Supplementary Materials

Investigation of 8-aza-7-deaza purine nucleoside derivatives

Hang Ren [1,2], Haoyun An [2,*] and Jingchao Tao [1,*]

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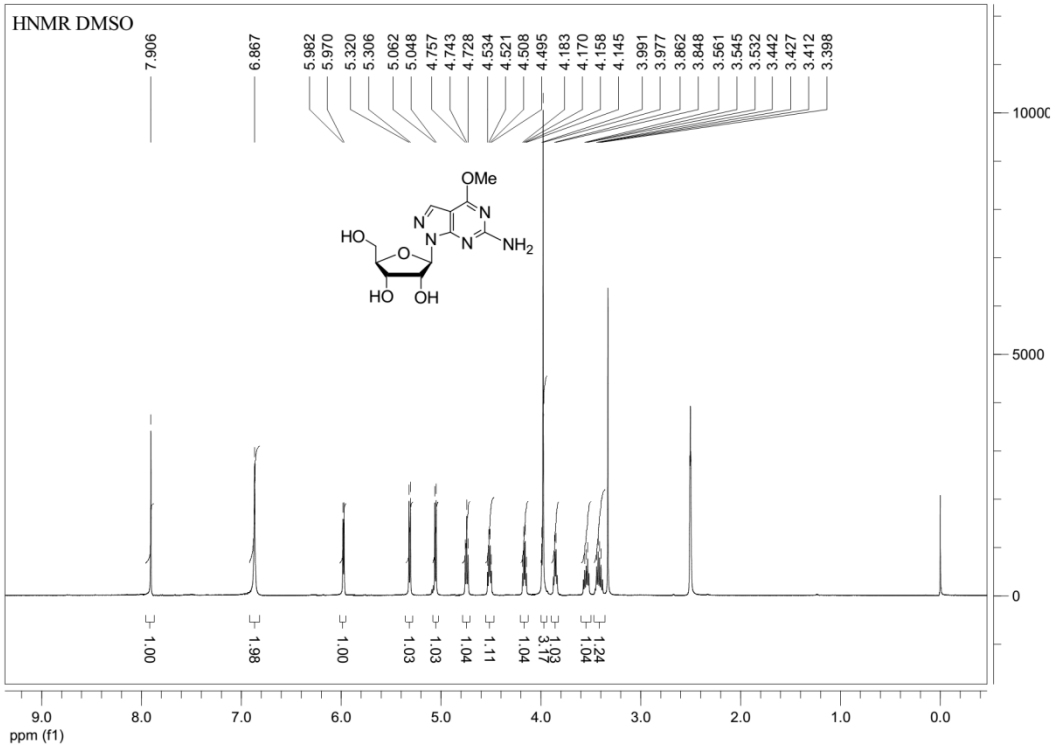
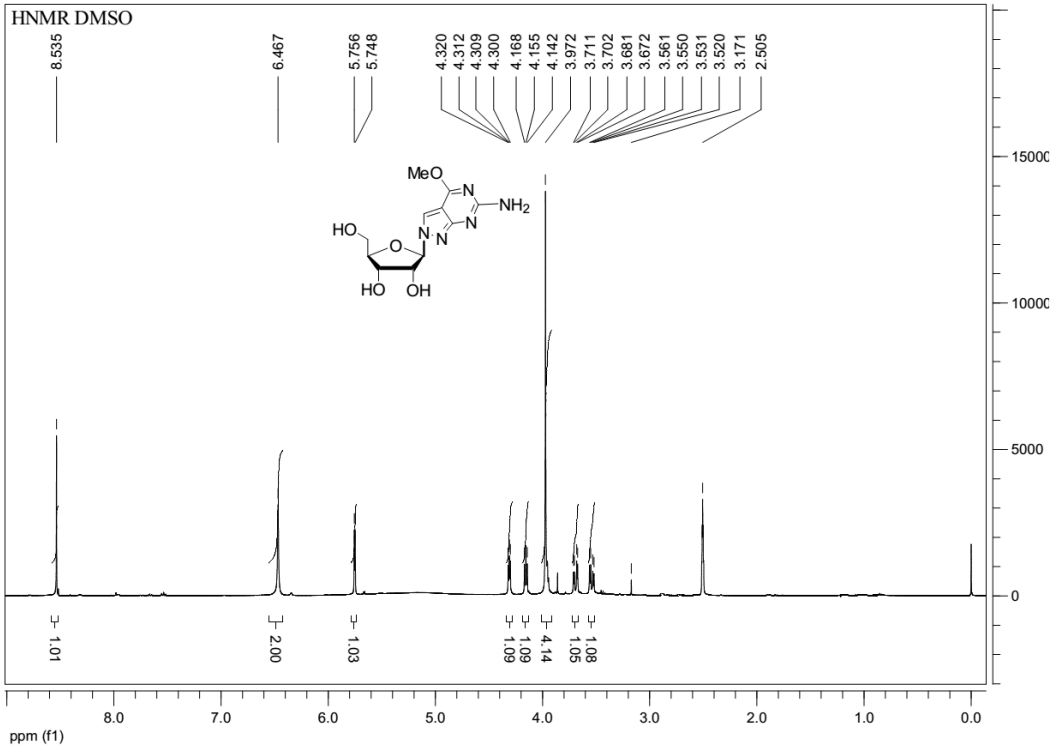
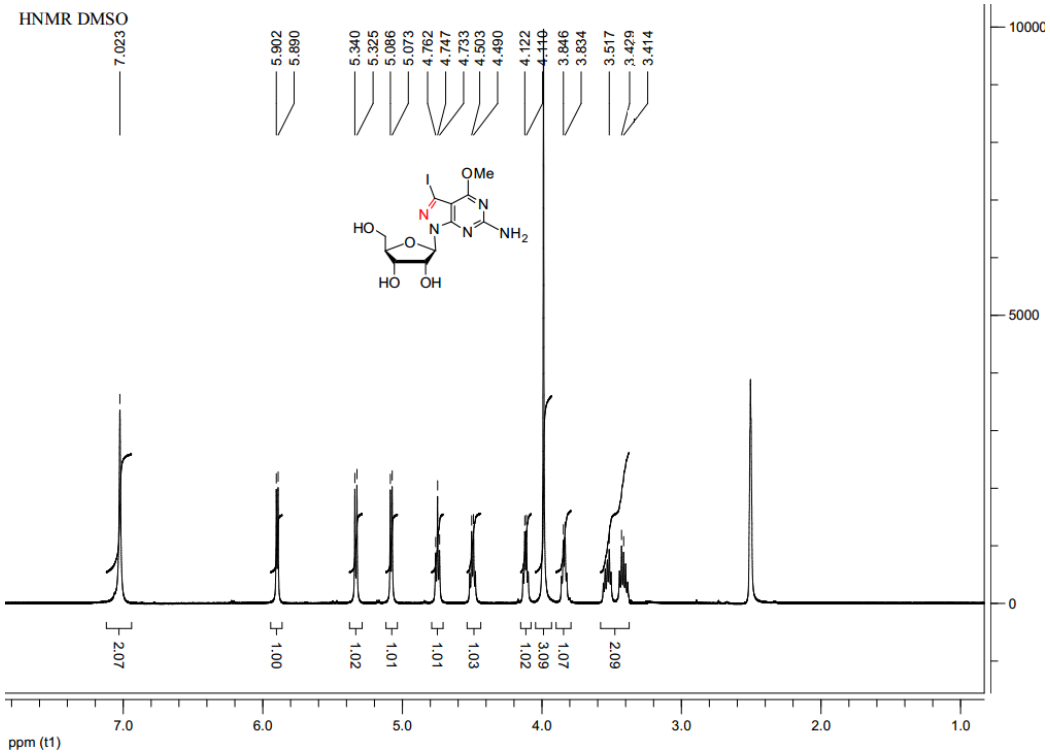
Product 1: ^{1}H NMR (400 MHz, DMSO-d_6)



