

Volume 72 (2016)

**Supporting information for article:** 

Novel protein-inhibitor interactions in Site 3 of Ca<sup>2+</sup>-bound S100B as discovered by X-ray crystallography

Michael C. Cavalier, Zephan Melville, Ehson Aligholizadeh, E. Prabhu Raman, Wenbo Yu, Lei Fang, Milad Alasady, Adam D. Pierce, Paul T. Wilder, Alexander D. MacKerell and David J. Weber

**Table S1** Calculated RMSD (Å) of Models from  $C^{\alpha}$  of **1MHO**.

S100B•SC0025	0.459 (0.327)
S100B•SC1990	0.351 (0.286)

Modeled protein chains are compared to that of <u>1MHO</u>. Numbers in parentheses are the calculated RMSD of only the globally conserved residues 1-84.



**Figure S1** Representative Western Blot Analysis. The control without drug was treated with an equivalent amount of DMSO. The addition of SC0025 (DMSO stock solution) did not affect the protein levels of S100B in the shRNA<sup>scrambled</sup> (High S100B) or shRNA<sup>S100B</sup> (Low S100B) WM115 cell lines. There was no measureable gain in total p53 levels in the presence of SC0025.