
Supplementary Materials

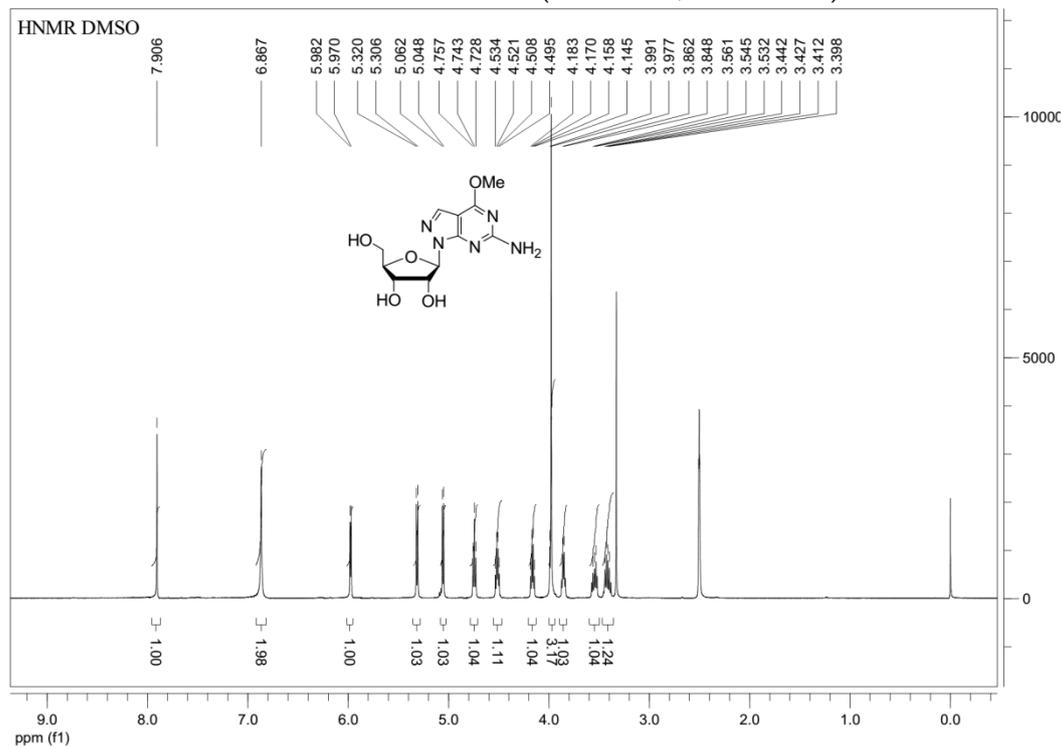
Investigation of 8-aza-7-deaza purine nucleoside derivatives

Hang Ren ^{1,2}, Haoyun An ^{2,*} and Jingchao Tao ^{1,*}

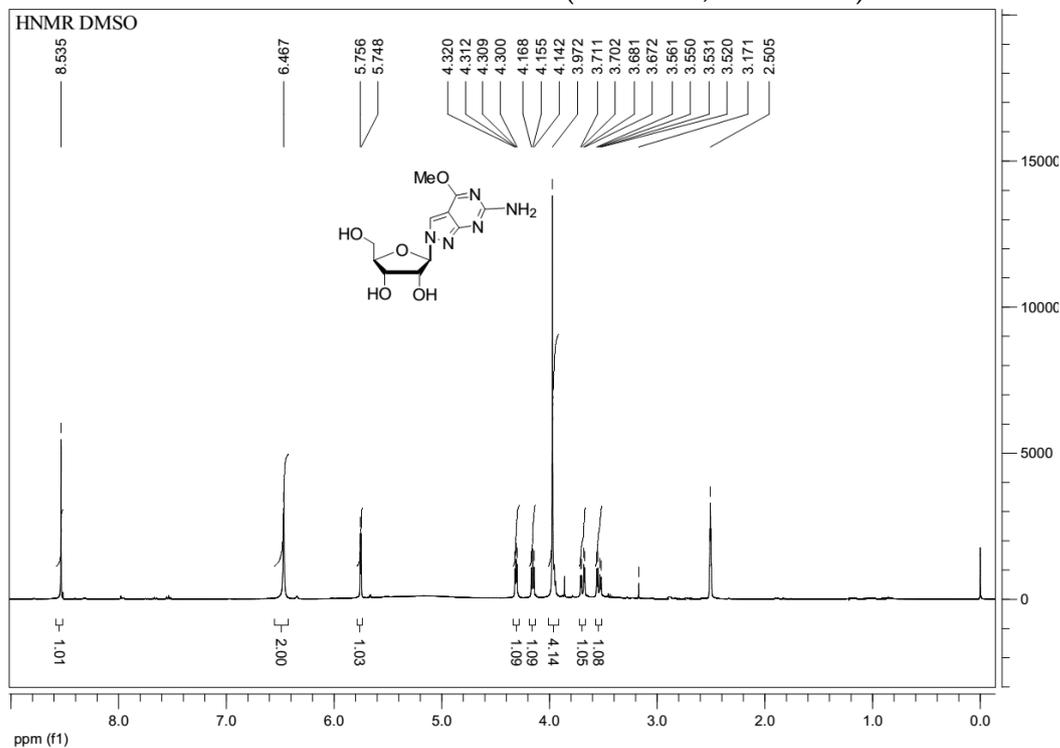
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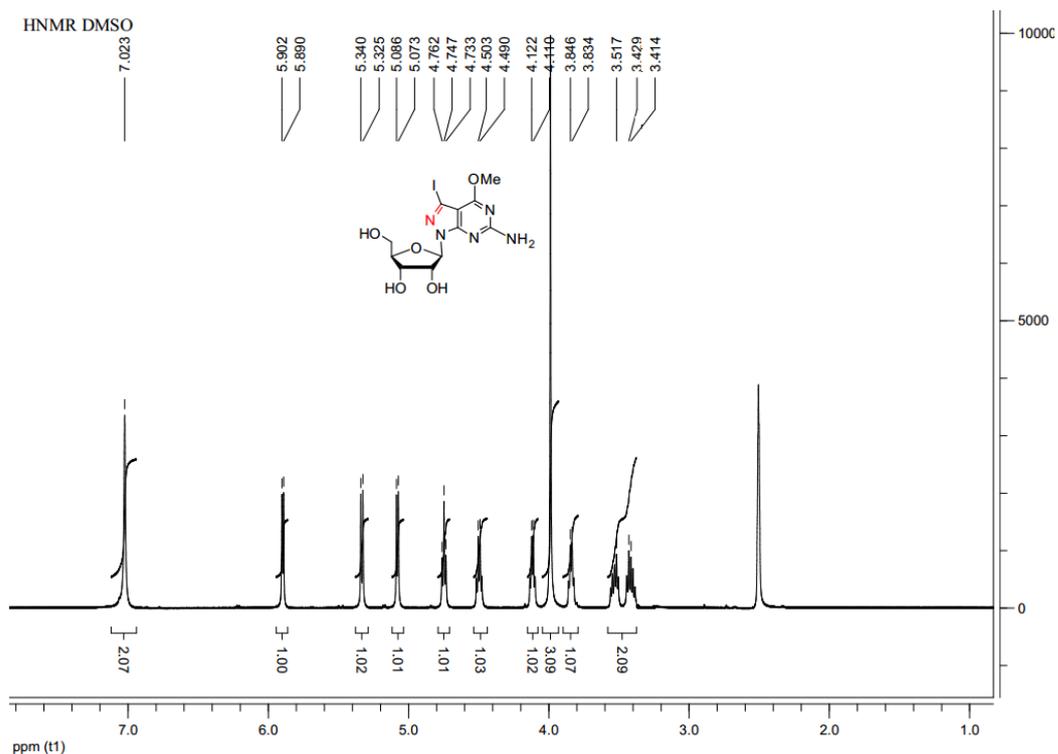
Product 1: ¹H NMR (400 MHz, DMSO-*d*₆)



