Supplemental Material

The Oriented Development of Antituberculotics: Salicylanilides

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Elemental analysis of halogenated *N*-(4-alkylphenyl)salicylamides.

Compounds	Analysis (found/calculated) (%)		
	C	H	N
1a	66.29/66.32	5.59/5.57	4.66/4.83
1b	67.51/67.21	6.18/5.97	4.34/4.61
1c	67.17/67.21	6.08/5.97	4.59/4.61
1f	69.54/69.45	6.97/6.99	3.93/4.05
1g	69.91/70.08	7.05/7.28	3.75/3.89
2a	65.92/66.32	5.35/5.57	4.61/4.83
2b	67.05/67.21	5.95/5.97	4.38/4.61
2c	67.08/67.21	5.93/5.97	4.42/4.61
2d	68.01/68.03	6.46/6.37	4.33/4.41
2e	68.91/68.77	6.76/6.68	4.08/4.22
2f	69.28/69.45	6.96/6.99	3.83/4.05
2g	69.85/70.08	7.33/7.28	3.69/3.89
3a	55.68/55.50	4.62/4.83	3.99/4.19
3b	58.48/58.63	5.13/5.21	3.85/4.02
3d	59.46/59.68	5.33/5.56	3.76/3.87
3e	60.50/60.65	5.80/5.89	3.59/3.72
3f	61.58/61.54	6.20/6.20	3.43/3.59
3g	62.26/62.38	6.47/6.48	3.33/3.46
4b	47.67/47.80	3.91/4.01	3.12/3.28
4d	48.83/49.01	4.10/4.39	2.95/3.17
4e	49.85/50.14	4.60/4.65	2.90/3.08
4f	51.04/51.20	4.79/4.94	2.86/2.99

^{1}H and ^{13}C NMR spectra of halogenated *N*-(4-alkylphenyl)salicylamides.

