Supporting Information



Supplementary Scheme 1: Synthesis of compound 4 reagents and conditions: (a) 20% piperidine in DMF, rt, 30 min, two times; (b) Fmoc-L-Ile-OH, oxyma pure, DIC, DIEA, DMF, rt, 2 h; (c) Fmoc-L-Glu(Otbu)-OH, oxyma pure, DIC, DIEA, DMF, rt, 2 h; (d) Fmoc-L-Cyclopentylglycine, oxyma pure, DIC, DIEA, DMF, rt, 2 h; (e) Fmoc-L-Obenzylphosphotyrosine, oxyma pure, DIC, DIEA, DMF, rt, 2 h; (f) Acetic anhydride, DIEA, DMF, rt, 2 h; (g) TFA, phenol, TIPS, water, rt, 3 h.



Supplementary Figure 1: Time course of full length GST-YopH dephosphorylation of Lck.



Supplementary Figure 2: Compound **14** (up to 60 µM) did not inhibit full length GST-YopH catalytic activity to hydrolyze DiFMUP.



Supplementary Figure 3: 1D proton NMR spectra for the indicated molecules are recorded in absence and presence of a catalytic amount of full length GST-YopH. In the bottom spectrum, the aromatic ¹H resonances of DiFMUP are shown in black (60 μ M, in absence of GST-YopH), while the hydrolyzed DiFMUP, obtained by adding 15 nM of GST-YopH and incubating for 60 minutes, is shown in red. Similarly, the aromatic region of the 1D NMR ¹H spectrum of compound **14** (60 μ M) is reported in blue, in absence of GST-YopH, and in green after incubation with 15 nM GST-YopH for 60 minutes. In aromatic region of compound **14** in the free form (blue), the aromatic resonances for the F residue are close to 7.25 ppm while the aromatic resonances for the and pY residue occur around 7 ppm. In green the spectrum showed F still at ~7.25 ppm while peaks of tyrosine have shifted.



Supplementary Figure 4: HPLC trace for compound 14.



Supplementary Figure 5: 1D 1H NMR spectrum for compound 14 in d6DMSO.



Supplementary Figure 6: MS spectrum for compound 14.