SUPPORTING INFORMATION

Inhibition of Siderophore Biosynthesis by 2-Triazole Substituted Analogues of 5'-O-[N-(Salicyl)sulfamoyl]adenosine: Antibacterial Nucleosides Effective Against Mycobacterium tuberculosis

*Amol Gupte, Helena I. Boshoff,b Daniel J. Wilson,a João Neres,a Nicholas P. Labello, a Ravindranadh V. Somu,a Chengguo Xing,c Clifton E. Barry III,b Courtney C. Aldricha**

[a]Center for Drug Design, Academic Health Center, University of Minnesota, Minneapolis, Minnesota 55455

[b]Tuberculosis Research Section, National Institute of Allergy and Infectious Diseases, Bethesda, Maryland 20892

[c]Department of Medicinal Chemistry, University of Minnesota, Minneapolis, Minnesota, MN 55455

Table S1. HPLC purity and conditions for the final compounds.

Compound	Conditions	Retention time (min)	Purity (%)
16	Method 2	7.3	95.4
	Method 4	7.4	95.6
17	Method 2	8.5	97.1
	Method 4	9.0	95.6
18	Method 1	12.8	95.0
	Method 3	13.0	95.5
19	Method 1	13.5	97.9
	Method 3	13.9	99.2
20	Method 1	13.9	97.8
	Method 3	14.5	98.3
21	Method 1	14.2	95.3
	Method 3	14.9	96.9
22	Method 1	14.5	99.9
	Method 3	15.2	98.4
23	Method 1	14.8	99.8
	Method 3	15.4	97.8
24	Method 1	15.2	99.9
	Method 3	16.0	97.4
25	Method 2	20.7	98.5
	Method 4	22.3	98.3
26	Method 2	10.7	97.0
	Method 4	10.8	96.7
27	Method 2	13.3	99.3
	Method 4	13.8	98.0
28	Method 2	8.1	99.3
	Method 4	8.1	99.4
29	Method 2	11.7	96.9
	Method 4	12.0	97.7
30	Method 2	13.6	99.2
	Method 4	14.2	98.5
31	Method 2	14.0	96.7
	Method 4	14.6	97.0
32	Method 2	13.9	95.2
	Method 4	14.6	95.1
33	Method 3	14.0	95.4
	Method 4	11.3	95.1
34	Method 2	10.4	98.6
	Method 4	11.0	96.9
35	Method 2	9.2	96.9
	Method 4	9.6	95.9

Compound	Conditions	Retention time (min)	Purity (%)
36	Method 2	8.9	96.3
	Method 4	9.0	97.4
37	Method 2	11.7	95.7
	Method 4	12.8	95.1
38	Method 2	12.0	98.1
	Method 4	12.9	96.5
39	Method 2	11.7	95.8
	Method 4	12.8	95.4
40	Method 2	11.0	98.3
	Method 4	12.7	96.2
41	Method 2	12.2	98.8
	Method 4	9.9	99.0
42	Method 2	8.9	95.0
	Method 4	9.6	95.3
43	Method 2	8.9	96.5
	Method 4	9.1	95.5
44	Method 2	10.6	95.8
	Method 4	7.7	97.0
45	Method 2	8.1	95.7
	Method 4	8.7	95.0

- HPLC solvents:

  A1: 20 mM Triethylammonium bicarbonate
  A2: 50 mM Triethylammonium bicarbonate
  B1: Methanol
  B2: Acetonitrile

- HPLC column:

  Analytical: Varian Microsorb MV100-5 C18, 250 × 4.6 mm, operated at 1 mL/min, detection at 220 nm.

- Methods:

  Method 1: Elution with A1 and 20-80% linear gradient of B1 in 20 min followed by isocratic elution with 80% B for 6 min.

  Method 2: Elution with A2 and 20-80% linear gradient of B2 in 20 min followed by isocratic elution with 80% B for 6 min.

  Method 3: Elution with A1 and 20-100% linear gradient of B1 in 30 min.

  Method 4: Elution with A2 and 20-100% linear gradient of B2 in 30 min.