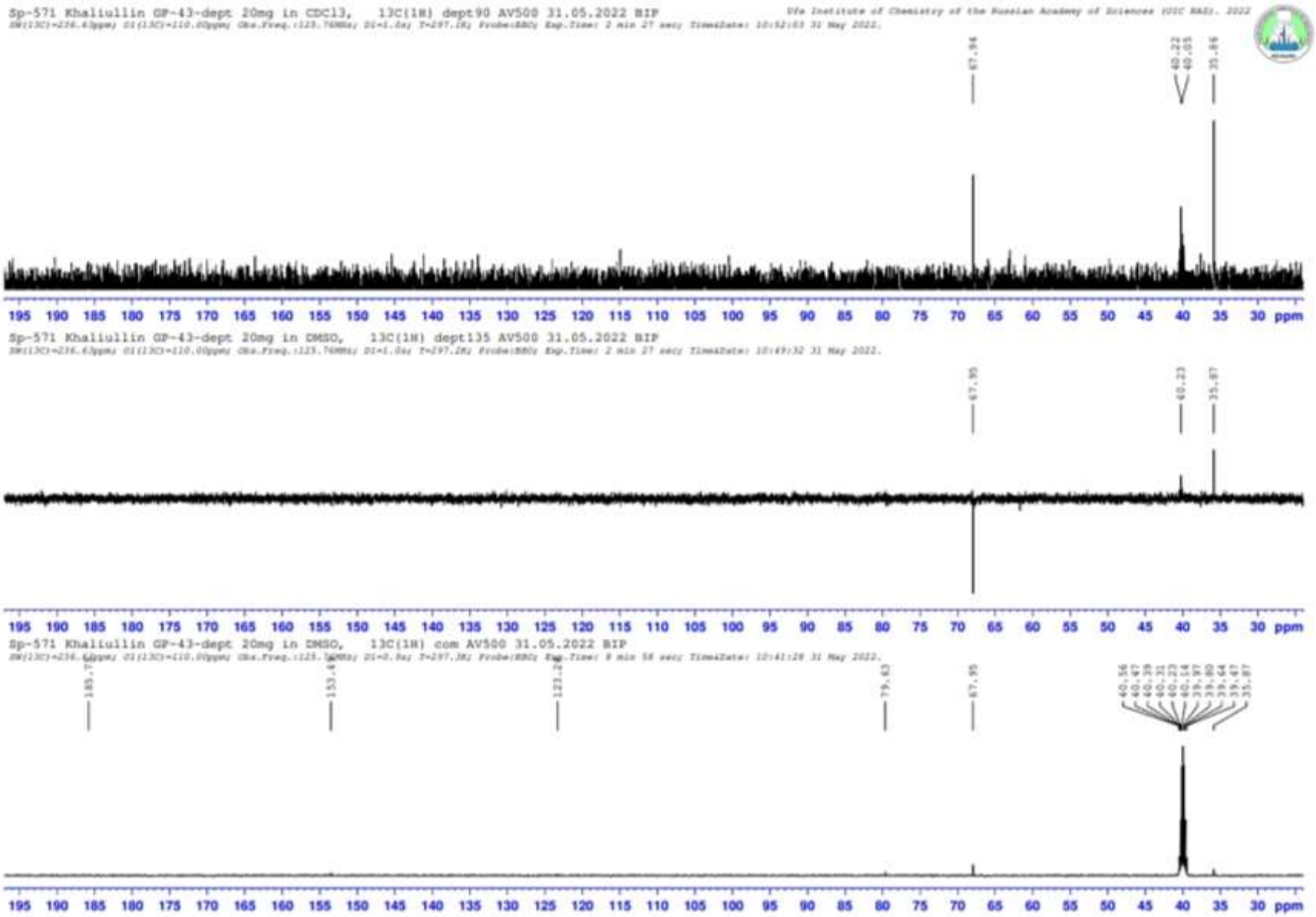


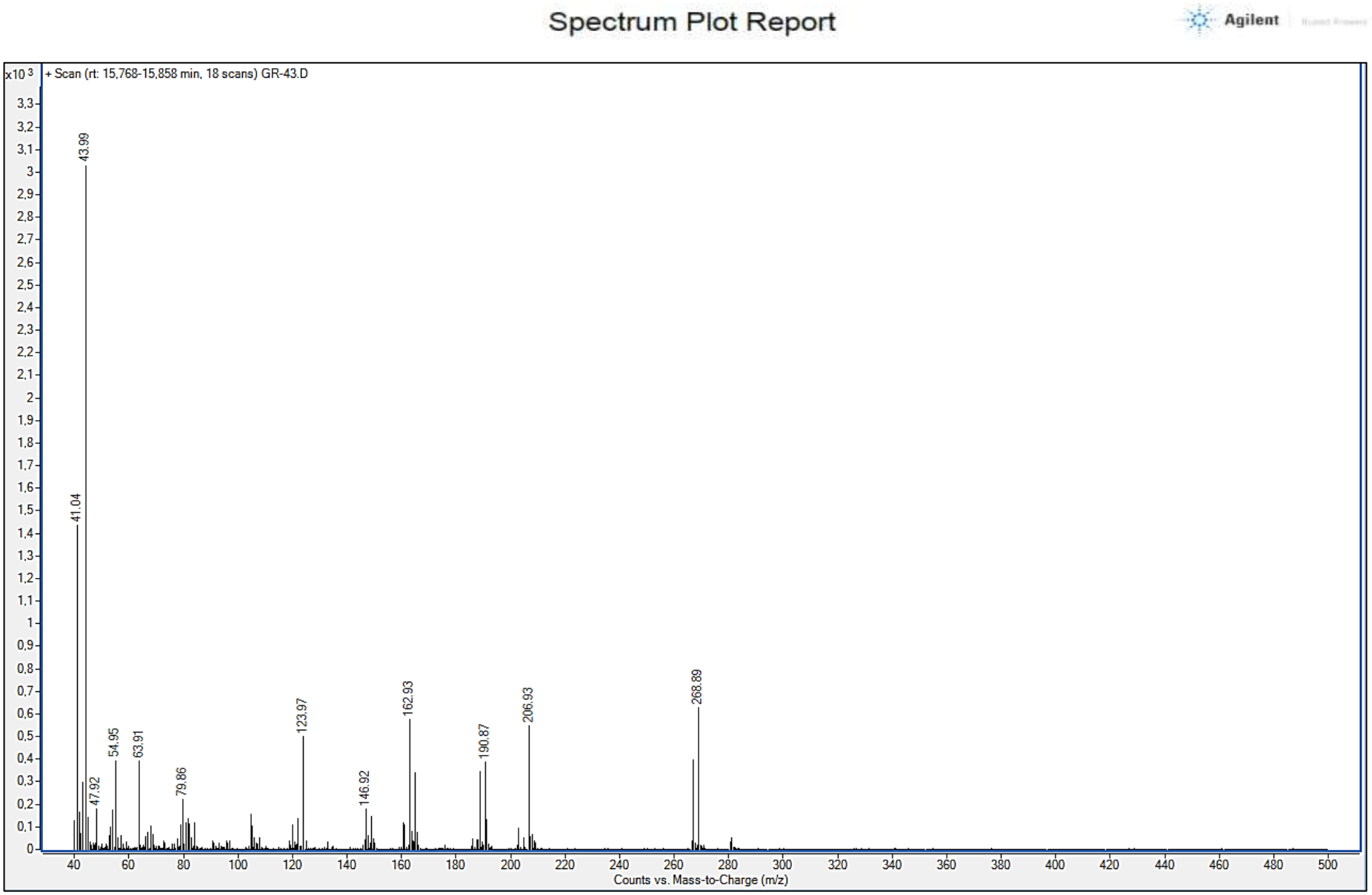
^{1}H NMR (500 MHz, DMSO-d_6) of 5-bromo-4-(1,1-dioxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