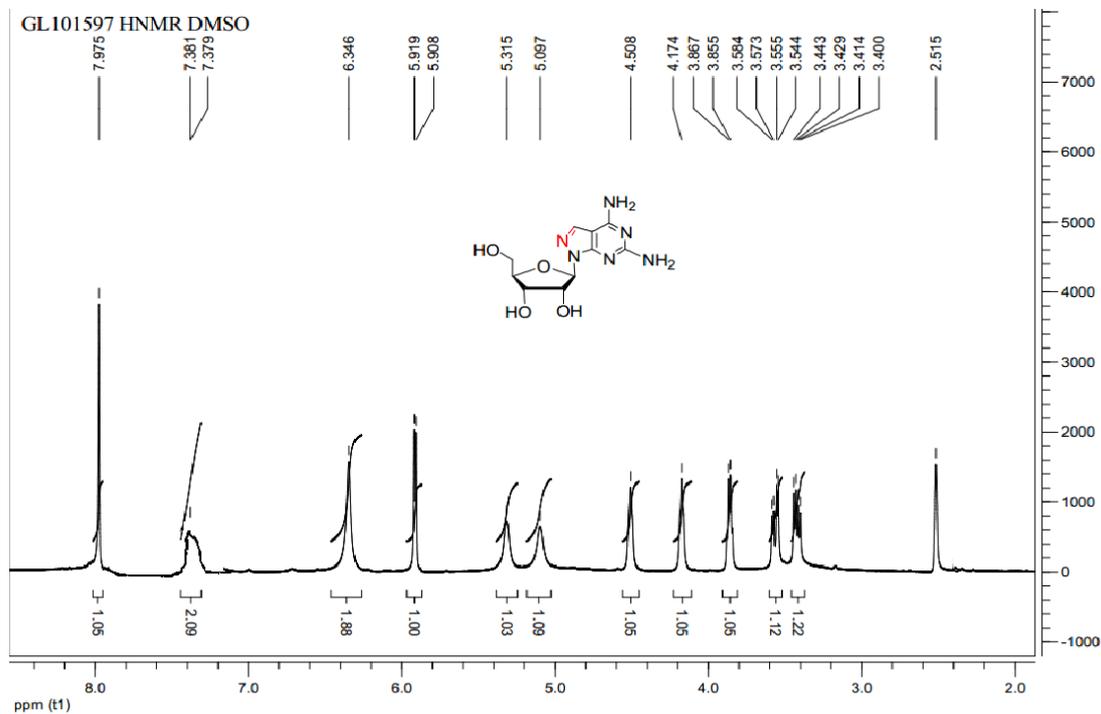
Product 2: ¹H NMR (400 MHz, DMSO-*d*₆)



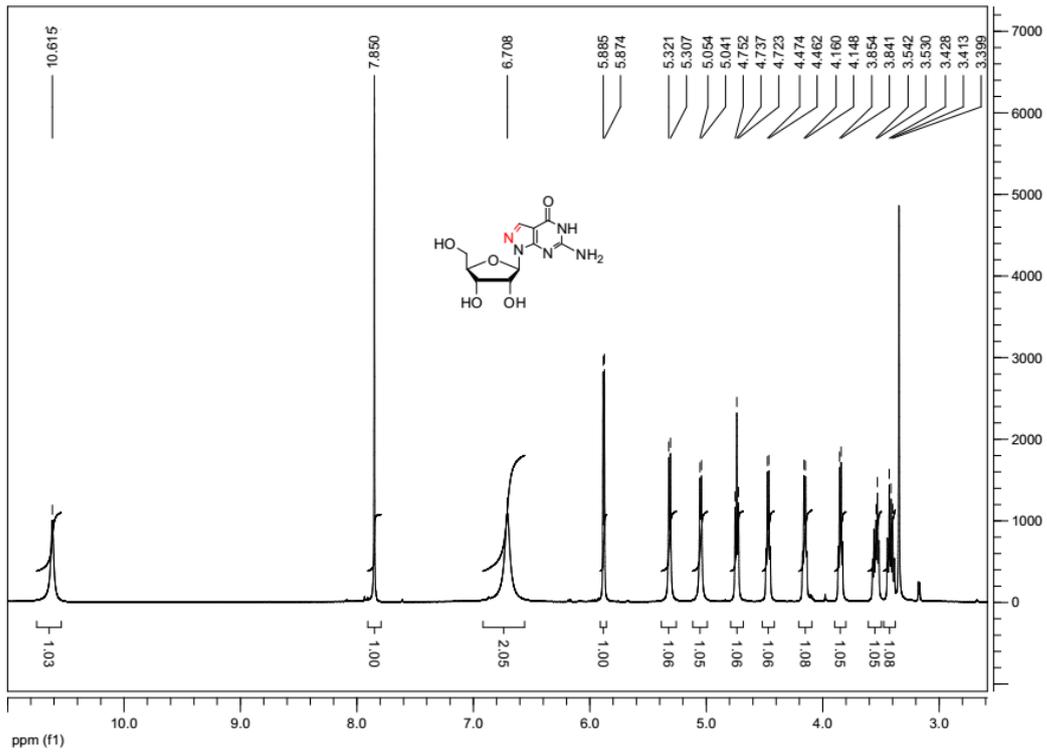
Product 3: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



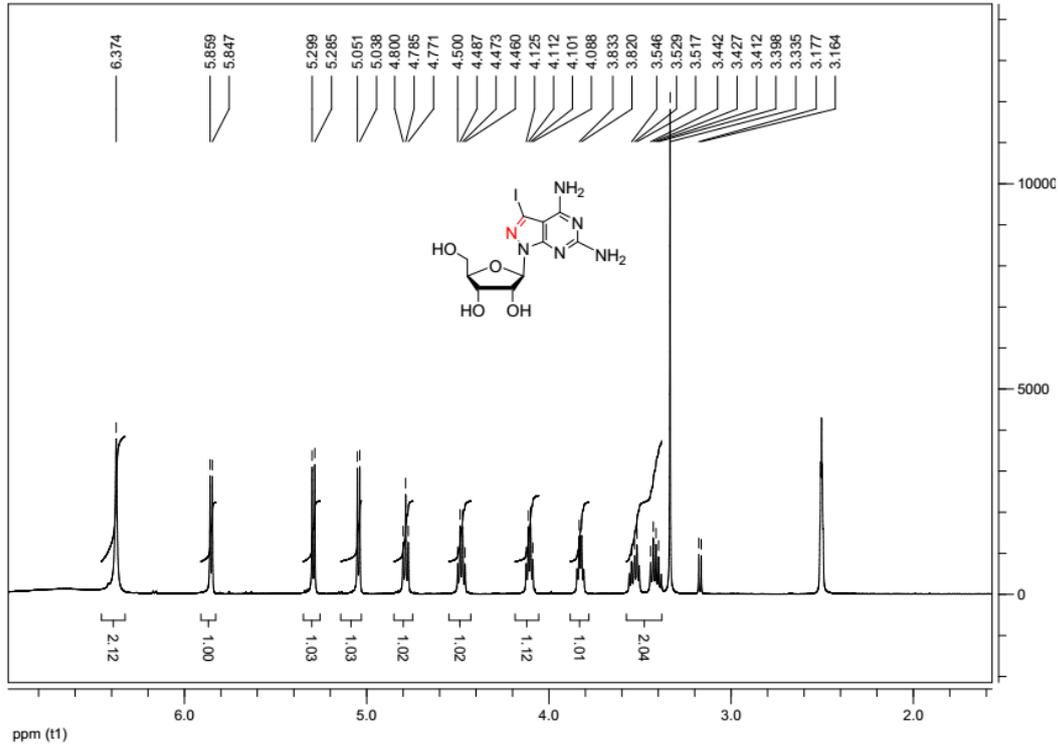
Product 5: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



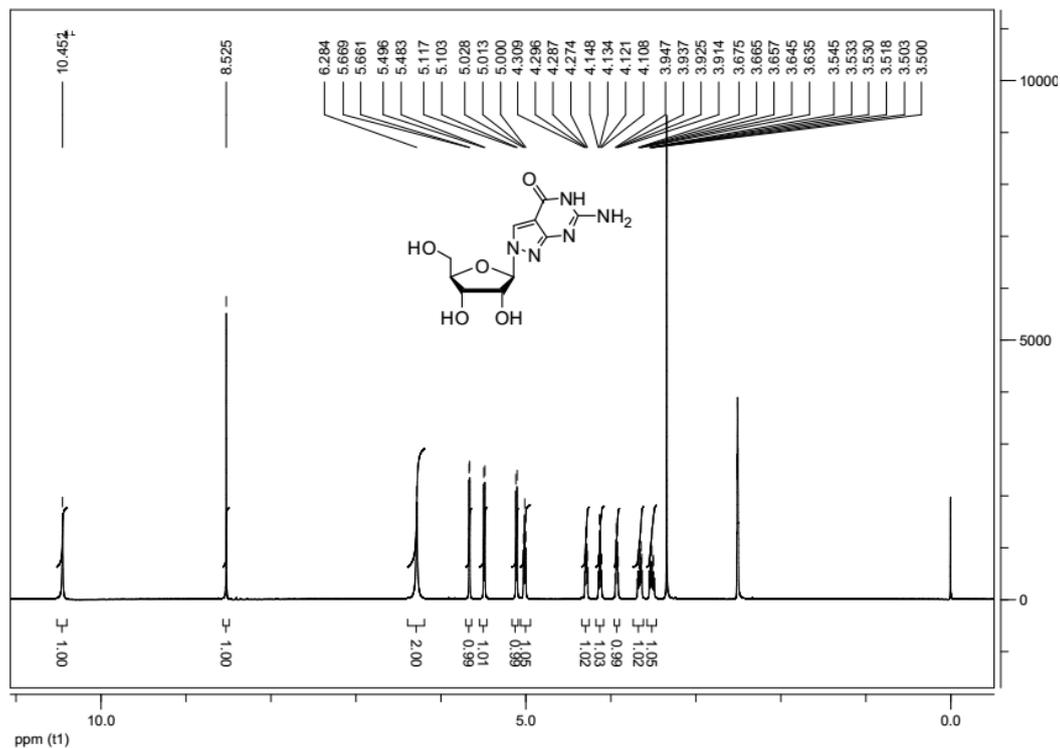
Product 7: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