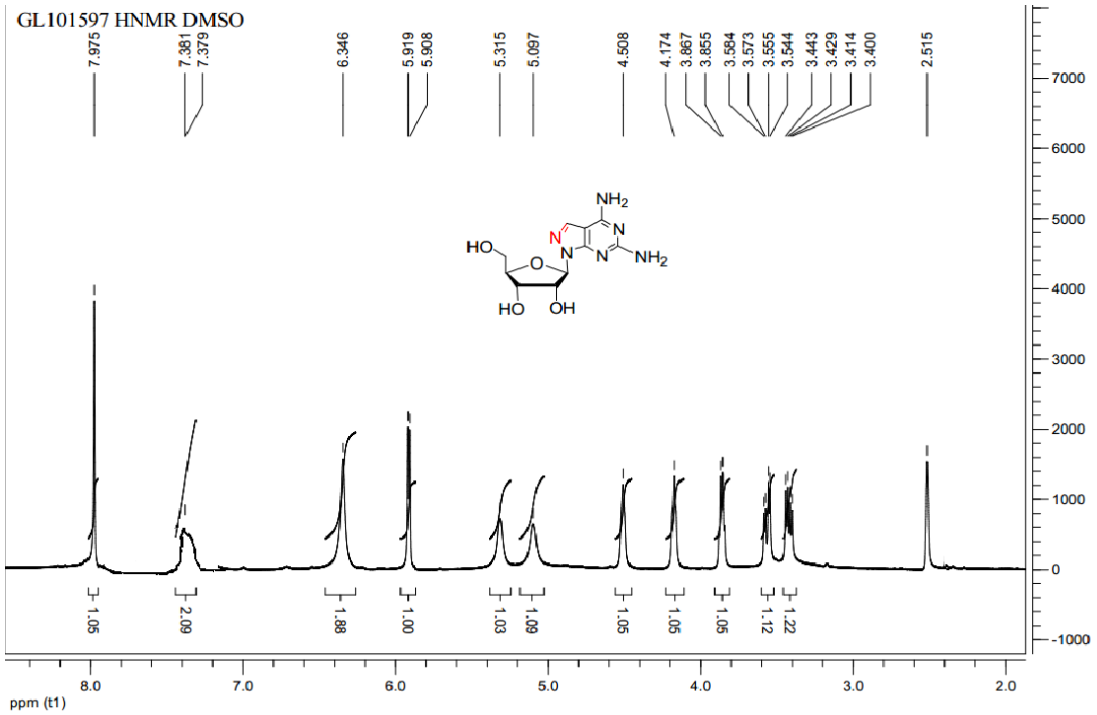
Product 2: ^{1}H NMR (400 MHz, DMSO-d_6)



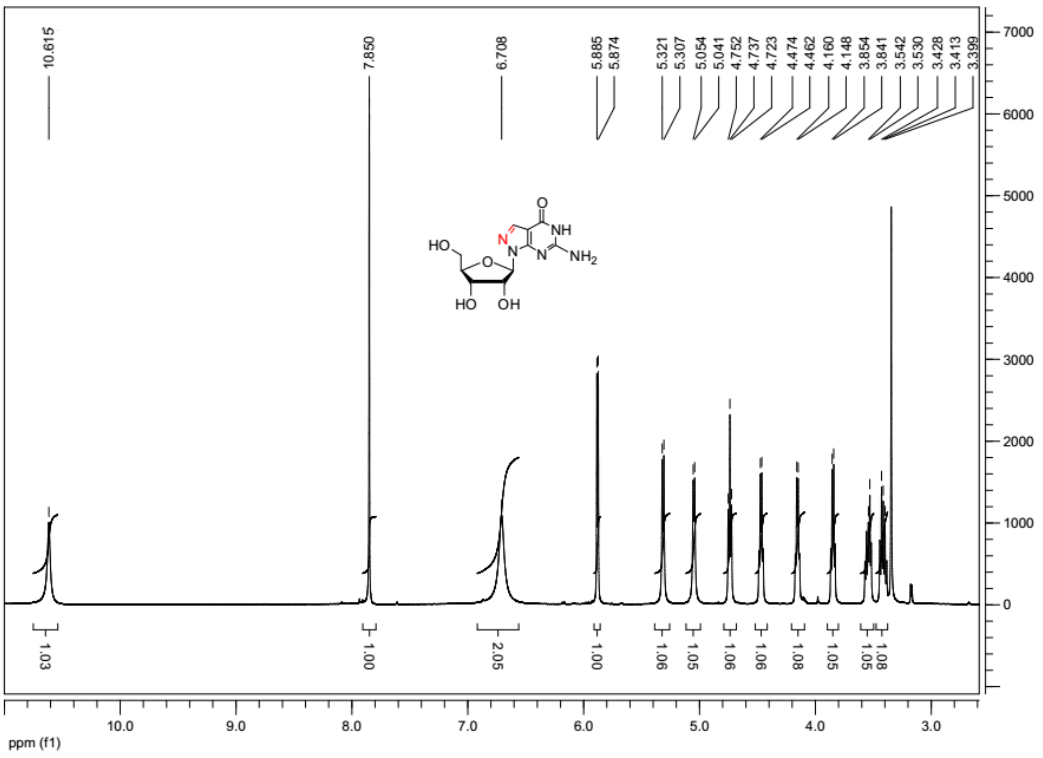
Product 3: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



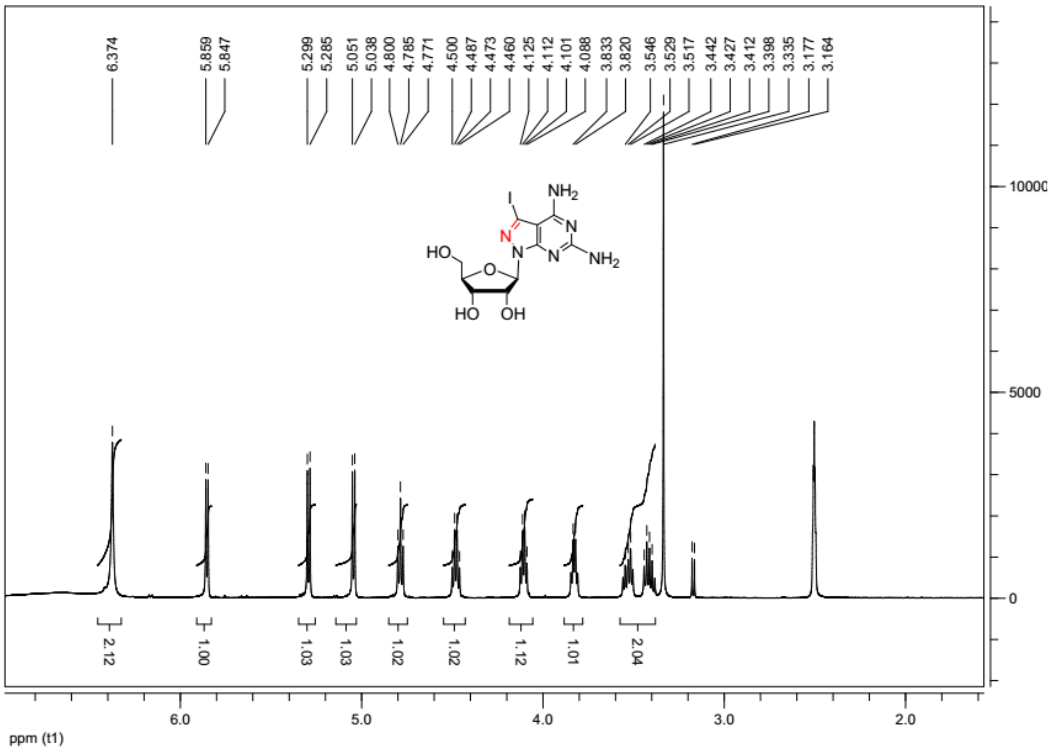
Product 5: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



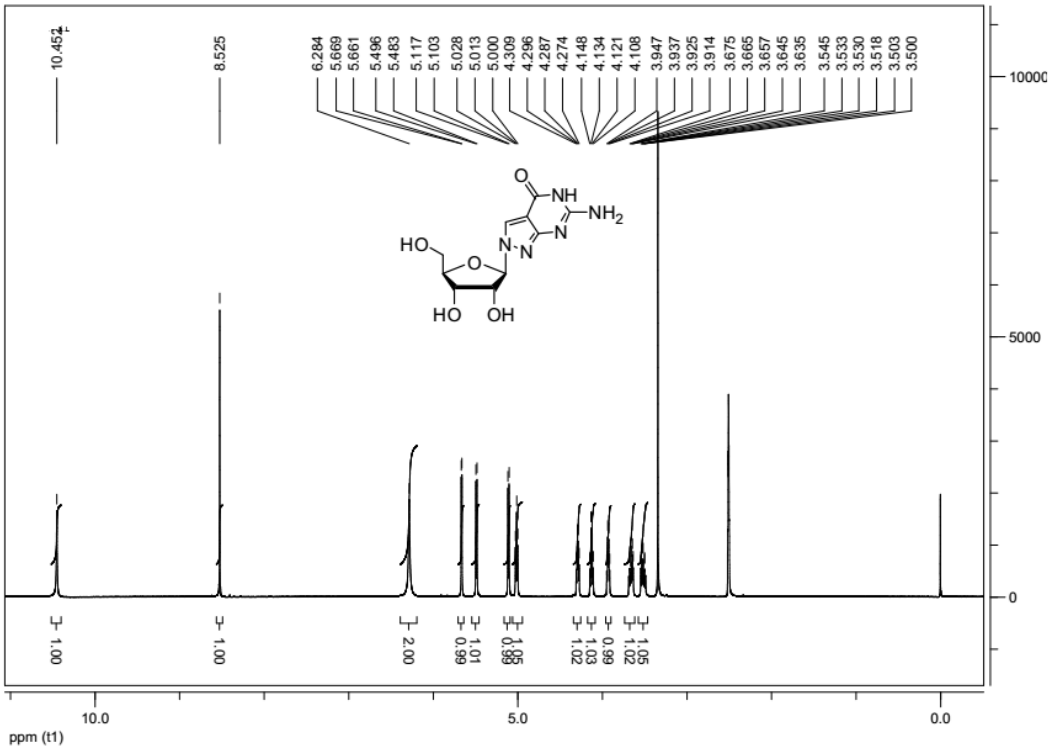
Product 7: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



