Authors: R. K. Ujjinamatada, P. Pathak, A. Burger, and R. S. Hosmane.* Inhibition of adenosine deaminase by analogues of adenosine and inosine incorporating a common heterocyclic base 4(7)-amino-6(5)*H*-imidazo[4,5-*d*]pyridazin-7(4)one.

SUPPORTING INFORMATION

General Experimental Procedure: ^{1}H and ^{13}C NMR spectra were recorded on a General Electric QE-300 NMR spectrometer or on an Oxford AS400 NMR spectrometer operating at 300/400 MHz for ^{1}H and 75/100 MHz for ^{13}C. The Chemical shift data are reported with reference to Me_4Si (internal standard) for ^{1}H and ^{13}C NMR spectra. The data are reported in the following format: Chemical shift, multiplicity (s=singlet, d=doublet, dt=double triplet, dd=double doublet, t=triplet, q=quartet, m=multiplet, br=broad, coupling constants, integration and assignment). Elemental Microanalyses were performed by Atlantic Microlab, Inc., Norcross, Georgia. The mass spectra were recorded at the Mass Spectrometry Facility, Department of Chemistry and Biochemistry, University of Maryland, Baltimore County or the Mass Spectrometry Analysis Laboratory, Department of Chemistry and Biochemistry, University of Maryland, College Park. Thin layer chromatography was performed on Merck Kieselgel 60 GF_{254} plates (0.2 mm thickness). Melting points were determined on a Thomas-Hoover capillary melting point apparatus, and are uncorrected. Dry solvents were prepared as follows: Methanol was distilled from calcium hydride and was stored over molecular sieves (type 3Å); methylene chloride was distilled from calcium hydride and was stored over molecular sieves (type 3Å); dimethylformamide was dried over calcium oxide and then distilled under reduced pressure from calcium hydride, and was subsequently stored over molecular sieves (type 3Å); acetonitrile was distilled from calcium hydride and was stored over molecular sieves (type 3Å). Starting materials were purchased from Aldrich Chemical Co., Acros or Lancaster. All solvents are reagent grade and were purchased from VWR Scientific or Fisher Scientific. All yields reported are for dry compounds that require no further purification for use in other reactions.

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Elemental microanalyses Data Sheet

Compd. #	Molecular Formula	M.W.	Calcd'			Found			HRMS (FAB) (MH+)
			C	H	N	C	H	N	
3	$C_{10}H_{13}N_5O_5$**.** H_2O	301	39.87	4.98	23.25	39.44	4.92	23.70	Calcd for $C_{10}H_{14}N_5O_5$: 284.0995 Found: 284.0995
4	$C_{10}H_{13}N_5O_5$ $2H_2O$	319	37.62	5.37	21.94	37.53	5.35	21.86	Calcd for $C_{10}H_{14}N_5O_5$: 284.0995 Found: 284.0997
7	$C_{33}H_{27}N_3O_9$	609	65.02	4.46	6.89	65.09	4.40	6.80	
8	$C_{33}H_{27}N_3O_9$	609	65.02	4.46	6.89	65.16	4.71	6.36	
9	$C_{11}H_{13}N_3O_6$.	283	46.65	4.63	14.84	46.66	4.60	14.75	
10	$C_{11}H_{13}N_3O_6$**.** 0.125 CH_3OH	287	46.47	4.87	14.62	46.39	4.79	14.26	
11	$C_{10}H_{17}N_7O_5$**.** 0.75 CH_3OH	339	38.05	5.42	29.05	37.62	5.89	28.89	Calcd for $C_{10}H_{18}N_7O_5$: 316.1369 Found: 316.1363