Supporting Information

Synthesis and *in vitro* Biological Evaluation of Novel Thymidine Analogs Containing 1*H*-1,2,3-Triazolyl, 1*H*- Tetrazolyl, and 2*H*-Tetrazolyl Fragments

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Contents

1. NMR spectra of compounds

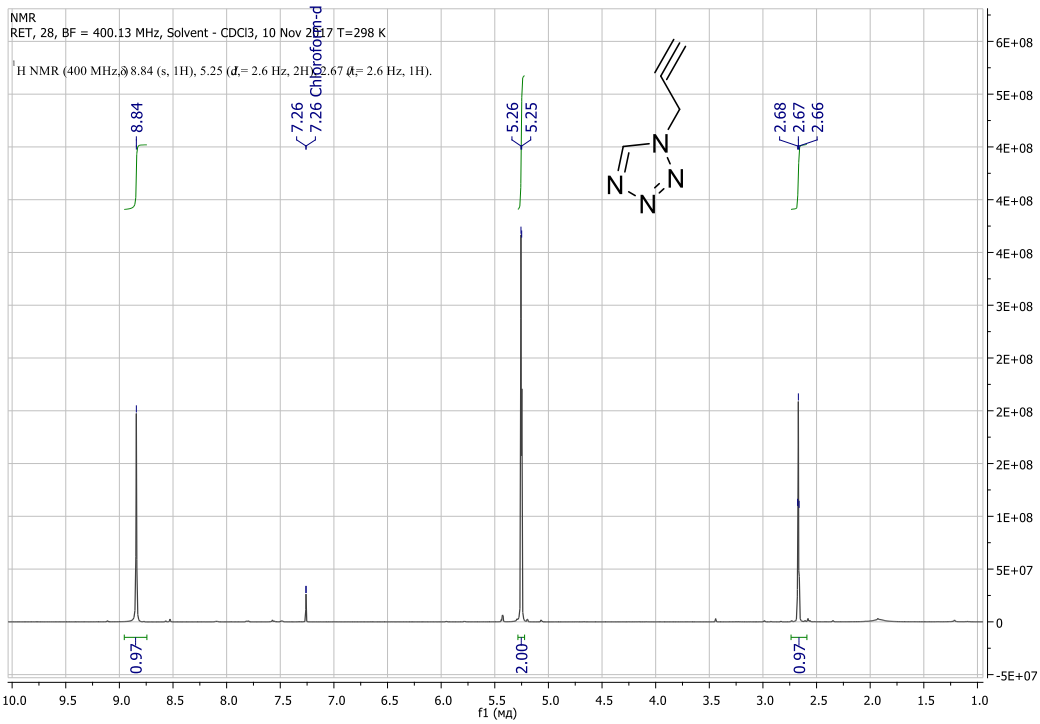


Fig. S1. ^{1}H NMR spectrum of 1-(prop-2-yn-1-yl)-1H-tetrazole (**8a**), 400 MHz, $CDCl_3$.

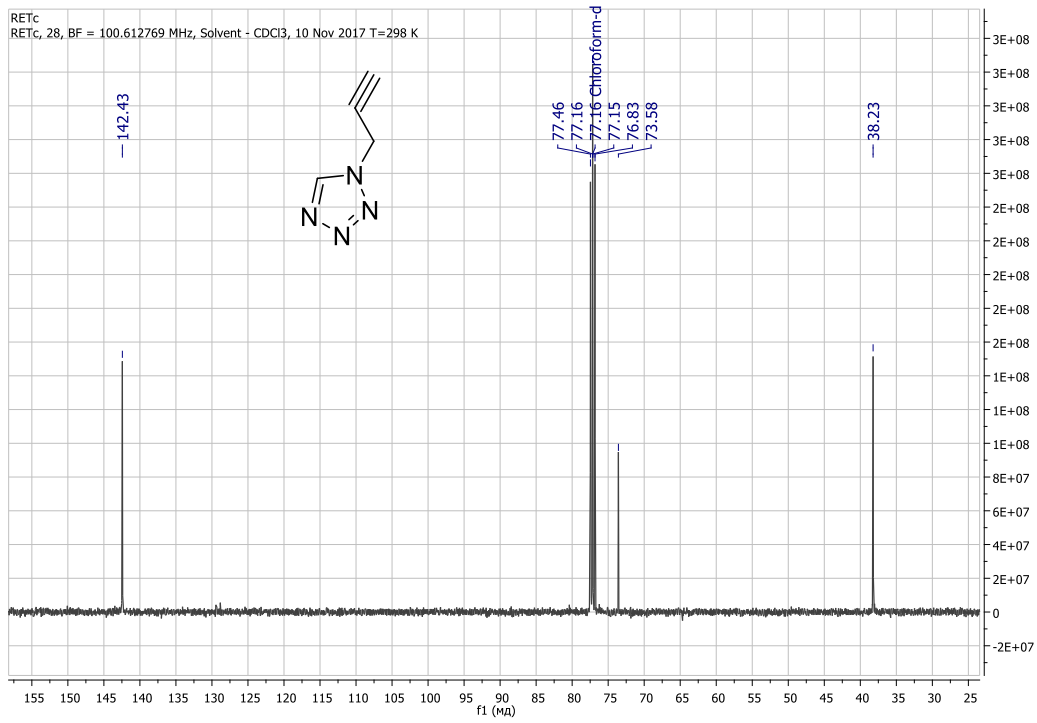


Fig. S2. ^{13}C{H} NMR spectrum of 1-(prop-2-yn-1-yl)-1H-tetrazole (**8a**), 101 MHz, $CDCl_3$.

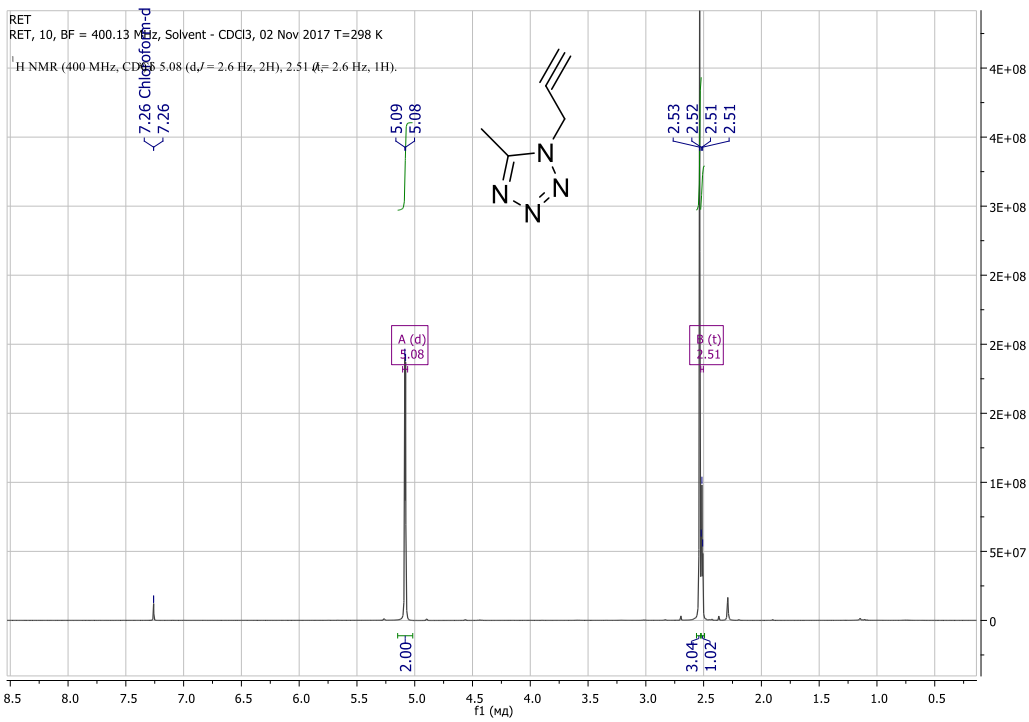


Fig. S3. ^{1}H NMR spectrum of 5-methyl-1-(prop-2-yn-1-yl)-1H-tetrazole (**8b**), 400 MHz, $CDCl_3$.

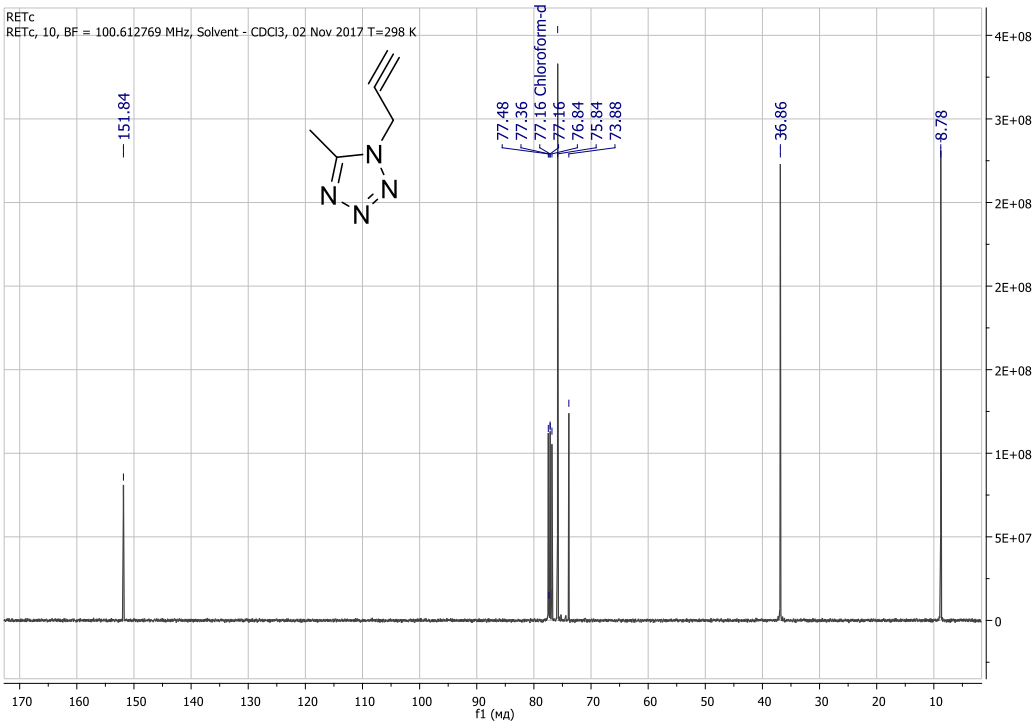


Fig. S4. ^{13}C{H} NMR spectrum of 5-methyl-1-(prop-2-yn-1-yl)-1H-tetrazole (**8b**), 101 MHz, $CDCl_3$.

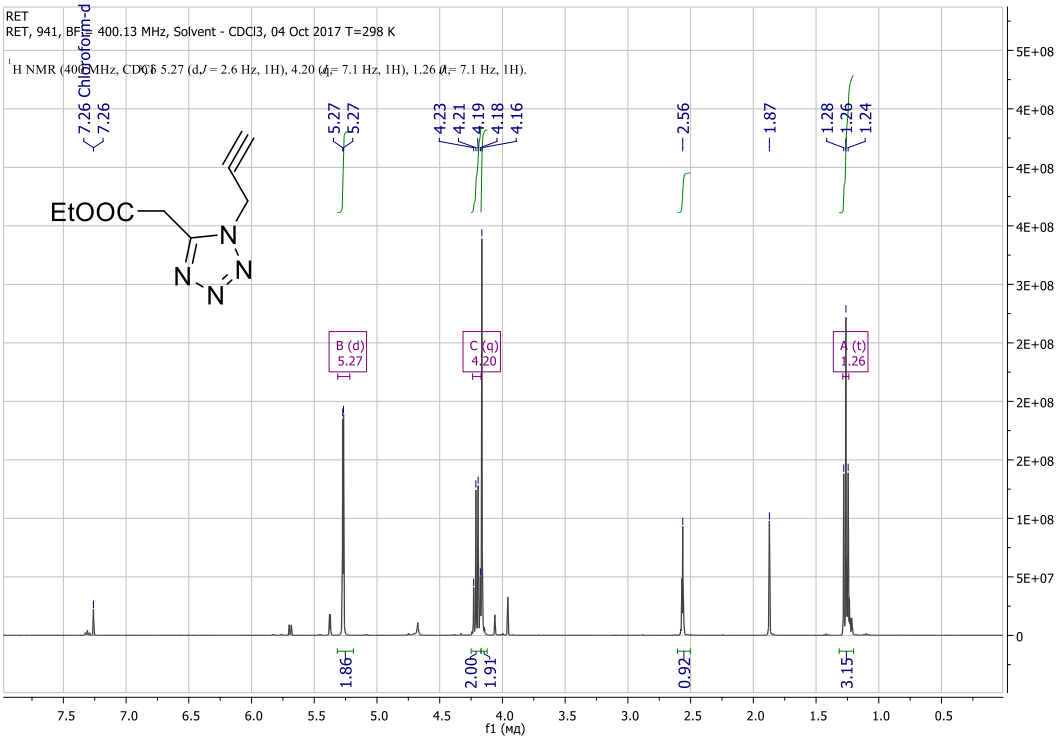


Fig. S5. ^{1}H NMR spectrum of ethyl 2-(1-(prop-2-yn-1-yl)-1H-tetrazol-5-yl)acetate (**8c**), 400 MHz, $CDCl_3$.

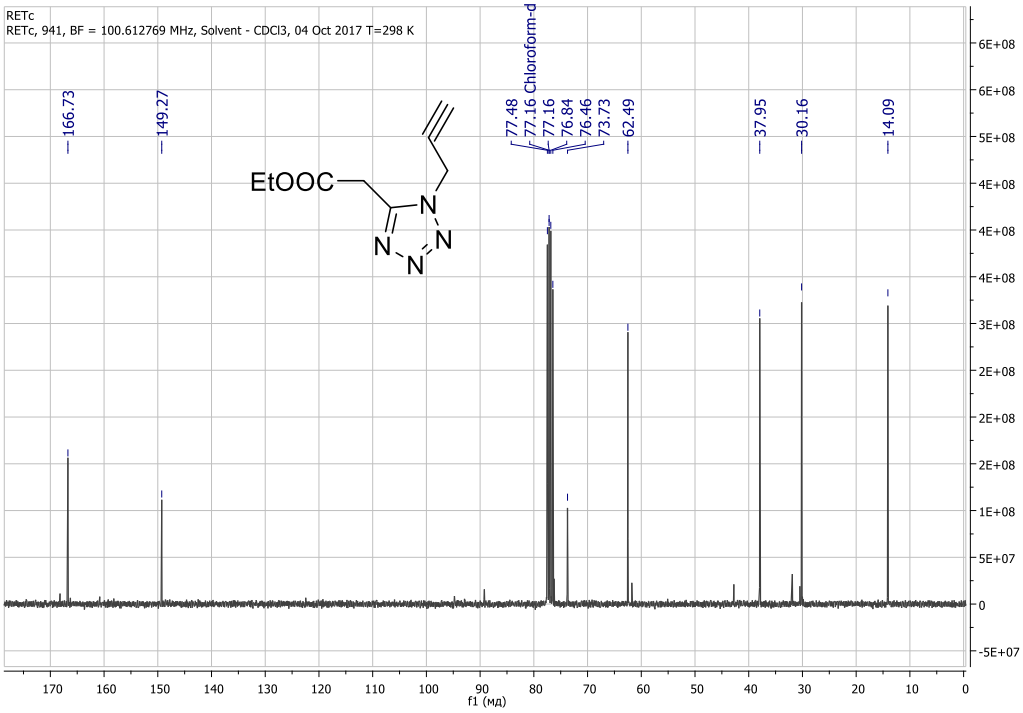


Fig. S6. ^{13}C{H} NMR spectrum of 2-(1-(prop-2-yn-1-yl)-1H-tetrazol-5-yl)acetate (**8c**), 101 MHz, $CDCl_3$.

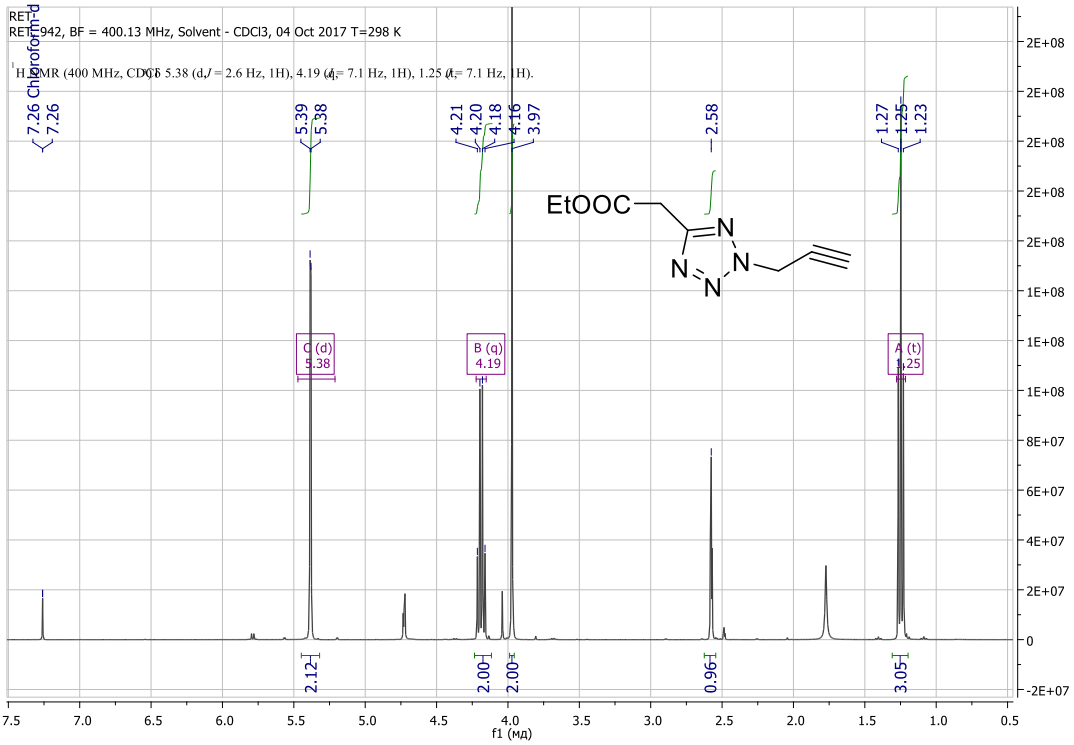


Fig. S7. ^{1}H NMR spectrum of ethyl 2-(2-(prop-2-yn-1-yl)-2H-tetrazol-5-yl)acetate (**9c**), 400 MHz, $CDCl_3$.

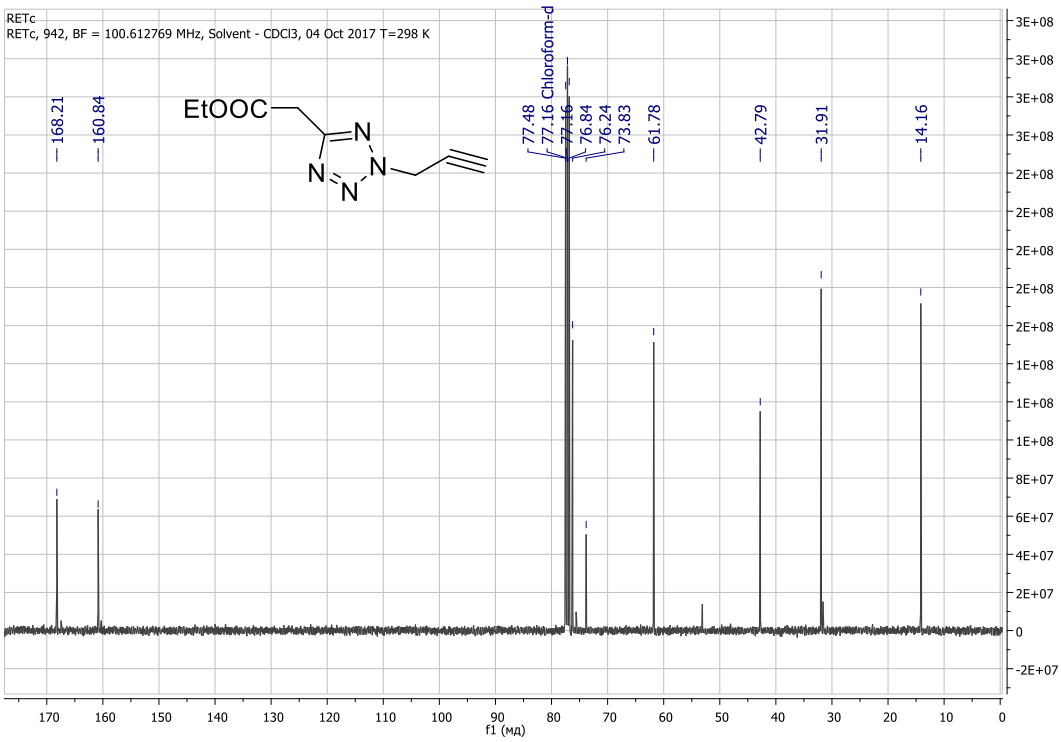


Fig. S8. ^{13}C{H} NMR spectrum of ethyl 2-(2-(prop-2-yn-1-yl)-2H-tetrazol-5-yl)acetate (**9c**), 101 MHz, $CDCl_3$.

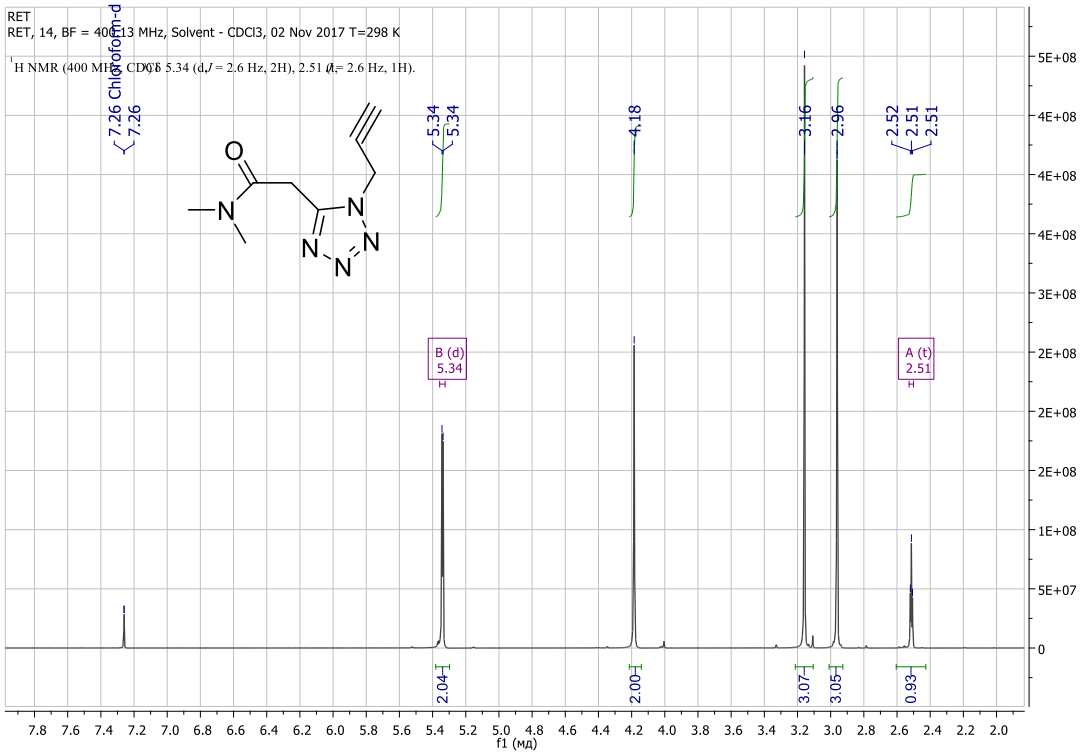


Fig. S9. ^{1}H NMR spectrum of N,N-dimethyl-2-(1-(prop-2-yn-1-yl)-1H-tetrazol-5-yl)acetamide (**8d**), 400 MHz, $CDCl_3$.