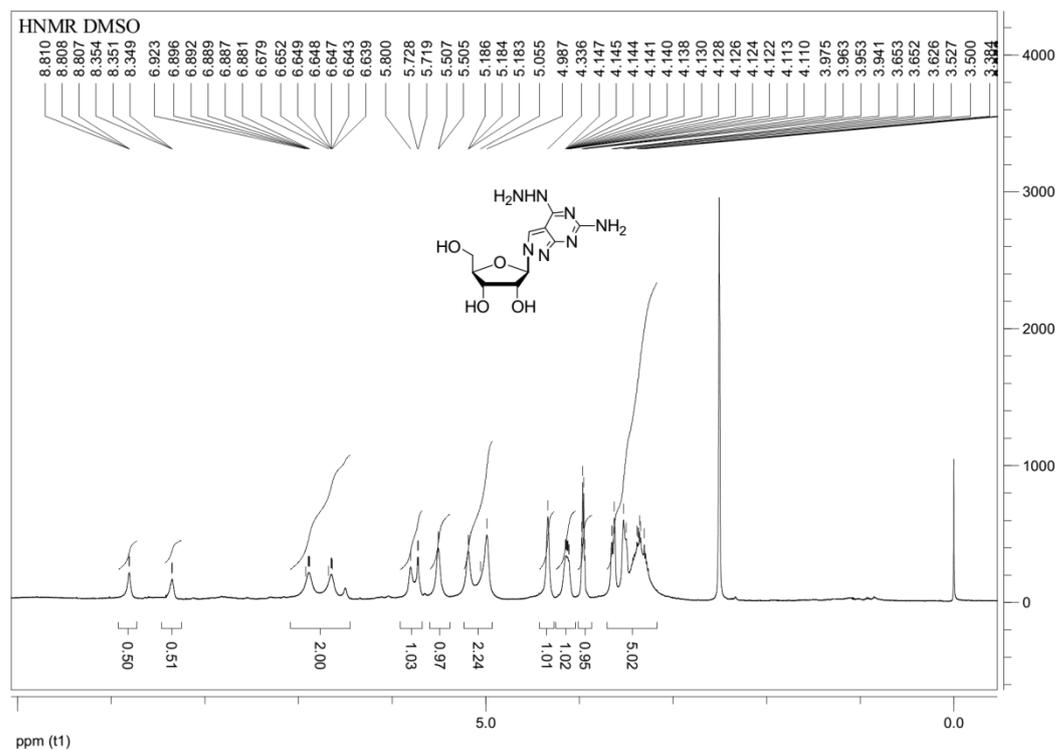
Product 8: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



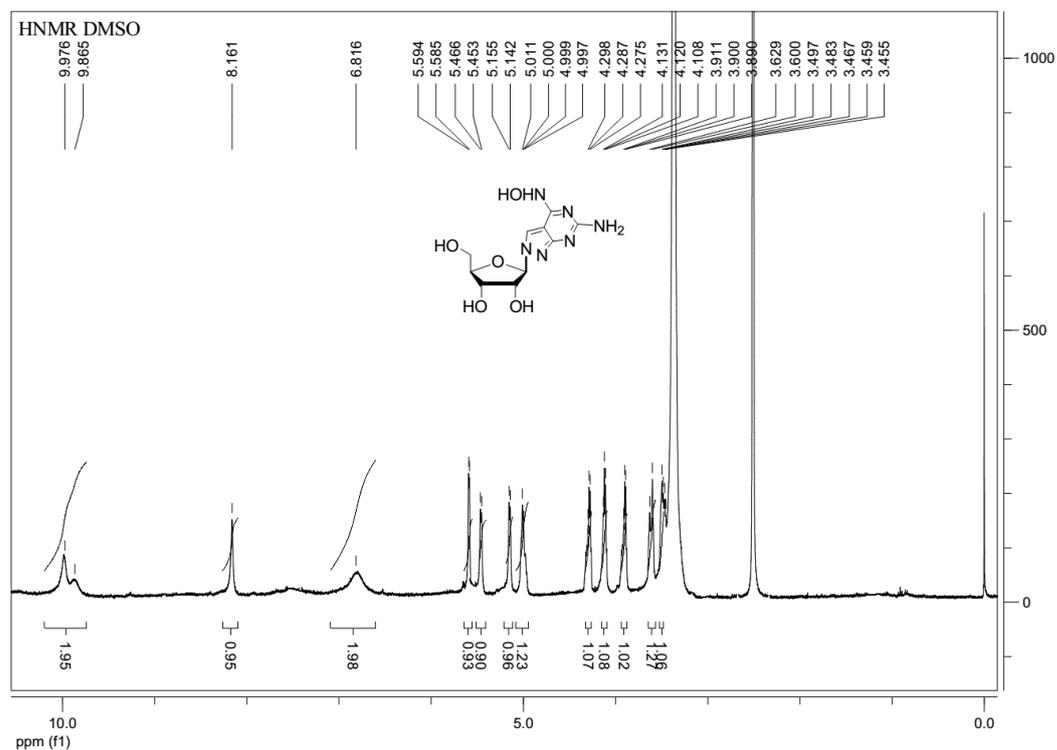
Product 10: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



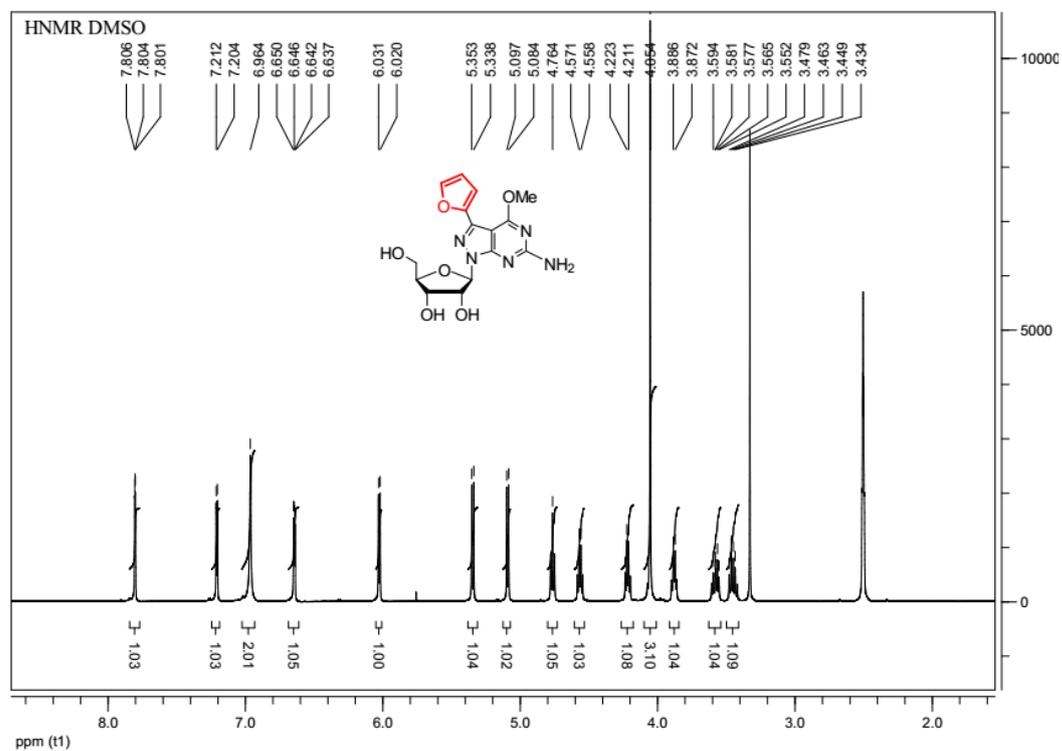
Product 12: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