**7c**)



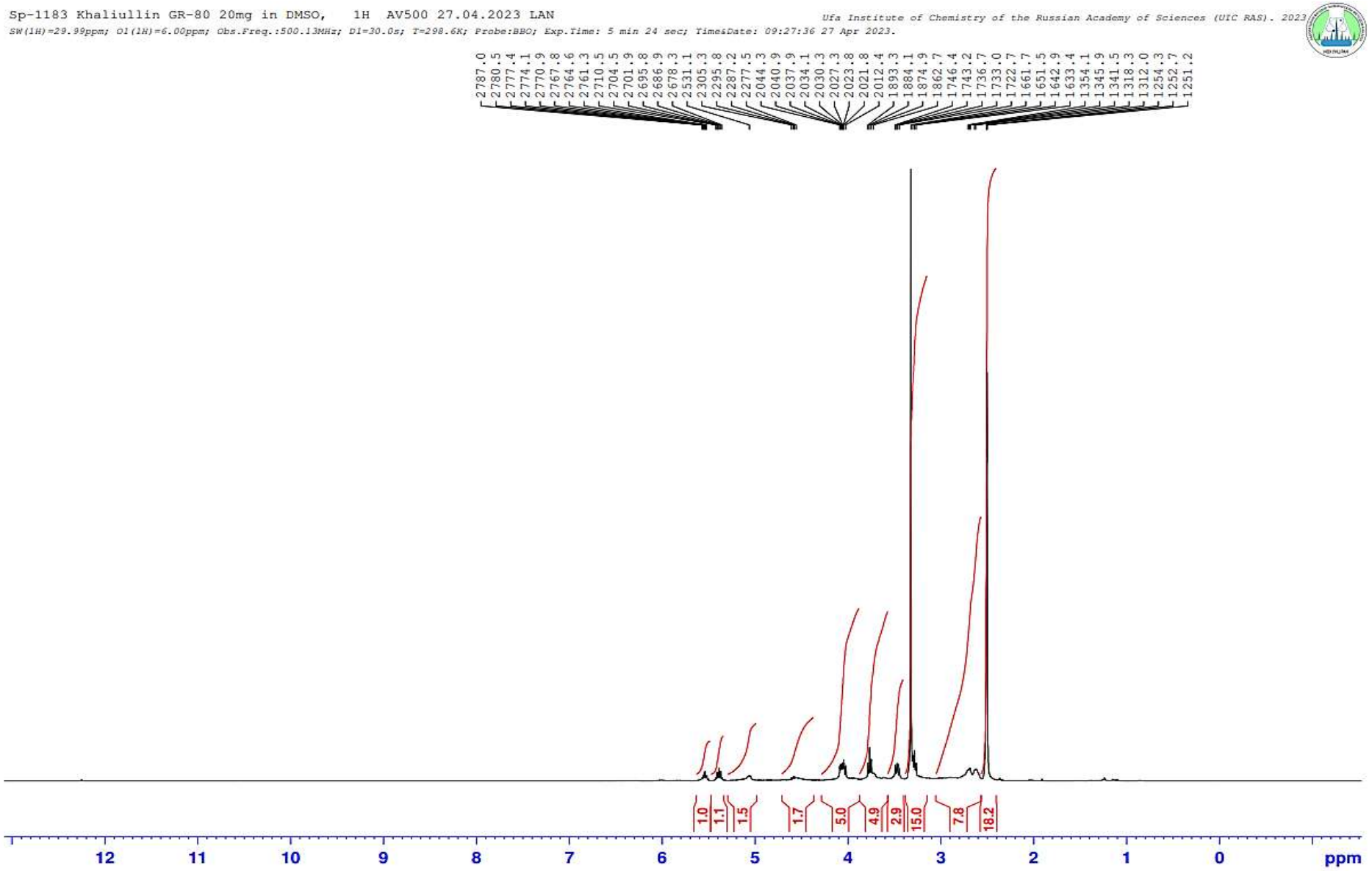
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-4-(1,1-dioxothietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**7c**)



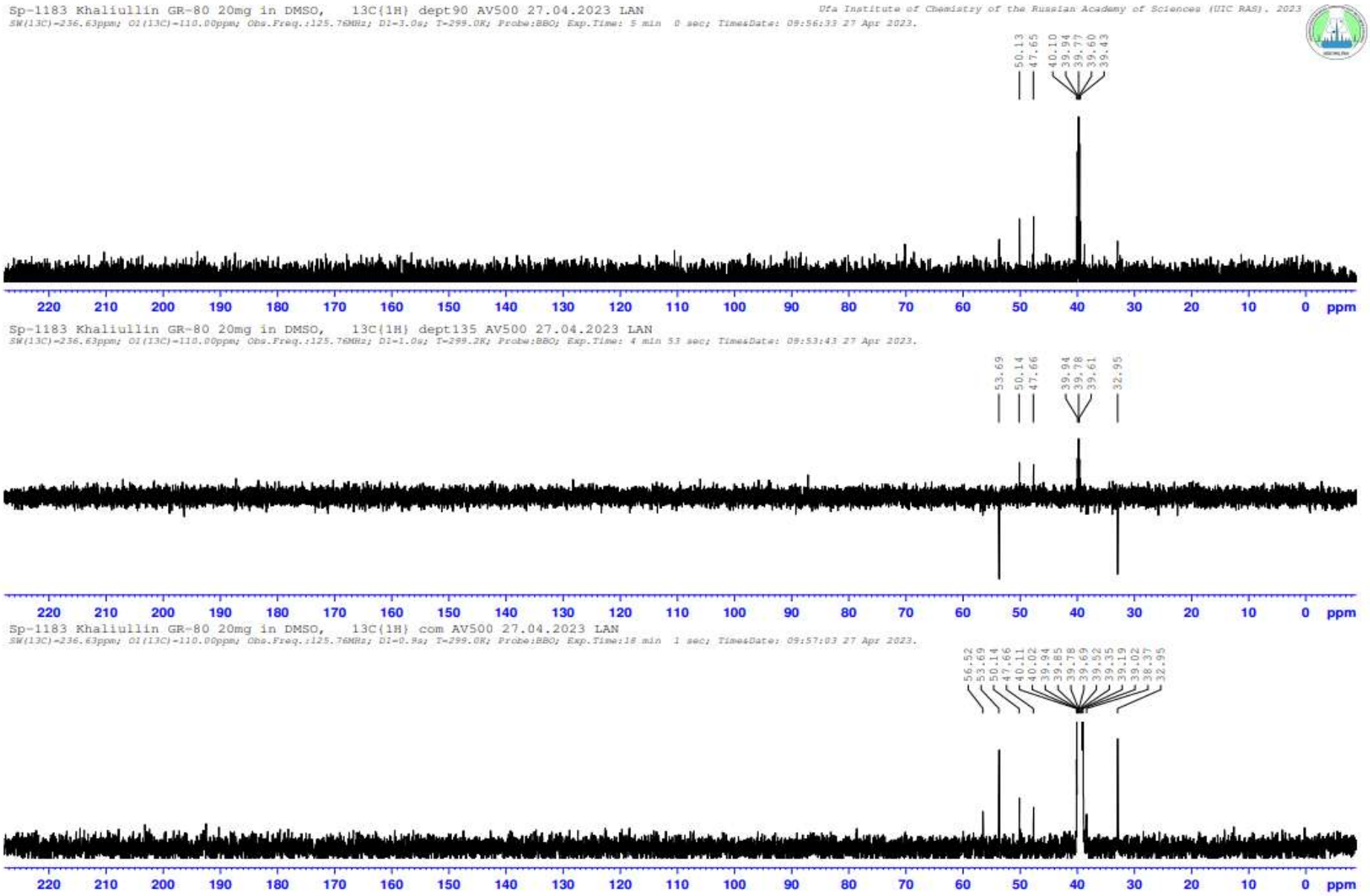
Mass spectrum (EI, 70 eV) of 5-bromo-4-(1,1-dioxothietanyl-3)-2,4-dihydro-3H-1,2,4-triazol-3-one (**7c**)