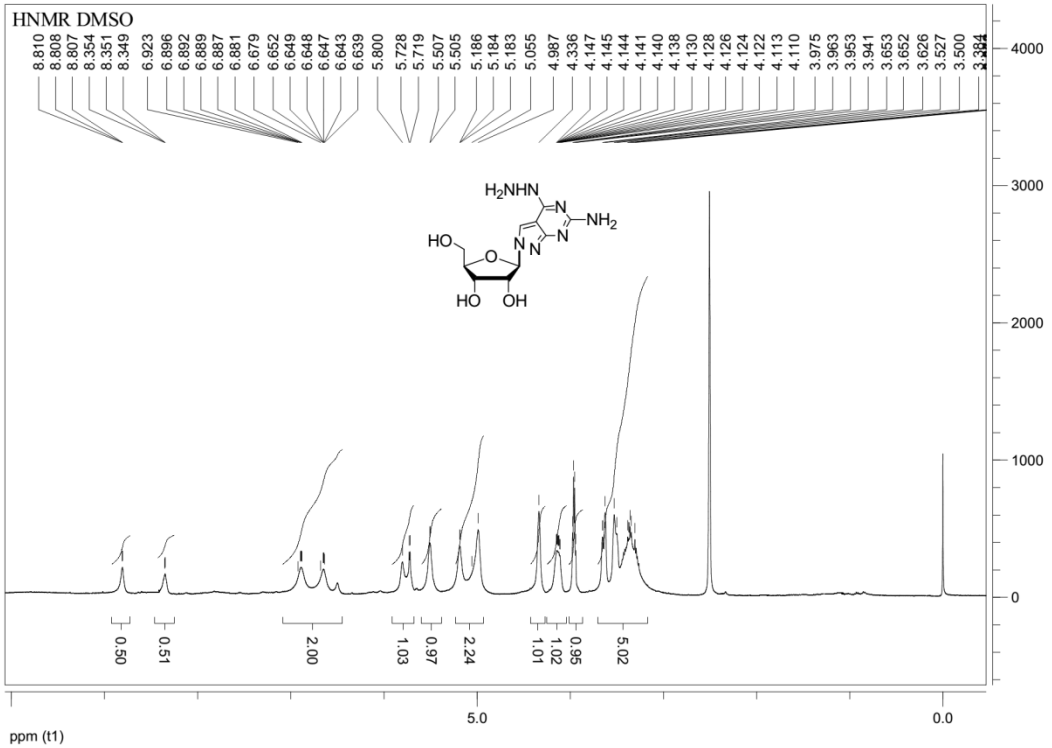
Product 8: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



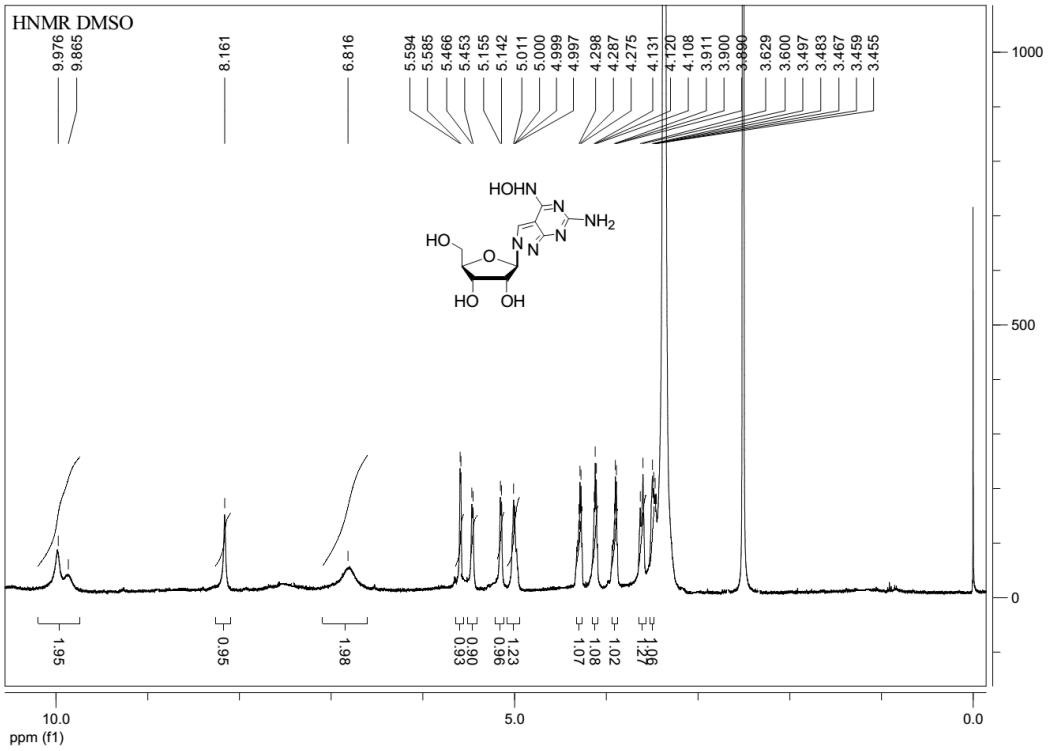
Product 10: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



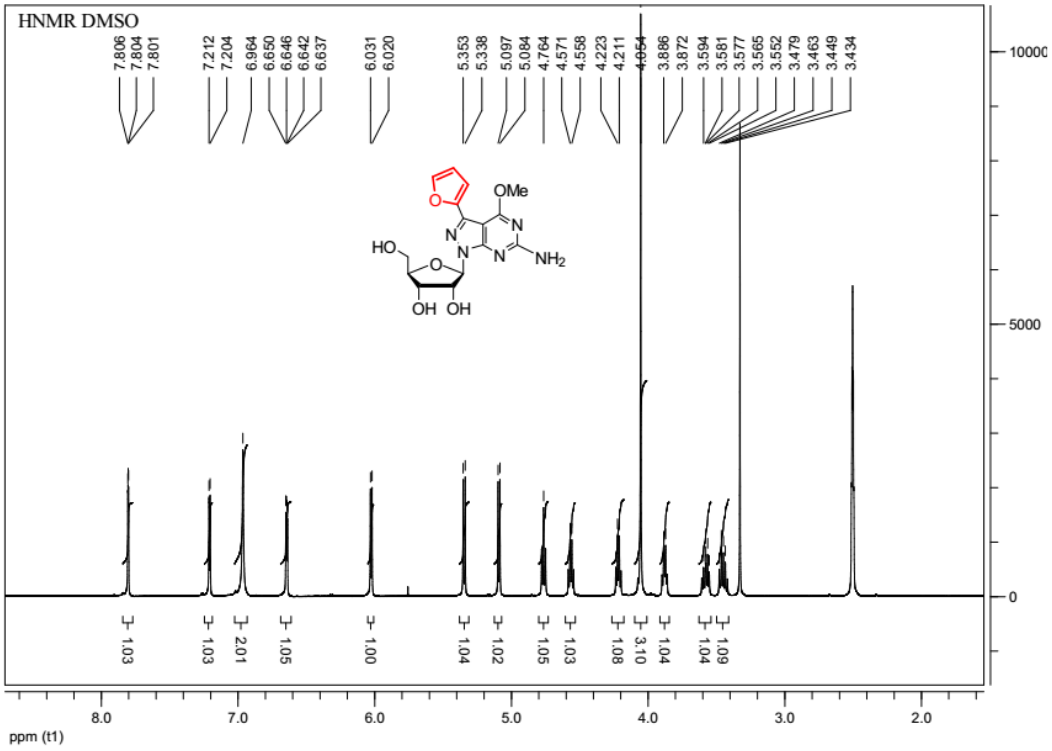
Product 12: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