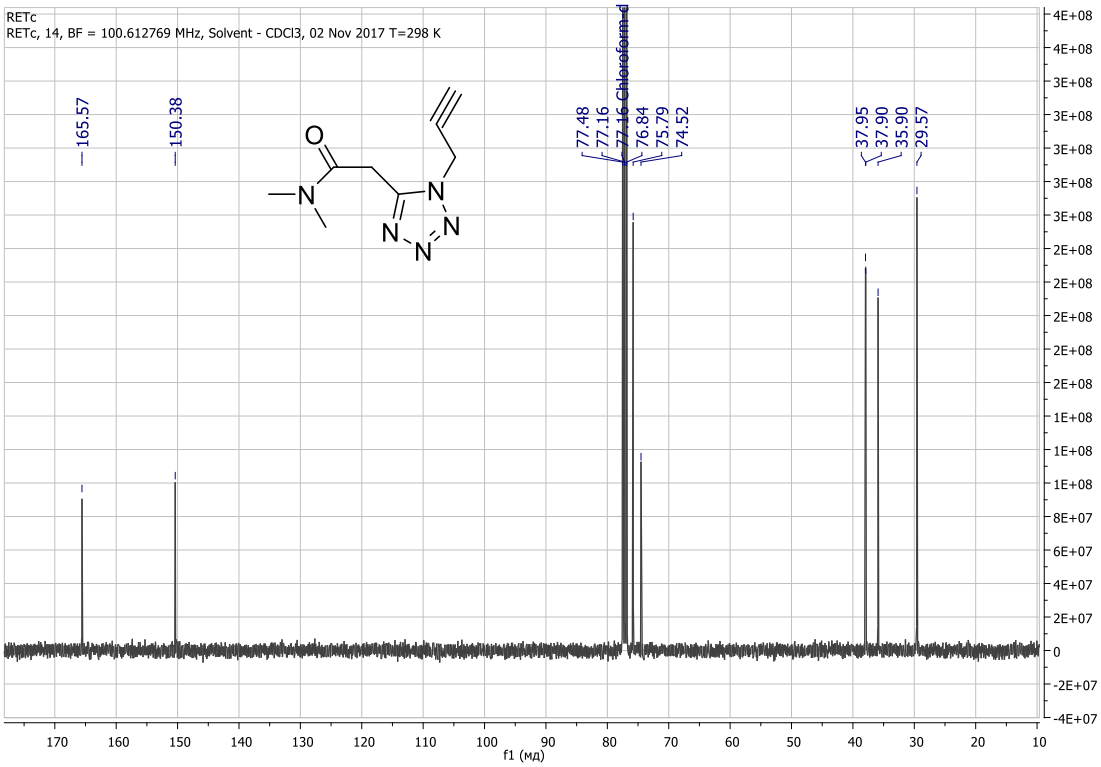


Fig. S10. ^{13}C{H} NMR spectrum of N,N-dimethyl-2-(1-(prop-2-yn-1-yl)-1H-tetrazol-5-yl)acetamide (**8d**), 101 MHz, $CDCl_3$.

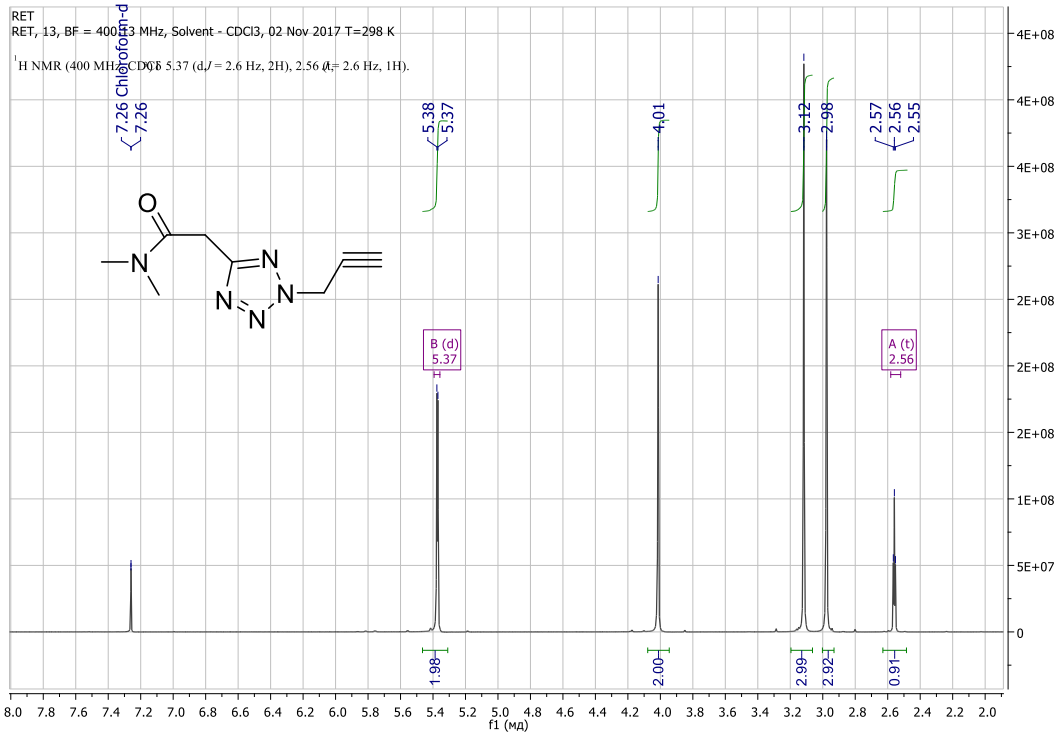


Fig. S11. ^{1}H NMR spectrum of N,N-dimethyl-2-(2-(prop-2-yn-1-yl)-2H-tetrazol-5-yl)acetamide (**9d**), 400 MHz, $CDCl_3$.

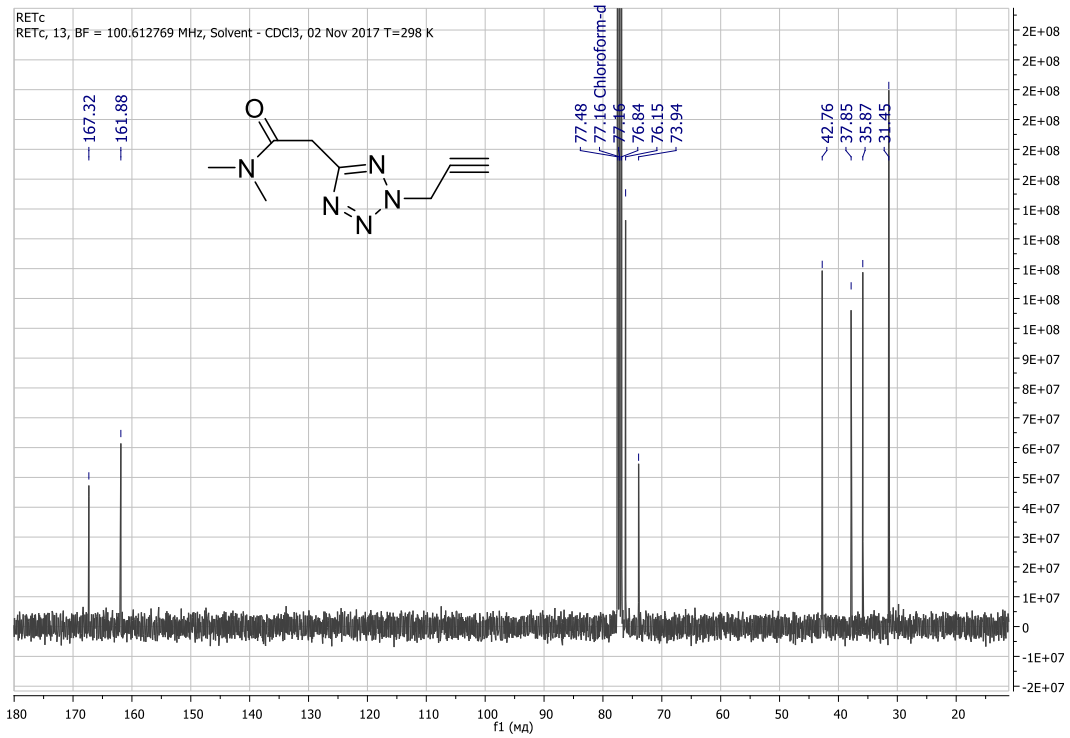


Fig. S12. ^{13}C{H} NMR spectrum of N,N-dimethyl-2-(2-(prop-2-yn-1-yl)-2H-tetrazol-5-yl)acetamide (**9d**), 101 MHz, $CDCl_3$.

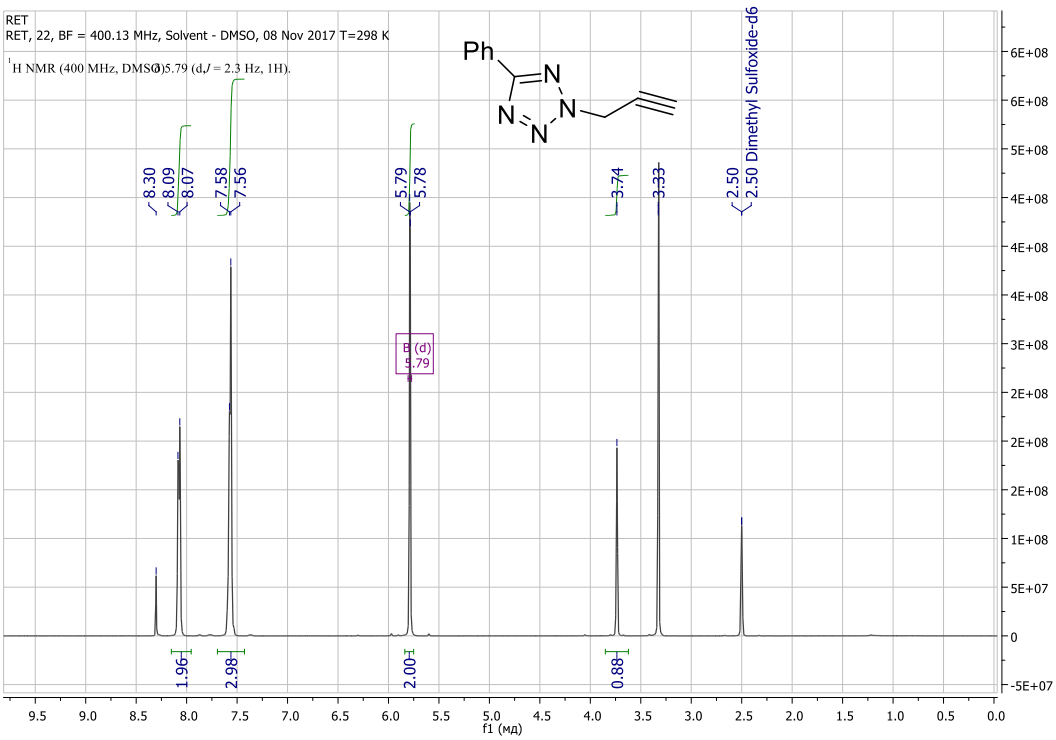


Fig. S13. ^{1}H NMR spectrum of 5-phenyl-2-(prop-2-yn-1-yl)-2H-tetrazole (**9e**), 400 MHz, DMSO-d_6.

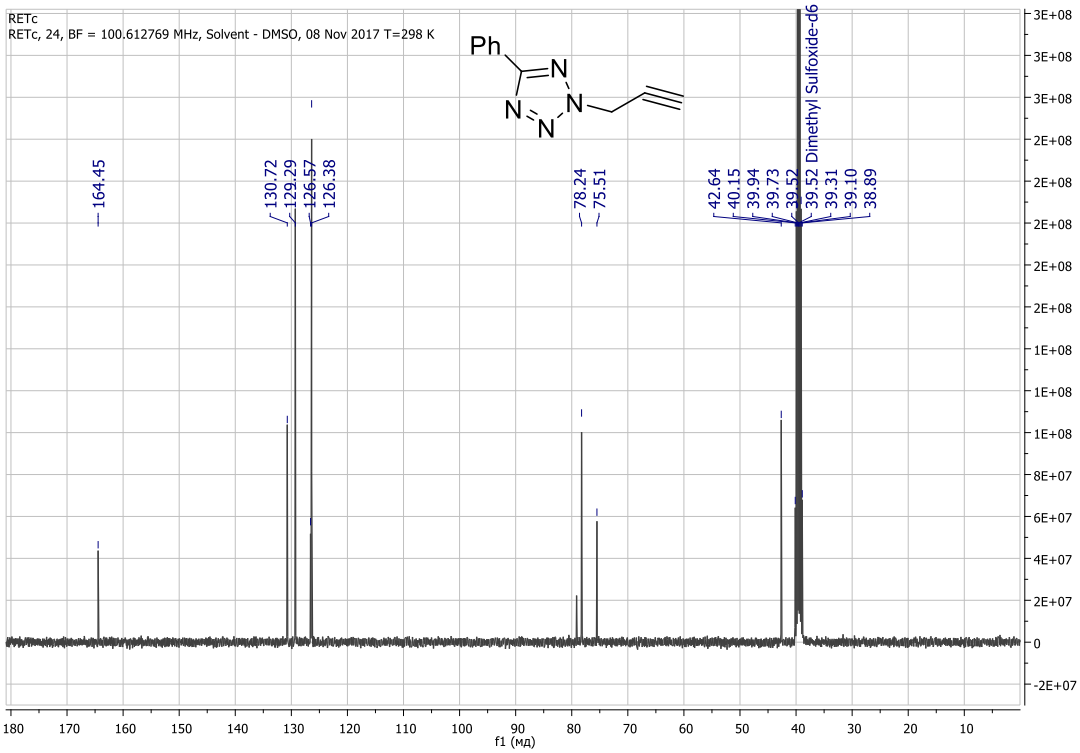


Fig. S14. ^{13}C{H} NMR spectrum of 5-phenyl-2-(prop-2-yn-1-yl)-2H-tetrazole (**9e**), 101 MHz, DMSO-d_6.

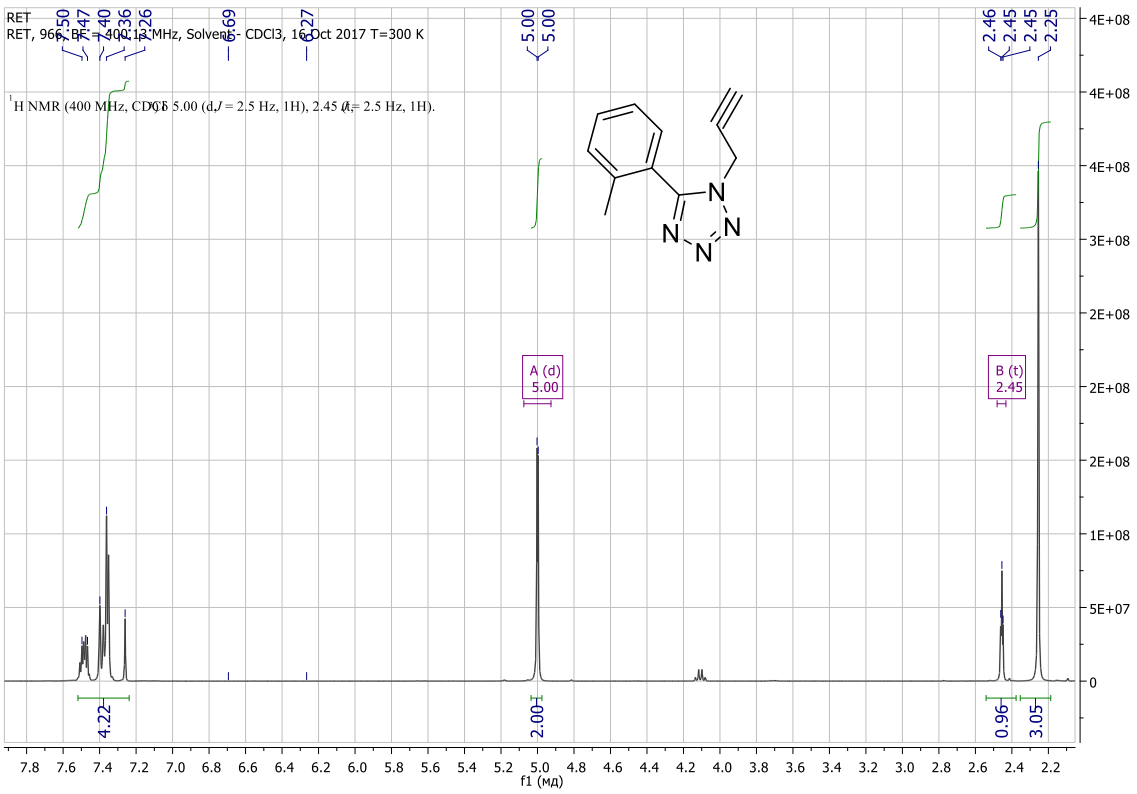


Fig. S15. ^{1}H NMR spectrum of 1-(prop-2-yn-1-yl)-5-(o-tolyl)-1H-tetrazole (**8f**), 400 MHz, $CDCl_3$.

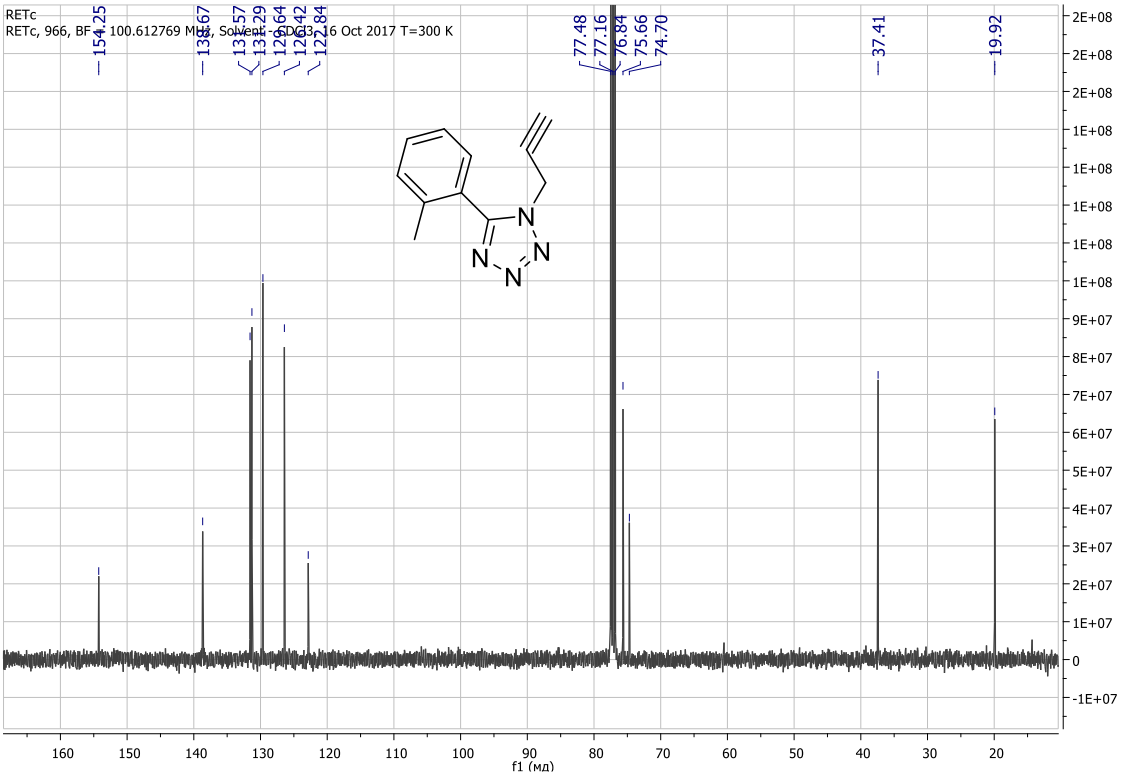


Fig. S16. ^{13}C{H} NMR spectrum of 1-(prop-2-yn-1-yl)-5-(o-tolyl)-1H-tetrazole (**8f**), 101 MHz, $CDCl_3$.

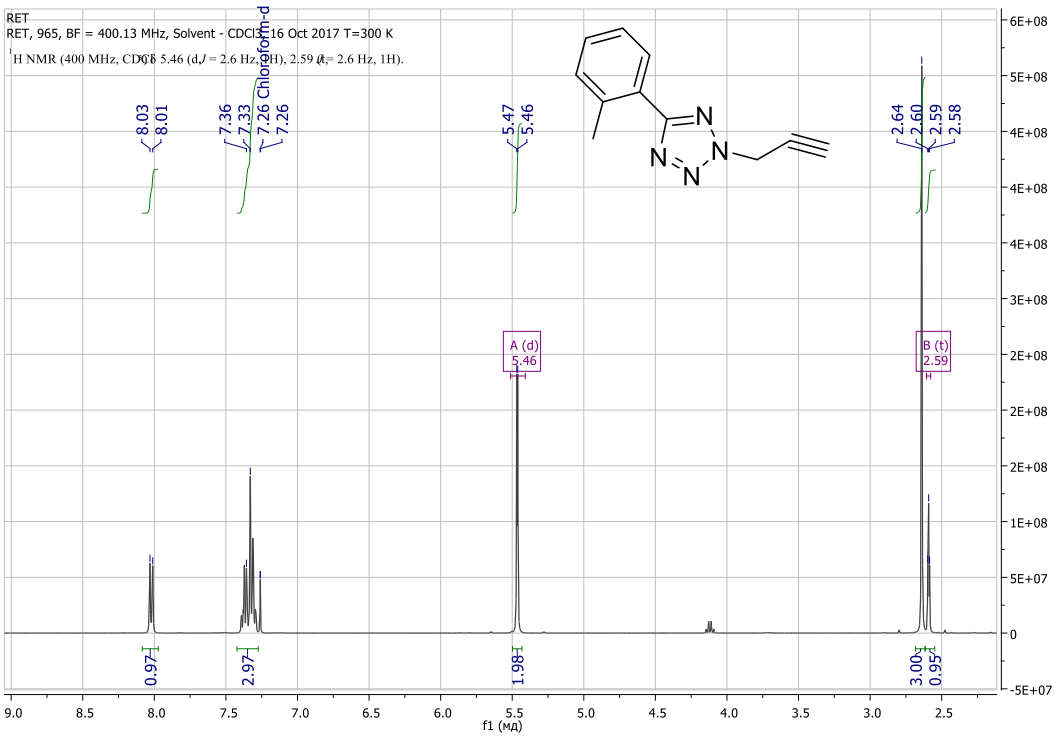


Fig. S17. ^{1}H NMR spectrum of 2-(prop-2-yn-1-yl)-5-(o-tolyl)-2H-tetrazole (**9f**), 400 MHz, $CDCl_3$.