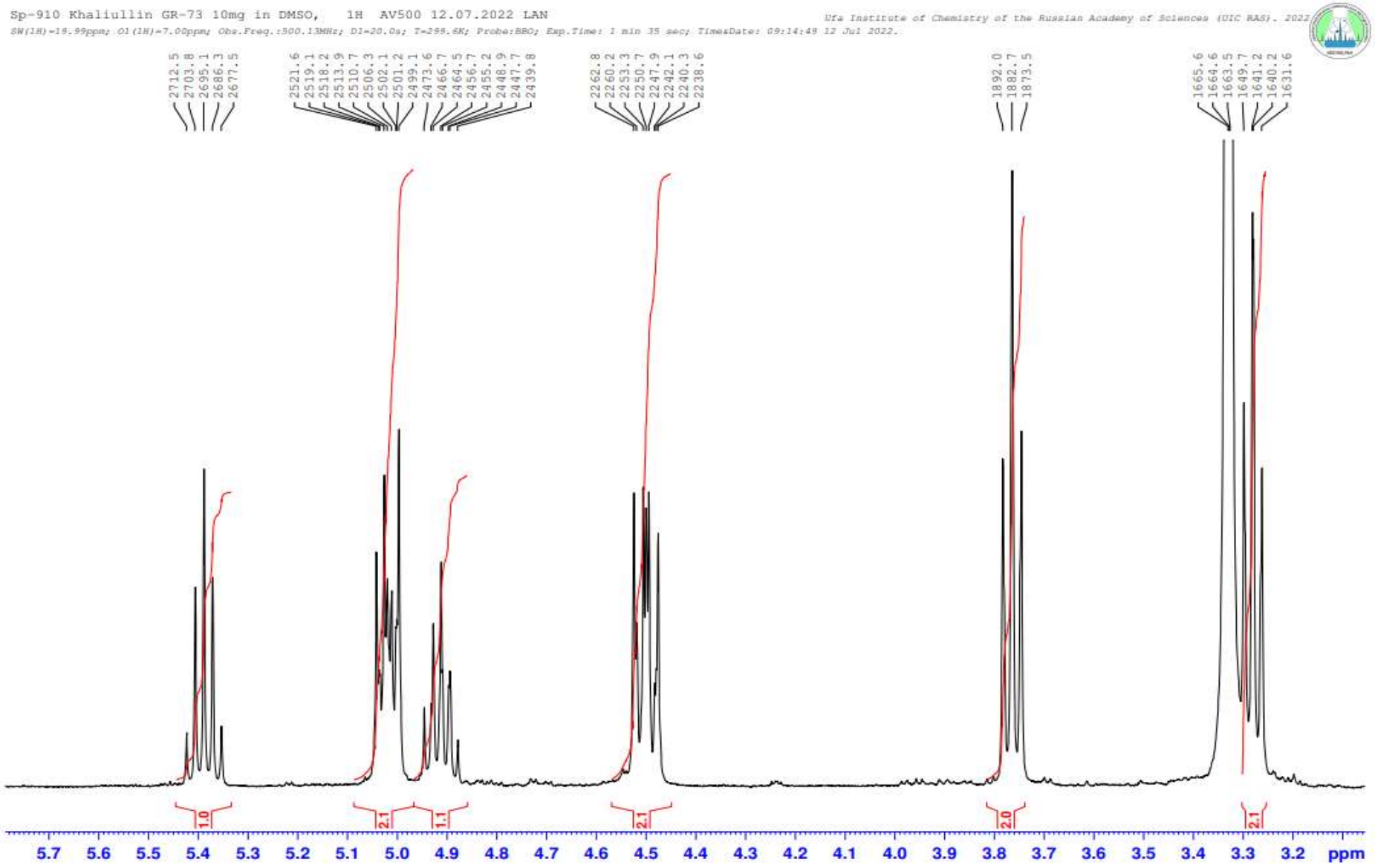
^{1}H NMR (300 MHz, DMSO-d_6) of 5-bromo-4-(1-oxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**8a**)