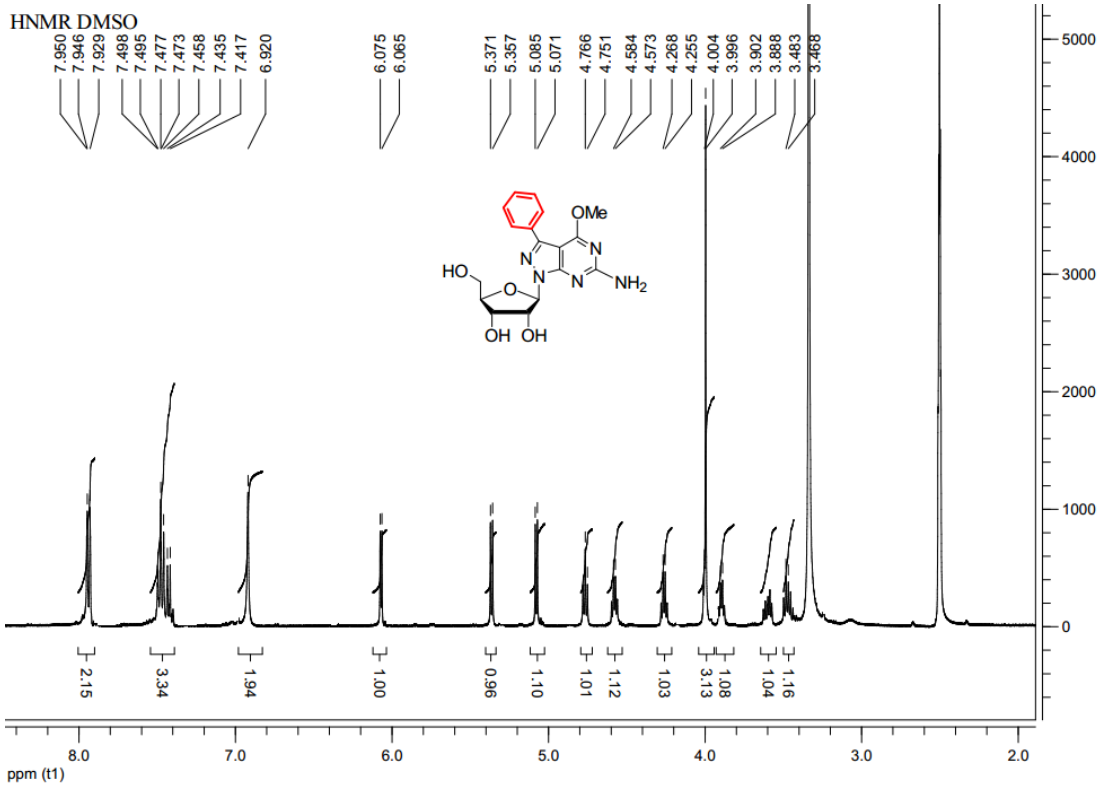
Product 13: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



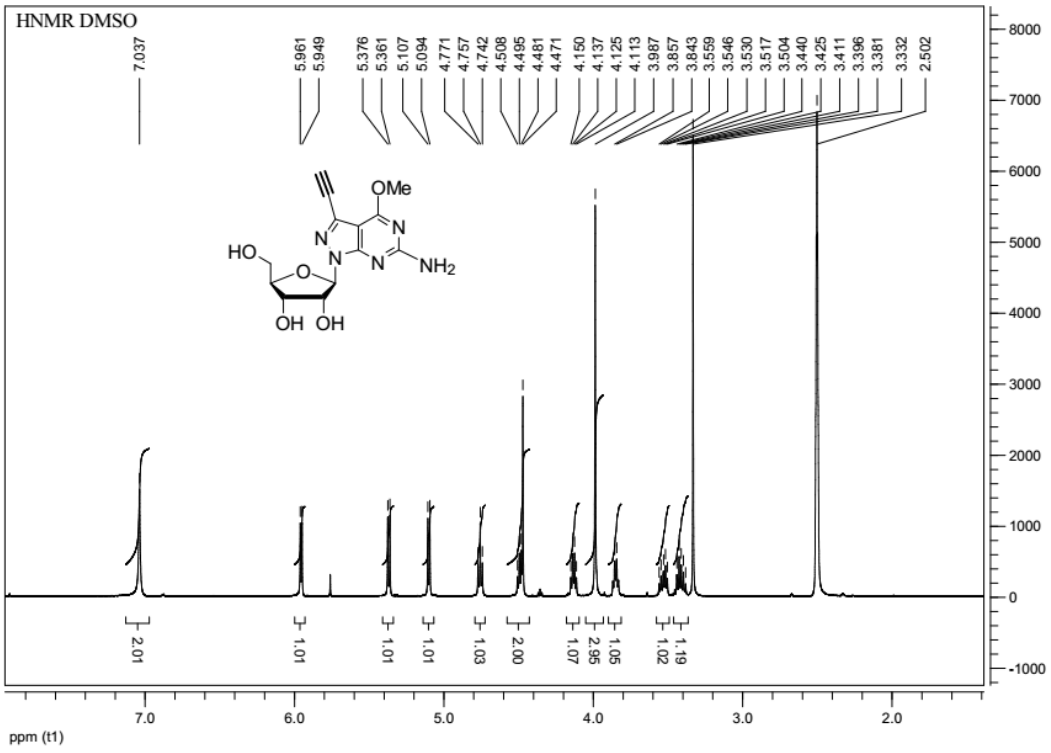
Product 14: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



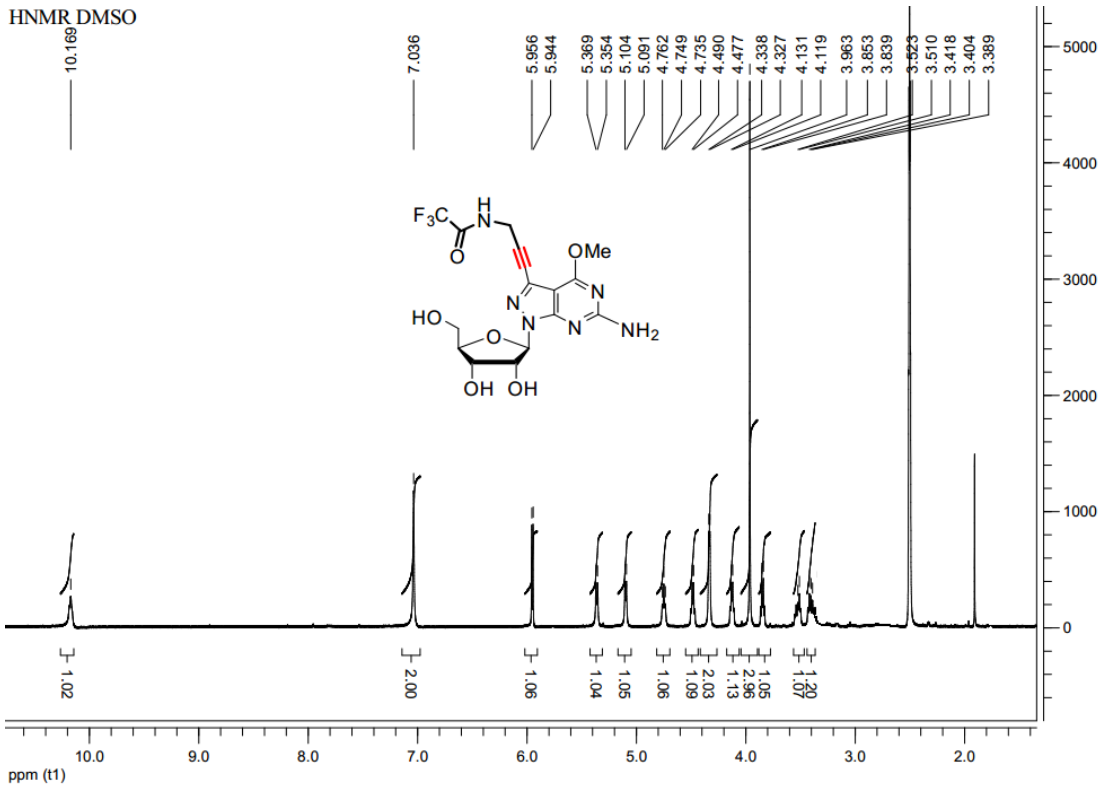
Product 15: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