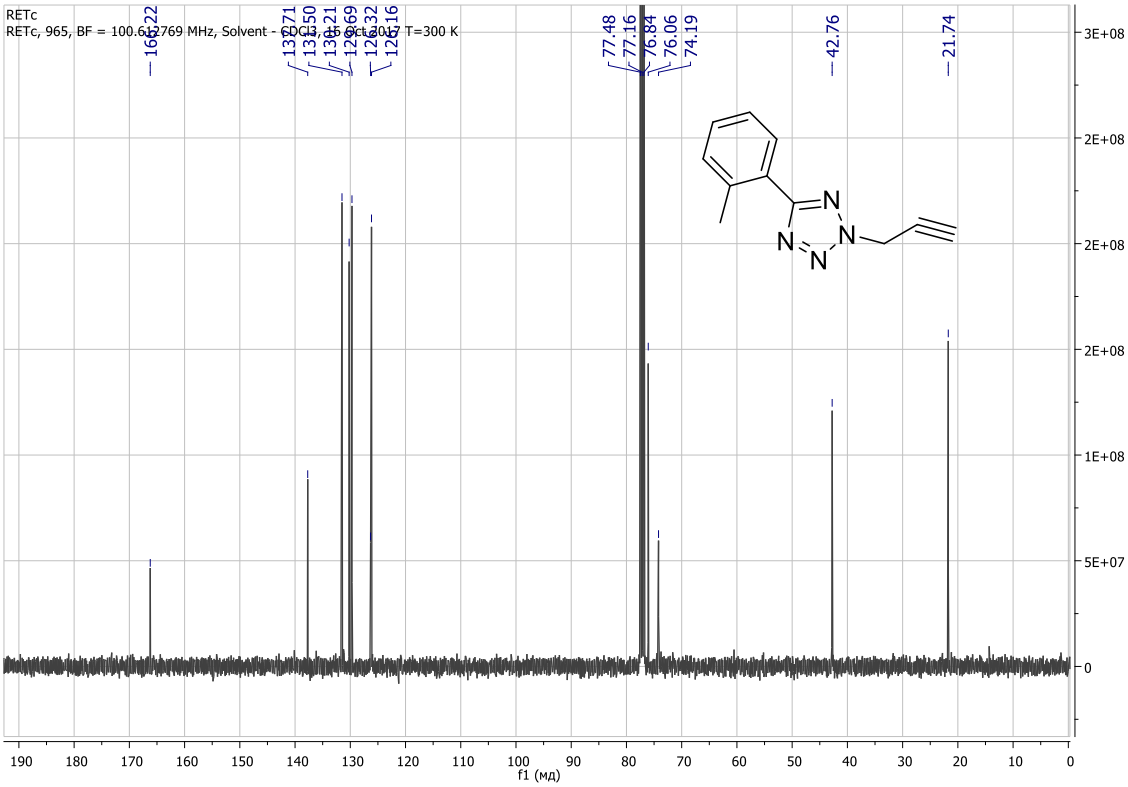


Fig. S18. ^{13}C{H} NMR spectrum of 2-(prop-2-yn-1-yl)-5-(o-tolyl)-2H-tetrazole (**9f**), 101 MHz, $CDCl_3$.

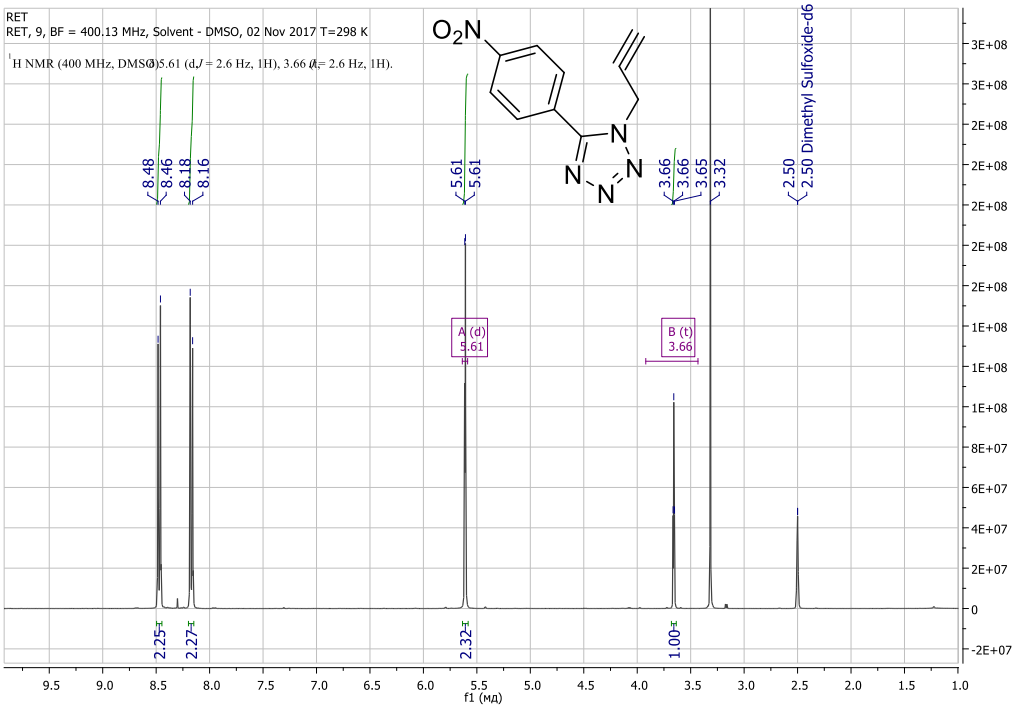


Fig. S19. ^{1}H NMR spectrum of 5-(4-nitrophenyl)-1-(prop-2-yn-1-yl)-1H-tetrazole (**8g**), 400 MHz, DMSO-d_6.

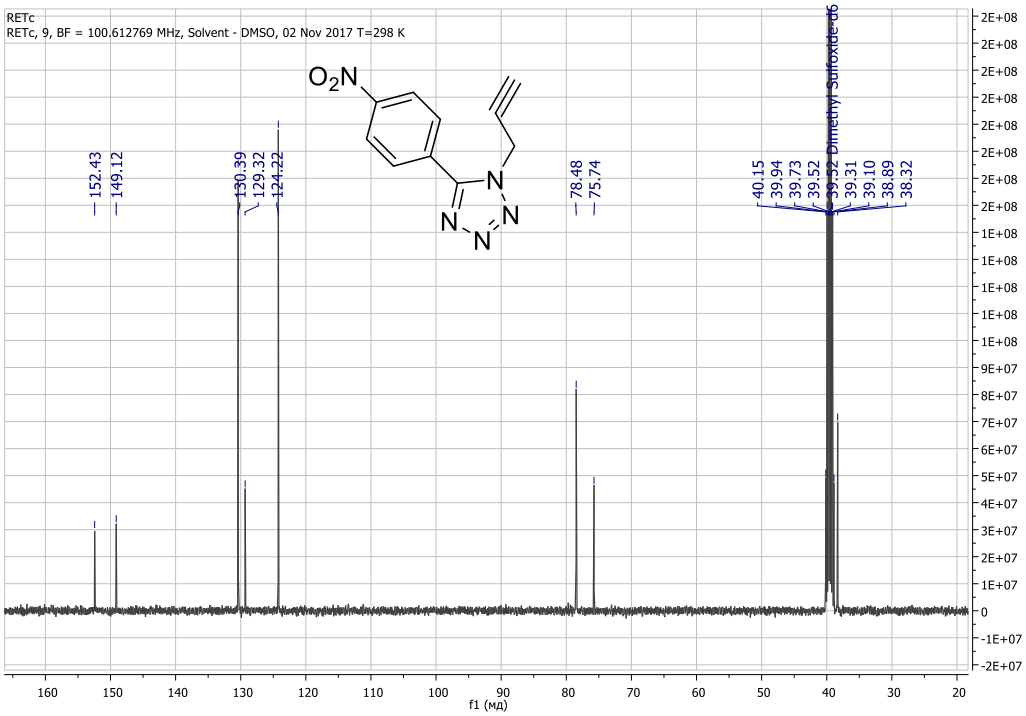


Fig. S20. ^{13}C{H} NMR spectrum of 5-(4-nitrophenyl)-1-(prop-2-yn-1-yl)-1H-tetrazole (**8g**), 101 MHz, DMSO-d_6.

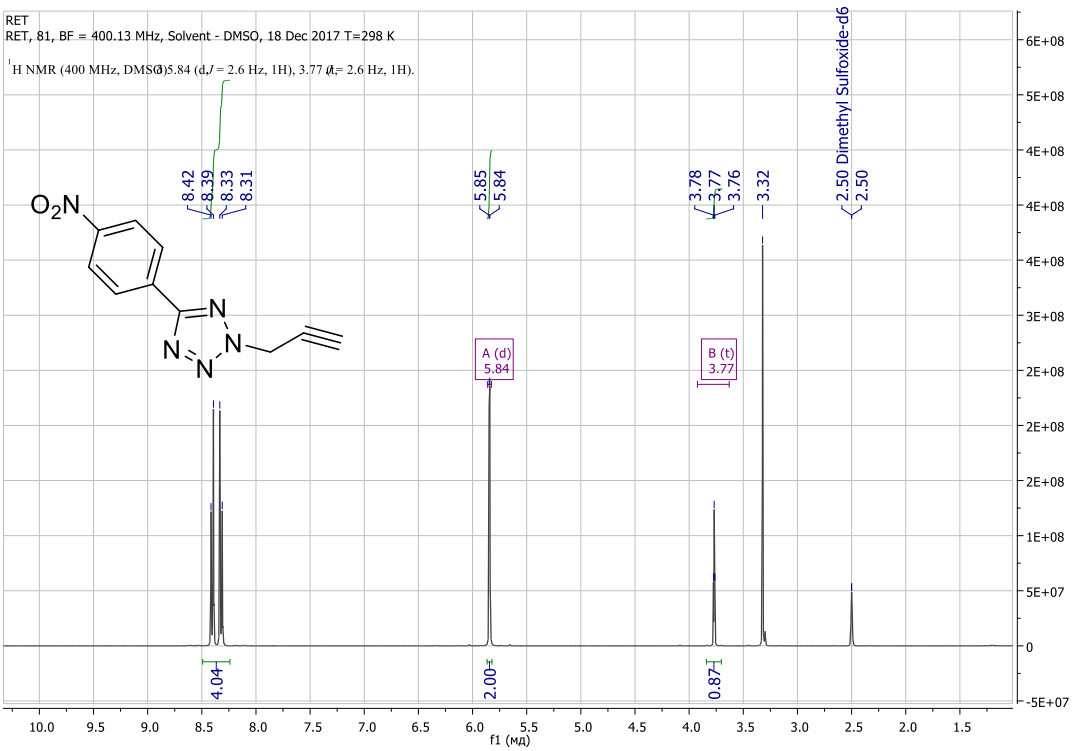


Fig. S21. ^{1}H NMR spectrum of 5-(4-nitrophenyl)-2-(prop-2-yn-1-yl)-2H-tetrazole (**9g**), 400 MHz, DMSO-d_6.

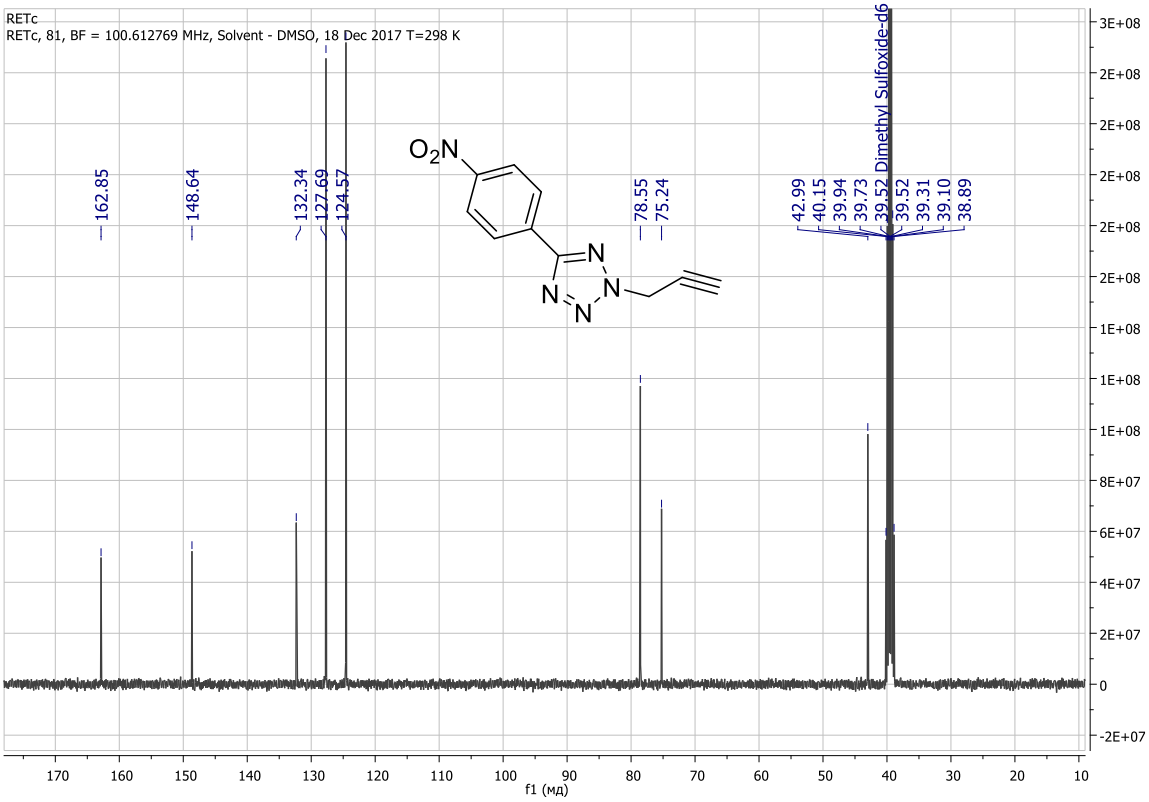


Fig. S22. ^{13}C{H} NMR spectrum of 5-(4-nitrophenyl)-2-(prop-2-yn-1-yl)-2H-tetrazole (**9g**), 101 MHz, DMSO-d_6.

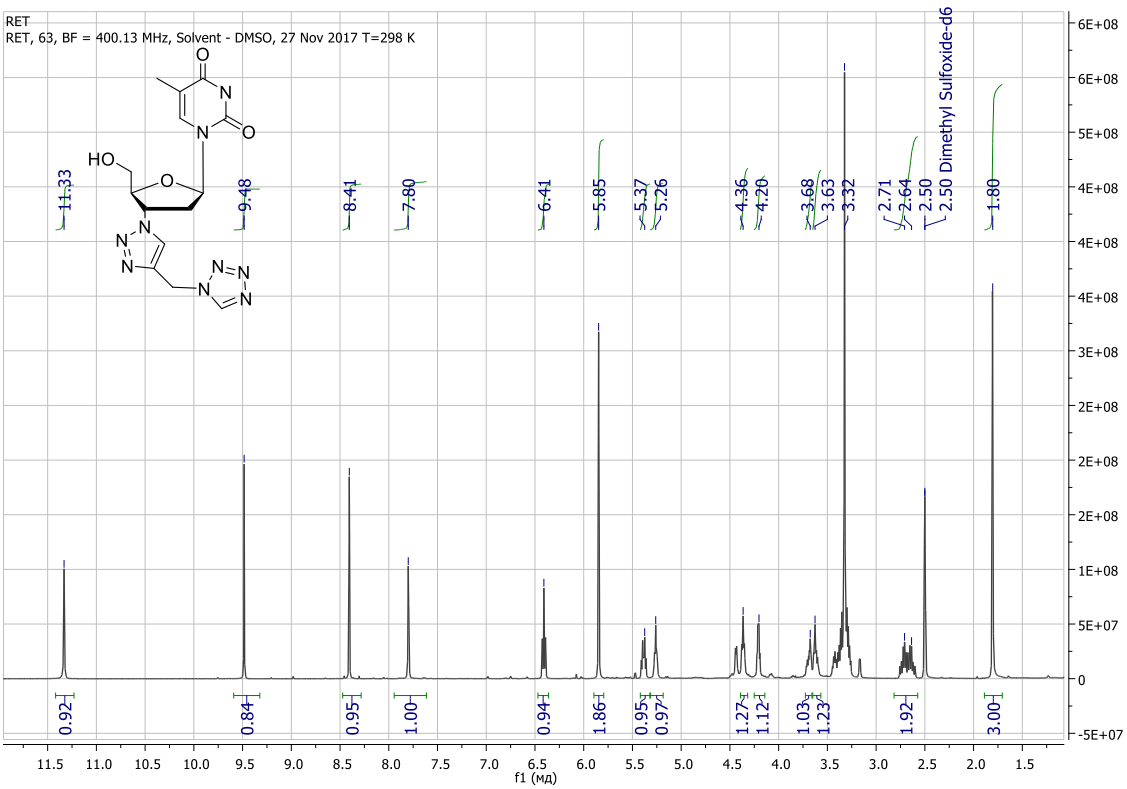


Fig. S23. ^{1}H NMR spectrum of 1-((2R,4S,5S)-4-(4-((1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10a**), 400 MHz, DMSO-d_6.

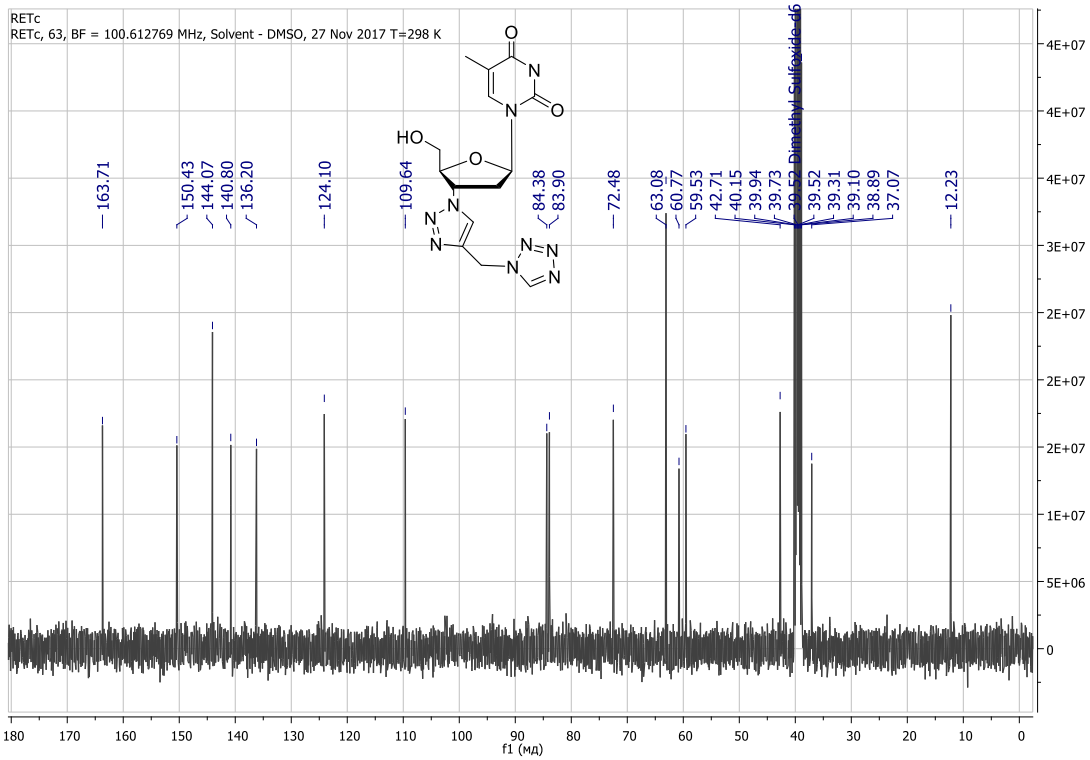


Fig. S24. ^{13}C{H} NMR spectrum of 1-((2R,4S,5S)-4-(4-((1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10a**), 101 MHz, DMSO-d_6.

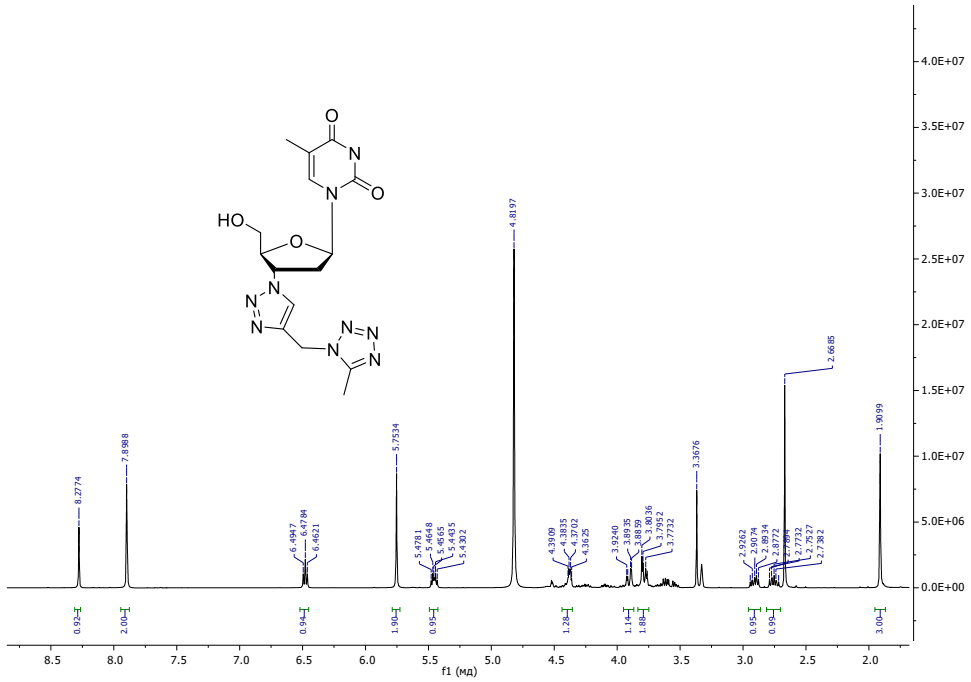


Fig. S25. ^{1}H NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-methyl-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10b**), 400 MHz, DMSO-d_6.

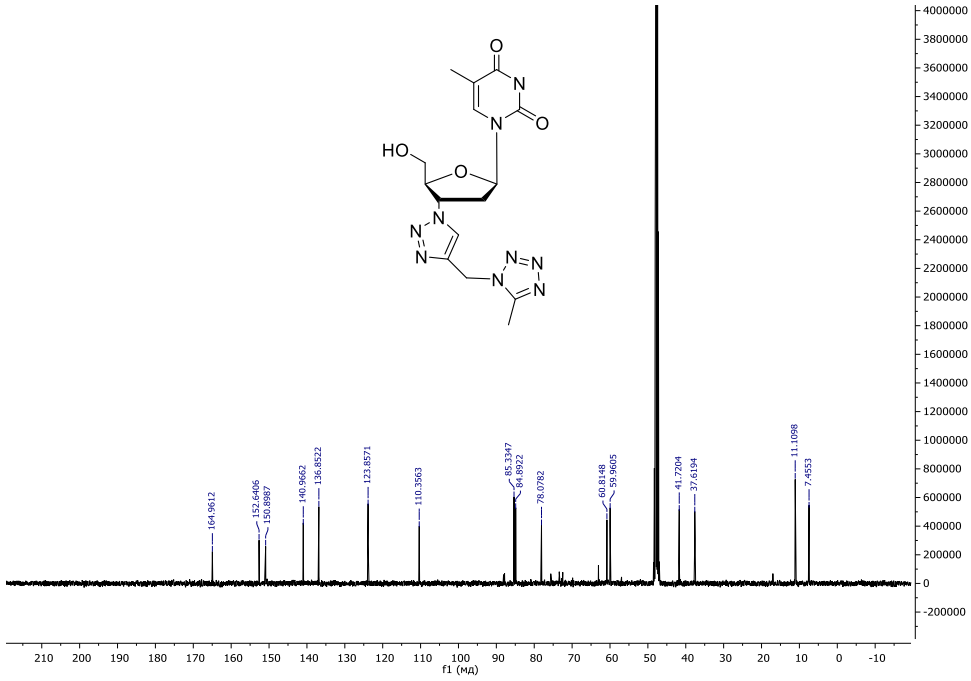


Fig. S26. ^{13}C NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-methyl-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10b**), 101 MHz, DMSO-d_6.