Compounds	NMR, δ
1a	^{1}H NMR (300 MHz, DMSO) δ 12.21 (1H, brs, NH), 10.31 (1H, s, OH), 7.96 (1H, d , *J*=8.2 Hz, H6), 7.63-7.53 (2H, m, AA′, BB′, H2′, H6′), 7.22-7.12 (2H, m, AA′, BB′, H3′, H5′), 7.07-6.98 (2H, m, H3, H5), 2.52 (2H, t, *J*=7.3 Hz, CH_2), 1.64-1.48 (2H, m, CH_2), 0.87 (3H, t, *J*=7.3 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.7, 159.4, 138.4, 137.6, 135.9, 130.9, 128.8, 121.2, 119.4, 117.1, 117.0, 36.9, 34.3, 13.8.
1b	^{1}H NMR (300 MHz, DMSO) δ 12.19 (1H, brs, NH), 10.31 (1H, s, OH), 7.95 (1H, d, *J*=8.5 Hz, H6), 7.61-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.21-7.12 (2H, m, AA′, BB′, H3′, H5′), 7.03 (1H, d overlapped, *J*=1.7 Hz, H3), 7.02 (1H, dd overlapped, *J*=8.5 Hz, *J*=1.7 Hz, H5), 2.54 (2H, t, *J*=7.5 Hz, CH_2), 1.60-1.46 (2H, m, CH_2), 1.36-1.20 (2H, m, CH_2), 0.88 (3H, t, *J*=7.5 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.7, 159.4, 138.6, 137.6, 135.8, 130.9, 128.7, 121.2, 119.4, 117.1, 117.0 34.5, 33.4, 21.9 14.0
1c	^{1}H NMR (300 MHz, DMSO) δ 12.21 (1H, brs, NH), 10.33 (1H, s, OH), 7.96 (1H, d, *J*=9.1 Hz, H6), 7.63-7.56 (2H, m, AA′, BB′, H2′, H6′), 7.41-7.33 (2H, m, AA′, BB′, H3′, H5′), 7.05-7.00 (2H, m, H3, H5), 1.27 (9H, s, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.7, 159.5, 146.9, 137.6, 135.6, 130.9, 125.6, 120.9, 119.4, 117.1, 34.3, 31.4.
1f	^{1}H NMR (300 MHz, DMSO) δ 12.21 (1H, brs, NH), 10.31 (1H, s, OH), 7.99-7.93 (1H, m, H6), 7.61-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.21-7.11 (2H, m, AA′, BB′, H3′, H5′), 7.05-7.00 (2H, m, H3, H5), 2.53 (2H, t, *J*=7.4 Hz, CH_2), 1.62-1.46 (2H, m, CH_2), 1.32-1.15 (8H, m, CH_2), 0.83 (3H, t, *J*=6.7 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.7, 159.4, 138.6, 137.6, 135.8, 130.9, 128.7, 121.2, 119.4, 117.1, 117.0, 34.8, 31.5, 31.3, 28.8, 28.8, 22.3, 14.2.
1g	^{1}H NMR (300 MHz, DMSO) δ 12.23 (1H, brs, NH), 10.32 (1H, s, OH), 7.95 (1H, d, *J*=8.8 Hz, H6), 7.61-7.53 (2H, m, AA′, BB′, H2′, H6′), 7.21-7.12 (2H, m, AA′, BB′, H3′, H5′), 7.04-7.00 (2H, m, H3, H5), 2.53 (2H, t, *J*=7.4 Hz, CH_2), 1.61-1.45 (2H, m, CH_2), 1.32-1.15 (10H, m, CH_2), 0.83 (3H, t, *J*=6.7 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.4, 159.2, 138.3, 137.3, 135.6, 130.6, 128.4, 120.9, 119.1, 116.8, 116.8, 34.5, 31.2, 31.0, 28.8, 28.6, 28.6, 22.0, 13.9.
2a	^{1}H NMR (300 MHz, DMSO) δ 11.94 (1H, brs, NH), 10.35 (1H, s, OH), 8.00-7.94 (1H, m, H6), 7.63-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.49-7.41 (1H, m, H4), 7.22-7.12 (2H, m, AA′, BB′, H3′, H5′), 6.99 (1H, d, *J*=8.8 Hz, H3), 2.52 (2H, t, *J*=7.3 Hz, CH_2), 1.65-1.47 (2H, m, CH_2), 0.87 (3H, t, *J*=7.3 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.3, 138.4, 135.8, 133.3, 128.8, 128.5, 1229. 121.1, 119.5, 119.3 36.9, 24.3 13.8..
2b	^{1}H NMR (300 MHz, DMSO) δ 11.93 (1H, bs, NH), 10.35 (1H, s, OH), 7.97 (1H, d, *J*=2.5 Hz, H6), 7.61-7.55 (2H, m, AA′, BB′, H2′, H6′), 7.46 (1H, dd, *J*=8.8 Hz, *J*=2.5 Hz, H4), 7.22-7.13 (2H, m, AA′, BB′, H3′, H5′), 7.00 (1H, d, *J*=8.8 Hz, H3), 2.54 (2H, t, *J*=7.4 Hz, CH_2), 1.60-1.45 (2H, m, CH_2), 1.36-1.21 (2H, m, CH_2), 0.88 (3H, t, *J*=7.4 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.3, 138.7, 135.8, 133.3, 128.7, 128.5, 122.9, 121.1, 119.5, 119.3, 34.5, 33.4, 21.9, 14.0.
2c	^{1}H NMR (300 MHz, DMSO) δ 11.97 (1H, brs, NH), 10.37 (1H, s, OH), 7.98 (1H, d, *J*=2.6 Hz, H6), 7.64-7.56 (2H, m, AA′, BB′, H2′, H6′), 7.46 (1H, dd, *J*=8.9 Hz, *J*=2.6 Hz, H4), 7.41-7.33 (2H, m, AA′, BB′, H3′, H5′), 7.00 (1H,

d, *J*=8.9 Hz, H3), 1.27 (9H, s, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.4, 147.0, 135.6, 133.3, 128.5, 125.6, 122.9, 120.9, 119.4, 34.3, 31.4.