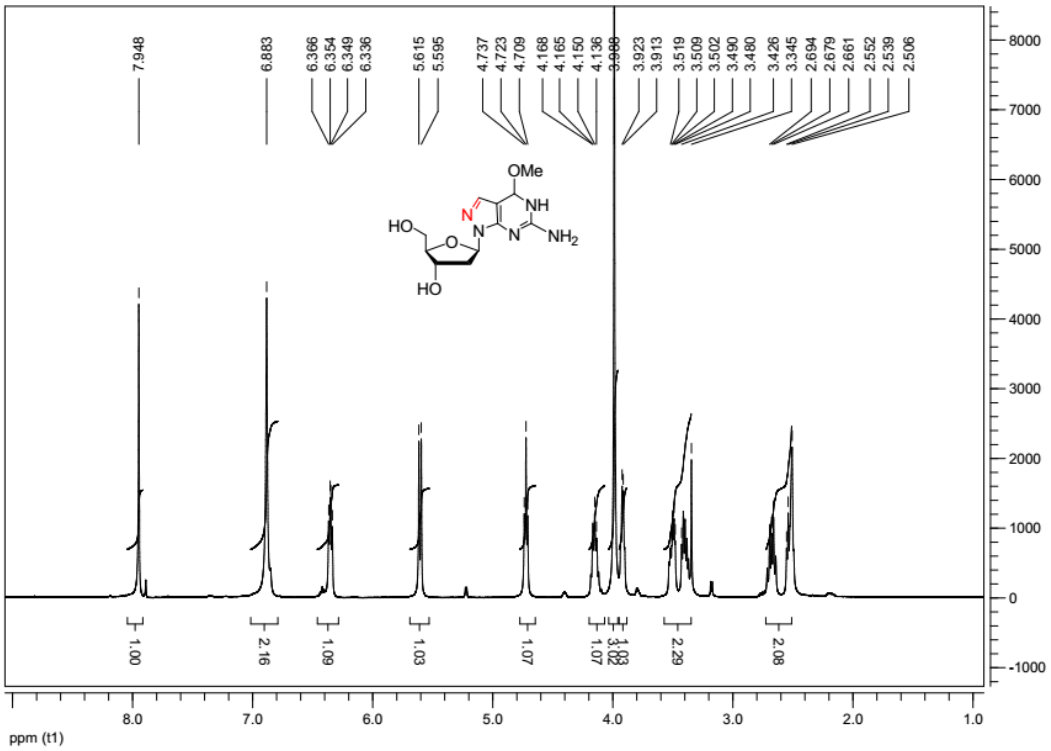
Product 16: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



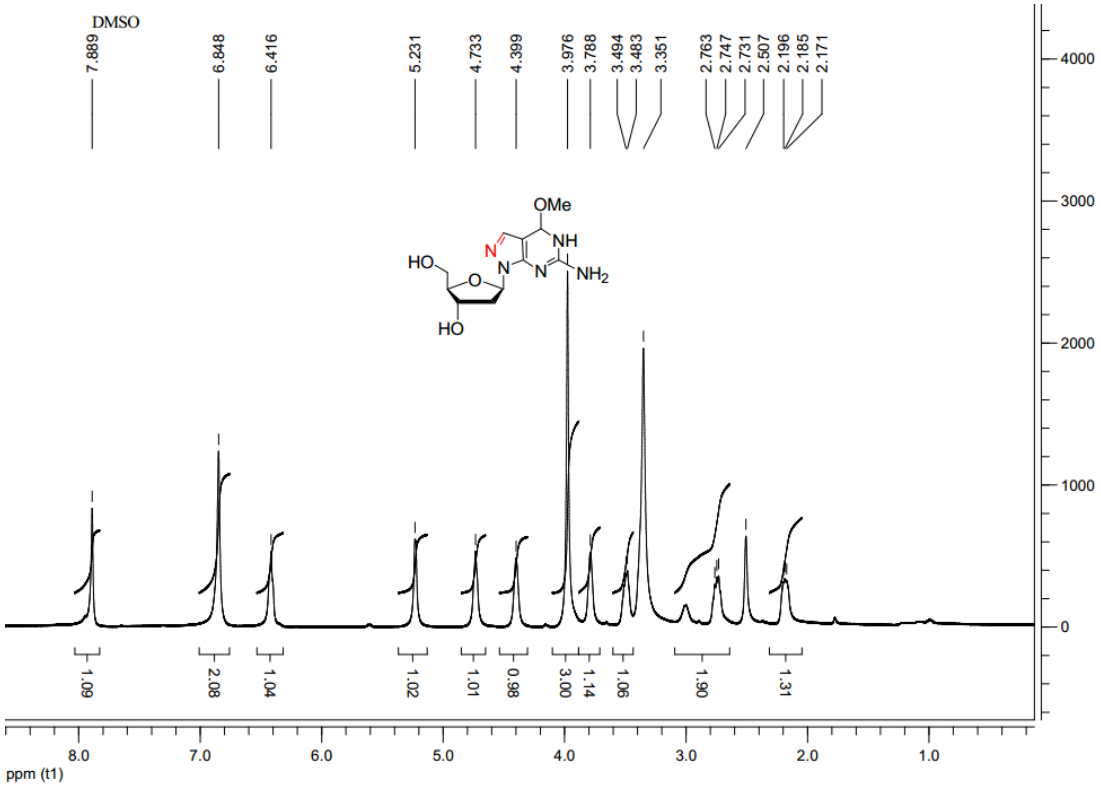
Product 17: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



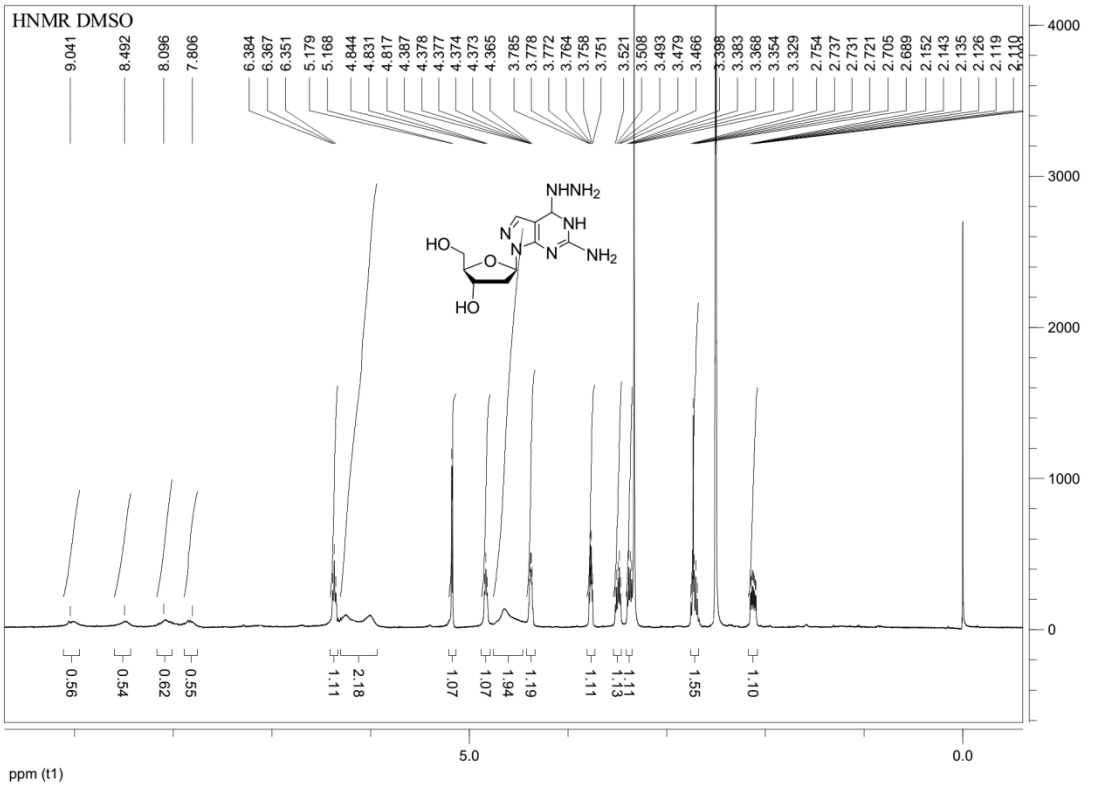
Product 18: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



