J. Med. Chem. 40, 11136-1148: Corrected Table 1. Chemical formulae and activities of the HSF-PLA_2 inhibitors[a]

Name	XLM	YLM	ZLM	SN1	SN2	SN3	SN4	SN5	RLM	GLI	% inhibition
LM1166	$-CH_2-$	-CONH-	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CH_2OH$	$-(CH_2)_3CH_3$	-	-	-	65±14(7)
LM1192	$-CH_2-$	-CONH-	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	-	6±9(3)
LM1216	$-CH_2-$	-CONH-	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CHNH_3COO$	$-(CH_2)_3CH_3$	-	-	-	31±27(3)
LM1220	-O-	$-PO_2O-$	$-OPO_2O-$	$-(CH_2)_4-$	$-C_6H_{12}$	$-CH_2CH_2NH_3$	$-CH_3$	$-(CH_2)_3CH_3$	-	R	33±3(3)
LM1228	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	R	78±12(6)
LM1230	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2OH$	$-(CH_2)_3CH_3$	-	-	-	49±3(3)
LM1240	-O-	$-PO_2O-$	$-OPO_2O-$	$-(CH_2)_4-$	$-C_6H_{12}$	$-CH_2CH_2N(CH_3)_3$	$-CH_3$	$-(CH_2)_3CH_3$	-	R	9(1)
LM1245	$-CH_2-$	-CONH-	$-OPOOCH_3CH_2-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CH_2CH_3$	$-(CH_2)_3CH_3$	-	-	-	24±36(3)
LM1246	$-CH_2-$	-CONH-	$-OPO_2CH_2-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CH_2CH_3$	$-(CH_2)_3CH_3$	-	-	-	45(1)
LM1258	$-CH_2-$	$-SO_2NH-$	$-OCH_2CF_3$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	-	$-(CH_2)_3CH_3$	-	-	-	0(1)
LM1261	$-CH_2-$	-CONH-	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CH_3$	$-(CH_2)_3CH_3$	-	-	-	80±6(3)
LM1265	$-CH_2-$	$-SO_2NH-$	$-OPO_2CH_2-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2CH_3$	$-(CH_2)_3CH_3$	-	-	-	30±18(3)
LM1277	$-CH_2-$	$-SO_2NH-$	$-OPO_2CH_2-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_3$	$-(CH_2)_3CH_3$	-	-	-	33±18(3)
LM1283	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-CH_2CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	R	45±26(3)
LM1284	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-CH_2CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	S	12±10(3)
LM1292	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2OH$	$-(CH_2)_3CH_3$	-	-	R	44±18(3)
LM1293	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2OH$	$-(CH_2)_3CH_3$	-	-	S	40±19(3)
LM1298	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2NH_3$	$-(CH_2)_3CH_3$	-	-	-	4±20(3)
LM1299	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_3$	$-(CH_2)_3CH_3$	-	-	-	0(3)
LM1300	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-C_6H_5$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	-	24±24(3)
LM1304	$-CH_2-$	$-SO_2NH-$	$-OSO_2CH_2-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	-	28±5(3)
LM1309	$-CH_2-$	-CONH-	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_7H_{14}$	$-CH_2CH_2NH_3$	$-(CH_2)_3CH_3$	-	-	-	28±28(3)
LM1313	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-(CH_2)_3C_6H_5$	$-CH_2CH_2O-$	-	-	$-CH_2C_6H_5$	-	36±12(3)
LM1338	$-CH_2-$	$-SO_2NH-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	S	46±15(7)
LM1339	$-CH_2-$	$-SO_2CH_2-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	$-CH_2C_6H_5$	-	79±17(3)
LM1340	$-CH_2-$	$-SO_2CH_2-$	$-OPO_2O-$	$-(CH_2)_3CH_3$	$-C_6H_{12}$	$-CH_2CH_2O-$	$-(CH_2)_3CH_3$	-	-	-	29±3(3)

[a]See figure 1 for a schematic diagram of the molecules' structure. The GLI fragment corresponds to the glycerol backbone. Its chirality is specified as follows: R indicates that both experiments and modeling were performed with the R structure; likewise for S. For the remaining compounds, a racemic mixture was used in the experiments, but the R form was modeled as the most potent chirally resolved compound had R-stereochemistry. Enzyme activities were measured as described in ref. 13b with enzyme isolated from human synovial fluid and the natural substrate, phosphatydylethanolamine so that the experimental conditions were as relevant to human proinflammatory situations as possible. Inhibitor activities (taken from ref. 13) are expressed as % enzyme inhibition (with standard deviation) at 0.01 mole fraction of inhibitor in the substrate vesicles. The number of activity measurements for each compound is shown in parentheses. XI(50) data available for 10 of these compounds (unpublished) show similar trends to the % inhibition data with a limited linear correlation (R=0.86). This provides support for the validity of correlating % inhibition data and receptor binding affinity.