2d ^{1}H NMR (300 MHz, DMSO) δ 11.94 (1H, brs, NH), 10.36 (1H, s, OH), 7.97 (1H, d, *J*=2.7 Hz, H6), 7.62-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.45 (1H, dd, *J*=8.8 Hz, *J*=2.7 Hz, H4), 7.21-7.13 (2H, m, AA′, BB′, H3′, H5′), 7.00 (1H, d, *J*=8.8 Hz, H3), 2.53 (2H, t, *J*=7.0 Hz, CH_2), 1.62-1.47 (2H, m, CH_2), 1.36-1.16 (4H, m, CH_2), 0.84 (3H, t, *J*=7.0 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.3, 138.7, 135.8, 133.3, 128.7, 128.5, 122.9, 121.1, 119.5, 119.3, 34.8, 31.1, 30.9, 22.2, 14.2.

2e ^{1}H NMR (300 MHz, DMSO) δ 11.94 (1H, brs, NH), 10.37 (1H, s, OH), 7.97 (1H, d, *J*=2.8 Hz, H6), 7.62-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.45 (1H, dd, *J*=8.8 Hz, *J*=2.8 Hz, H4), 7.21-7.12 (2H, m, AA′, BB′, H3′, H5′), 7.00 (1H, d, *J*=8.8 Hz, H3), 2.53 (2H, t, *J*=7.4 Hz, CH_2), 1.60-1.46 (2H, m, CH_2), 1.33-1.17 (6H, m, CH_2), 0.84 (3H, t, *J*=6.7 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.4, 138.7, 135.8, 133.3, 128.7, 128.5, 122.8, 121.1, 119.5, 119.3, 34.8, 31.3, 31.2, 28.5, 22.3, 17.2.

2f ^{1}H NMR (300 MHz, DMSO) δ 11.97 (1H, brs, NH), 10.35 (1H, s, OH), 7.98 (1H, d, *J*=2.6 Hz, H6), 7.63-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.45 (1H, dd, *J*=8.8 Hz, *J*=2.6 Hz, H4), 7.20-7.12 (2H, m, AA′, BB′, H3′, H5′), 6.99 (1H, d, *J*=8.8 Hz, H3), 2.52 (2H, t, *J*=7.1 Hz, CH_2), 1.61-1.44 (2H, m, CH_2), 1.33-1.12 (8H, m, CH_2), 0.83 (3H, t, *J*=6.7 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.4, 138.7, 135.8, 133.3, 128.7, 128.5, 122.9, 121.1, 119.4, 119.3, 34.8, 31.5, 31.3, 28.8, 28.8, 22.3, 14.2.

2g ^{1}H NMR (300 MHz, DMSO) δ 11.94 (1H, brs, NH), 10.35 (1H, s, OH), 7.97 (1H, d, *J*=2.6 Hz, H6), 7.61-7.54 (2H, m, AA′, BB′, H2′, H6′), 7.45 (1H, dd, *J*=8.8 Hz, *J*=2.6 Hz, H4), 7.20-7.12 (2H, m, AA′, BB′, H3′, H5′), 7.00 (1H, d, *J*=8.8 Hz, H3), 2.53 (2H, t, *J*=7.4 Hz, CH_2), 1.62-1.47 (2H, m, CH_2), 1.34-1.14 (10H, m, CH_2), 0.83 (3H, t, *J*=6.6 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.3, 138.7, 135.8, 133.2, 128.7, 128.5, 122.9, 121.1, 119.4, 119.3, 34.8, 31.5, 31.2, 29.1, 28.9, 28.8, 22.3 14.2.

3a ^{1}H NMR (300 MHz, DMSO) δ 11.95 (1H, brs, NH), 10.35 (1H, s, OH), 8.09 (1H, d *J*=2.6 Hz, H6), 7.62-7.54 (2H, m, AA′, BB′ overlapped, H2′, H6′), 7.57 (1H, dd overlapped, *J*=8.8 Hz, *J*=2.6 Hz, H4), 7.22-7.13 (2H, m, AA′, BB′, H3′, H5′), 6.95 (1H, d, *J*=8.8 Hz, H3), 2.52 (2H, t, *J*=7.3 Hz, CH_2), 1.66-1.48 (2H, m, CH_2), 0.88 (3H, t, *J*=7.3 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.1, 157.7, 138.4, 136.1, 135.8, 131.3, 128.8, 121.1, 120.0, 119.7, 110.3, 36.9, 24.3, 13.8.