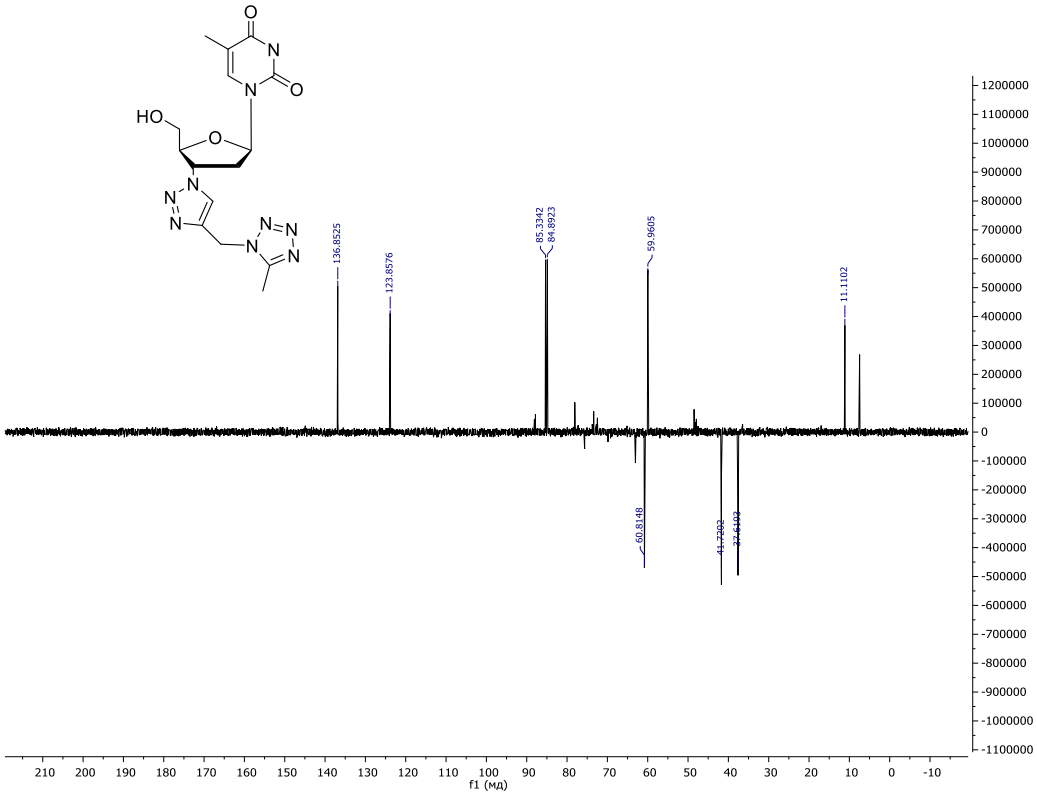


Fig. S27. ^{13}C{dept} NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-methyl-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10b**), 101 MHz, DMSO-d_6.

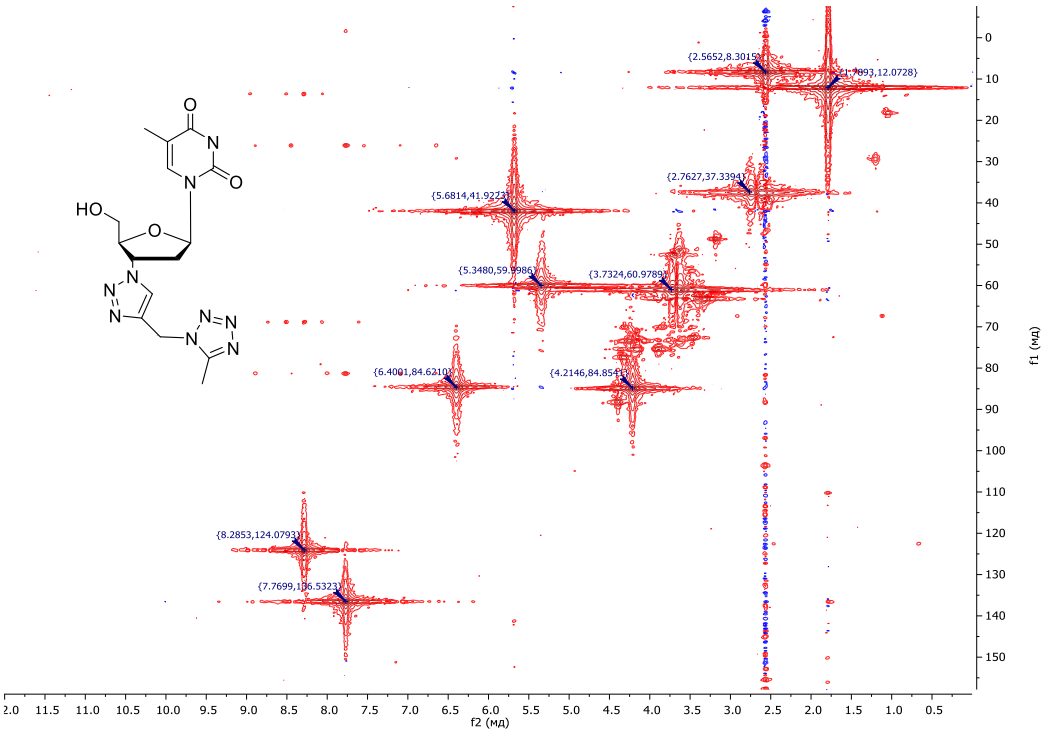


Fig. S28. HMQC NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-methyl-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10b**).

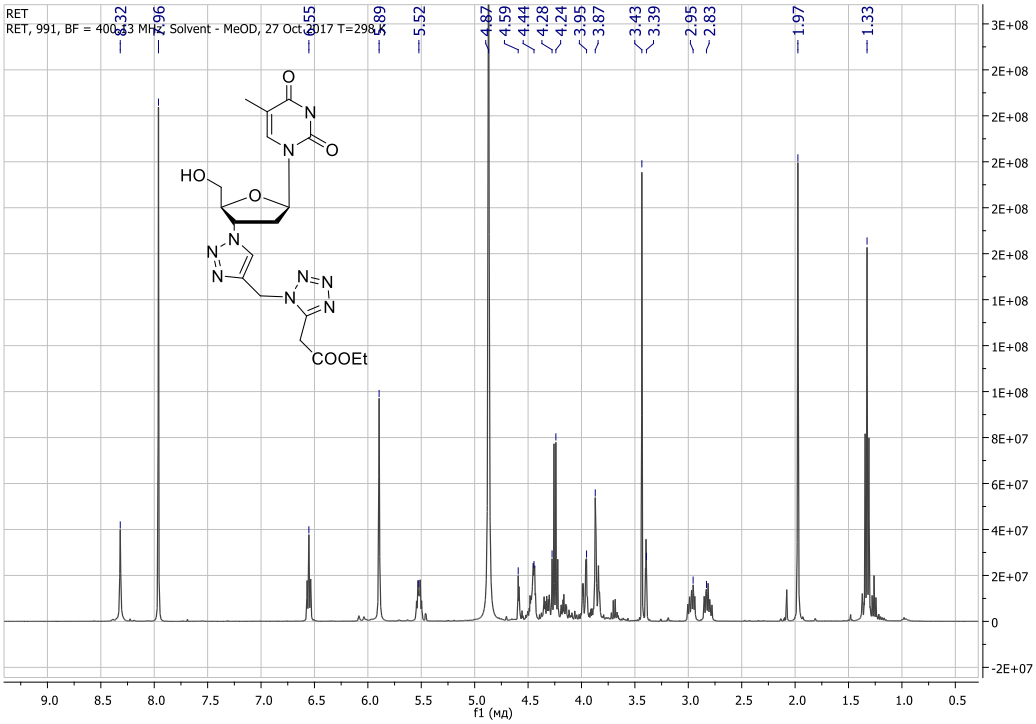


Fig. S29. ^{1}H NMR spectrum of ethyl 2-(1-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-1H-tetrazol-5-yl)acetate (**10c**), 400 MHz, DMSO-d_6.

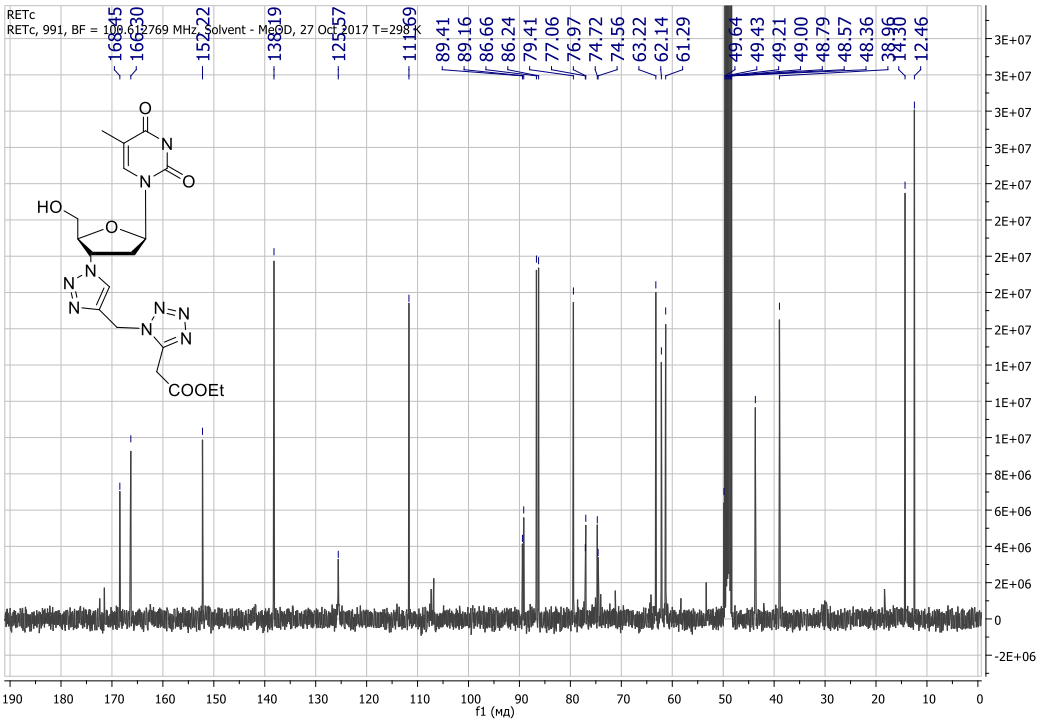


Fig. S30. ^{13}C{H} NMR spectrum of ethyl 2-(1-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-1H-tetrazol-5-yl)acetate (**10c**), 101 MHz, DMSO-d_6.

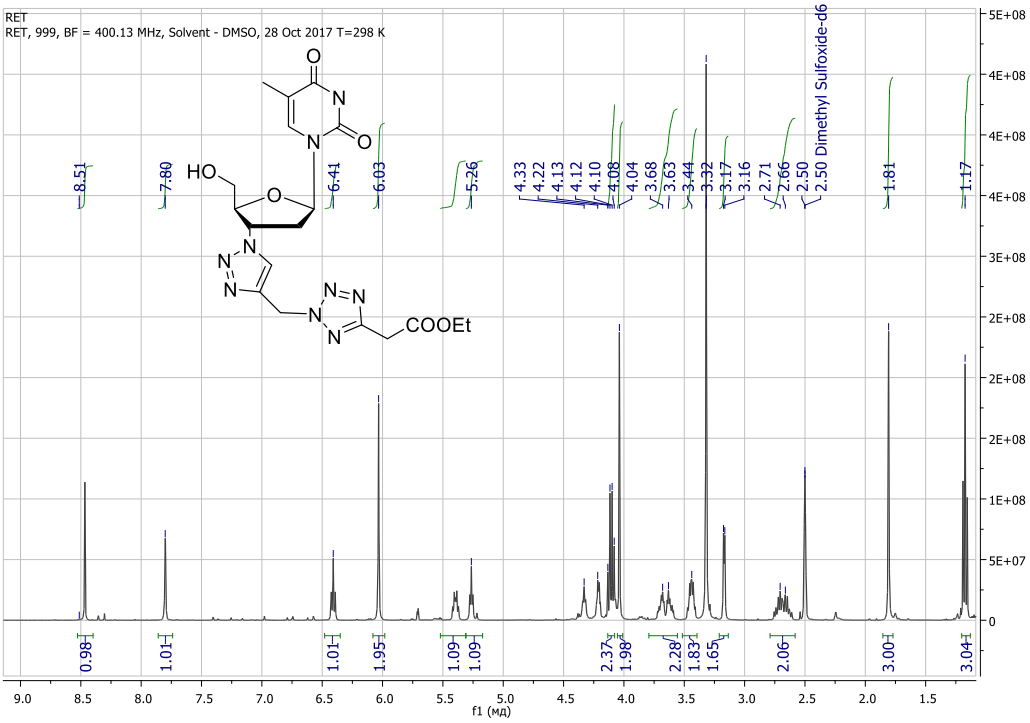


Fig. S31. ^{1}H NMR spectrum of ethyl 2-(2-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-2H-tetrazol-5-yl)acetate (**11c**), 400 MHz, DMSO-d_6.

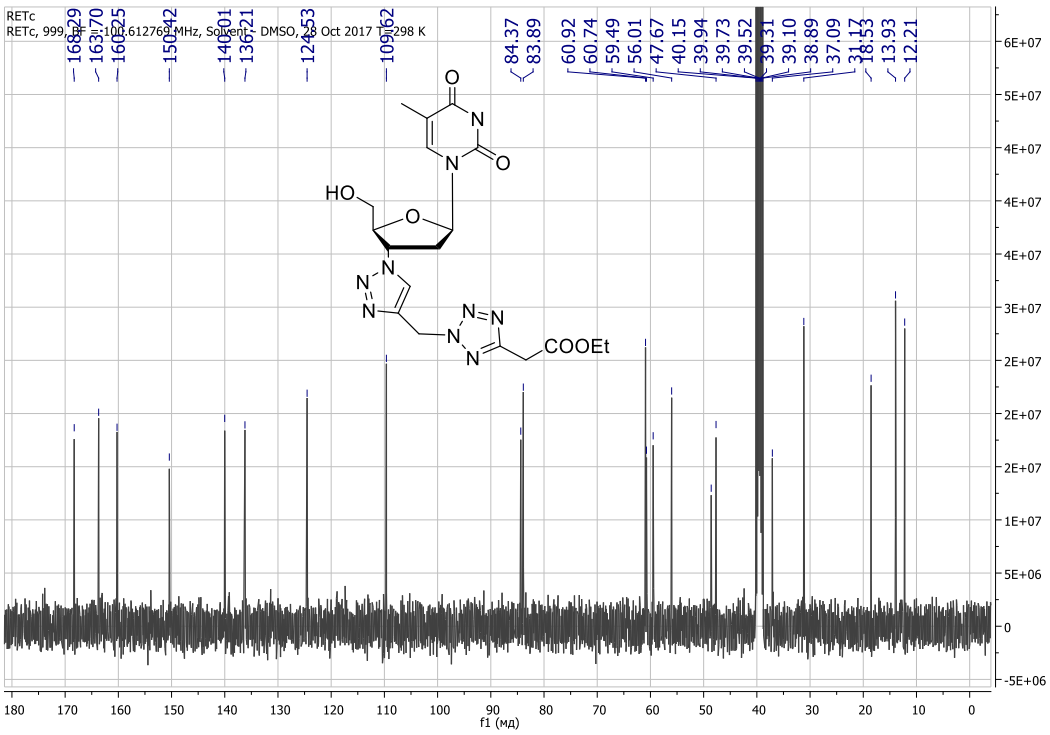


Fig. S32. ^{13}C{H} NMR spectrum of ethyl 2-(2-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-2H-tetrazol-5-yl)acetate (**11c**), 101 MHz, DMSO-d_6.

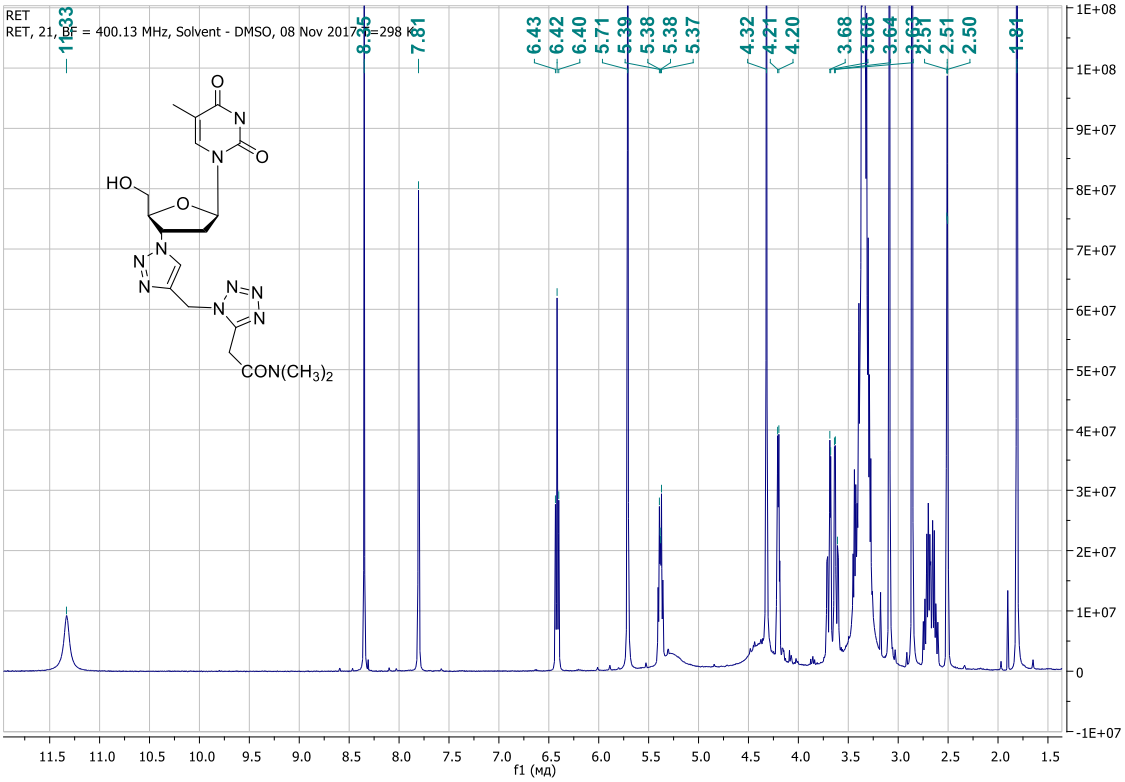


Fig. S33. ^{1}H NMR spectrum of 2-(1-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-1H-tetrazol-5-yl)-N,N-dimethylacetamide (**10d**), 400 MHz, DMSO-d_6.

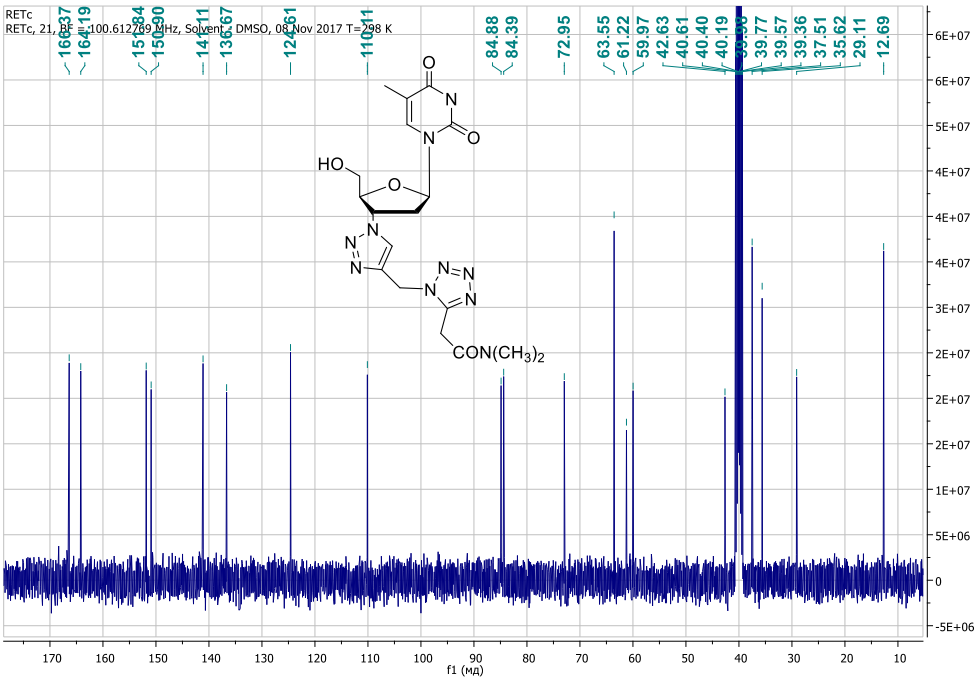


Fig. S34. ^{13}C{H} NMR spectrum of 2-(1-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-1H-tetrazol-5-yl)-N,N-dimethylacetamide (**10d**), 101 MHz, DMSO-d_6.

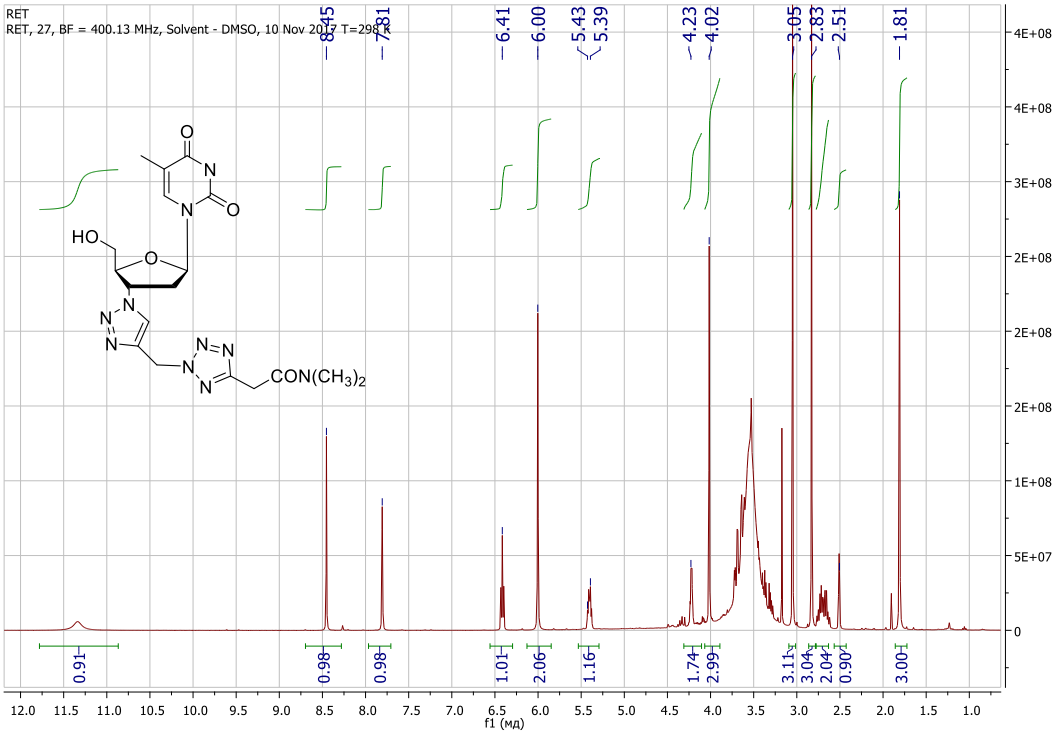


Fig. S35. ^{1}H NMR spectrum of ((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-2H-tetrazol-5-yl)-N,N-dimethylacetamide (**11d**), 400 MHz, DMSO-d_6.

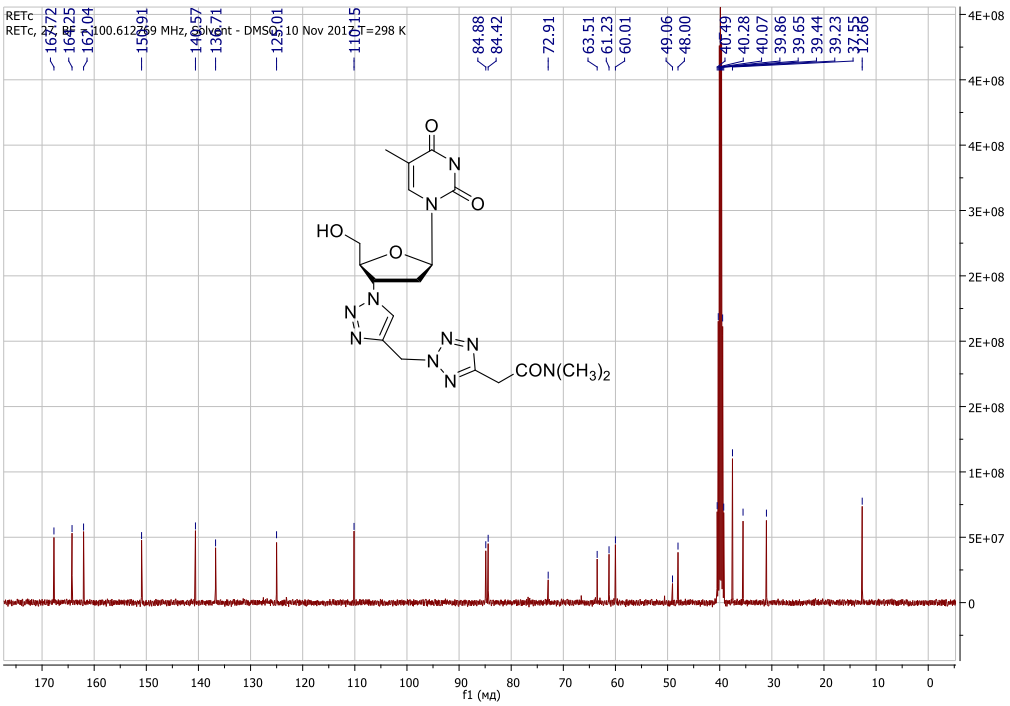


Fig. S36. ^{13}C{H} NMR spectrum of ((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-2H-tetrazol-5-yl)-N,N-dimethylacetamide (**11d**), 101 MHz, DMSO-d_6.