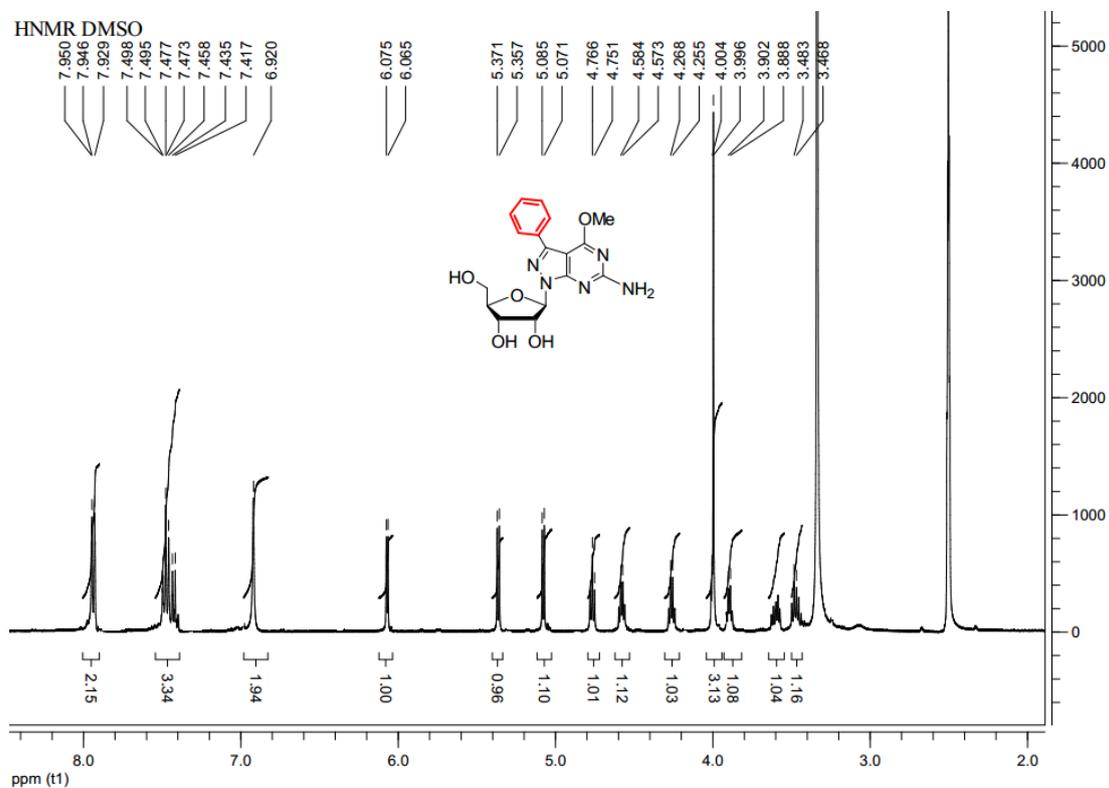
Product 13: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



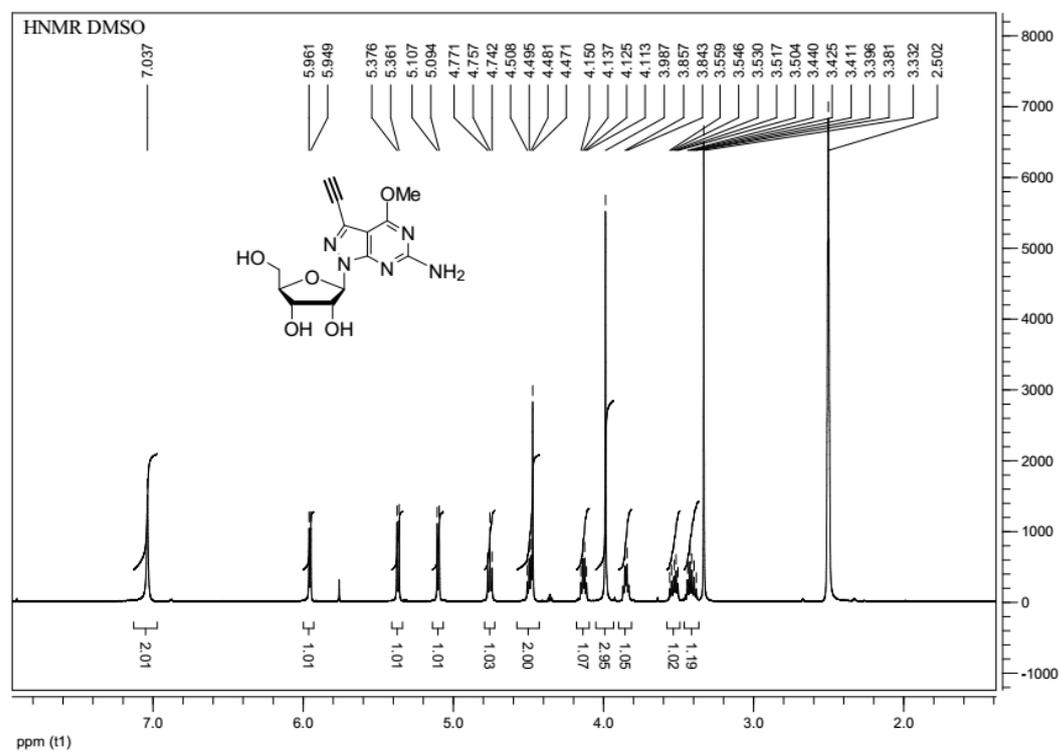
Product 14: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



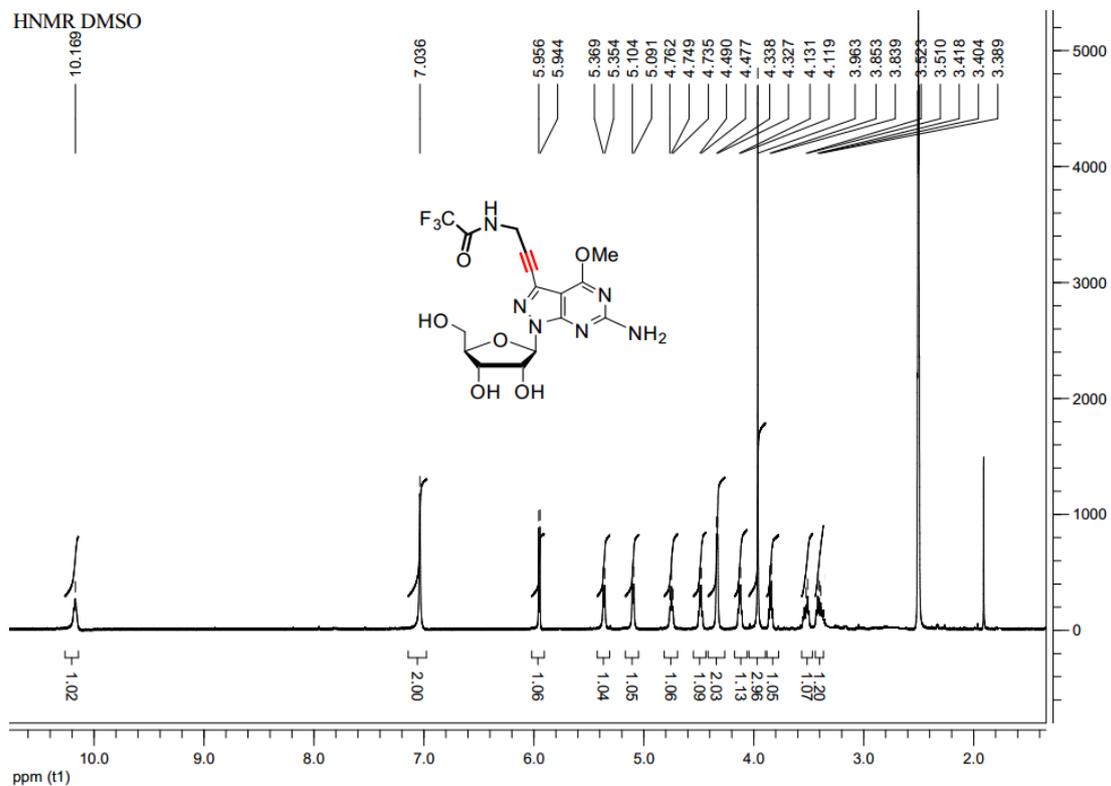
Product 15: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