3b ^{1}H NMR (300 MHz, DMSO) δ 11.97 (1H, brs, NH), 10.35 (1H, s, OH), 8.09 (1H, d, *J*=2.2 Hz, H6), 7.63-7.52 (3H, m, H4, H2′, H6′), 7.22-7.14 (2H, m, AA′, BB′, H3′, H5′), 6.95 (1H, d, *J*=8.8 Hz, H3), 2.54 (2H, t, *J*=7.5 Hz, CH_2), 1.61-1.45 (2H, m, CH_2), 1.36-1.21 (2H, m, CH_2), 0.88 (3H, t, *J*=7.5 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.2, 157.8, 138.6, 136.1, 135.8, 131.3, 128.7, 121.1, 120.0, 119.7, 110.3, 34.5, 33.4, 21.9, 14.0.

3d ^{1}H NMR (300 MHz, DMSO) δ 11.95 (1H, brs, NH), 10.35 (1H, s, OH), 8.09 (1H, d, *J*=2.5 Hz, H6), 7.62-7.53 (3H, m, H4, H2′, H6′), 7.21-7.13 (2H, m, AA′, BB′, H3′, H5′), 6.95 (1H, d, *J*=8.8 Hz, H3), 2.53 (2H, t, *J*=7.4 Hz, CH_2), 1.62-1.47 (2H, m, CH_2), 1.37-1.18 (4H, m, CH_2), 0.85 (3H, t, *J*=6.9 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.1, 157.7, 138.7, 136.1, 135.8, 131.3, 128.7, 121.1, 120.0, 119.8, 110.3, 34.8, 31.1, 30.9, 22.2, 14.2.

3e ^{1}H NMR (300 MHz, DMSO) δ 11.97 (1H, brs, NH), 10.35 (1H, s, OH), 8.09 (1H, d, *J*=2.5 Hz, H6), 7.61-7.53 (3H, m, H4, H2′, H6′), 7.20-7.13 (2H, m, AA′, BB′, H3′, H5′), 6.94 (1H, d, *J*=8.8 Hz, H3), 2.53 (2H, t, *J*=7.4 Hz, CH_2), 1.62-1.46 (2H, m, CH_2), 1.32-1.18 (6H, m, CH_2), 0.84 (3H, t, *J*=6.9 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.1, 157.7, 138.7, 136.1, 135.8, 131.3, 128.7, 121.1, 120.0, 119.8, 110.3, 34.8, 31.3, 31.2, 28.5, 22.3, 14.2,

3f ^{1}H NMR (300 MHz, DMSO) δ 11.99 (1H, bs, NH), 10.35 (1H, s, OH), 8.10 (1H, d, *J*=2.5 Hz, H6), 7.62-7.52 (3H, m, H4, H2′, H6′), 7.19-7.12 (2H, m, AA′, BB′, H3′, H5′), 6.94 (1H, d, *J*=8.8 Hz, H3), 2.52 (2H, t, *J*=7.1 Hz, CH_2), 1.61-1.45 (2H, m, CH_2), 1.32-1.15 (8H, m, CH_2), 0.83 (3H, t, *J*=6.7 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 165.1, 157.8, 138.7, 136.1, 135.8, 131.3, 128.7, 121.1, 119.9, 119.8, 110.3, 34.8, 31.5, 31.3, 28.8, 28.8, 22.3, 14.2.