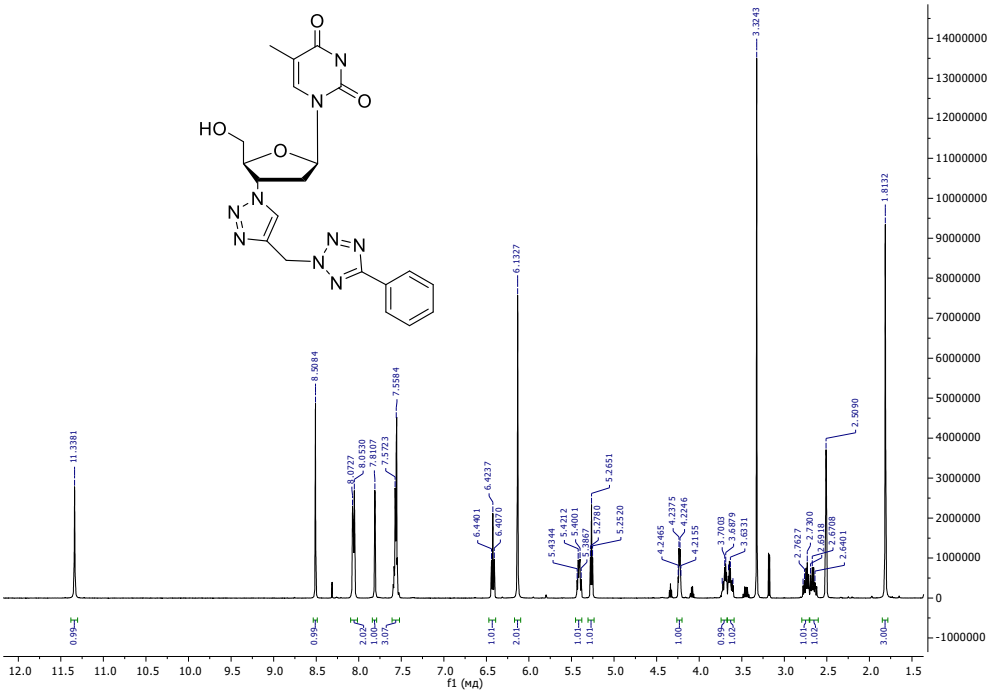


Fig. S37. ^{1}H NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-phenyl-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11e**), 400 MHz, DMSO-d_6.

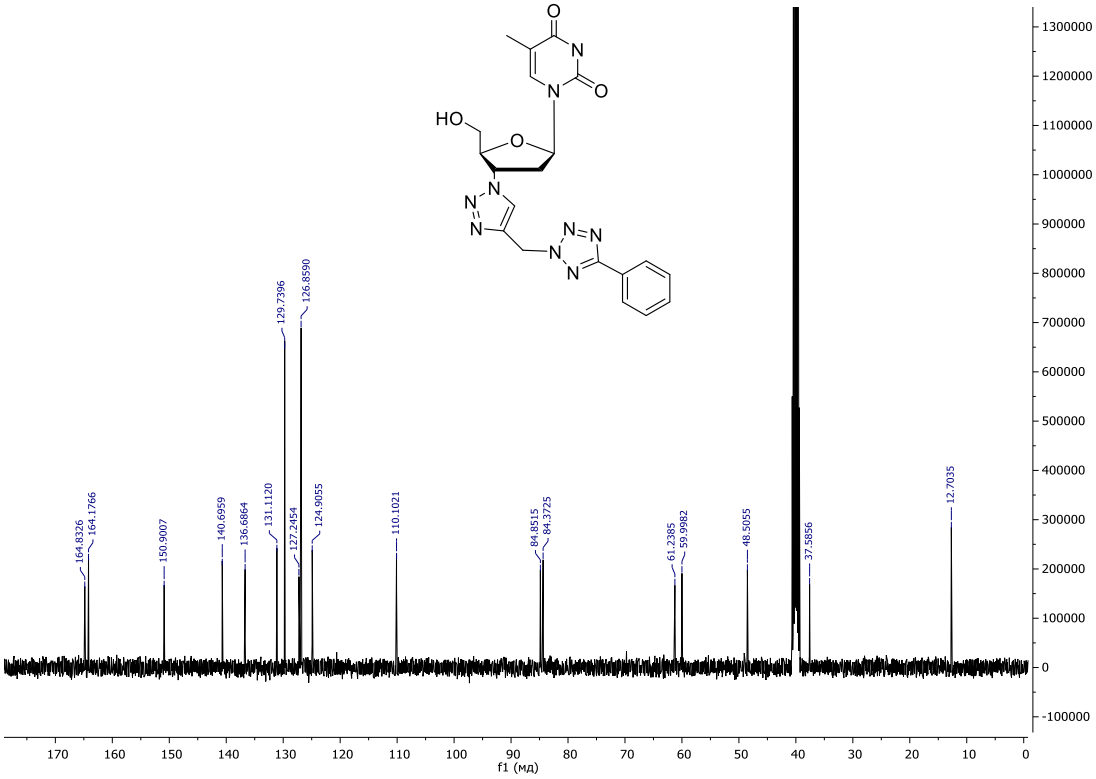


Fig. S38. ^{13}C NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-phenyl-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11e**), 101 MHz, DMSO-d_6.

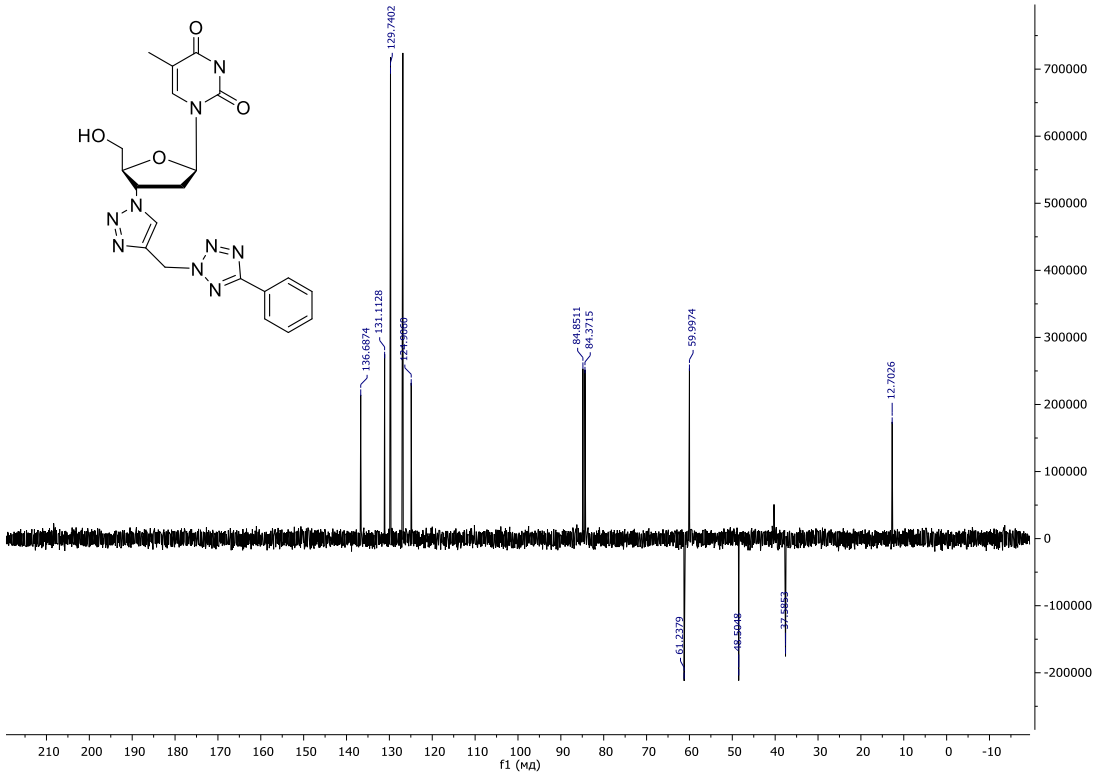


Fig. S39. ^{13}C{dept} NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-phenyl-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11e**), 101 MHz, DMSO-d_6.

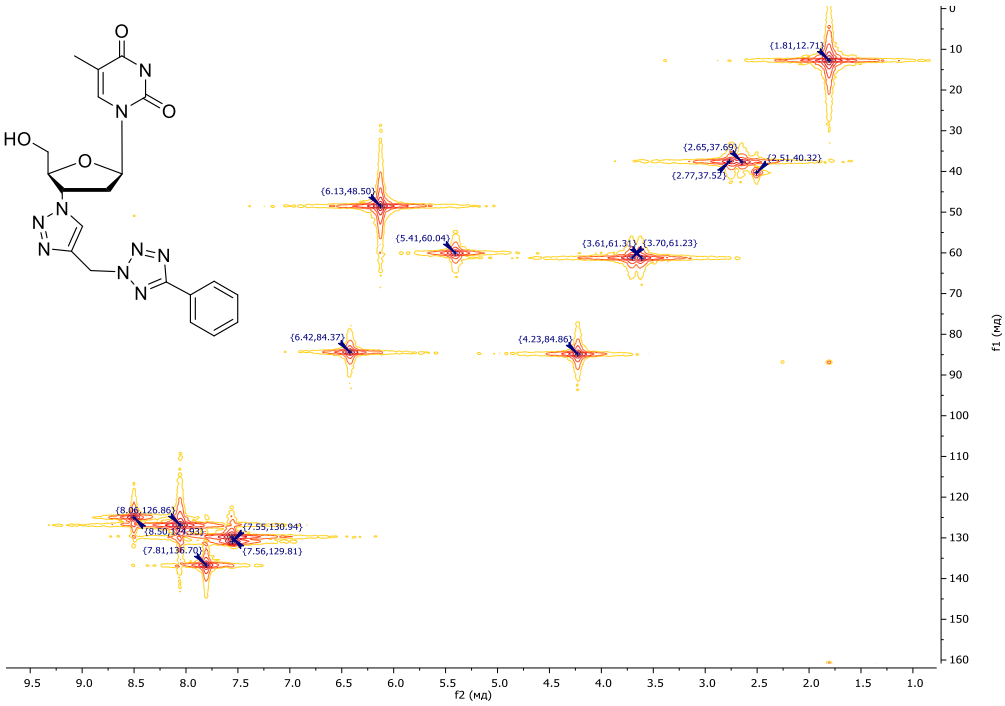


Fig. S40. HMQC{^{1}H-^{13}C} spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-phenyl-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11e**), DMSO-d_6.

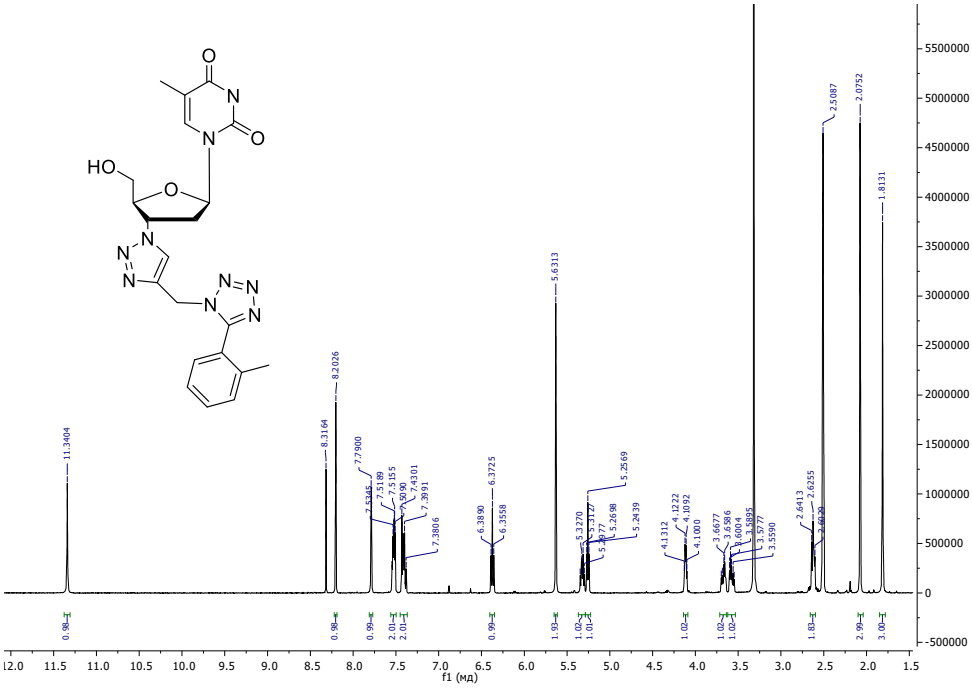


Fig. S41. ^{1}H NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10f**), 400 MHz, DMSO-d_6.

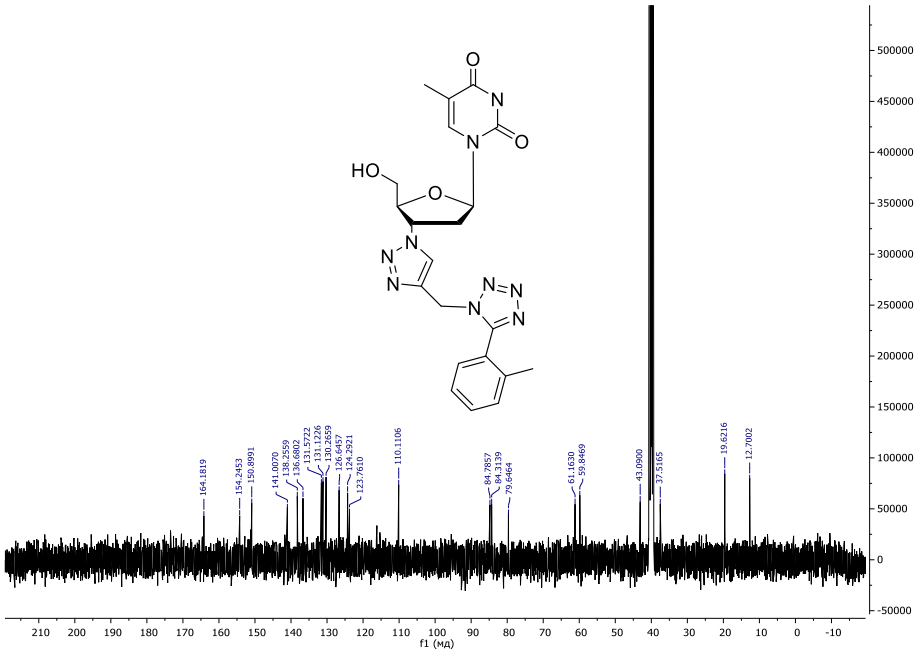


Fig. S42. ^{13}C NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10f**), 101 MHz, DMSO-d_6.

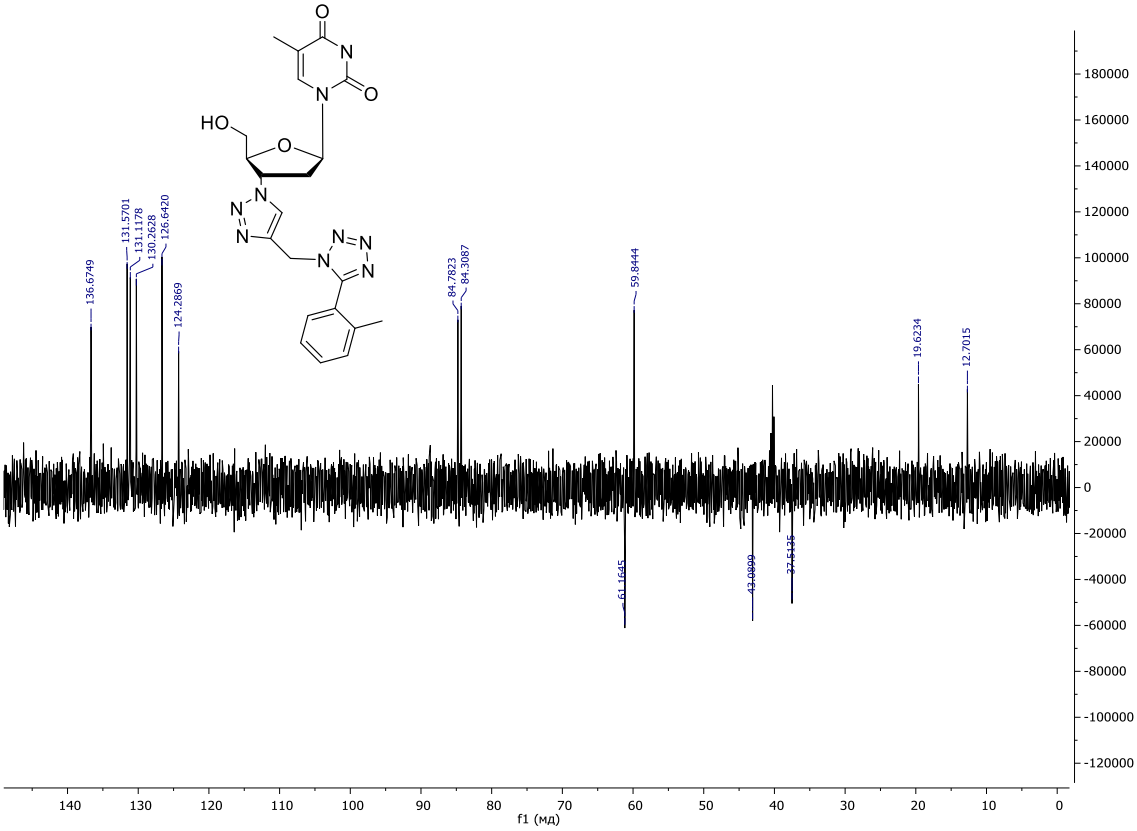


Fig. S43. ^{13}C{dept} NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10f**), 101 MHz, DMSO-d_6.

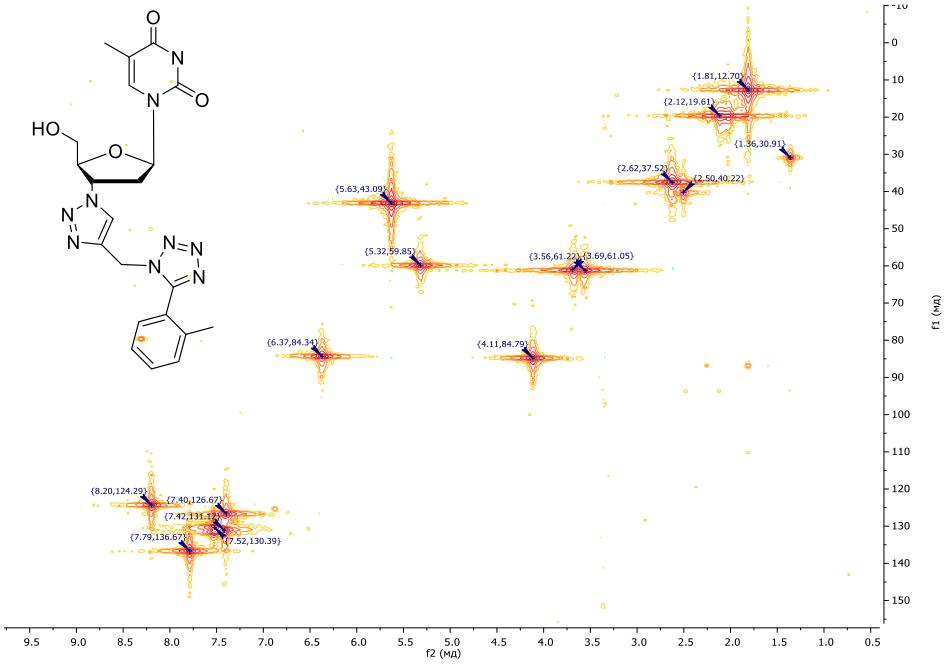


Fig. S44. HMQC{^{1}H-^{13}C} NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10f**), DMSO-d_6.

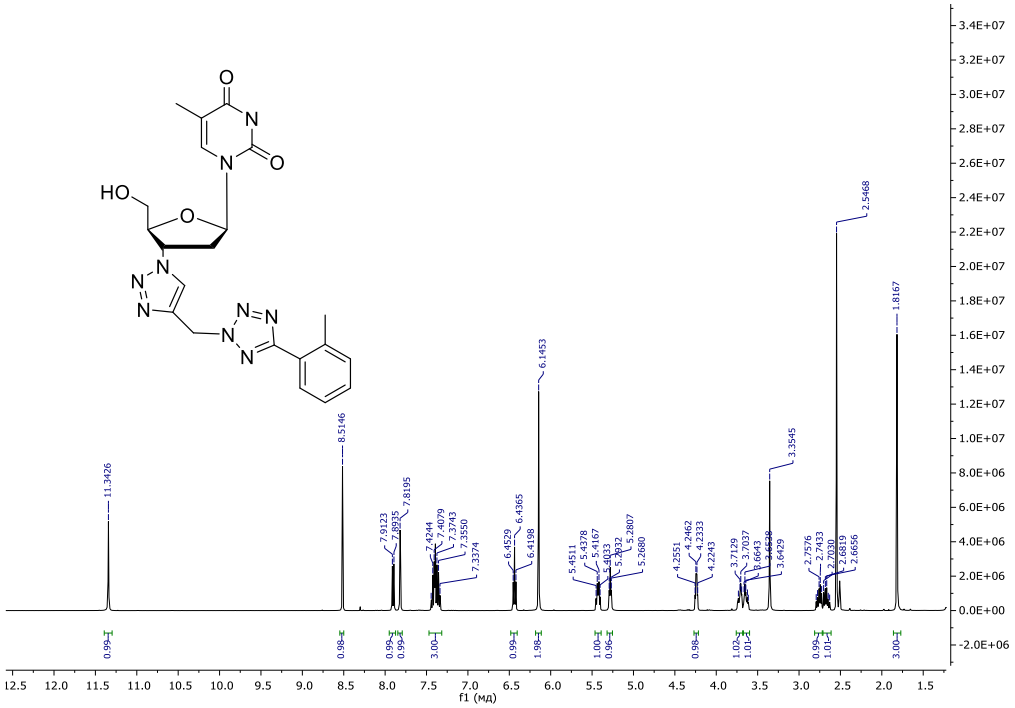


Fig. S45. ^{1}H NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11f**), 400 MHz, DMSO-d_6.