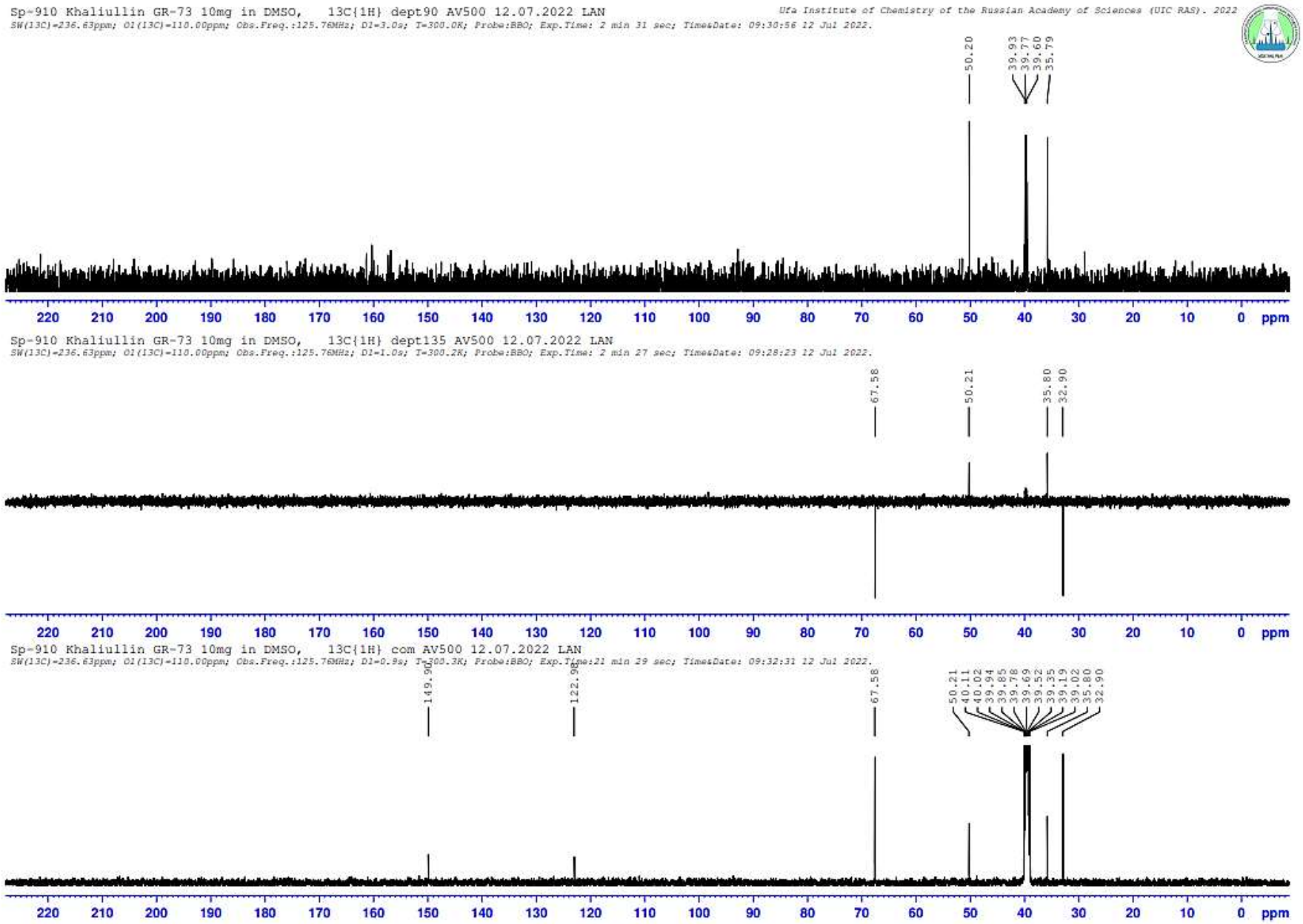
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-4-(1-oxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**8a**)



