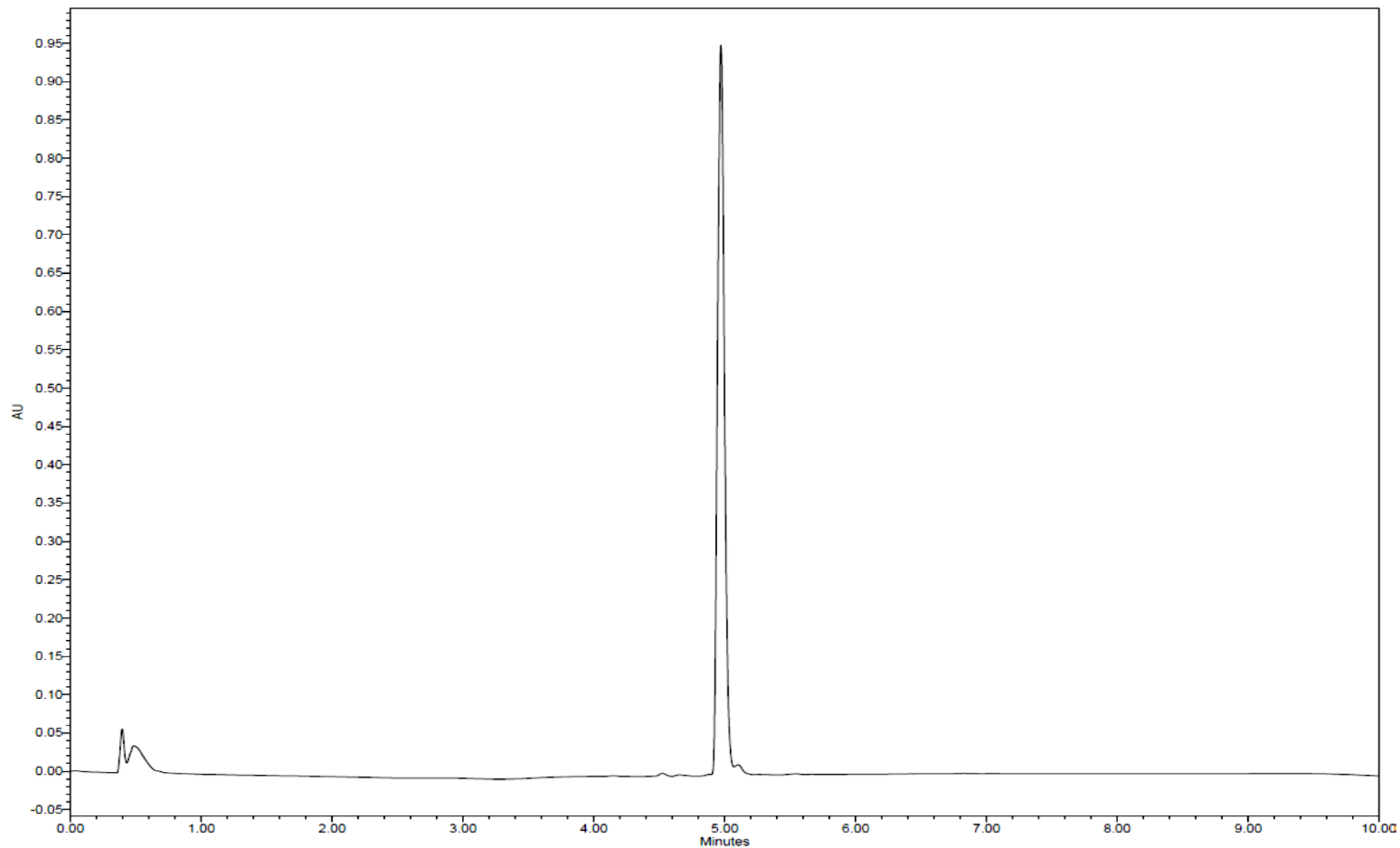
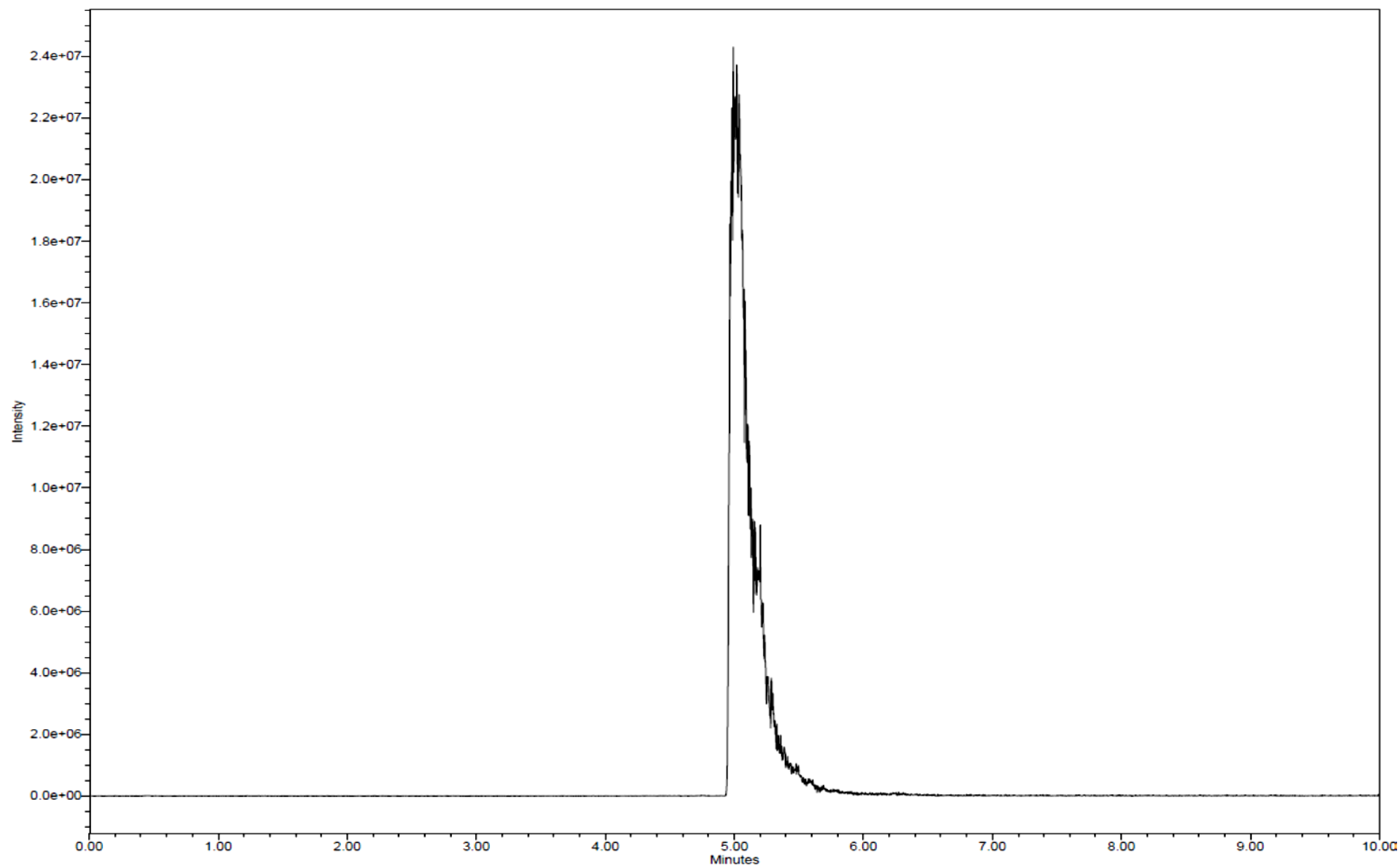


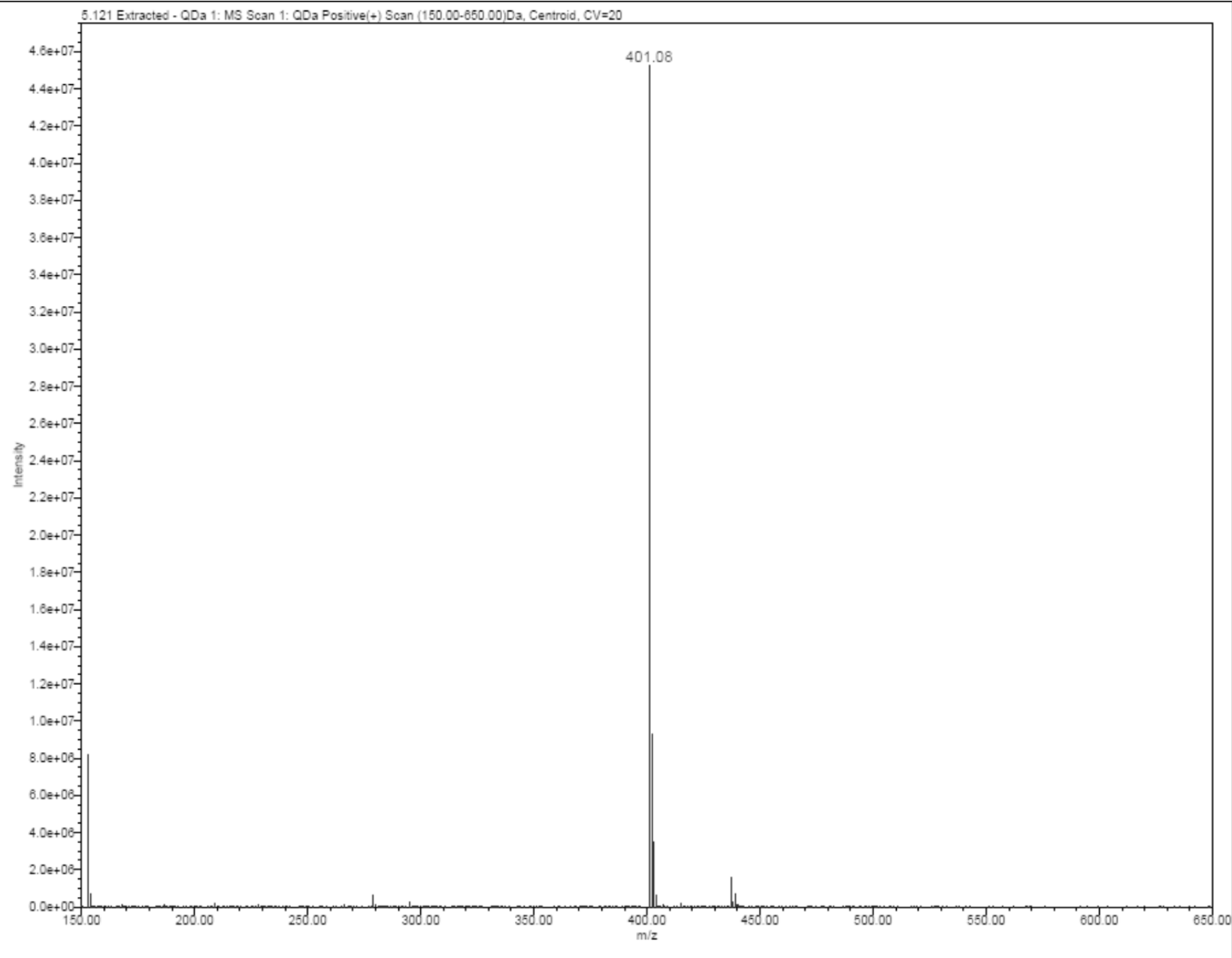
**Figure S1.** Protein NMR Spectra of UCUF-728. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.80 (d, *J* = 8.6 Hz, 2H), 7.60 (d, *J* = 8.6 Hz, 2H), 7.19 (d, *J* = 3.0 Hz, 1H), 7.08 (s, 1H), 6.67 (d, *J* = 8.9 Hz, 1H), 6.58 (dd, *J* = 8.9, 3.0 Hz, 1H), 3.77 (s, 3H), 3.62 (s, 3H), 2.18 – 2.06 (m, 1H), 1.19 – 1.06 (m, 4H).