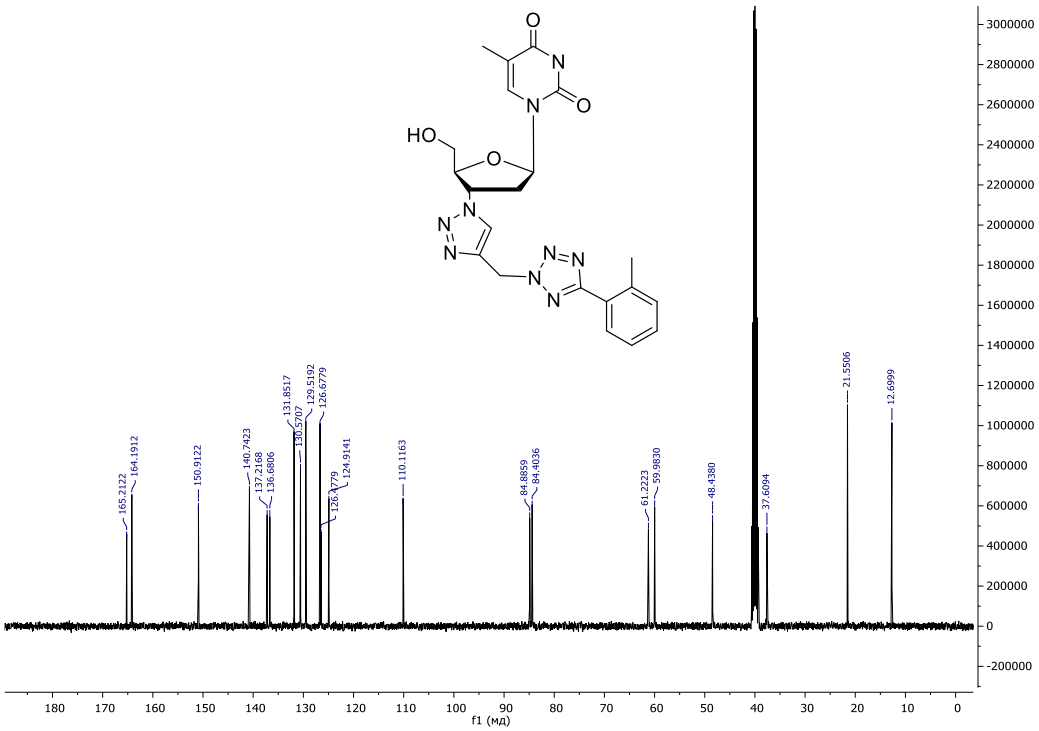


Fig. S46. ^{13}C NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11f**), 101 MHz, DMSO-d_6.

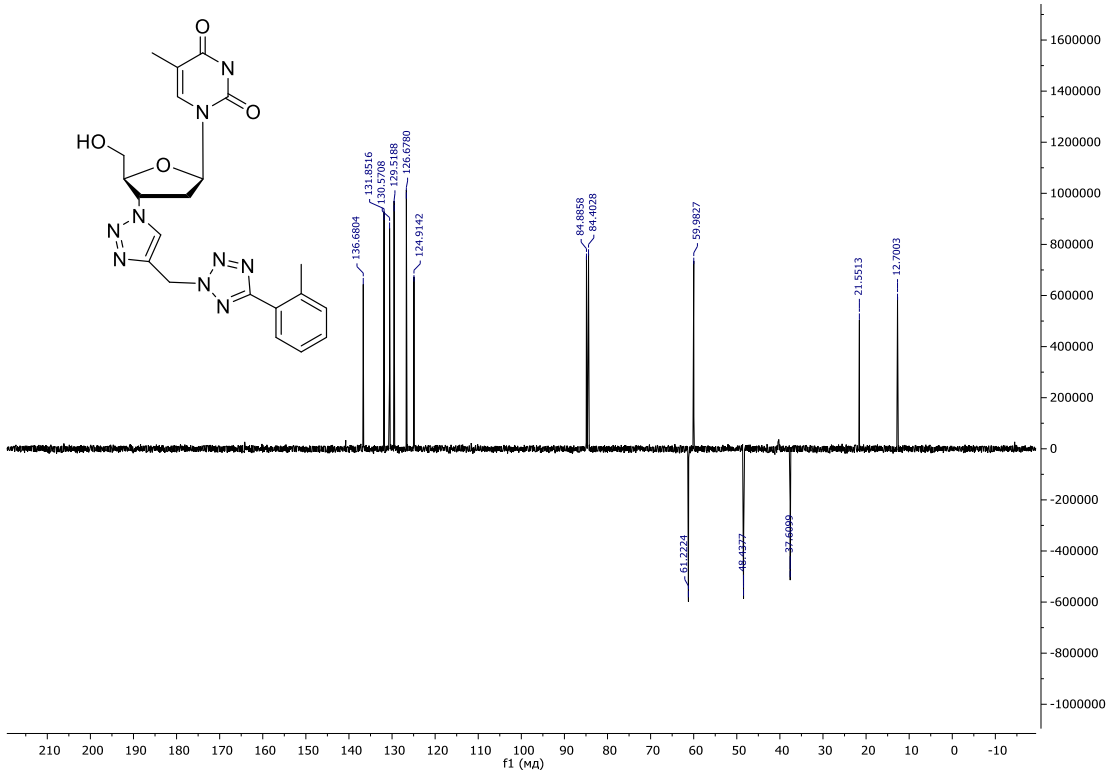


Fig. S47. ^{13}C{dept} NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11f**), 101 MHz, DMSO-d_6.

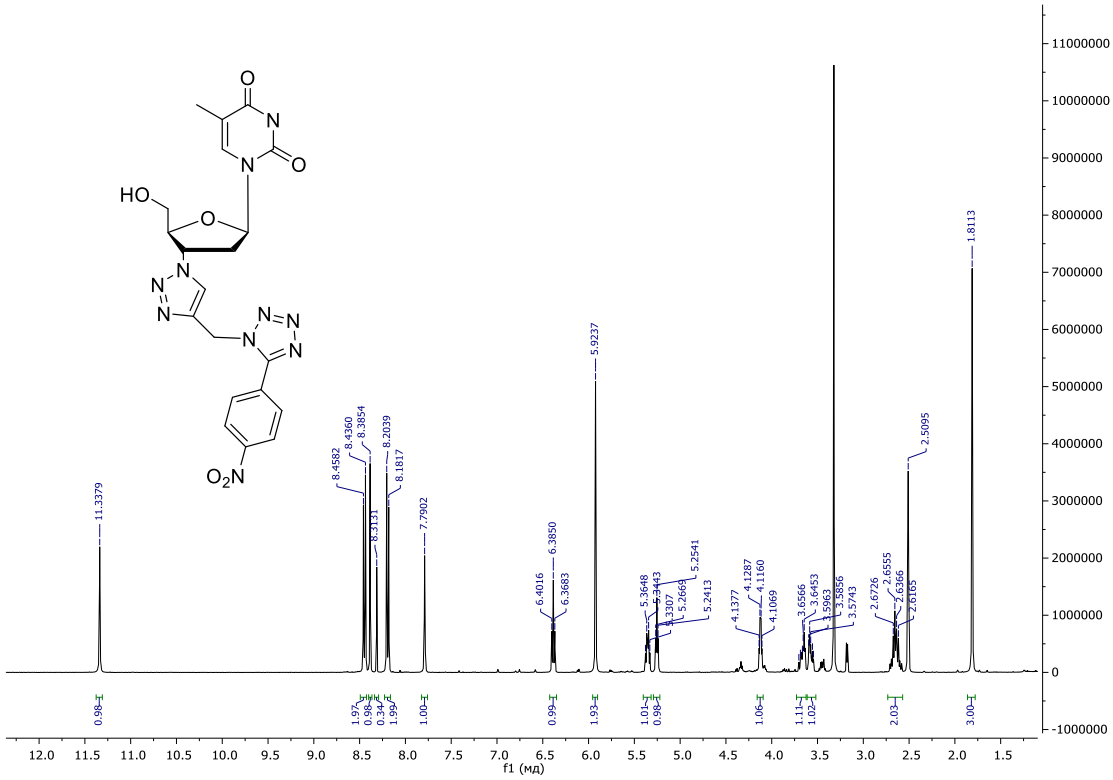


Fig. S48. ^{1}H NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10g**), 400 MHz, DMSO-d_6.

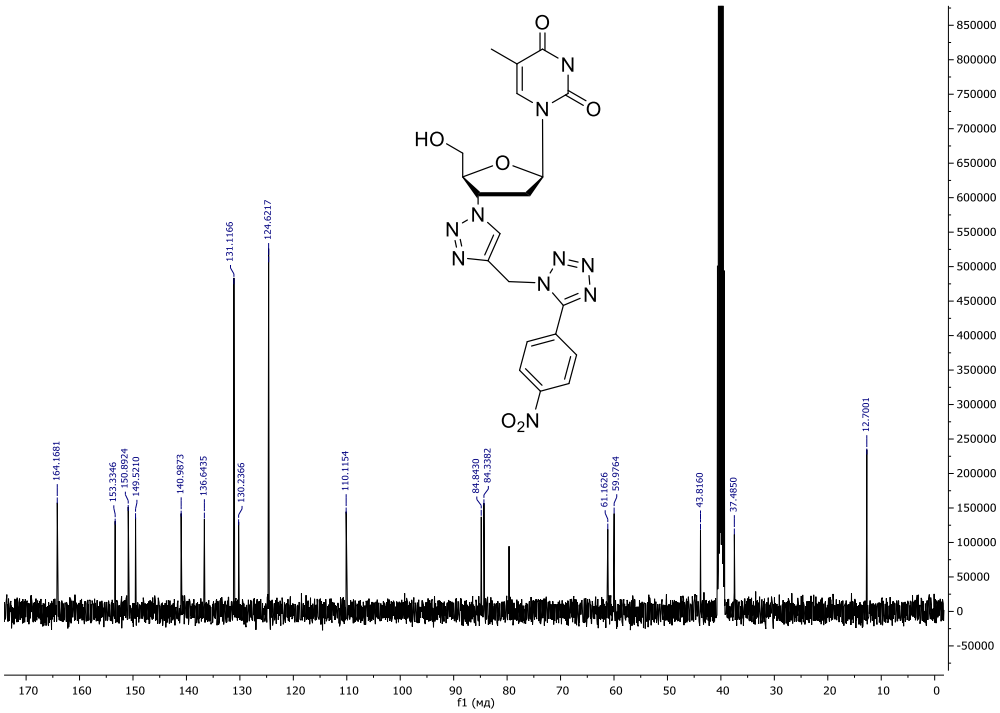


Fig. S49. ^{13}C NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10g**), 101 MHz, DMSO-d_6.

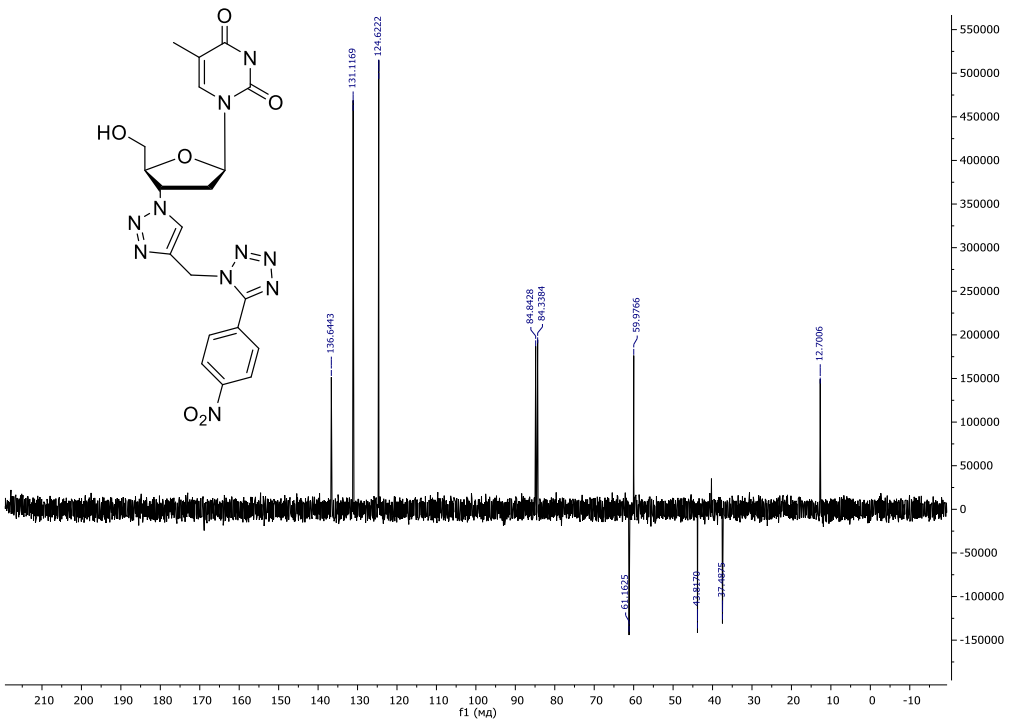


Fig. S50. ^{13}C{dept} NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10g**), 101 MHz, DMSO-d_6.

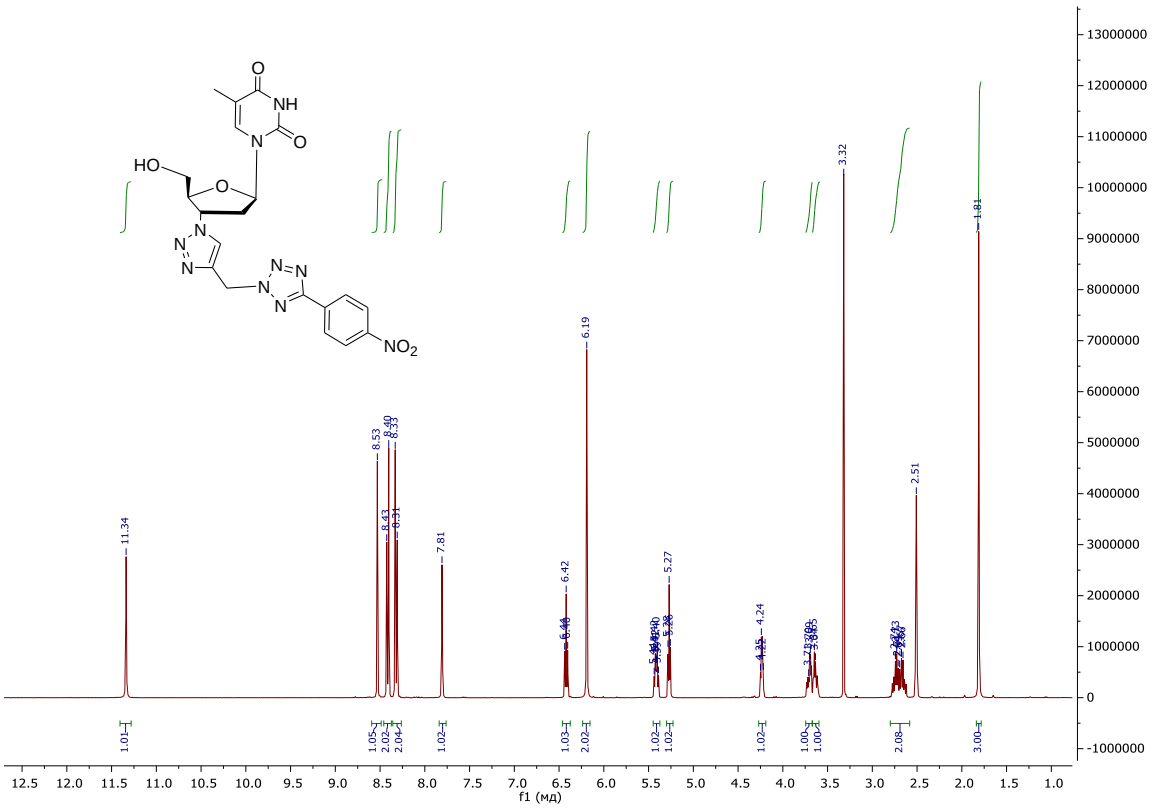


Fig. S51. ^{1}H NMR spectrum (DMSO-d_6) of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11g**), 400 MHz, DMSO-d_6.

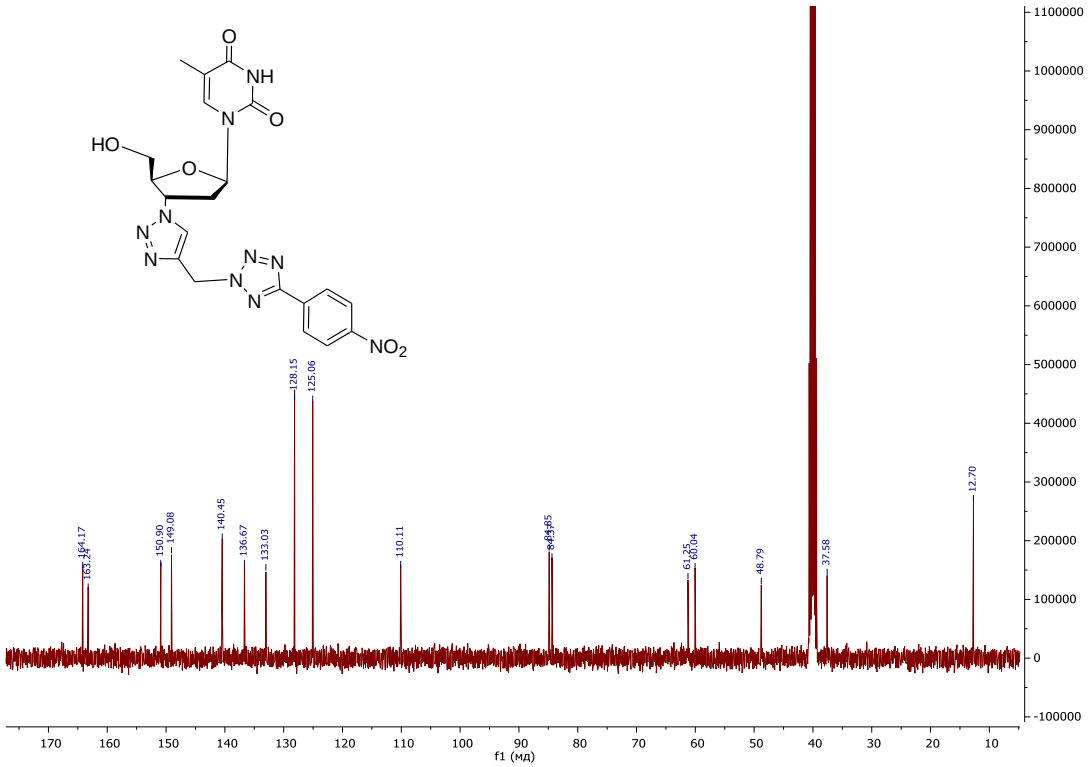


Fig. S52. ^{13}C NMR spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11g**), 101 MHz, DMSO-d_6.

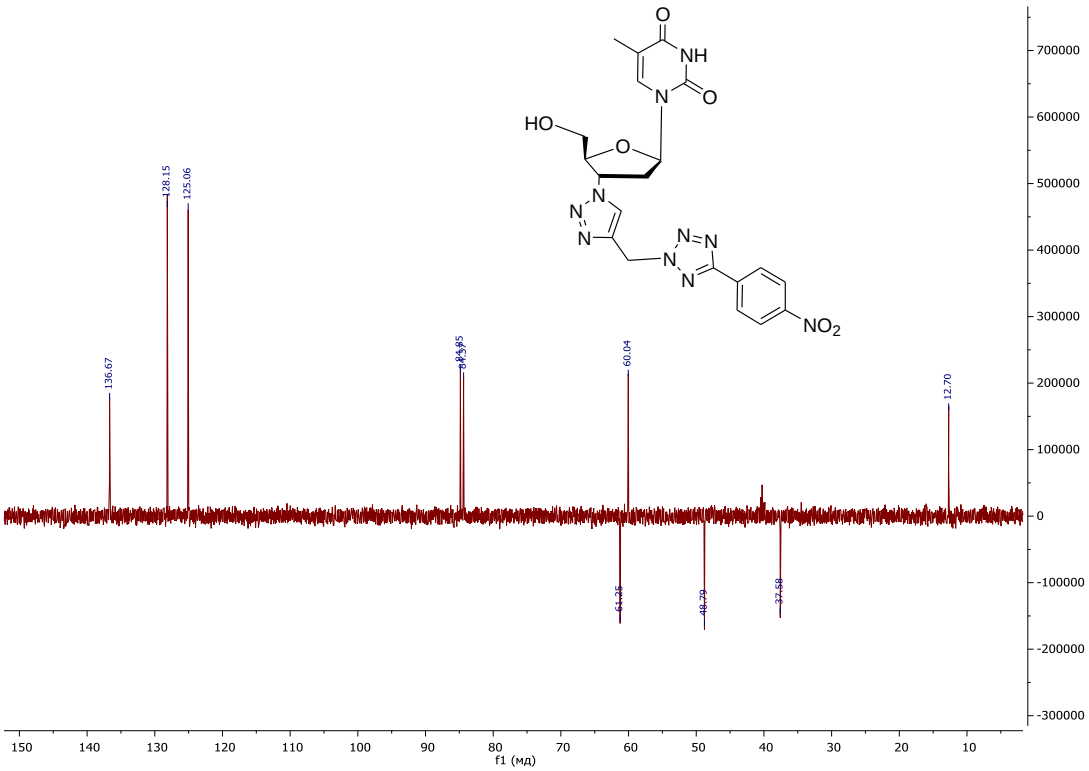


Fig. S53. ^{13}C NMR {dept} spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11g**), 101 MHz, DMSO-d_6.

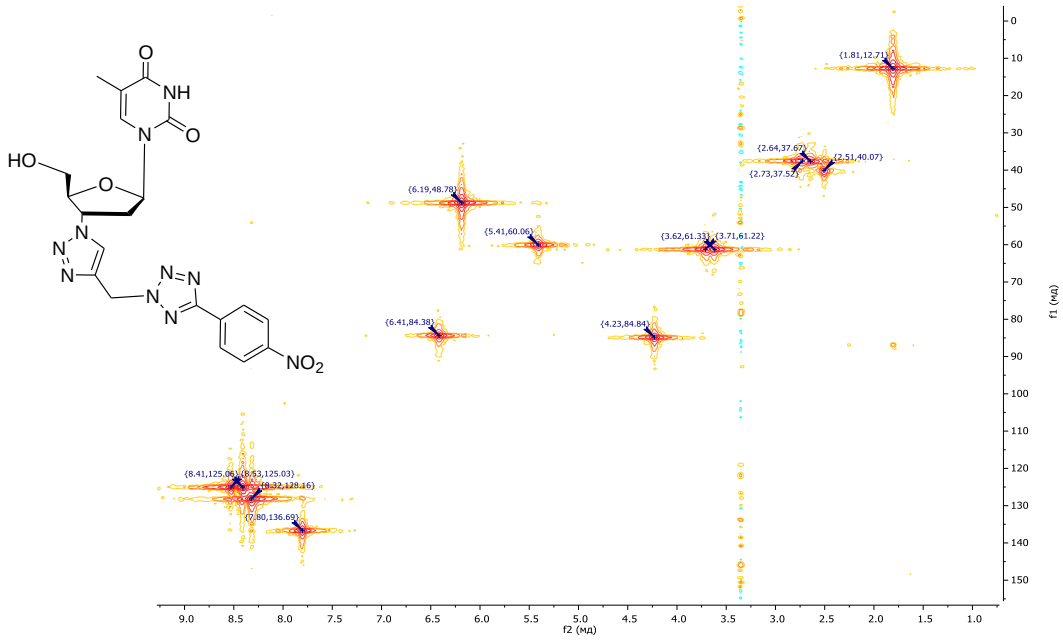


Fig. S54. HMQC{^{1}H-^{13}C} NMR spectrum (DMSO-d_6) of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11g**).