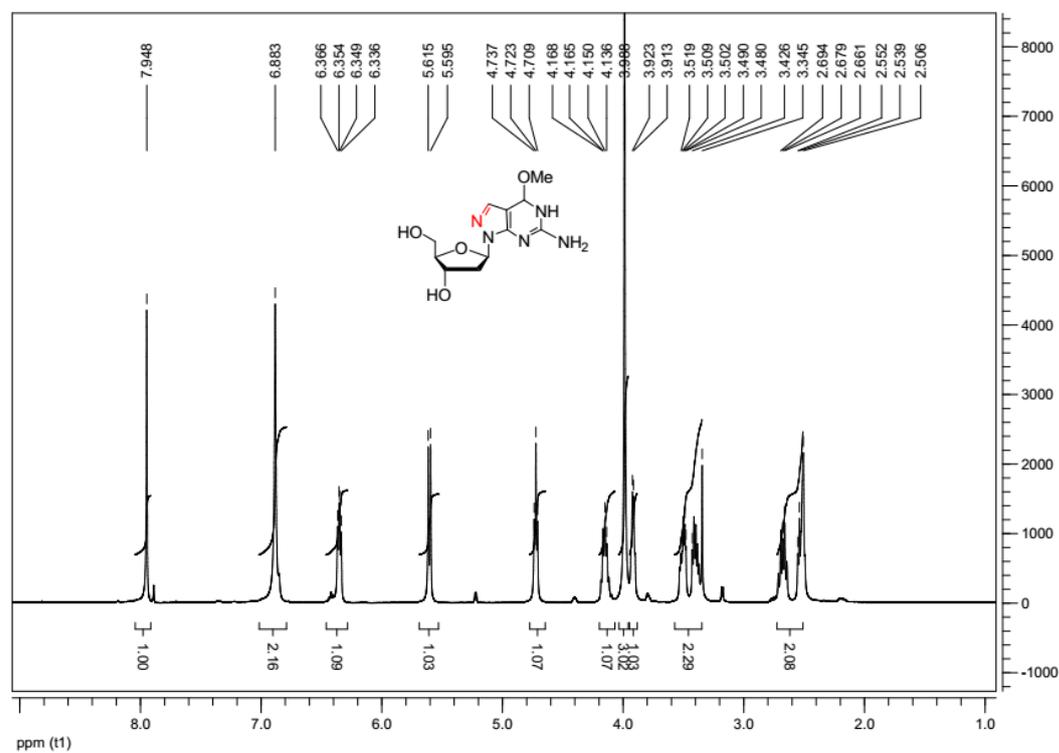
Product 16: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



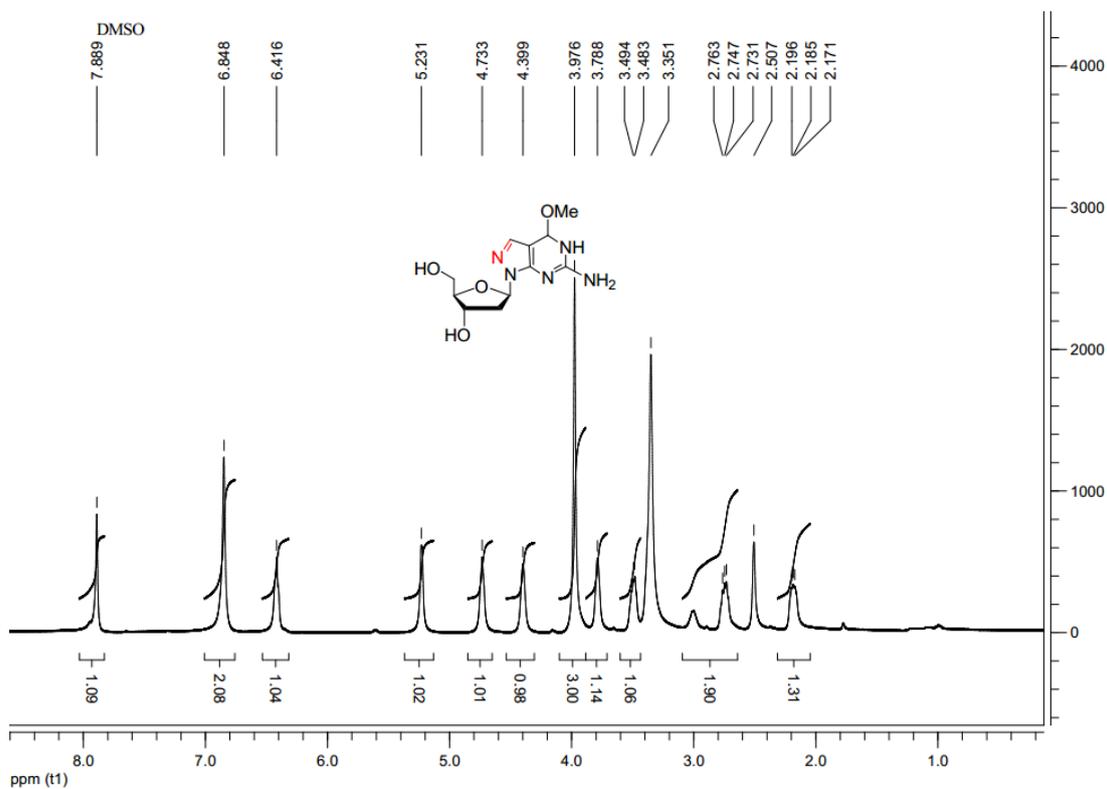
Product 17: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



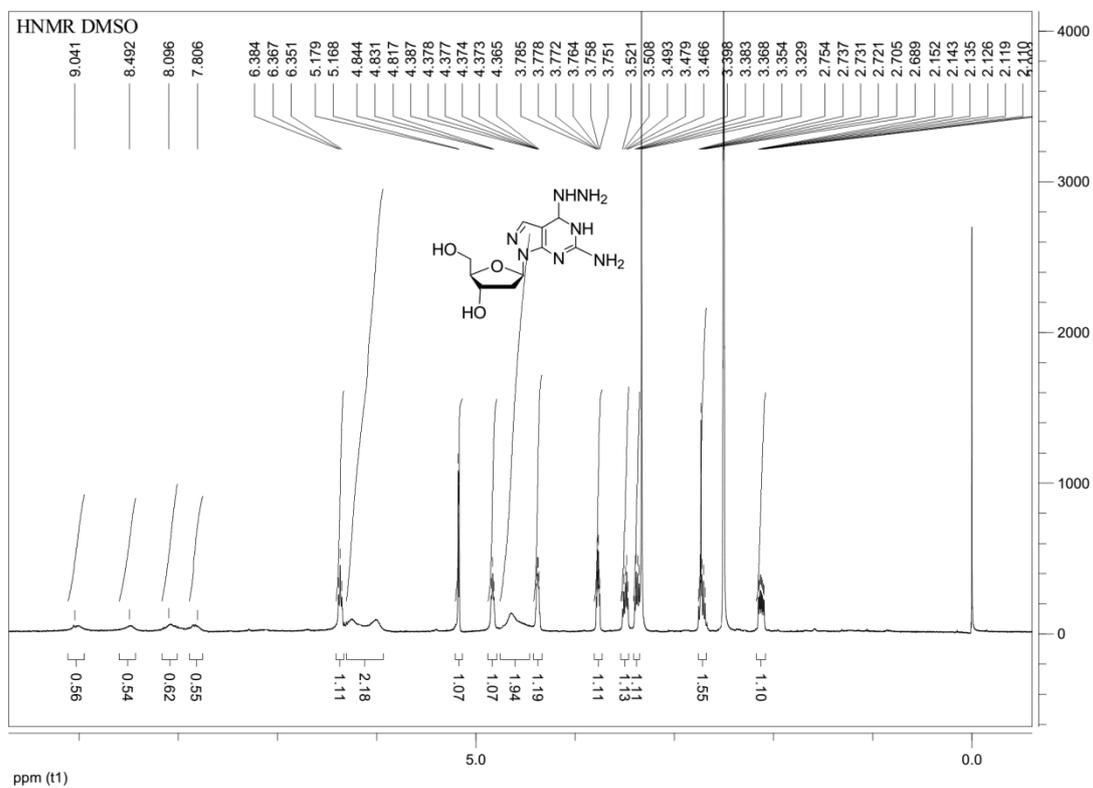
Product 18: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



