

## Supplementary Data

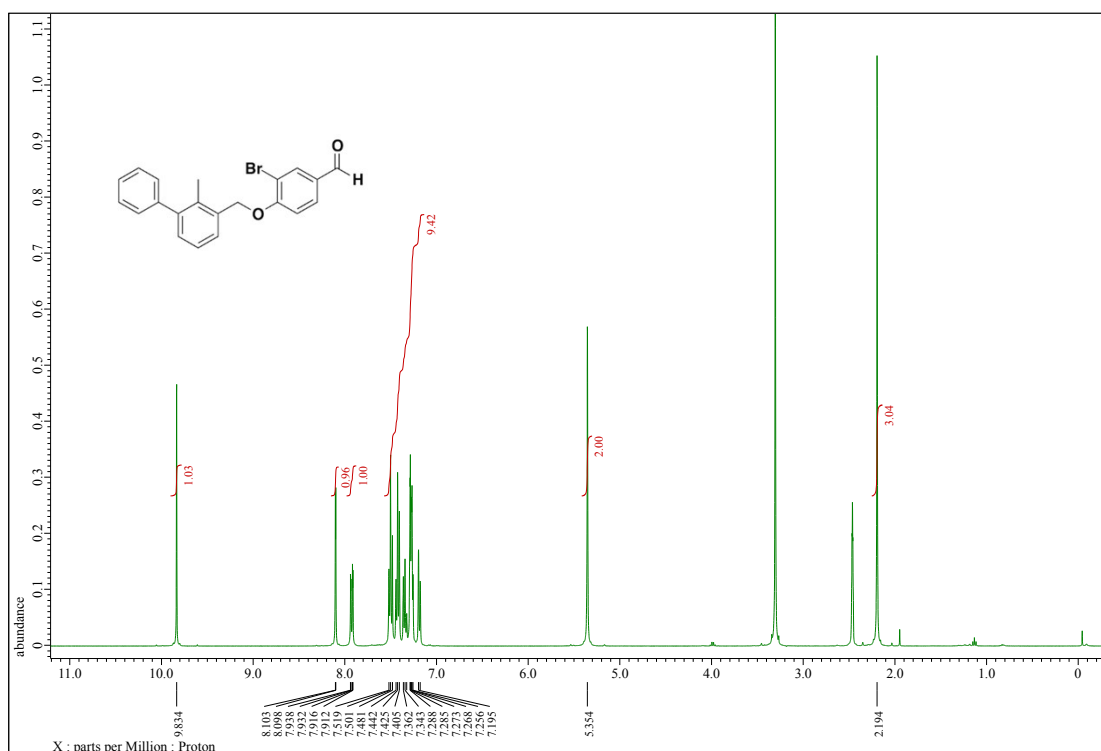


Figure S1.  $^1\text{H}$  NMR spectrum of **C1** in  $\text{DMSO-d}_6$