2. Mass spectra of compounds

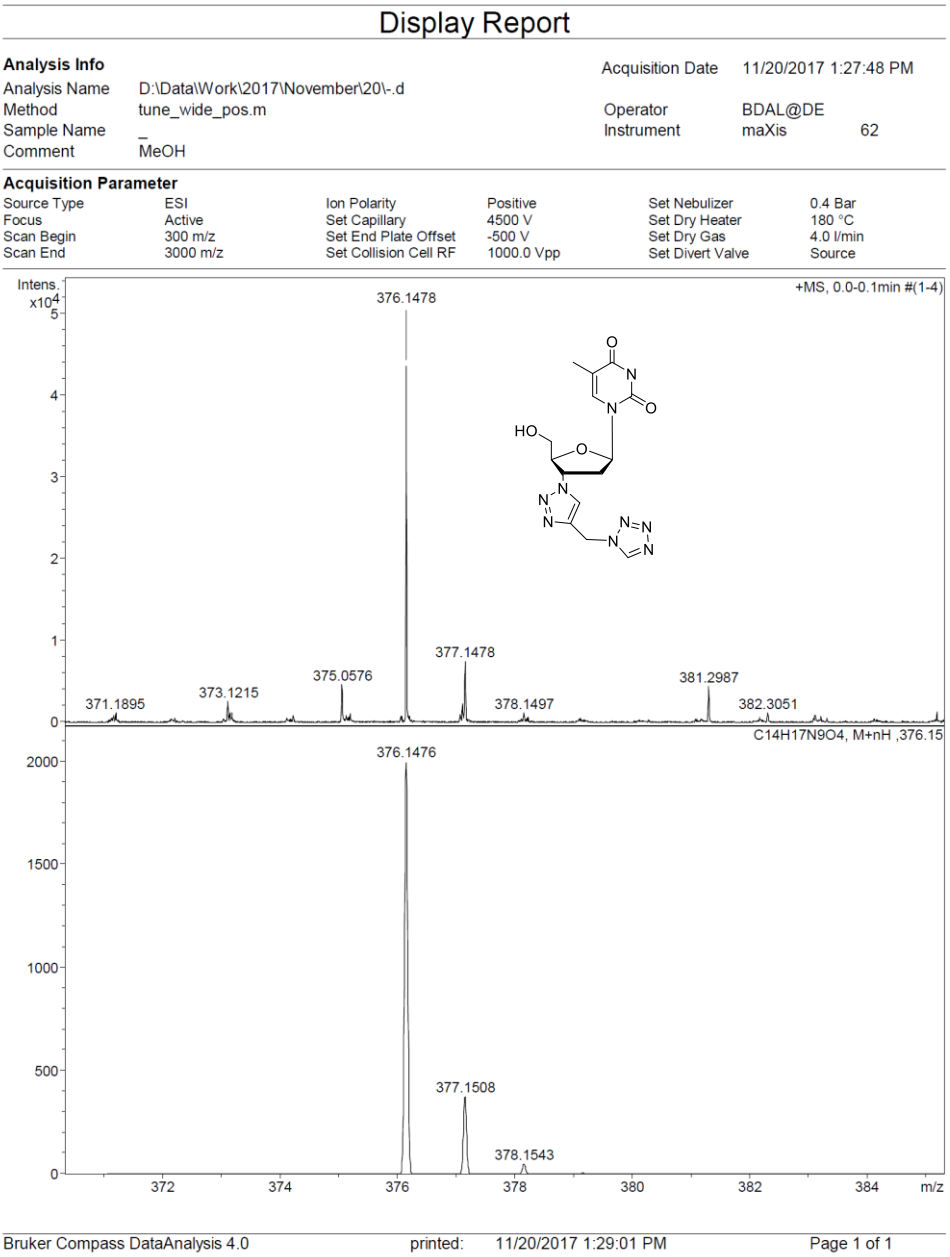


Fig. S55. Mass spectrum of 1-((2R,4S,5S)-4-(4-((1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10a**).

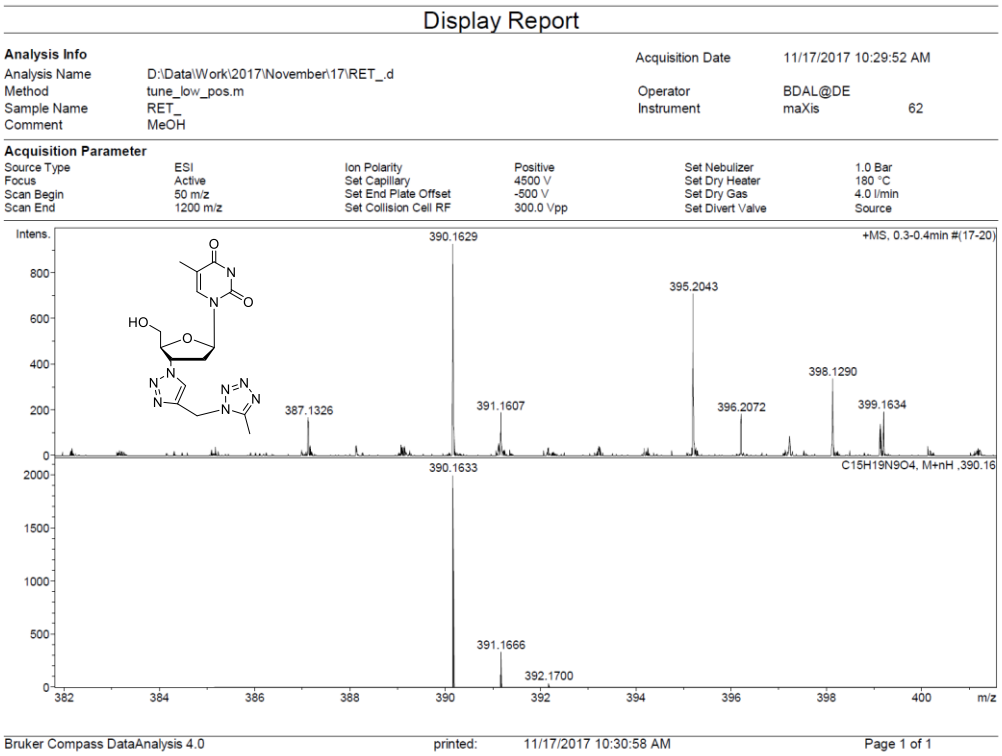


Fig. S56. Mass spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-methyl-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10b**).

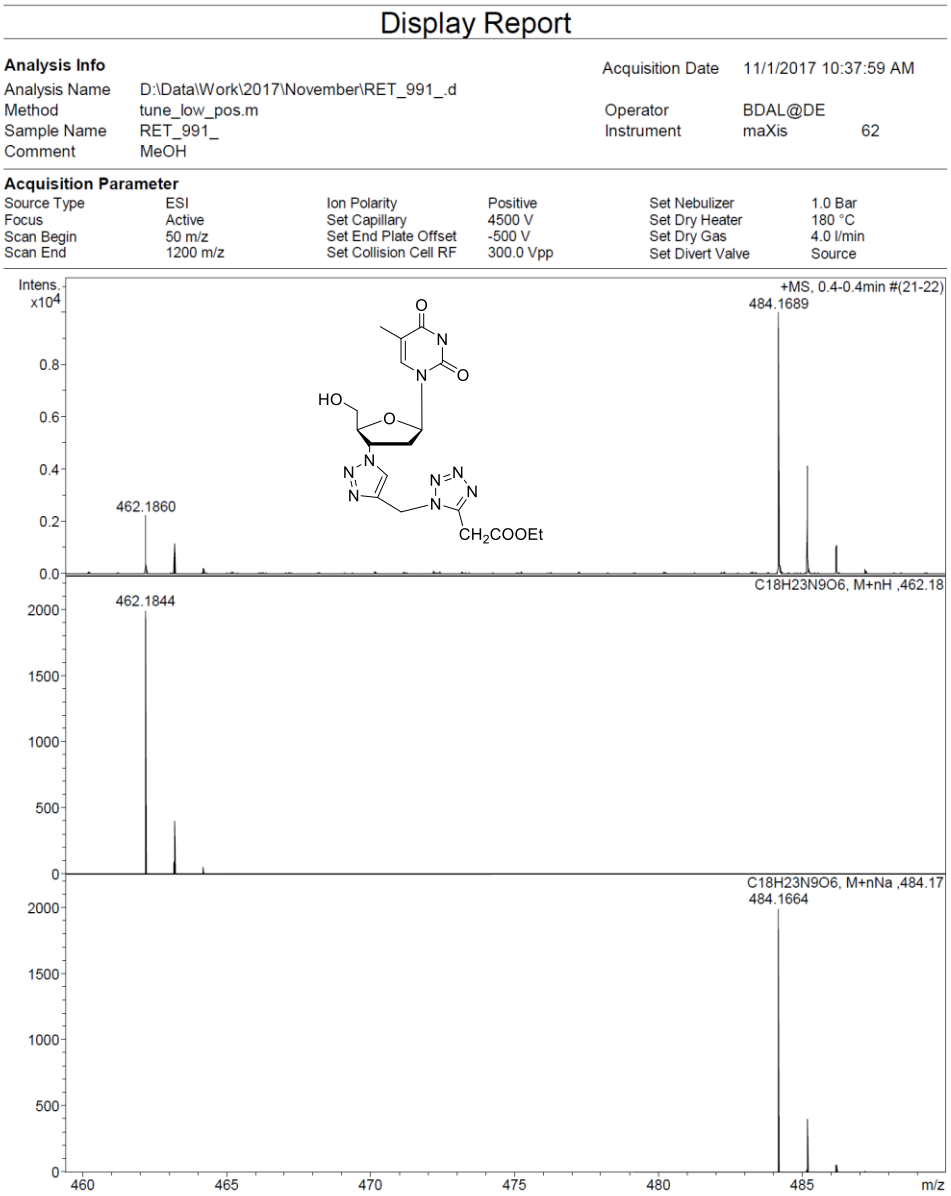


Fig. S57. Mass spectrum of ethyl 2-(1-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-1H-tetrazol-5-yl)acetate (**10c**).

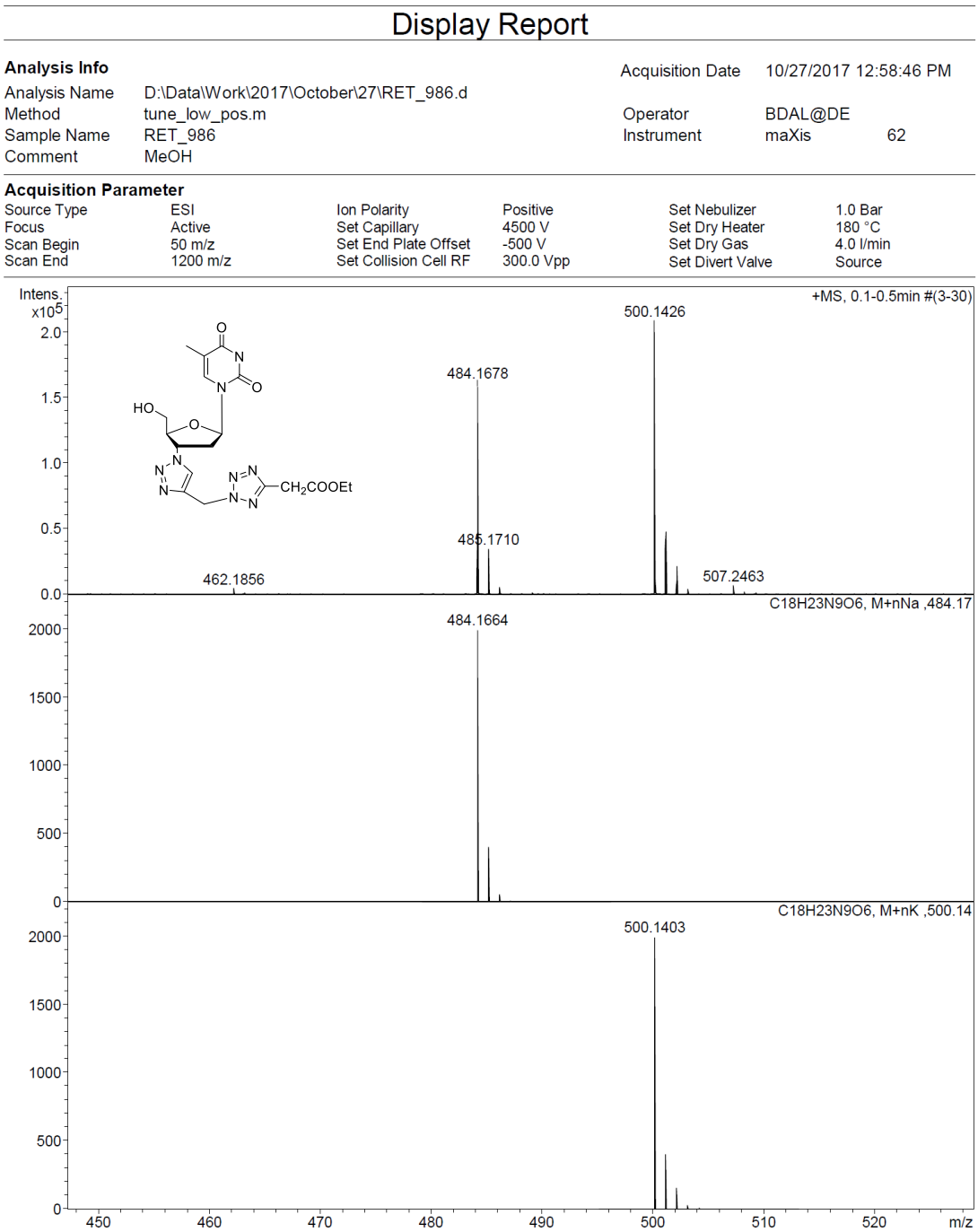


Fig. S58. Mass spectrum of ethyl 2-(2-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-2H-tetrazol-5-yl)acetate (**11c**).

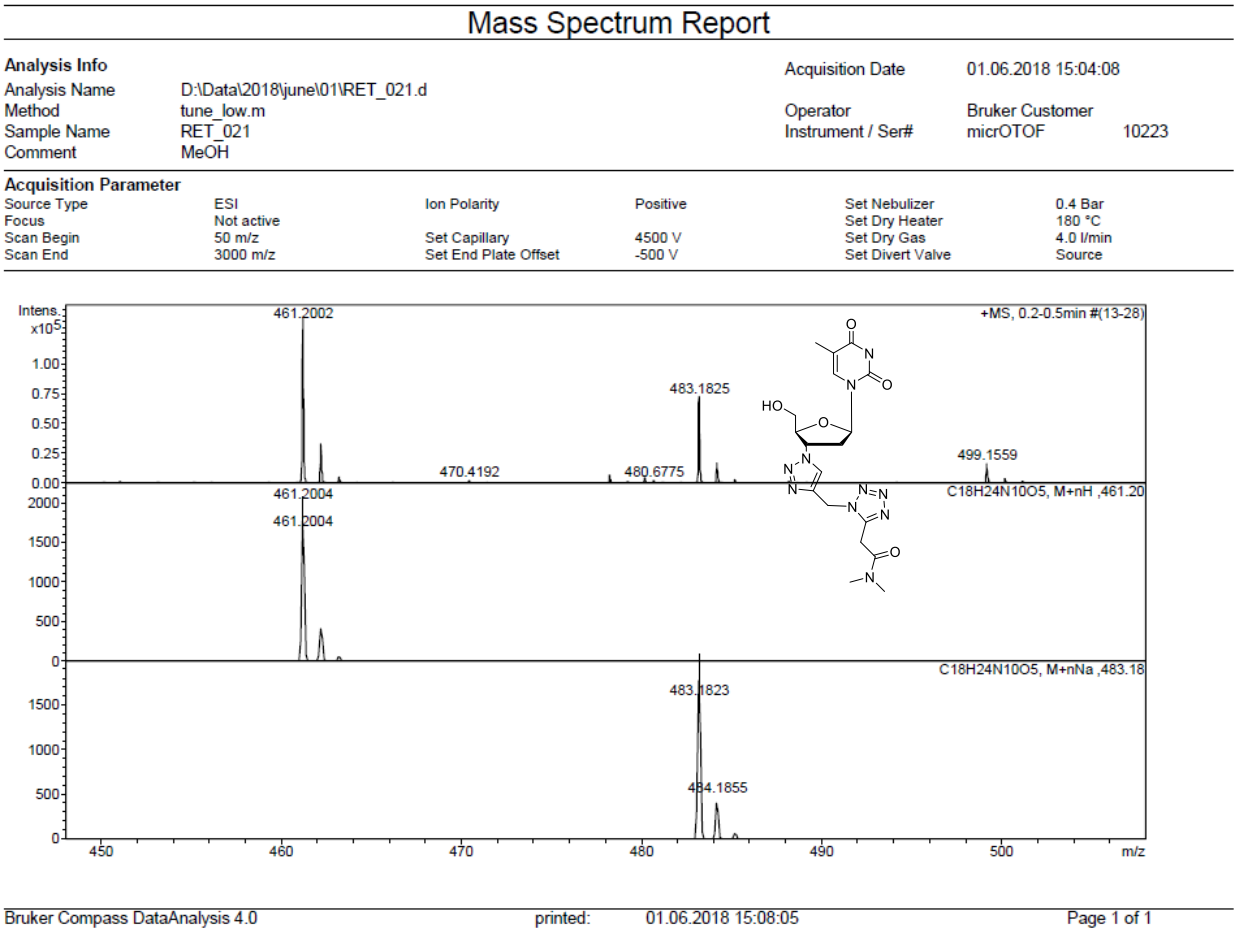


Fig. S59. Mass spectrum of 2-(1-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-1H-tetrazol-5-yl)-N,N-dimethylacetamide (**10d**).

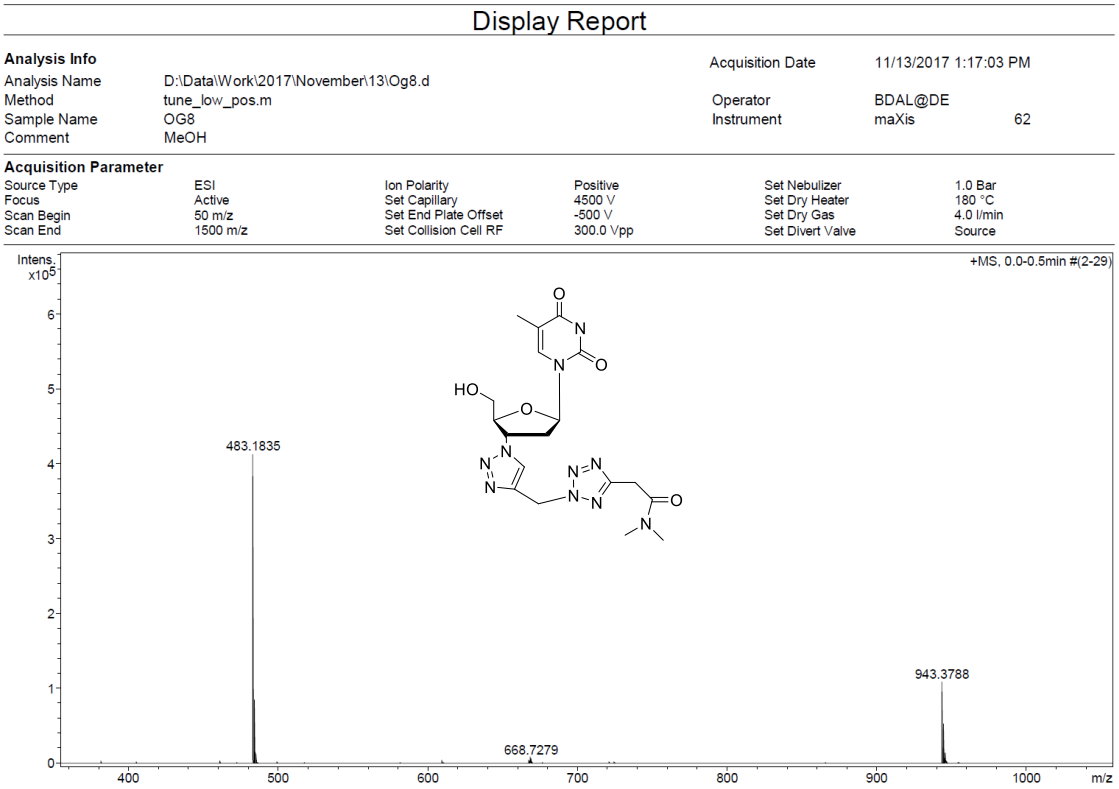


Fig. S60. Mass spectrum of 2-(2-((1-((2S,3S,5R)-2-(hydroxymethyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-3-yl)-1H-1,2,3-triazol-4-yl)methyl)-2H-tetrazol-5-yl)-N,N-dimethylacetamide (**11d**).

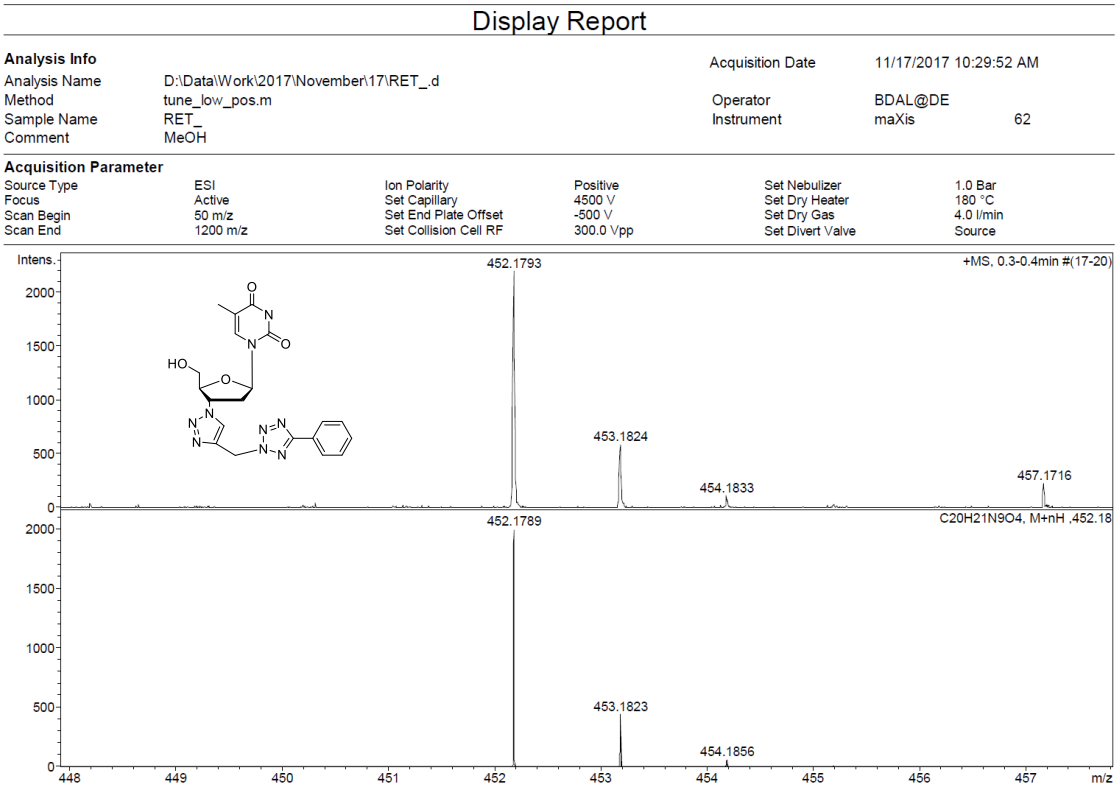


Fig. S61. Mass spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-phenyl-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11e**).

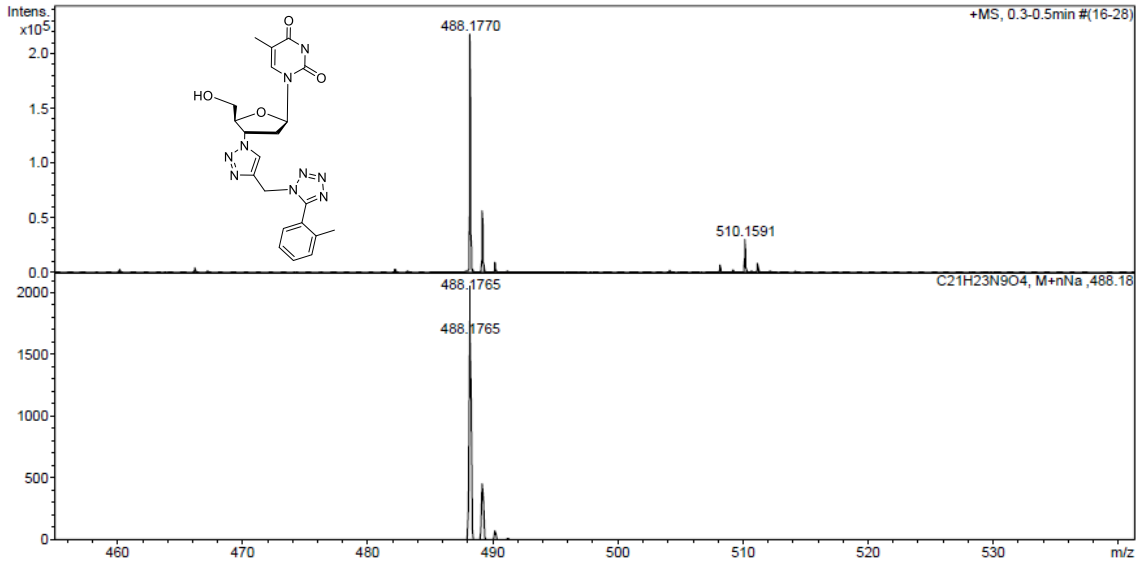
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\2018\june\01\RET_004.d	Acquisition Date	01.06.2018 14:50:06
Method	tune_low.m	Operator	Bruker Customer
Sample Name	RET_004	Instrument / Ser#	micrOTOF 10223
Comment	MeOH		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Bruker Compass DataAnalysis 4.0 printed: 01.06.2018 14:56:01 Page 1 of 1

Fig. S62. Mass spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10f**).