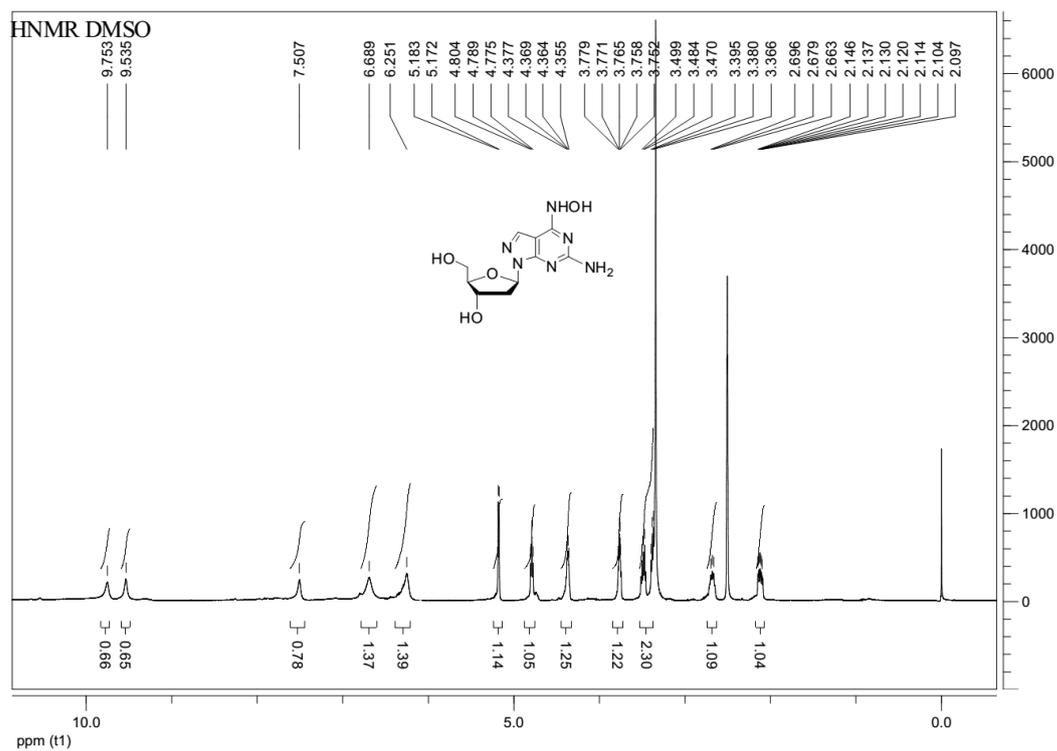
Product 19: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



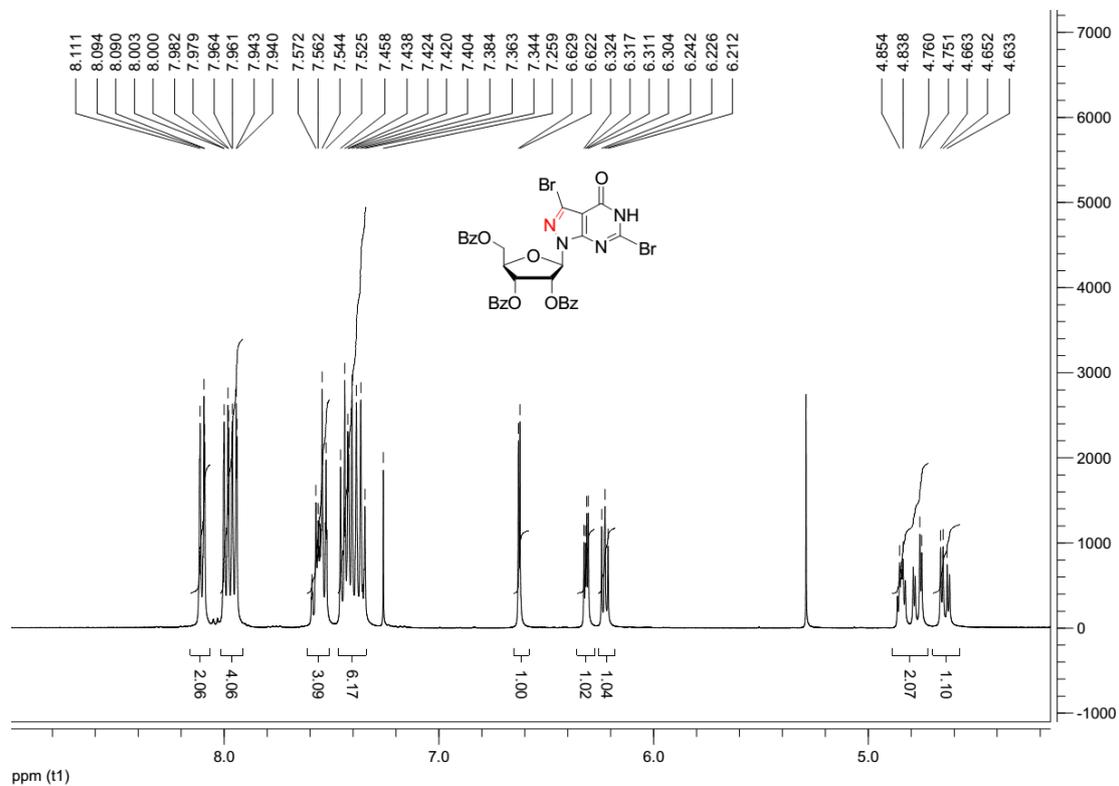
Product 22: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



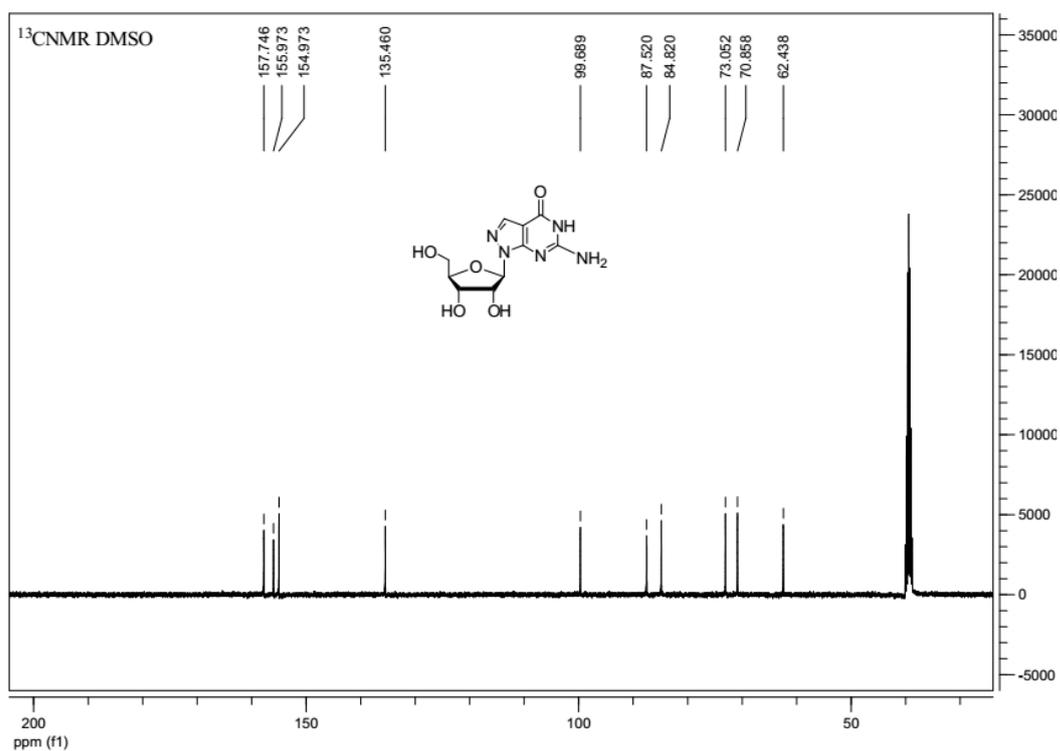
Product 23: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