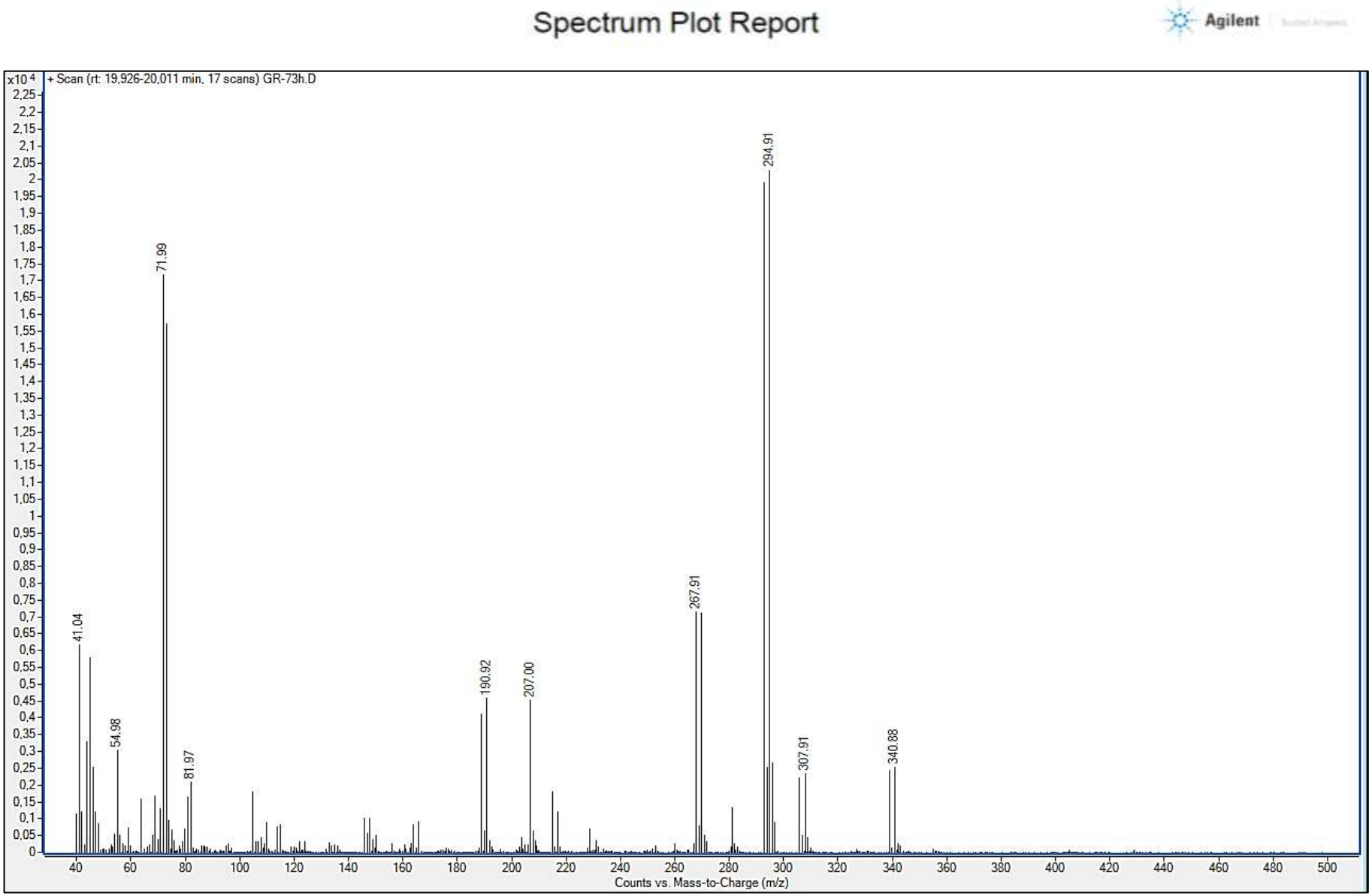
^{1}H NMR (300 MHz, DMSO-d_6) of 5-bromo-4-(1,1-dioxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**8b**)