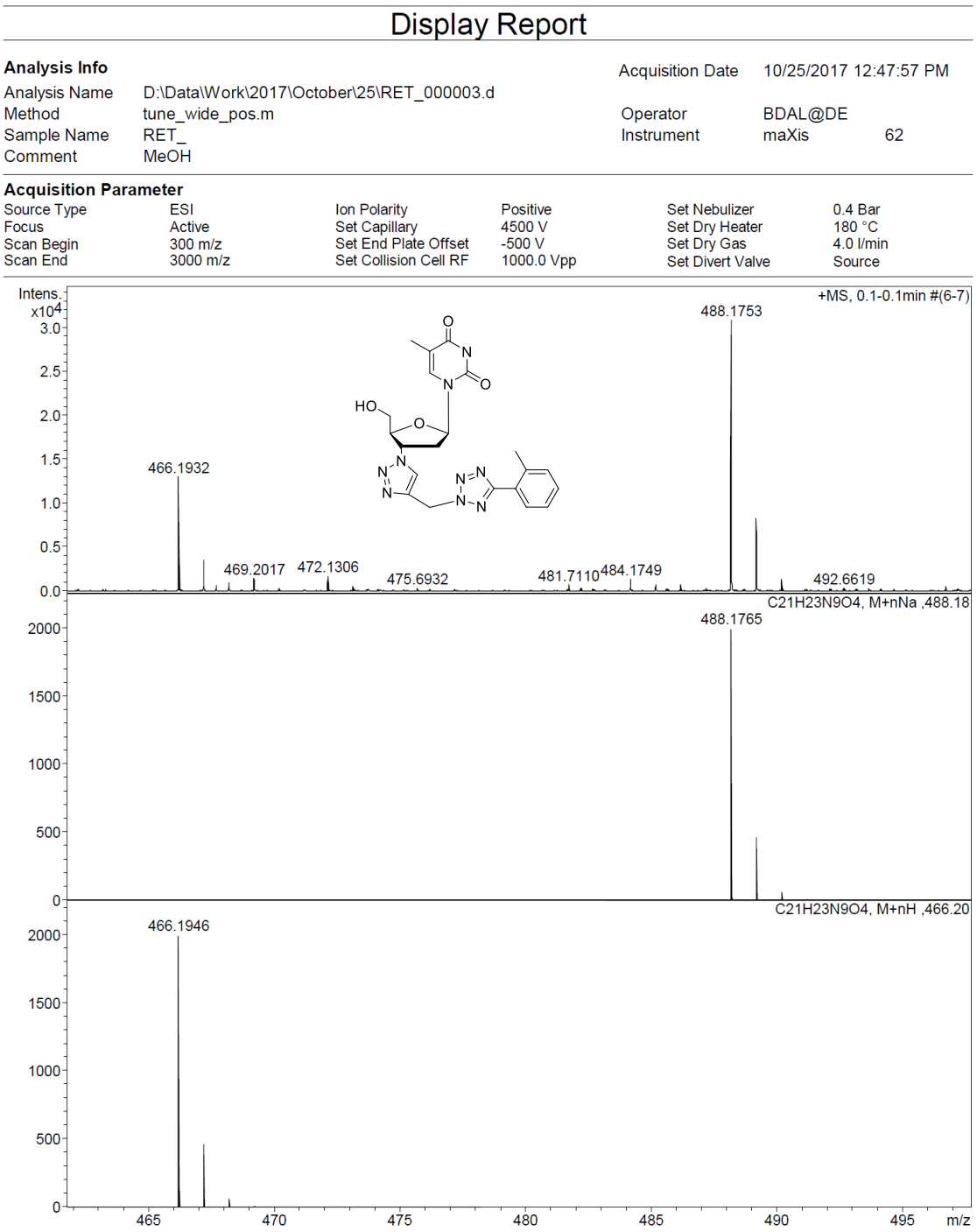


Fig. S63. Mass spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(o-tolyl)-2H-tetrazol-2-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**11f**).

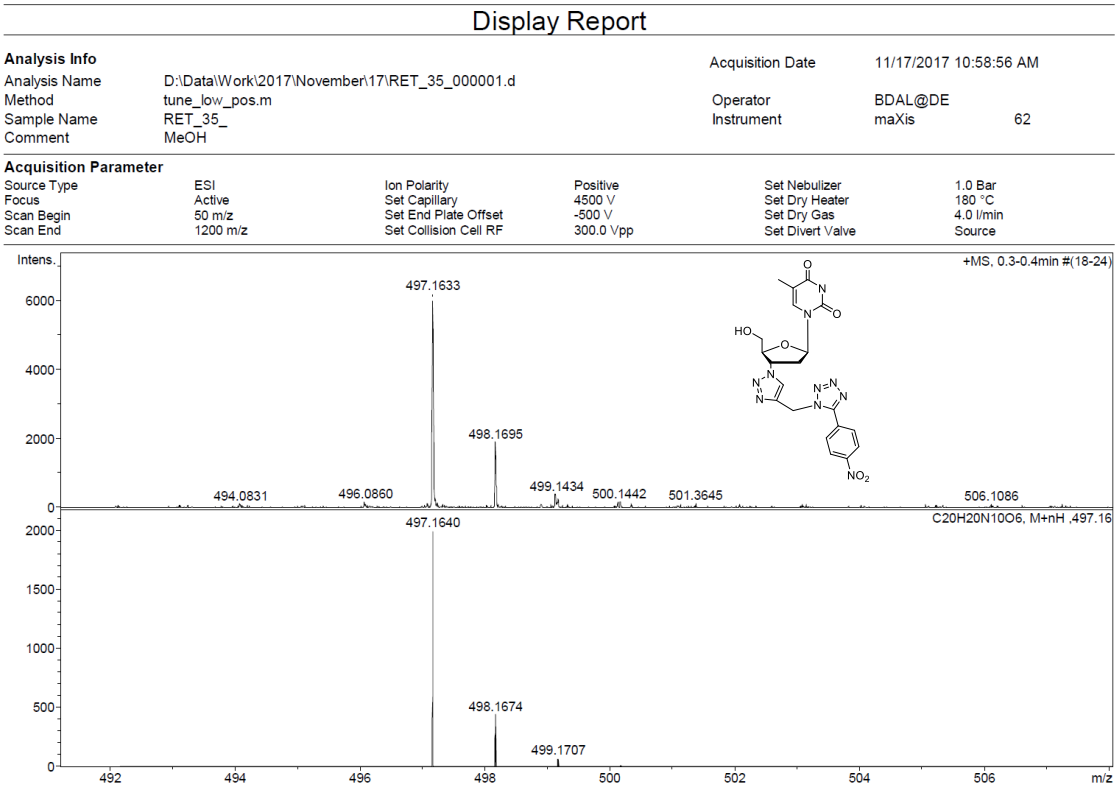


Fig. S64. Mass spectrum of 1-((2R,4S,5S)-5-(hydroxymethyl)-4-(4-((5-(4-nitrophenyl)-1H-tetrazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (**10g**).

3. Crystal structure of compound 10d

Table S1. Crystal data and structure refinement for **10d**

Identification code	**10d**
Empirical formula	$C_{19}H_{28}N_{10}O_6$
Formula weight	492.51
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	4.72153(19)
b/Å	15.4366(7)
c/Å	31.4484(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2292.09(16)
Z	4
ρ_{calc}g/cm^3	1.427
μ/mm^{-1}	0.109
F(000)	1040.0
Crystal size/mm^3	0.2 × 0.2 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.556 to 54.998
Index ranges	$-6 \leq h \leq 4$, $-19 \leq k \leq 20$, $-40 \leq l \leq 40$
Reflections collected	17747
Independent reflections	5228 [R_{int} = 0.0566, R_{sigma} = 0.0492]
Data/restraints/parameters	5228/0/322
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0462, wR_2 = 0.1113
Final R indexes [all data]	R_1 = 0.0521, wR_2 = 0.1153
Largest diff. peak/hole / e Å^{-3}	0.50/-0.30
CCDC number	1846759

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **10d.** U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O2	-4171(5)	6660.5(12)	109.5(5)	19.2(4)
O3	1927(4)	6125.1(12)	1784.3(5)	15.5(4)
O4	-2706(4)	5022.3(12)	2106.6(6)	18.3(4)
O1	2034(4)	7960.8(12)	1012.3(6)	20.3(4)
O5	1239(5)	6107.5(12)	4008.3(6)	22.9(5)
O1S	-2194(6)	5566.5(15)	3336.8(8)	38.6(6)

N3	1467(5)	7132.0(13)	2687.7(6)	13.3(5)
N2	-730(5)	6854.5(14)	1272.5(6)	13.5(5)
N6	3894(5)	8038.7(14)	3921.6(6)	14.5(5)
N4	2319(5)	7914.5(14)	2553.7(7)	16.3(5)
N7	2175(5)	8733.9(14)	3892.1(7)	18.1(5)
N5	3994(5)	8227.1(15)	2853.8(7)	18.0(5)
N1	-1032(5)	7275.8(14)	566.8(6)	14.5(5)
N9	1345(6)	8049.3(16)	4489.1(7)	21.5(5)
N8	655(6)	8735.1(16)	4234.7(7)	22.6(5)
N10	4029(6)	5256.8(15)	4425.1(8)	22.3(5)
C4	-3135(6)	6683.6(16)	470.3(7)	13.4(5)
C1	234(6)	7405.0(17)	957.8(8)	14.3(5)
C14	3372(6)	7626.5(17)	4288.2(8)	16.0(5)
C3	-3929(6)	6097.7(16)	809.2(8)	13.5(5)
C2	-2676(6)	6204.5(16)	1190.5(8)	13.0(5)
C8	-342(6)	6560.1(16)	2427.9(8)	13.0(5)
C12	4200(6)	7640.3(17)	3171.7(8)	13.9(5)
C16	3185(6)	6023.8(18)	4272.8(8)	18.1(6)
C6	511(6)	6917.9(17)	1698.7(7)	13.7(5)
C9	1493(6)	5850.7(16)	2219.0(7)	13.4(5)
C11	2611(6)	6933.4(17)	3069.9(8)	16.8(6)
C13	5848(6)	7826.5(18)	3570.9(8)	16.7(5)
C10	192(6)	4965.3(18)	2228.6(9)	18.2(6)
C15	4739(6)	6818.8(17)	4439.1(8)	18.1(6)
C5	-6062(6)	5403.1(17)	724.9(8)	16.3(6)
C7	-1674(6)	7035.9(17)	2052.5(7)	13.8(5)
C17	6191(7)	5181(2)	4759.7(10)	28.3(7)
C1S	-3633(9)	4767(2)	3295.7(11)	42.5(9)
C18	2660(8)	4453.8(19)	4302.8(11)	31.5(8)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **10d**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O2	29.0(11)	18.5(10)	10.0(8)	0.9(7)	-5.2(8)	1.9(9)
O3	17.1(9)	22.0(9)	7.5(8)	0.1(7)	1.0(7)	3.2(8)
O4	15.4(10)	14.1(9)	25.4(10)	-1.3(8)	-2.0(8)	-1.8(8)
O1	24.2(11)	21(1)	15.7(9)	2.5(7)	0.1(8)	-7.8(9)
O5	30.9(12)	19.4(10)	18.5(9)	0.1(8)	-3.0(9)	-0.7(9)
O1S	43.4(15)	39.8(13)	32.8(12)	15.7(11)	-15.1(12)	-16.5(12)
N3	15.8(12)	15(1)	9.2(9)	-0.2(8)	0.1(9)	-2.0(9)
N2	16.7(12)	16.9(11)	7.1(9)	0.7(8)	-0.9(9)	-3.1(9)
N6	18.3(12)	14.1(10)	11.2(10)	-0.2(8)	-5.1(9)	-0.5(9)
N4	21.9(12)	15.1(11)	11.9(10)	0.1(8)	-3.5(9)	-2(1)
N7	22.4(13)	14.7(10)	17.2(10)	-1.6(9)	-6(1)	2.3(10)

N5	22.7(13)	19.1(11)	12.1(10)	-0.2(9)	-4(1)	-2.9(10)
N1	20.5(12)	14.6(10)	8.4(9)	3.8(8)	0.0(9)	-2.5(9)
N9	23.6(13)	23.1(12)	17.6(11)	-1.3(9)	-0.9(10)	1.7(10)
N8	25.8(14)	21.3(12)	20.6(11)	-2.4(9)	-3.6(11)	3.3(11)
N10	27.0(14)	19.3(12)	20.8(12)	4.6(9)	7.4(11)	4.4(10)
C4	16.8(13)	13.8(12)	9.6(10)	-0.2(9)	-0.4(10)	2.8(10)
C1	16.5(13)	14.4(12)	11.9(11)	0.6(9)	2.1(11)	1(1)
C14	18.5(14)	16.3(13)	13.3(12)	-2.4(10)	-3.2(11)	-1.5(11)
C3	14.6(13)	15.3(12)	10.6(11)	0.6(9)	0.3(10)	1.8(10)
C2	12.5(13)	14.8(12)	11.7(11)	1.4(9)	2.5(10)	-1.2(10)
C8	13.3(13)	16.3(13)	9.3(11)	0.4(9)	-1.6(10)	-2(1)
C12	13.4(13)	17.0(12)	11.3(11)	-0.3(9)	-0.2(10)	0.9(10)
C16	23.8(15)	20.3(13)	10.2(11)	1.5(10)	7.7(11)	2.1(12)
C6	16.6(13)	15.3(12)	9.1(11)	-1.0(9)	-2.4(10)	-0.9(10)
C9	13.8(13)	18.5(12)	8.0(11)	1.0(9)	-2(1)	0.5(10)
C11	23.2(15)	17.2(12)	9.9(11)	1.8(10)	-2.1(11)	-2.7(11)
C13	17.2(14)	22.7(13)	10.2(11)	-0.6(10)	-1.3(10)	-4.1(11)
C10	14.8(13)	18.6(14)	21.2(13)	1.6(11)	-2.2(11)	0.5(11)
C15	19.5(14)	20.3(14)	14.5(12)	4.1(10)	-1.1(11)	1.9(11)
C5	16.1(13)	17.3(13)	15.6(12)	-1.4(10)	-1.6(11)	-0.8(10)
C7	14.4(13)	17.2(12)	10.0(11)	-0.9(9)	-0.8(10)	0.7(10)
C17	29.5(17)	28.0(16)	27.4(15)	12.7(12)	4.6(14)	9.4(14)
C1S	55(2)	44(2)	29.2(17)	4.6(15)	1.7(18)	-12.5(19)
C18	43(2)	16.6(14)	34.9(17)	0.7(12)	13.0(16)	1.5(14)

Table S4. Bond Lengths for **10d**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C4	1.236(3)	N1	C4	1.383(3)
O3	C6	1.420(3)	N1	C1	1.382(3)
O3	C9	1.446(3)	N9	N8	1.366(3)
O4	C10	1.424(3)	N9	C14	1.320(4)
O1	C1	1.220(3)	N10	C16	1.338(3)
O5	C16	1.246(3)	N10	C17	1.471(4)
O1S	C1S	1.415(4)	N10	C18	1.450(4)
N3	N4	1.341(3)	C4	C3	1.447(3)
N3	C8	1.475(3)	C14	C15	1.482(4)
N3	C11	1.353(3)	C3	C2	1.347(3)
N2	C1	1.382(3)	C3	C5	1.495(4)
N2	C2	1.385(3)	C8	C9	1.543(4)
N2	C6	1.466(3)	C8	C7	1.526(3)
N6	N7	1.349(3)	C12	C11	1.362(4)
N6	C14	1.340(3)	C12	C13	1.505(3)
N6	C13	1.475(3)	C16	C15	1.523(4)
N4	N5	1.323(3)	C6	C7	1.528(4)

N7	N8	1.295(3)	C9	C10	1.499(4)
N5	C12	1.352(3)			

Table S5. Bond Angles for **10d**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	O3	C9	111.40(18)	N9	C14	N6	108.1(2)
N4	N3	C8	122.6(2)	N9	C14	C15	125.4(2)
N4	N3	C11	111.3(2)	C4	C3	C5	119.5(2)
C11	N3	C8	126.0(2)	C2	C3	C4	117.7(2)
C1	N2	C2	122.1(2)	C2	C3	C5	122.8(2)
C1	N2	C6	118.8(2)	C3	C2	N2	123.1(2)
C2	N2	C6	118.9(2)	N3	C8	C9	109.6(2)
N7	N6	C13	120.1(2)	N3	C8	C7	112.3(2)
C14	N6	N7	109.1(2)	C7	C8	C9	104.1(2)
C14	N6	C13	130.8(2)	N5	C12	C11	108.9(2)
N5	N4	N3	106.5(2)	N5	C12	C13	121.7(2)
N8	N7	N6	106.1(2)	C11	C12	C13	129.3(2)
N4	N5	C12	109.0(2)	O5	C16	N10	123.4(3)
C1	N1	C4	127.0(2)	O5	C16	C15	120.1(2)
C14	N9	N8	106.0(2)	N10	C16	C15	116.5(2)
N7	N8	N9	110.7(2)	O3	C6	N2	107.70(19)
C16	N10	C17	122.2(3)	O3	C6	C7	106.41(19)
C16	N10	C18	121.9(3)	N2	C6	C7	113.8(2)
C18	N10	C17	115.6(2)	O3	C9	C8	105.92(19)
O2	C4	N1	120.3(2)	O3	C9	C10	110.1(2)
O2	C4	C3	123.8(2)	C10	C9	C8	114.1(2)
N1	C4	C3	115.9(2)	N3	C11	C12	104.3(2)
O1	C1	N2	124.2(2)	N6	C13	C12	110.0(2)
O1	C1	N1	121.9(2)	O4	C10	C9	109.4(2)
N1	C1	N2	114.0(2)	C14	C15	C16	111.0(2)
N6	C14	C15	126.5(2)	C8	C7	C6	103.2(2)

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **10d**.

Atom	*x*	*y*	*z*	U(eq)
H4	-3407	4523	2095	27
H1S	-1331	5579	3570	58
H1	-437	7605	357	17
H2	-3151	5816	1414	16
H8	-1847	6291	2608	16
H6	1902	7406	1707	16
H9	3368	5829	2367	16

H11	2362	6418	3231	20
H13A	6998	7314	3648	20
H13B	7151	8319	3521	20
H10A	1218	4577	2031	22
H10B	337	4720	2519	22
H15A	4742	6810	4754	22
H15B	6731	6804	4341	22
H5A	-7784	5663	606	25
H5B	-6521	5106	991	25
H5C	-5280	4986	522	25
H7A	-1961	7657	2118	17
H7B	-3515	6775	1973	17
H17A	7744	5585	4701	42
H17B	6925	4588	4766	42
H17C	5344	5321	5036	42
H1SA	-4000	4650	2994	64
H1SB	-5433	4794	3450	64
H1SC	-2461	4302	3414	64
H18A	1790	4186	4553	47
H18B	4068	4058	4182	47
H18C	1194	4575	4090	47

Crystal structure determination of compound 10d

Crystal Data for $C_{19}H_{28}N_{10}O_6$ (*M* =492.51 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), *a* = 4.72153(19) Å, *b* = 15.4366(7) Å, *c* = 31.4484(12) Å, *V* = 2292.09(16) Å^3, *Z* = 4, *T* = 100(2) K, μ(MoKα) = 0.109 mm^{-1}, *Dcalc* = 1.427 g/cm^3, 17747 reflections measured (6.556° ≤ 2Θ ≤ 54.998°), 5228 unique (R_{int} = 0.0566, R_{sigma} = 0.0492) which were used in all calculations. The final R_1 was 0.0462 (I > 2σ(I)) and wR_2 was 0.1152 (all data).

4. Anti-HIV activity

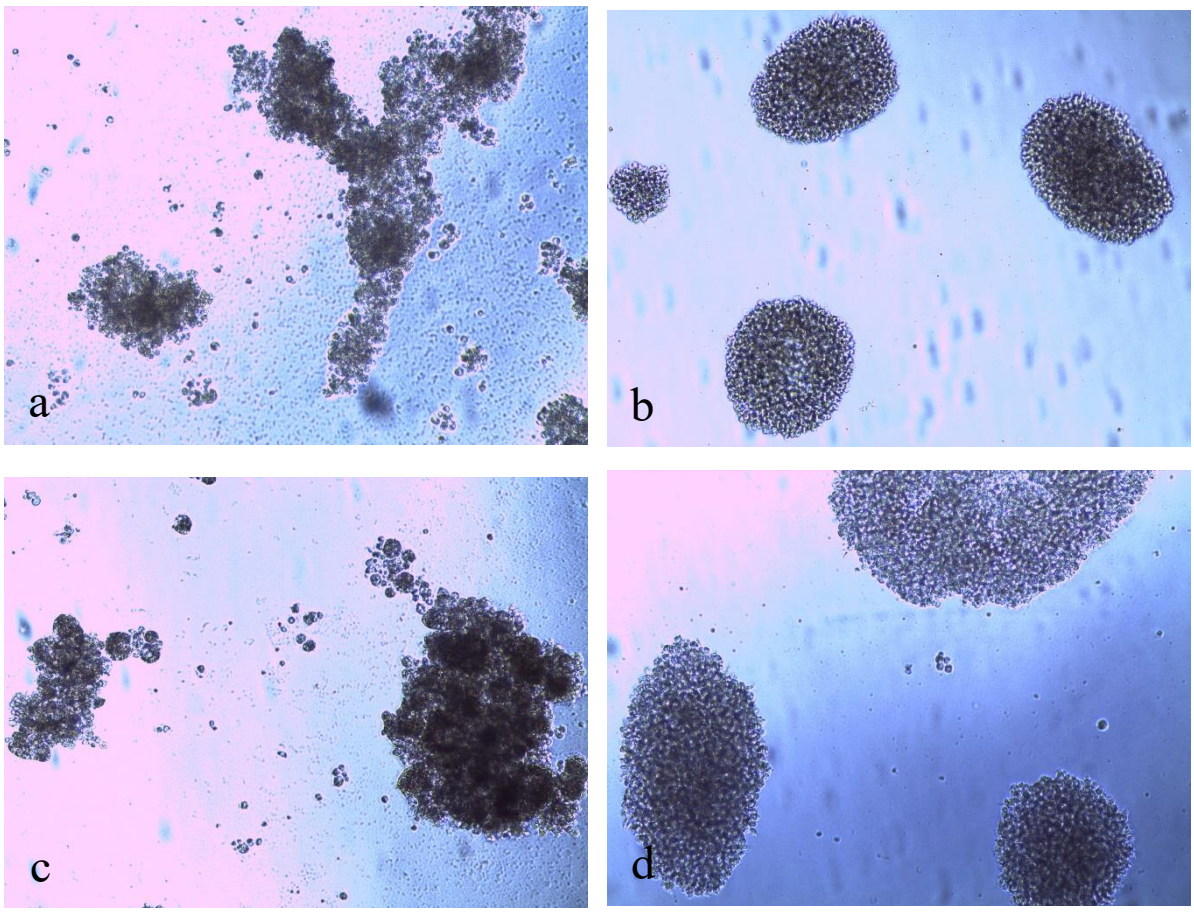


Fig. S65. The photo of MT-4 cells: a) cells without protection; b) cells control; c) protection of MT-4 cells by **10d** (50 μM); d) protection of MT-4 cells by AZT (0.1 μM).