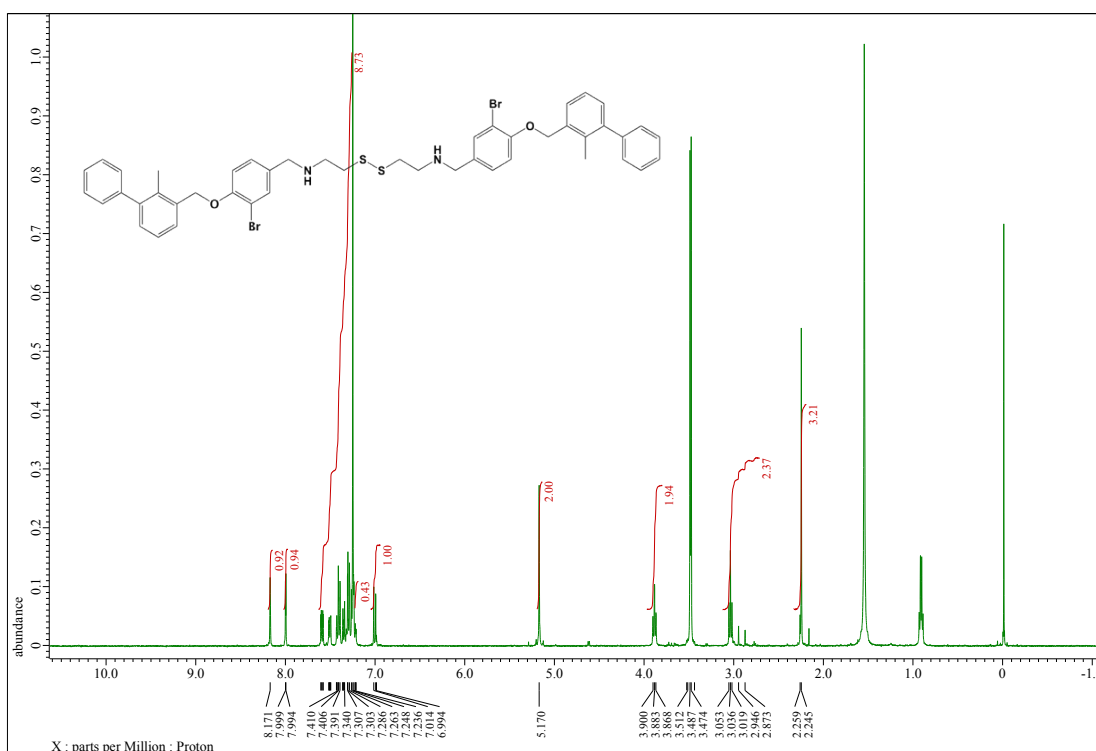


Figure S2.  $^1\text{H}$  NMR spectrum of **C2** in  $\text{CDCl}_3$