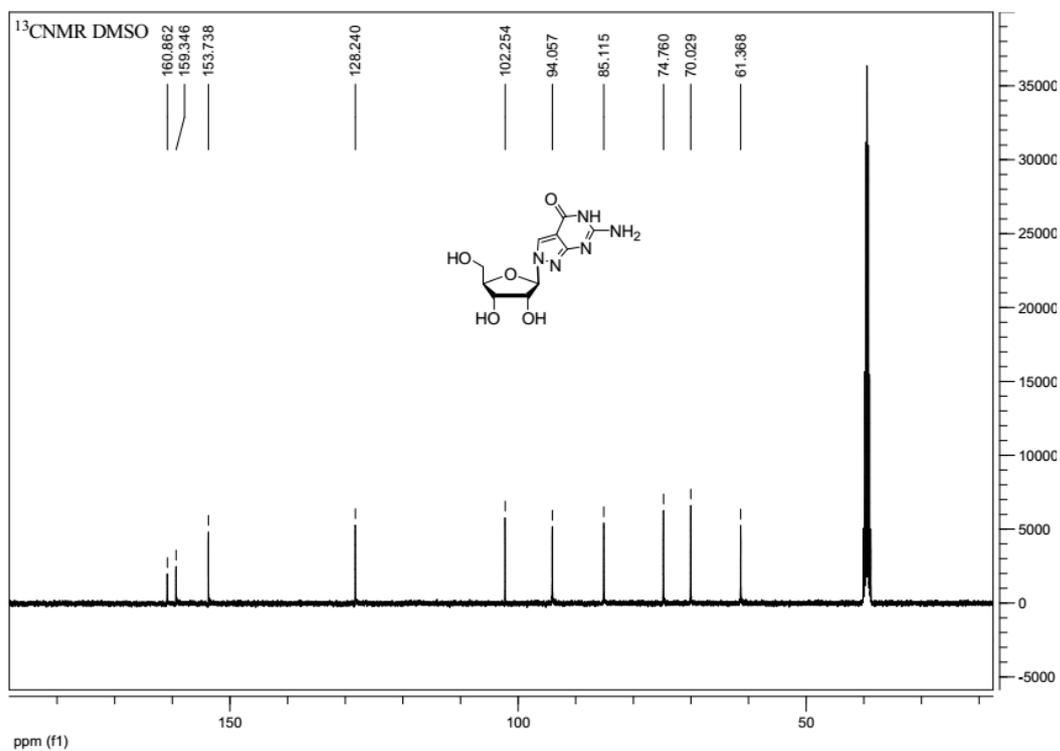
Product 27: ^1H NMR (400 MHz, $\text{DMSO-}d_6$)



Product 7: ^{13}C NMR (400 MHz, $\text{DMSO-}d_6$)



Product 10: ^{13}C NMR (400 MHz, $\text{DMSO-}d_6$)

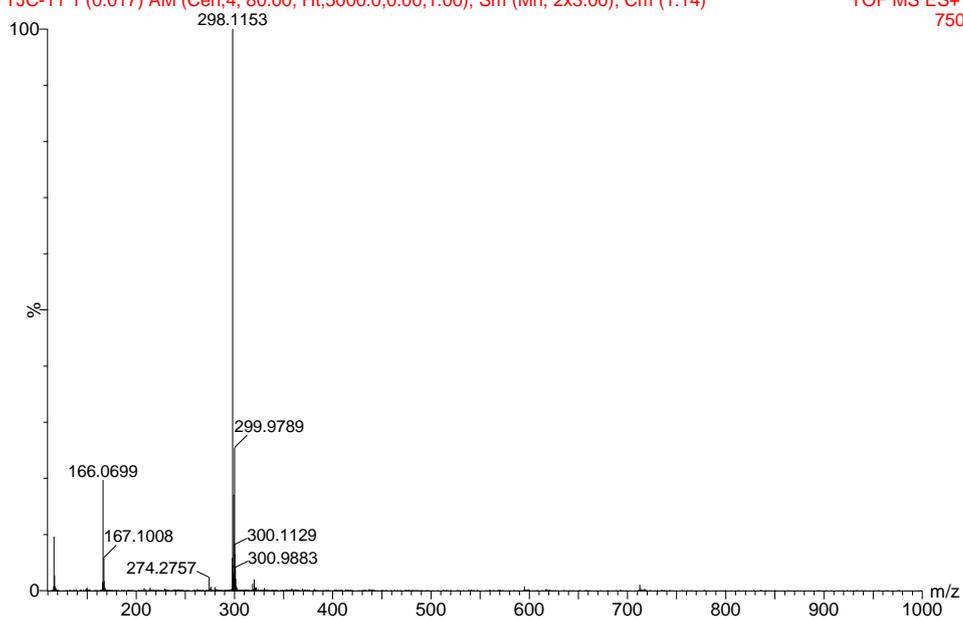


Product 2: HRMS spectra

2

TJC-11 1 (0.017) AM (Cen,4, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:14)

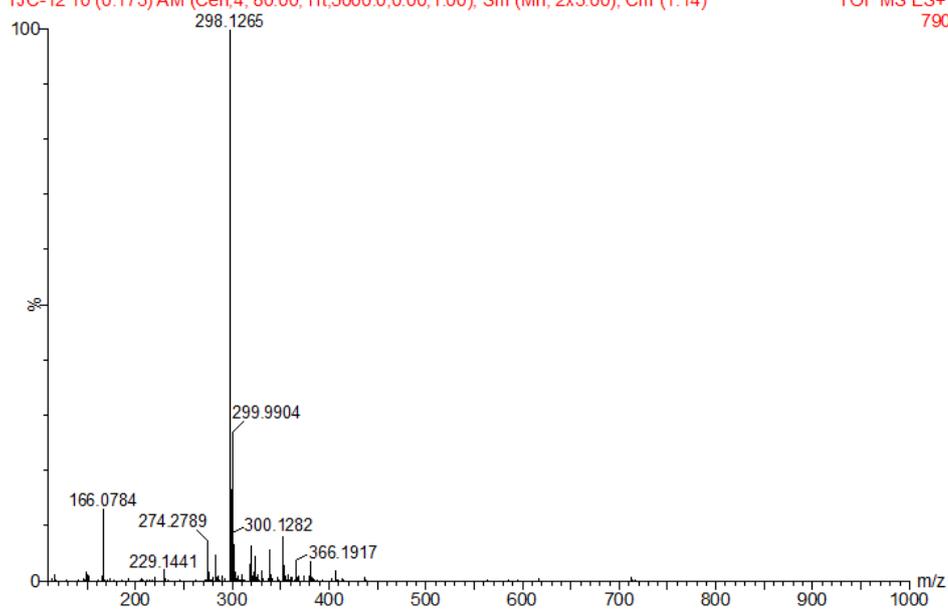
TOF MS ES+
750



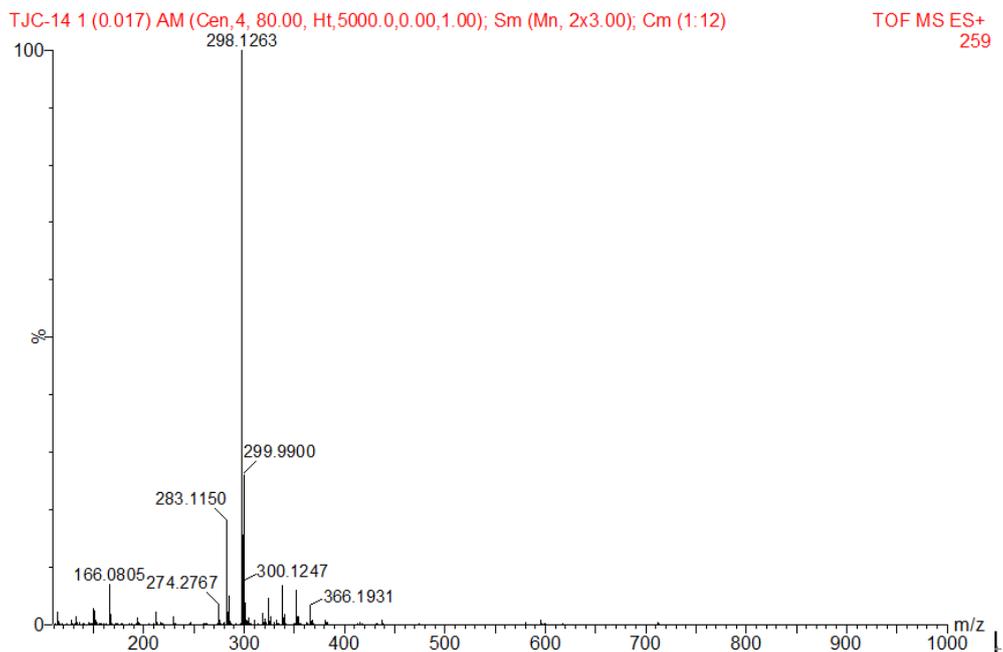
Product 6: HRMS spectra

TJC-12 10 (0.173) AM (Cen,4, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:14)