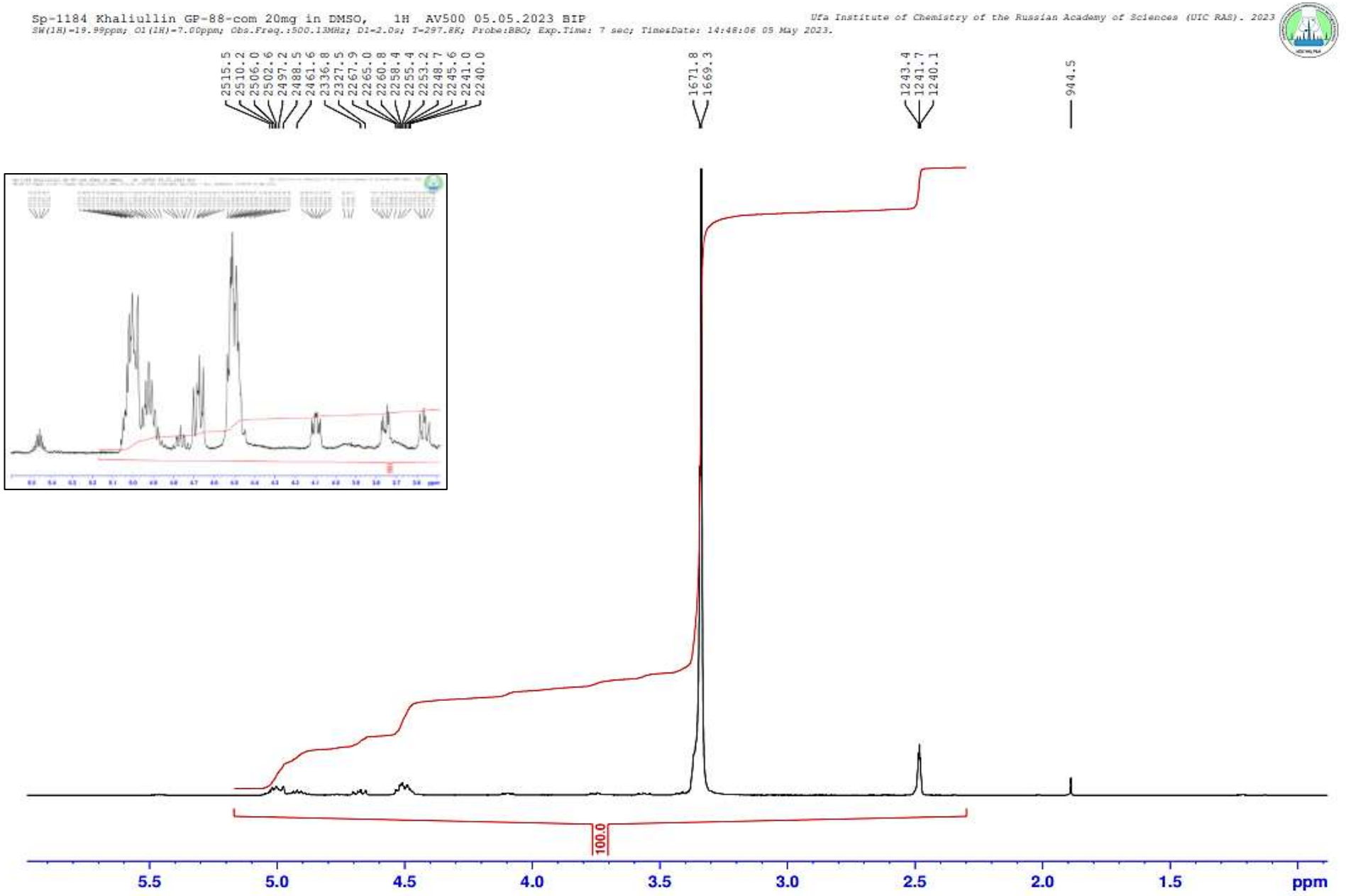
^{13}C NMR (125 MHz, DMSO-d_6) of 5-bromo-4-(1,1-dioxothietanyl-3)-2-(thietanyl-3)-2,4-dihydro-3*H*-1,2,4-triazol-3-one (**8b**)



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



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



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