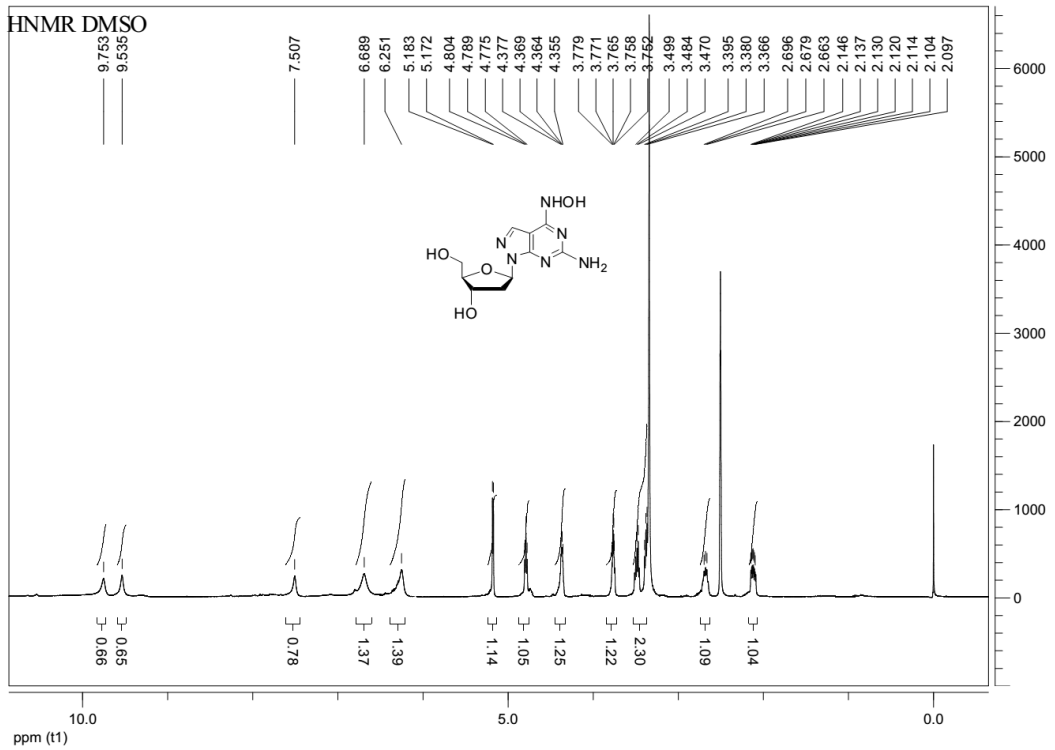
Product 19: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



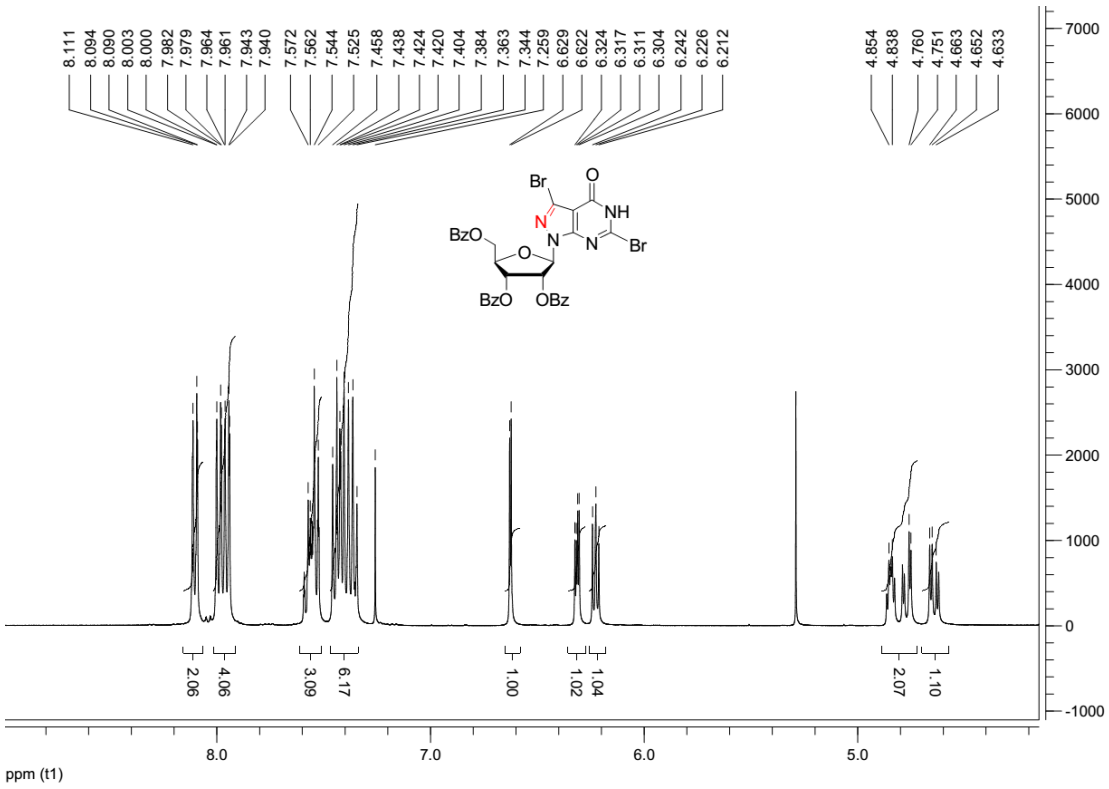
Product 22: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



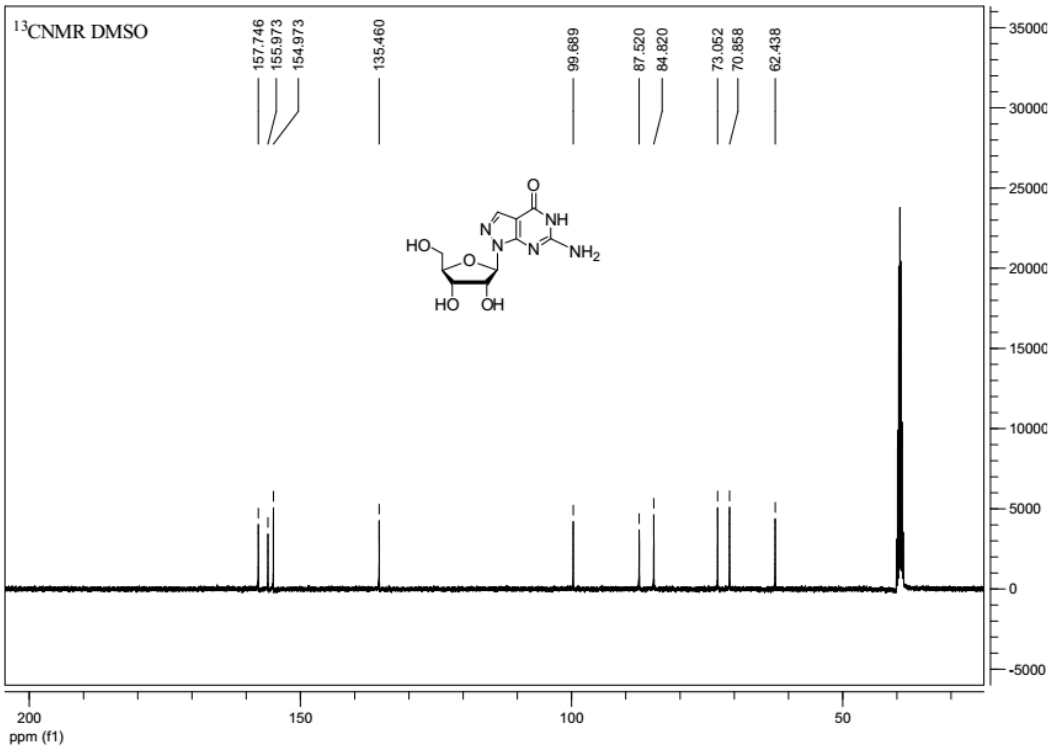
Product 23: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



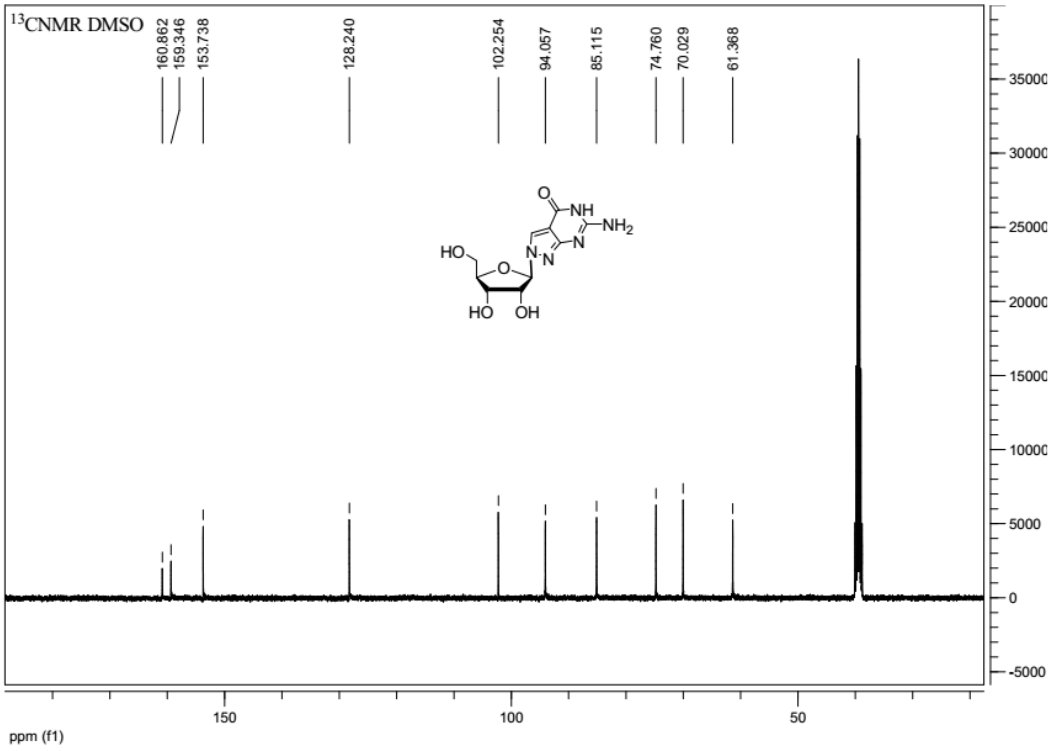
Product 27: ^{1}H NMR (400 MHz, DMSO-*d*$_6$)