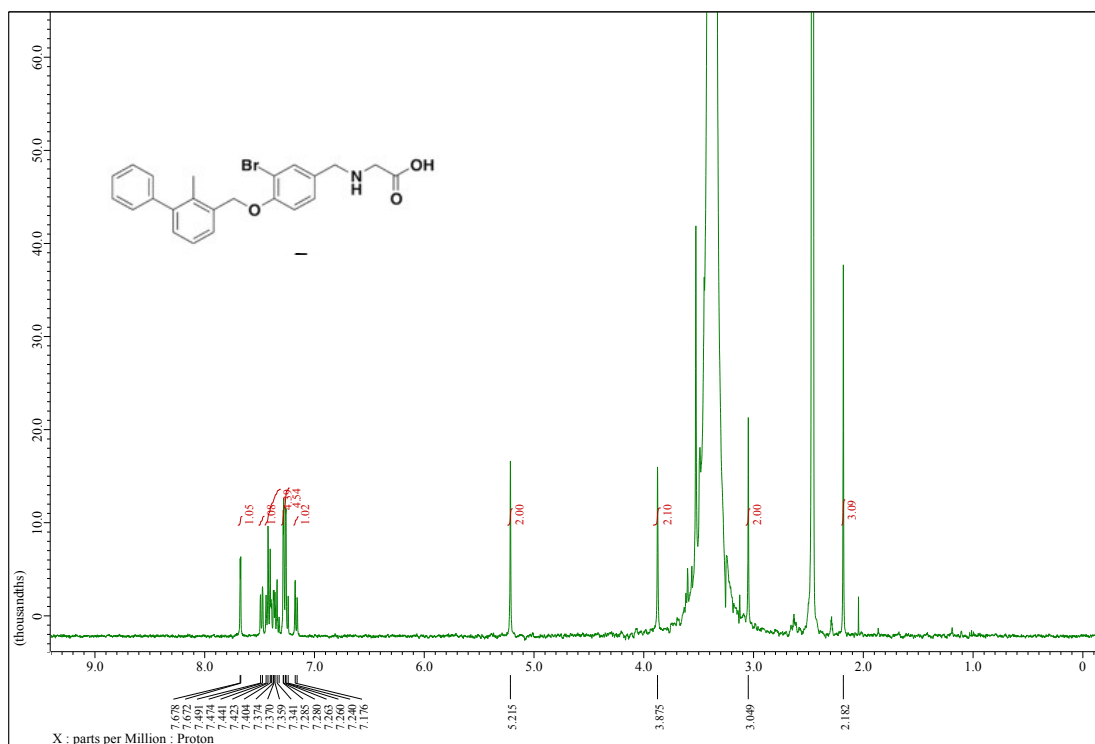


Figure S3.  $^1\text{H}$  NMR spectrum of C3 in  $\text{DMSO-d}_6$

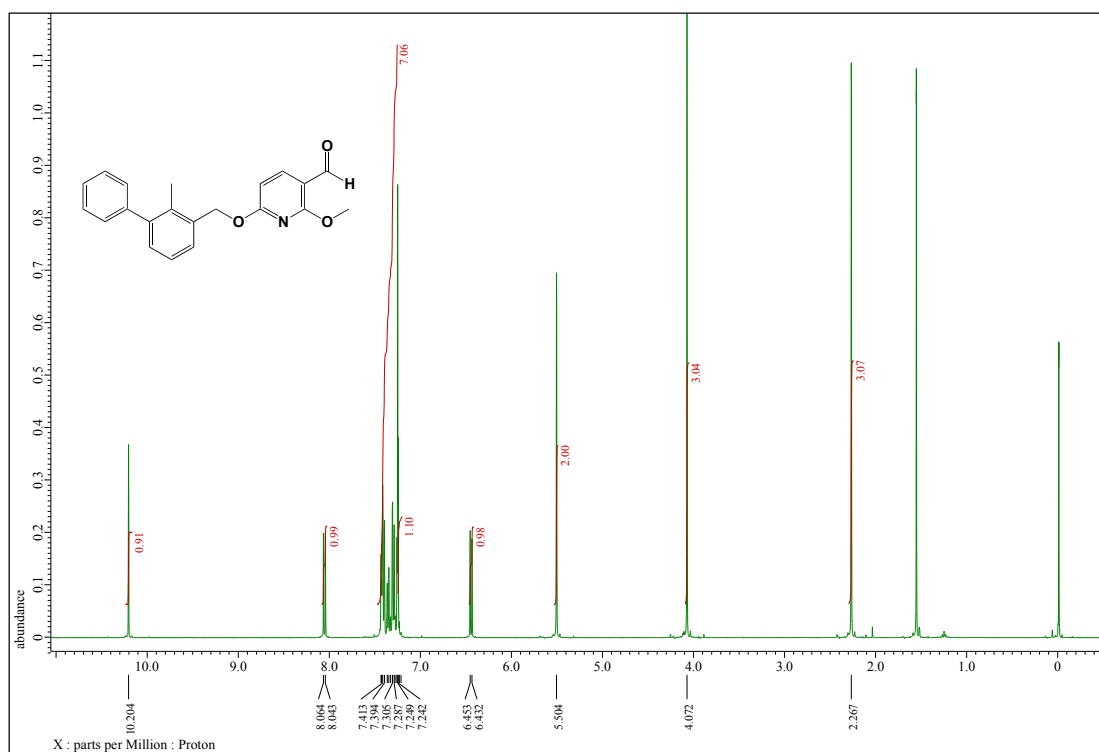
