SUPPORTING INFORMATION

5'-*O*-[(*N*-Acyl)sulfamoyl]adenosines as Antitubercular Agents that Inhibit MbtA: An Aryl Adenylating Enzyme Required for Siderophore Biosynthesis of the Mycobactins

*Chunhua Qiao,[a] Amol Gupte[a], Helena I. Boshoff,[b] Daniel J. Wilson,[a] Eric M. Bennett,[a] Ravindranadh V. Somu,[a] Clifton E. Barry III,[b] Courtney C. Aldrich[a]**

[a]*Center for Drug Design, University of Minnesota, Minneapolis, Minnesota 55455,* [b]*Tuberculosis Research Section, National Institute of Allergy and Infectious Diseases, Bethesda, Maryland 20892.*

HPLC Purity of Inhibitors. HPLC purity was determined by two methods using a Varian Microsorb MV 100-5 C18 column (4.6 × 150 mm, 5 μm particle size) with detection at 254 nm and the indicated HPLC conditions (Methods A–E) as described below.

HPLC Conditions:

Solvent A: 50 mM aqueous triethylammonium bicarbonate (TEAB) buffer.
Solvent B1: CH_3CN/H_2O (9:1)
Solvent B2: CH_3CN/H_2O (7:3)
Flowrate: 0.5 mL/min.
Detection 254 ± 4 nm
HPLC column: Varian Microsorb MV 100-5 C18 250 × 4.6 mm

HPLC Methods:

Method A: 0–25 min: gradient 5%–100% B1; isocratic 25–29 min: 100% B1
Method B: 0–20 min: gradient 20%–80% B1; isocratic 20–25 min: 80 % B1
Method C: 0–30 min: gradient 2%–100% B1; isocratic 30–34 min: 100% B1
Method D: 0–25 min: gradient 5%–100% B2; isocratic 25–28 min: 100% B2; 28–33 min: gradient 100%–5% B2; 33–35 min: isocratic 5% B2.
Method E: 0–20 min: gradient 20%–80% B2; isocratic 20–26 min: 80% B2; 26–28 min: gradient 80%–20% B2; 28–37 min: isocratic 20% B2.

Table S1. HPLC Purity of Inhibitors

Compound Number	Method	t_{ret} (min)	Purity (%)
9	D	15.6	96.2
	E	15.0	95.8
10	D	14.8	97.2
	E	15.5	96.9
11	D	15.7	98.5
	E	15.0	99.1
12	D	12.5	98.5
	E	14.4	97.9
13	D	15.8	98.5
	E	15.0	99.1
14	D	13.7	97.9
	E	15.1	98.3
15	A	14.2	95.9
	B	16.0	98.9
16	A	13.6	95.1
	B	17.4	95.2
17	A	16.6	99.0
	B	16.1	98.9
18	A	10.8	97.7
	B	10.4	97.6
19	D	14.8	99.2
	E	12.9	98.9
20	D	12.8	99.0
	E	11.4	98.7
23	D	14.3	98.7
	E	13.8	98.1
24	D	14.5	98.4
	E	12.5	99.0
25	D	13.2	97.5
	E	12.6	97.8
26	A	9.81	98.4
	C	7.44	99.0
27	A	15.8	97.6
	B	10.5	95.5
28	A	16.1	95.9
	B	11.4	95.3
29	A	15.7	98.8
	B	10.7	97.3
30	A	15.1	98.5
	B	10.6	98.7
31	A	15.7	98.3
	B	10.4	95.8
32	A	17.5	99.7
	B	12.8	98.3
58	A	15.8	99.1
	B	10.8	98.3
63	A	21.9	95.4
	B	15.9	96.3