

Supporting Information

Potent Benzimidazole Sulfonamide PTP1B Inhibitors Containing the Heterocyclic (S)-Isothiazolidinone Phosphotyrosine Mimetic

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1-HPLC Purity Analysis

1– HPLC Purity Analysis: HPLC Purity Analysis

HPLC purity was determined to be >95% for all final products by the following two HPCL conditions (See Table below); 1) HPLC method A utilized a Phenomenex Luna C18 column (6 x 75 mm, 3 μ M particle size), with a gradient of 95% water/0.05% TFA to 5% acetonitrile/0.05% TFA at a flow rate of 1.5 mL/min over a total run time of 7 min. with UV monitoring at 220 nm and 254 nm. 2) HPLC method B utilized a Zorbax Eclipse XDB-C8 column (6 x 50 mm, 3.5 μ M particle size), with a gradient of 95% water/0.05% TFA to 5% acetonitrile/0.05% TFA at a flow rate of 1.5 mL/min over a total run time of 5 min. with UV monitoring at 225 nm and 254 nm.

Compound	Formula	HPLC Analysis Data
2	$C_{20}H_{20}N_4O_4S$	Method A: $t_R = 2.23$ min (99.9%)
		Method B: $t_R = 1.74$ min (99.9%)
10	$C_{29}H_{29}N_5O_5S$	Method A: $t_R = 2.99$ min (95.0%)
		Method B: $t_R = 2.27$ min (99.9%)
12	$C_{20}H_{20}N_4O_4S$	Method A: $t_R = 2.23$ min (100%)

		Method B: $t_R = 1.74$ min (100%)
14	$C_{24}H_{22}N_4O_5S_2$	Method A: $t_R = 2.75$ min (99.7%) Method B: $t_R = 2.25$ min (100%)
16	$C_{24}H_{21}FN_4O_5S_2$	Method A: $t_R = 2.84$ min (95.9%) Method B: $t_R = 2.34$ min (99.1%)
67a	$C_{24}H_{21}FN_4O_5S_2$	Method A: $t_R = 2.67$ min (96.9%) Method B: $t_R = 2.19$ min (98.6%)
67b	$C_{24}H_{20}F_2N_4O_5S_2$	Method A: $t_R = 2.77$ min (95.6%) Method B: $t_R = 2.28$ min (97.2%)
67c	$C_{25}H_{19}ClF_4N_4O_5S_2$	Method A: $t_R = 3.66$ min (97.6%) Method B: $t_R = 2.96$ min (98.2%)
67d	$C_{20}H_{15}ClF_4N_4O_4S$	Method A: $t_R = 3.28$ min (98.7%) Method B: $t_R = 2.60$ min (97.8%)
79a	$C_{25}H_{24}N_4O_5S_2$	Method A: $t_R = 2.71$ min (96.0%) Method B: $t_R = 2.27$ min (98.5%)
79b	$C_{25}H_{24}N_4O_5S_2$	Method A: $t_R = 2.82$ min (98.7%) Method B: $t_R = 2.37$ min (99.0%)
79c	$C_{26}H_{22}BrF_3N_4O_5S_2$	Method A: $t_R = 3.32$ min (97.2%) Method B: $t_R = 2.82$ min (99.5%)

79d	$C_{26}H_{23}N_5O_5S_2$	Method A: $t_R = 2.69$ min (95.2%) Method B: $t_R = 2.82$ min (96.5%)
79e	$C_{25}H_{24}ClN_4O_5S_2$	Method A: $t_R = 3.02$ min (95.1%) Method B: $t_R = 2.82$ min (95.5%)
87	$C_{24}H_{21}ClN_4O_5S_2$	Method A: $t_R = 2.77$ min (97.2%) Method B: $t_R = 2.27$ min (98.0%)