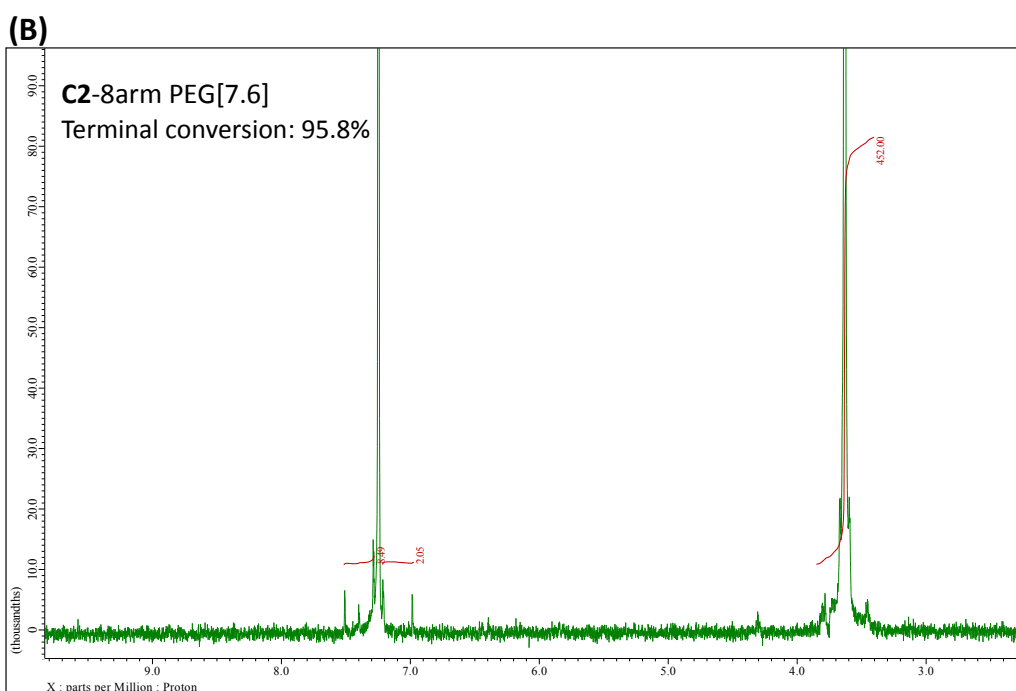
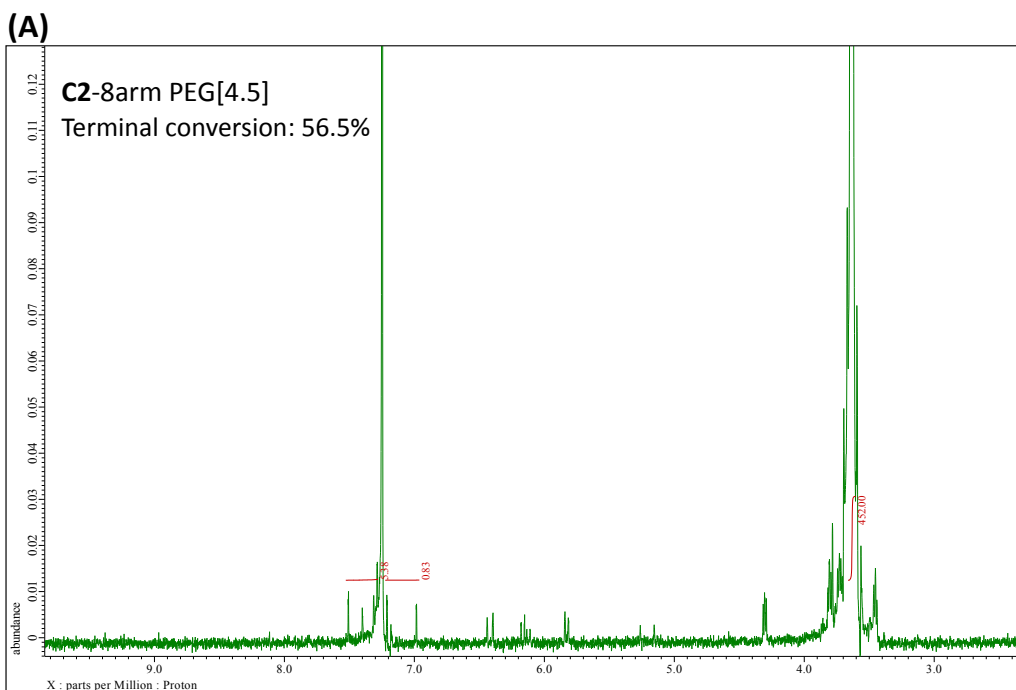
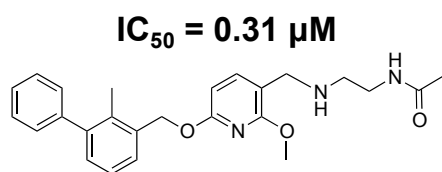


