Supporting Information for:

Novel Bromotyrosine Alkaloids: Inhibitors of Mycothiol S-Conjugate Amidase

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General procedures

UV spectra were obtained using a Beckman DU-600 spectrophotometer; optical rotations were measured on a Perkin Elmer 341 polarimeter in CH_3OH; CD spectra were measured on a Jasco-700 spectropolarimeter using a 0.2 cm cell; IR spectra were obtained with a Bio-Rad-FTS-45 FT-IR spectrophotometer. Low- and high-resolution FAB mass spectra were obtained on a Jeol-SX102 instrument. Reverse-phase (C18) HPLC was carried out using a GBC LC1150 pump, a GBC LC5100 photodiode array detector and a Waters μBondapak C18 column (7.8 x 300 mm) at a flow rate of 3 mL/min.

Compound 1.

^{1}H NMR (CD_3OD, 300MHz) 7.72 (s, H2'), 6.90 (s, H7'), 6.33 (s, H5), 3.98 (br s, H1), 3.70 (s, H15), 3.64 (d, *J*= 18.0 Hz, H7b), 3.50 (m, H10), 2.92 (d, *J*= 17.7 Hz, H7a), 2.91 (m, H11). **^{13}C NMR** (CD_3OD, 75 MHz) δ_C 175.0 (C4'), 161.7 (C9), 155.0 (C8), 151.5 (C5'), 149.4 (C3), 147.9 (C14), 141.9, 139.1, 133.7, 132.3 (C5), 124.8 (C2'), 122.9 (C4), 121.9, 121.5, 114.9 (C7'), 114.3, 114.2, 104.9 (C6'), 92.4 (C6), 75.5 (C1), 60.5 (C15), 40.0 (C7), 39.6 (C10), 25.7 (C11). **IR** (ZnSe, film) 3166 (broad), 1715, 1694, 1679, 1674, 4653, 1588, 1557, 1539, 1438, 1263, 1219, 1025, 994 cm^{-1}.

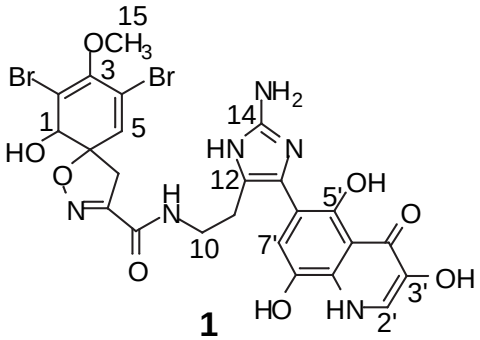

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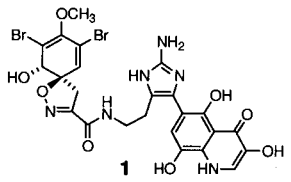
Table of full NMR data for compound **1**, including data obtained from the COSY, HMBC, and ROESY spectra in DMSO- d_6.

Atom	δ_C	δ_H, **multiplicity,** ***J*** **(Hz)**[a]	**COSY**	**HMBC (20 Hz)**	**HMBC (13 Hz)**	**HMBC (8 Hz)**	**ROESY**
1	73.5	3.89, d, 0.6		147.1, 131.2, 113.1, 90.1	147.1, 131.2, 113.1, 90.1	147.1, 131.2, 113.1, 90.1	6.42, 3.60
2	113.1						
3	147.1						
4	120.8						
5	131.2	6.56, d, 0.6		147.1, 120.8, 73.5	147.1, 120.8, 113.1, 73.5, 39.4	147.1, 120.8, 113.1, 90.1, 73.5, 39.4	3.12
6	90.1						
7a	39.4	3.12, d, 18.0	3.60	131.2	154.4, 131.2, 90.1, 73.5	131.2, 90.1, 73.5	6.56
7b		3.60, -	3.12	--	154.4, 131.2, 90.1, 73.5	73.5 weak	8,62, 3.89
8	154.4						
9	158.9						
10	38.1	3.40, -	8.62, 2.75	--	--	120.4, 158.9 (weak)	8.62
11	24.6	2.75, m	3.40	120.4, 38.1	120.4	120.4, 118.7	8.62, 6.96
12	120.4						
13	118.7						
14	146.2						
15	59.6	3.69, s		147.1	147.1	147.1	--
2’	124.2	7.70, s		173.2, 128.9	173.2, 128.9	173.2, 128.9	11.81, 9.00
3’	137.7						
4’	173.2						
4a’	112.2						
5’	149.3						
6’	103.1						
7’	113.8	6.96, s		149.3, 128.9, 118.7	137.0	137.0	10.36, 8.62
8’	137.0						
8a’	128.9						
1-OH		6.42, br s		--	113.8	--	3.89, 3.60
9-NH		8.62, br t, 5.7	3.40	158.9, 38.1	158.9	158.9	2.75, 3.12, 6.96
12-NH		11.95, br s		--	146.2, 120.4	--	7.27
14-NH_2		7.27, br s		--	--	--	11.95
1’-NH		9.00, br s		--	--	--	7.67
3’-OH		11.81, br s		--	139.9, 124.2, 112.2	--	7.67
5’-OH		14.42, br s		149.3, 112.2, 103.1	149.3, 112.2	--	--
8’-OH		10.36, br s		--	128.9	--	6.96

a. s=singlet, d=doublet, m=multiplet, br=broad, (--)=overlapped.

^{1}H and ^{13}C NMR spectra of compound **1** in CD_3OD run on a Mercury300 spectrometer.

^{1}H NMR spectrum of compound **1** (CD_3OD).



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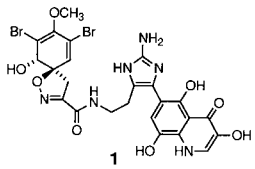
^{13}C NMR spectrum of compound **1** (CD_3OD).



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CD spectra of compounds **1** and **2** run on a Jasco-700 spectropolarimeter in CH_3OH.