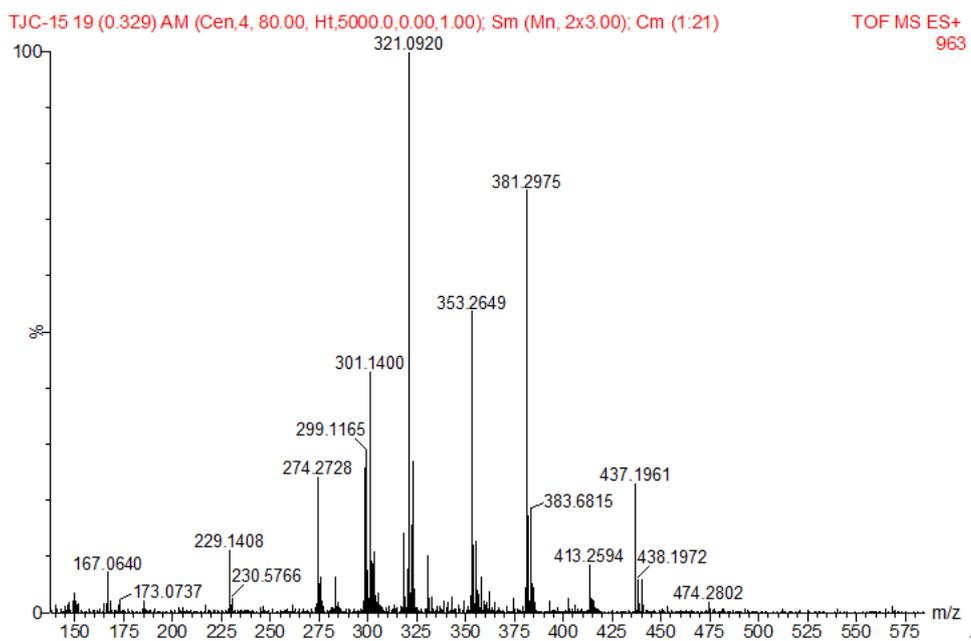
TOF MS ES+
790



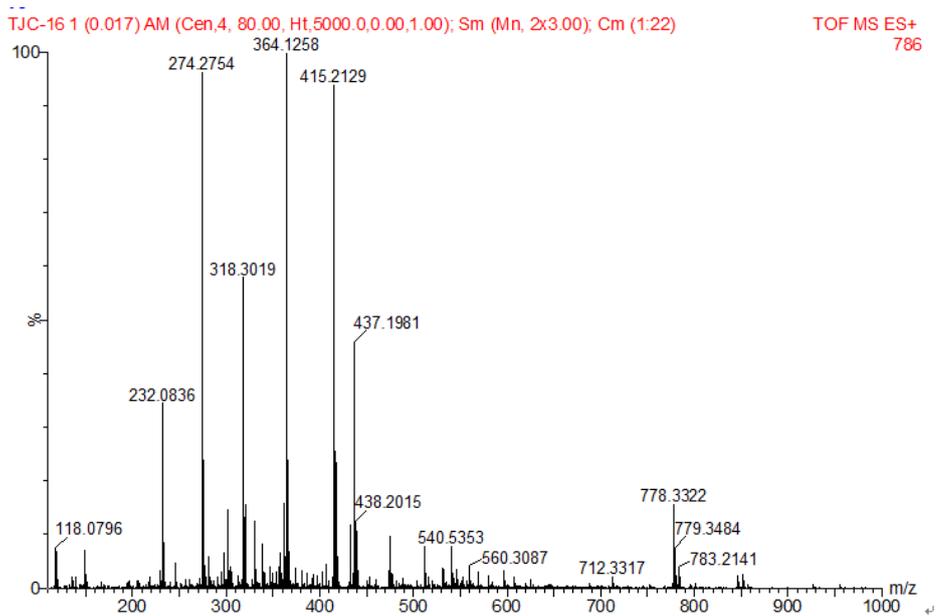
Product 12: HRMS spectra



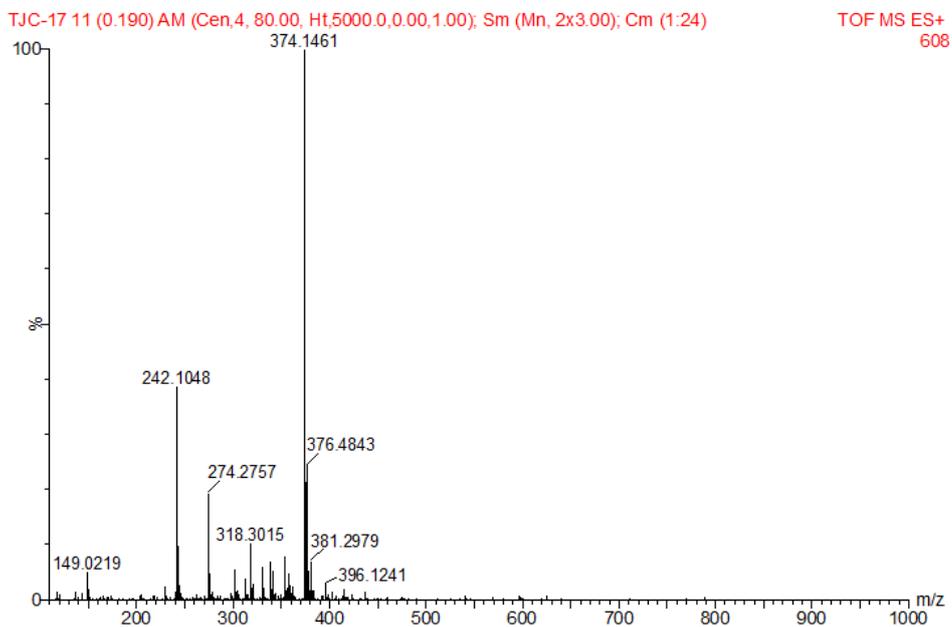
Product 13: HRMS spectra



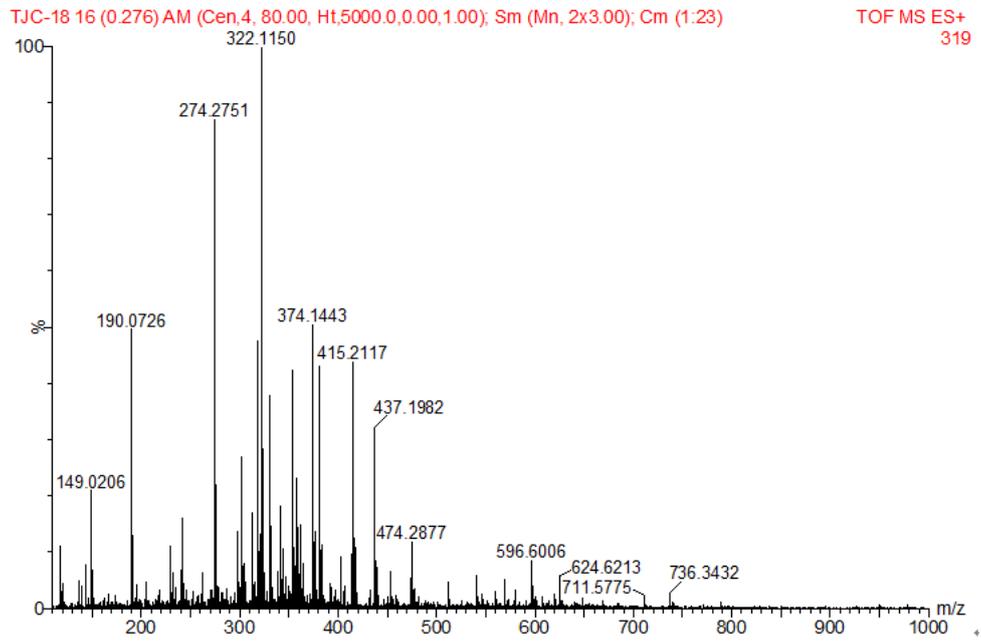
Product 14: HRMS spectra



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 ₅ O ₅
Formula weight	283.25
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 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} /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 ≤ h ≤ 5, -13 ≤ k ≤ 13, -25 ≤ l ≤ 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 ₆ O 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} /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 ≤ h ≤ 6, -15 ≤ k ≤ 15, -13 ≤ l ≤ 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)