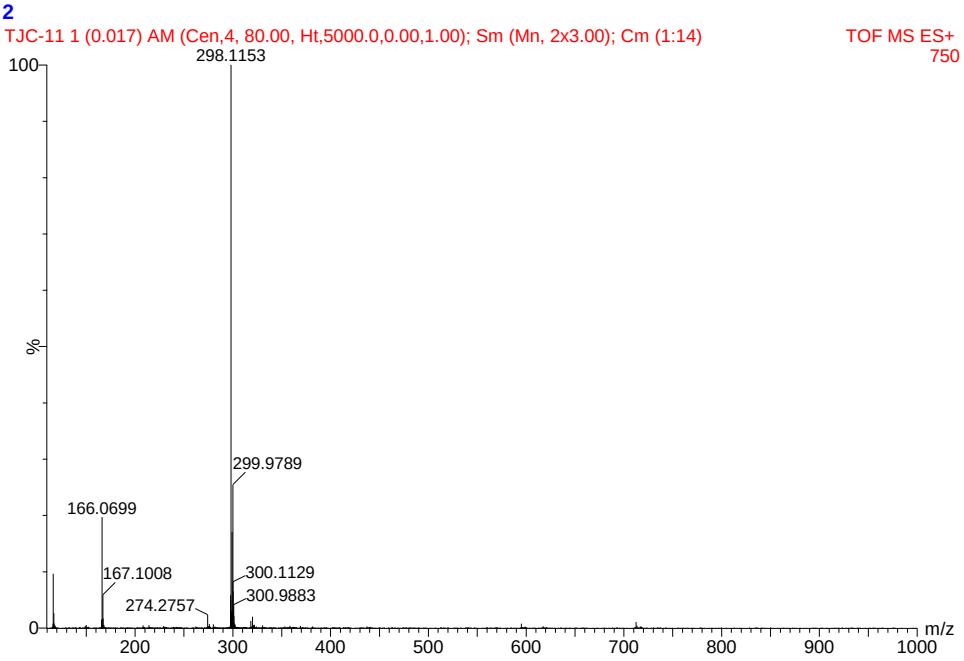
Product 7: ^{13}C NMR (400 MHz, DMSO-*d*$_6$)



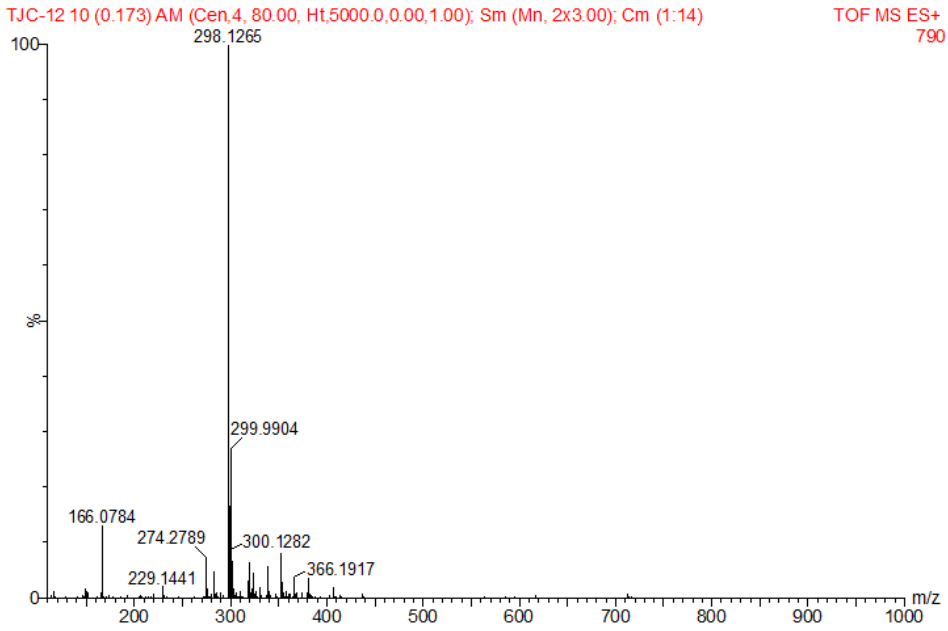
Product 10: ^{13}C NMR (400 MHz, DMSO-*d*$_6$)