3g ^{1}H NMR (300 MHz, DMSO) δ 11.98 (1H, brs, NH), 10.35 (1H, s, OH), 8.09 (1H, d, *J*=2.5 Hz, H6), 7.61-7.54 (3H, m, H4, H2′, H6′), 7.20-7.13 (2H, m, AA′, BB′, H3′, H5′), 6.94 (1H, d, *J*=8.8 Hz, H3), 2.53 (2H, t, *J*=7.1 Hz, CH_2), 1.61-1.45 (2H, m, CH_2), 1.32-1.16 (10H, m, CH_2), 0.85 (3H, t, *J*=6.6 Hz, CH_3).^{13}C NMR (75 MHz, DMSO) δ 165.1, 157.8, 138.7, 136.1, 135.8, 131.3, 128.7, 121.1, 119.9, 119.7, 110.3, 34.8, 31.5, 31.2, 29.1, 28.9, 28.8, 22.3, 14.2.

4b ^{1}H NMR (300 MHz, DMSO) δ 10.59 (1H, s, OH), 8.30 (1H, d, *J*=2.3 Hz, H6), 8.00 (1H, d, *J*=2.3 Hz, H4),7.59-7.51 (2H, m, AA′, BB′, H2′, H6′), 7.24-7.16 (2H, m, AA′, BB′, H3′, H5′), 2.55 (2H, t, *J*=7.5 Hz, CH_2), 1.60-1.47 (2H, m, CH_2), 1.36-1.22 (2H, m, CH_2), 0.88 (3H, t, *J*=7.5 Hz, CH_3).^{13}C NMR (75 MHz, DMSO) δ 166.8, 156.8, 139.4, 138.8, 135.1, 129.8, 128.7, 122.1, 118.3, 112.5, 110.0, 34.5, 33.3, 21.9, 14.0.

4d ^{1}H NMR (300 MHz, DMSO) δ 10.61 (1H, s, OH), 8.30 (1H, d, *J*=2.3 Hz, H6), 8.00 (1H, d, *J*=2.3 Hz, H4),7.60-7.55 (2H, m, AA′, BB′, H2′, H6′), 7.24-7.16 (2H, m, AA′, BB′, H3′, H5′), 2.55 (2H, t, *J*=7.4 Hz, CH_2), 1.62-1.47 (2H, m, CH_2), 1.37-1.17 (4H, m, CH_2), 0.85 (3H, t, *J*=6.9 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 166.8, 156.9, 139.5, 138.8, 135.0, ,129.8, 128.7, 122.1, 118.3, 112.6, 110.0, 34.8, 31.1, 30.9, 22.2, 14.1

4e ^{1}H NMR (300 MHz, DMSO) δ 10.59 (1H, s, OH), 8.30 (1H, d, *J*=2.3 Hz, H6), 8.00 (1H, d, *J*=2.3 Hz, H4), 7.60-7.51 (2H, m, AA′, BB′, H2′, H6′), 7.23-7.15 (2H, m, AA′, BB′, H3′, H5′), 2.54 (2H, t, *J*=7.0 Hz, CH_2), 1.62-1.46 (2H, m, CH_2), 1.33-1.18 (6H, m, CH_2), 0.83 (3H, t, *J*=7.0 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 166.8, 156.9, 139.5, 138.8, 135.0, 129.8, 128.7, 122.1, 118.3, 112.5, 110.0, 34.8, 31.3, 31.1, 28.5, 22.3, 14.2.

4f ^{1}H NMR (300 MHz, DMSO) δ 10.59 (1H, s, OH), 8.30 (1H, d, *J*=2.2 Hz, H6), 8.00 (1H, d, *J*=2.2 Hz, H4),7.59-7.51 (2H, m, AA′, BB′, H2′, H6′), 7.23-7.16 (2H, m, AA′, BB′, H3′, H5′), 2.54 (2H, t, *J*=7.4 Hz, CH_2), 1.63-1.47 (2H, m, CH_2), 1.34-1.15 (8H, m, CH_2), 0.84 (3H, t, *J*=6.7 Hz, CH_3). ^{13}C NMR (75 MHz, DMSO) δ 166.8, 156.8, 139.5, 138.8, 135.0, 129.8, 128.7, 122.1, 118.3, 112.5, 110.0, 34.8, 31.5, 31.2, 28.8, 28.8, 22.3, 14.2.