Figure S4.  $^1\text{H}$  NMR spectrum of C4 in  $\text{CDCl}_3$

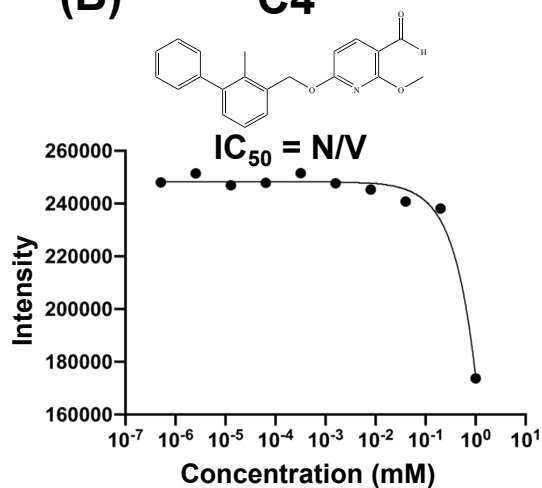


**Figure S5.**  $^1\text{H}$  NMR spectra in  $\text{DMF-d}_7$  of (A) **C2-8arm PEG[4.5]** and (B) **C2-8arm PEG[7.6]**.

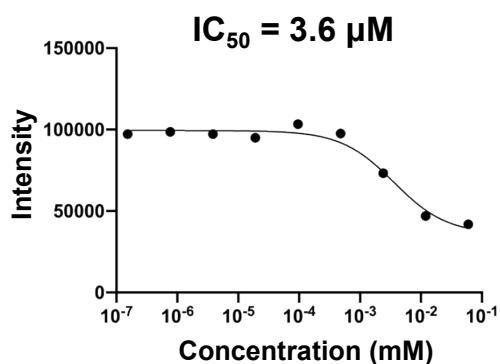
**(A) BMS-202**



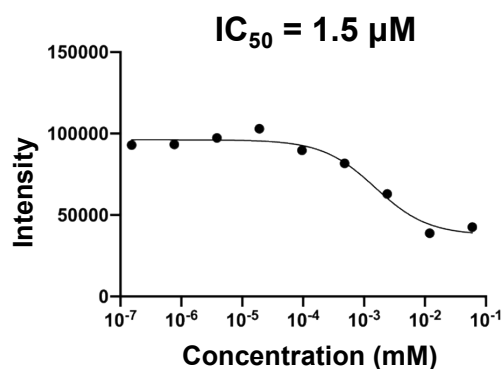
**(B) C4**



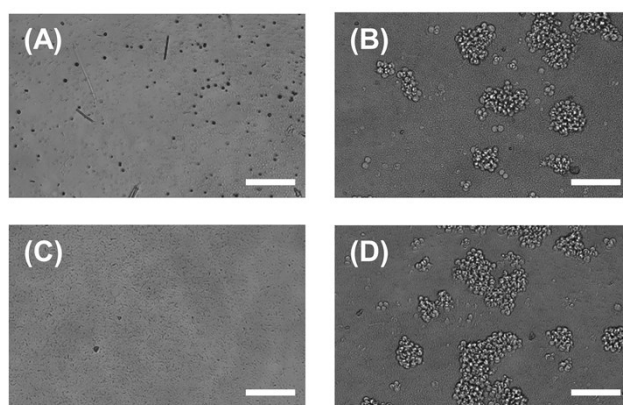
**(C) C4-8arm PEG[1.5]**



**(D) C4-8arm PEG[3.7]**



**Figure S6.** (A) BMS-202 which was previously reported small molecular inhibitor, (B) BMS-202 derivative, (C) and (D) Multivalent C4 (C4-8arm PEG conjugates)



**Figure S7.** Photos of (A, B) BMS-8 and (C,D) C4 in the cell culture medium (A,C) in the absence of Jurkat T cells and (B,D) in the presence of Jurkat T cells. Concentration: 50 μM. Scale bars=100 μm.