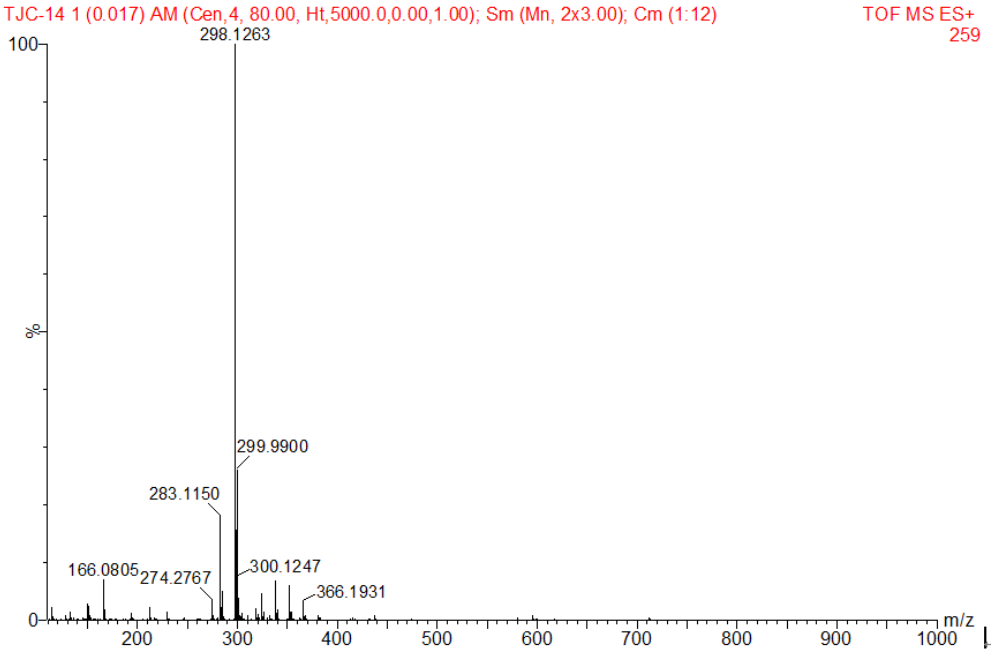
Product 2: HRMS spectra



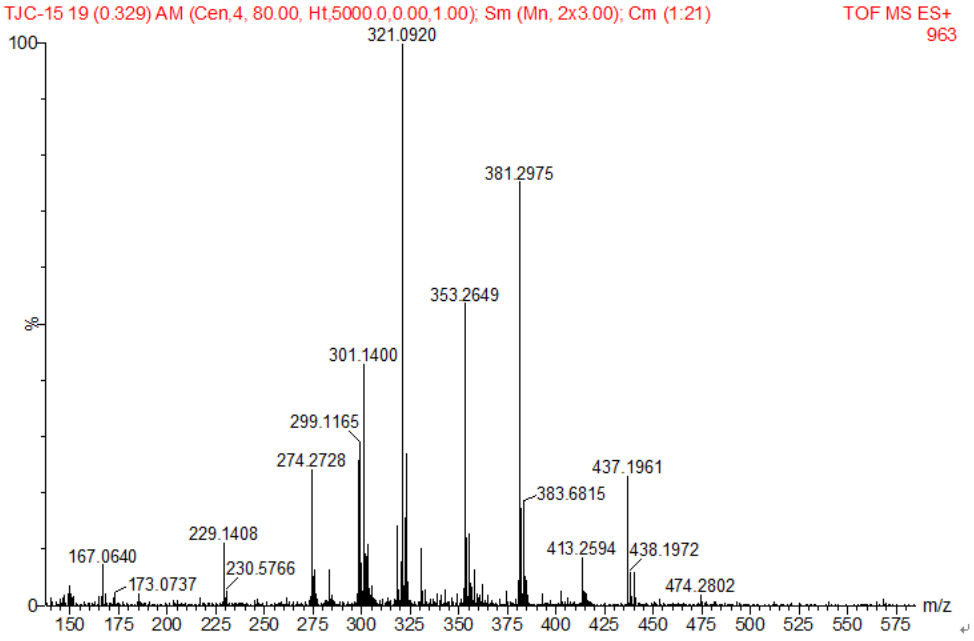
Product 6: HRMS spectra



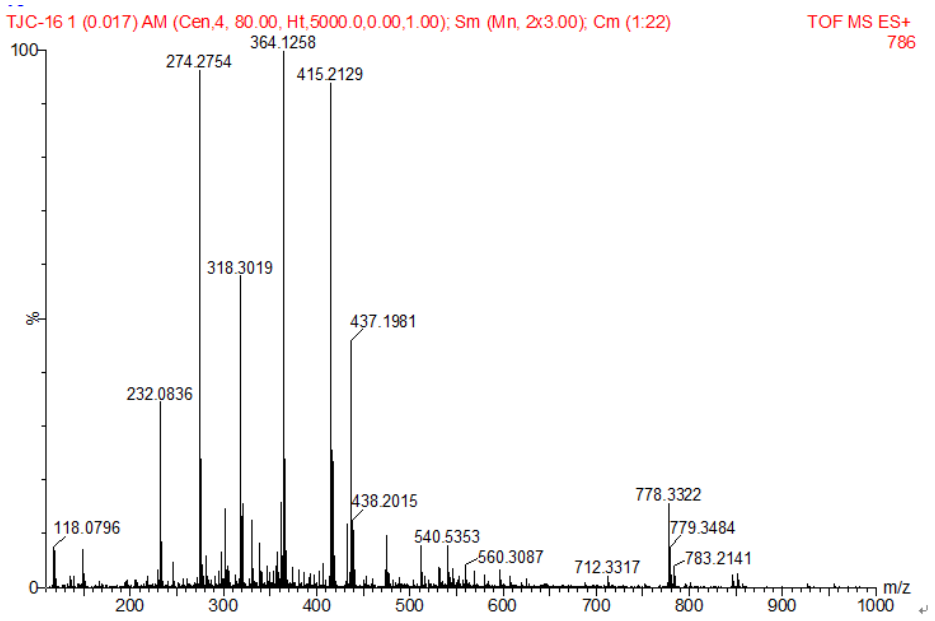
Product 12: HRMS spectra



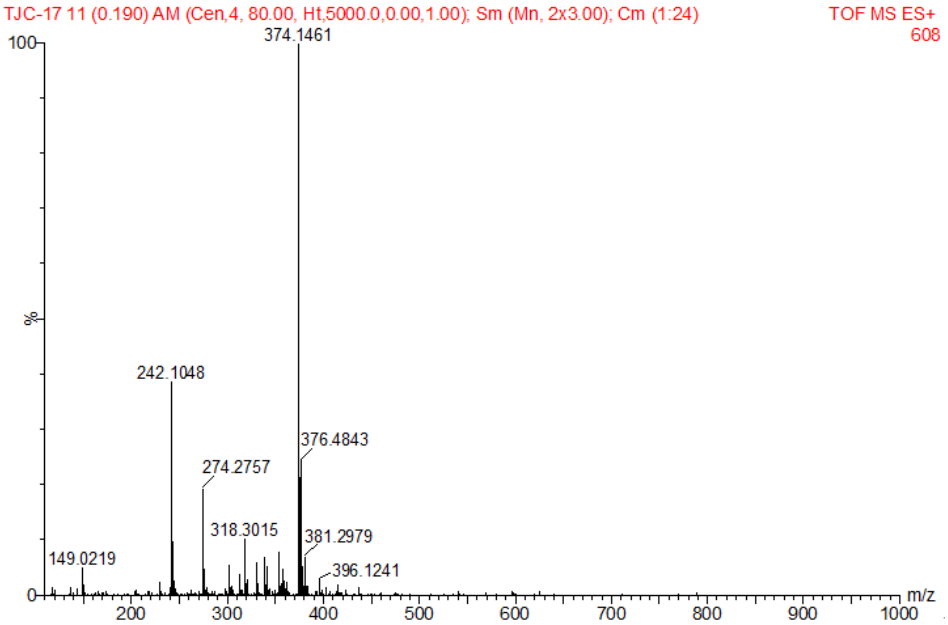
Product 13: HRMS spectra



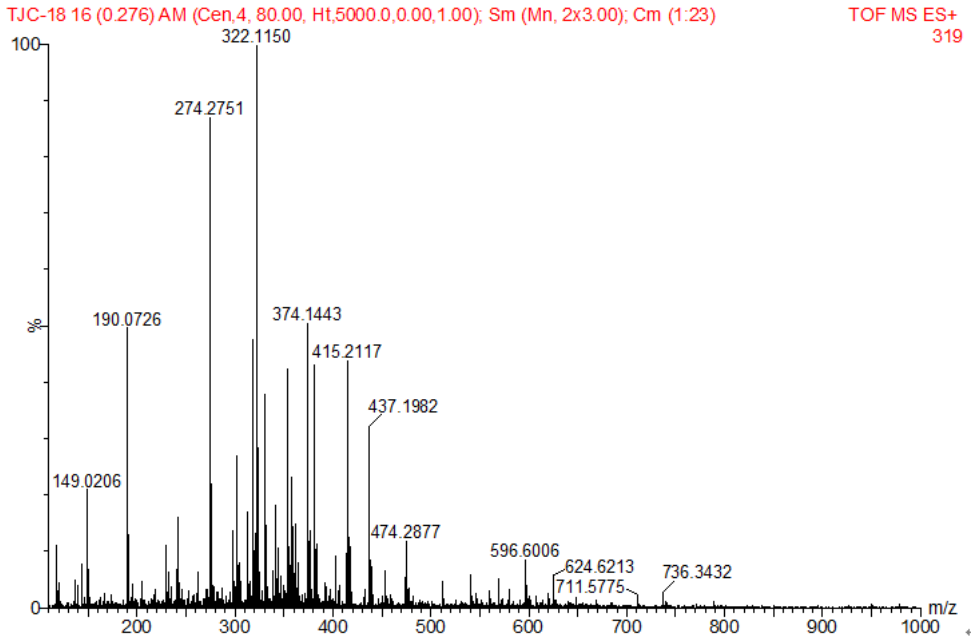
Product 14: HRMS spectra



Product 15: HRMS spectra



Product 16: HRMS spectra



Crystal data and structure refinement for compound 7

Identification code	201804211
Empirical formula	$C_{10}H_{13}N_5O_5$
Formula weight	283.25
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	4.7669(2)
b/Å	11.0409(5)
c/Å	21.6334(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1138.59(8)
Z	4
ρ_{calc}g/cm^3	1.652
μ/mm^{-1}	1.157
F(000)	592.0
Crystal size/mm^3	0.15 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.174 to 134.138
Index ranges	$-3 \le h \le 5$, $-13 \le k \le 13$, $-25 \le l \le 25$
Reflections collected	4100
Independent reflections	2032 [R_{int} = 0.0304, R_{sigma} = 0.0405]
Data/restraints/parameters	2032/0/184
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0366, wR_2 = 0.0880
Final R indexes [all data]	R_1 = 0.0408, wR_2 = 0.0924
Largest diff. peak/hole / e Å^{-3}	0.14/-0.21
Flack parameter	0.2(2)

Crystal data and structure refinement for compound 8

Identification code	201804210
Empirical formula	$C_{10}H_{15}IN_6O_5$
Formula weight	426.18
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.08845(13)
b/Å	12.7514(2)
c/Å	11.3200(2)
α/°	90
β/°	91.4146(19)
γ/°	90
Volume/Å^3	734.28(3)
Z	2
ρ_{calc}g/cm^3	1.928
μ/mm^{-1}	17.478
F(000)	420.0
Crystal size/mm^3	0.15 × 0.13 × 0.11
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.812 to 134.094
Index ranges	$-3 \le h \le 6$, $-15 \le k \le 15$, $-13 \le l \le 12$
Reflections collected	5309
Independent reflections	2616 [R_{int} = 0.0300, R_{sigma} = 0.0391]
Data/restraints/parameters	2616/3/213
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0286, wR_2 = 0.0701
Final R indexes [all data]	R_1 = 0.0296, wR_2 = 0.0711
Largest diff. peak/hole / e Å^{-3}	0.56/-0.62
Flack parameter	-0.021(5)