Antimicrobial Dialkylresorcinols from *Pseudomonas* sp. Ki19

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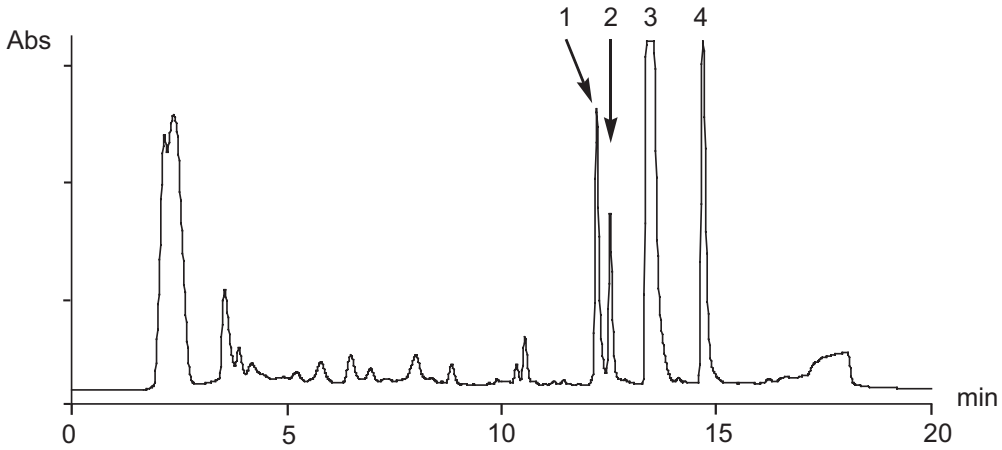
Figure 1. HPLC chromatogram of lipophilic 95% SPE eluate



Numbers indicate peaks corresponding to compounds **1**-**4**. HPLC system: 20 to 100% CH_3CN in H_2O in 10 min with an 8 min hold at 100%. The eluate was monitored at 210 nm.

Table 1. NMR Spectroscopic Data (CD_3OD, 100/400 MHz) for 2,5-dialkylresorcinols **1** and **2**

		2-butyl-5-propylresorcinol (**1**)			2-hexyl-5-methylresorcinol (**2**)	
position		δ_C, mult.	δ_H (*J* in Hz)	HMBC	δ_C, mult.	δ_H (*J* in Hz)
	1	157.2, qC			157.2, qC	
	2	114.8, qC			114.5, qC	
	3	157.2, qC			157.2, qC	
	4	108.0, CH	6.13, s	1, 2, 6, 1´´	108.6, CH	6.12, s
	5	142.1, qC			137.1, qC	
	6	108.0, CH	6.13, s	2, 3, 4, 1´´	108.6, CH	6.12, s
2-alkyl	1´	23.9, CH_2	2.55, t (7.6)	1, 2, 3, 2', 3'	24.1, CH_2	2.53, t (7.7)
	2´	32.8, CH_2	1.48, m	1´, 3´, 4´	30.5, CH_2	1.48, m
	3´	24.1, CH_2	1.36, m		30.7, CH_2	1.34, m
	4´	14.7, CH_3	0.922, t (7.3)		33.3, CH_2	1.32, m
	5´				23.9, CH_2	1.32, m
	6´			4´, 5´	14.6, CH_3	0.89, t (6.9)
5-alkyl	1´´	39.1, CH_2	2.38, t (7.6)	4, 5, 6, 2´´, 3´´	21.4, CH_3	2.13, s
	2´´	25.7, CH_2	1.58, tq (7.3, 7.6)	5, 1´´, 3´´		
	3´´	14.3, CH_3	0.917, t (7.3)	1´´, 2´´		

Compound Data for **3** (DB-2073) and **4** (resorstatin)

2-Hexyl-5-propylresorcinol [**3** (DB-2073)]: white powder; UV (CH_3OH/H_2O 1:1) λ_{max} (log ε) 207 (2.67), 271 (2.28), 279 (sh) (2.20) nm; ^{1}H NMR (CH_3OH-d_4, 400 MHz) δ 6.13 (2H, s, H-4, H-6), 2.54 (2H, t, J = 7.6 Hz, H-1´), 2.38 (2H, t, J = 7.6 Hz, H-1´´), 1.58 (2H, tq, J = 7.4, 7.7 Hz), H-2´´, 1.49 (2H, m, H-2´), 1.34 (2H, m, H-3´), 1.32 (4H, m, H-4´, H-5´), 0.92 (3H, t, J = 7.5 Hz, H-6´), 0.90 (3H, t, J = 6.9 Hz, H-3´´); ^{13}C NMR (CH_3OH-d_4, 100 MHz) δ 157.1 (C, C-1, C-3), 142.1 (C, C-5), 114.8 (C, C-2), 108.0 (C, C-4, C-6), 39.1 (CH_2, C-1´´), 33.2 (CH_2, C-4´), 30.7 (CH_2, C-3´), 30.5 (CH_2, C-2´), 25.7 (CH_2, C-2´´), 24.1 (CH_2, C-1´), 23.9 (CH_2, C-5´), 14.6 (CH_3, C-6´), 14.3 (CH_3, C-3´´); diagnostic H2BC connectivities, H-2´´→C-1´´, C-3´´; H-2´→C-1´, C-3´; H-3´→C-4´; HRFABMS *m/z* 237.1894 (calcd for $C_{15}H_{25}O_2$ 237.1855).

2-Hexyl-5-pentylresorcinol [**4** (Resorstatin)]: white powder; UV (CH_3OH/H_2O 1:1) λ_{max} (log ε) 207 (2.82), 271 (0.42), 280 (sh) (0.35) nm; ^{1}H NMR (CH_3OH-d_4, 400 MHz) δ 6.14 (2H, s, H-4, H-6), 2.54 (2H, t, J = 7.6 Hz, H-1´), 2.40 (2H, t, J = 7.6 Hz, H-1´´), 1.56 (2H, m, H-2´´), 1.49 (2H, m, H-2´), 1.34 (2H, m, H-3´), 1.32 (4H, m, H-5´, H-4´´), 1.31 (4H, m, H-4´, H-3´´), 0.91 (3H, t, J = 7.5 Hz, H-5´´)*, 0.90 (3H, t, J = 6.9 Hz, H-6´)*; ^{13}C NMR (CH_3OH-d_4, 100 MHz) δ 157.2 (C, C-1, C-3), 142.4 (C, C-5), 114.8 (C, C-2), 108.0 (C, C-4, C-6), 36.9 (CH_2, C-1´´), 33.2 (CH_2, C-3´´), 32.8 (CH_2, C-4´), 32.3 (CH_2, C-2´´), 30.7 (CH_2, C-3´), 30.5 (CH_2, C-2´), 24.1 (CH_2, C-1´), 23.7 (CH_2, C-5´), 23.9 (CH_2, C-4´´), 14.6 (CH_3, C-5´´)**, 14.5 (CH_3, C-6´)**; diagnostic HMBC connectivities, H-2´→C-3´; H-3´→C-4´; H-2´´→C-3´´; C-4´´; HRFABMS *m/z* 265.2146 (calcd for $C_{17}H_{29}O_2$ 265.2168); */** may be interchanged.

Figure 2. ^{1}H NMR spectra of **1**, **2**, **3**, **4** and **4a** (CD_3OD, 400 MHz)