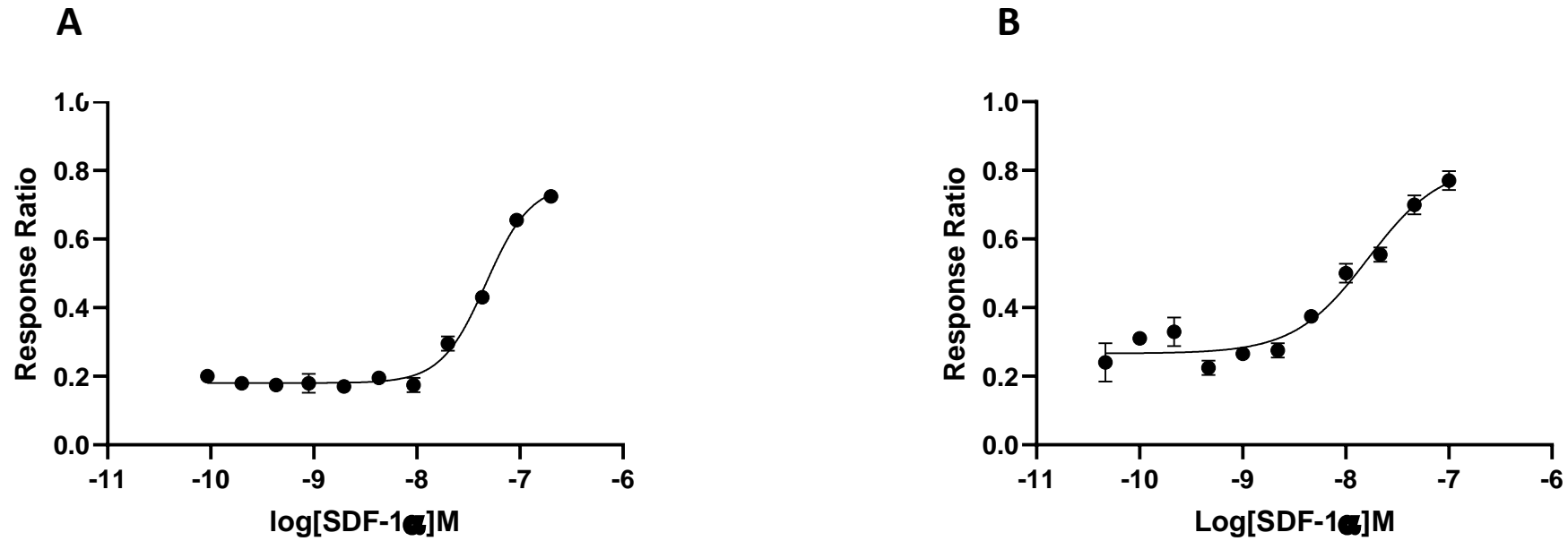
**Figure S2.** Liquid chromatography Spectra of UCUF-728 at 254 nm.



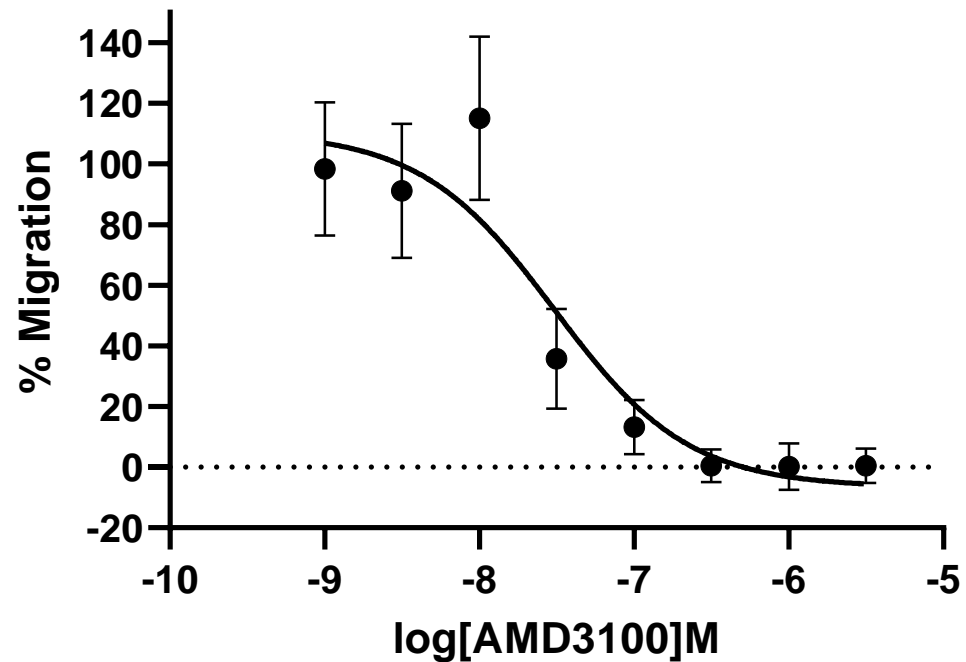
**Figure S3.** Mass Spectrometry Chromatogram of UCUF-728.



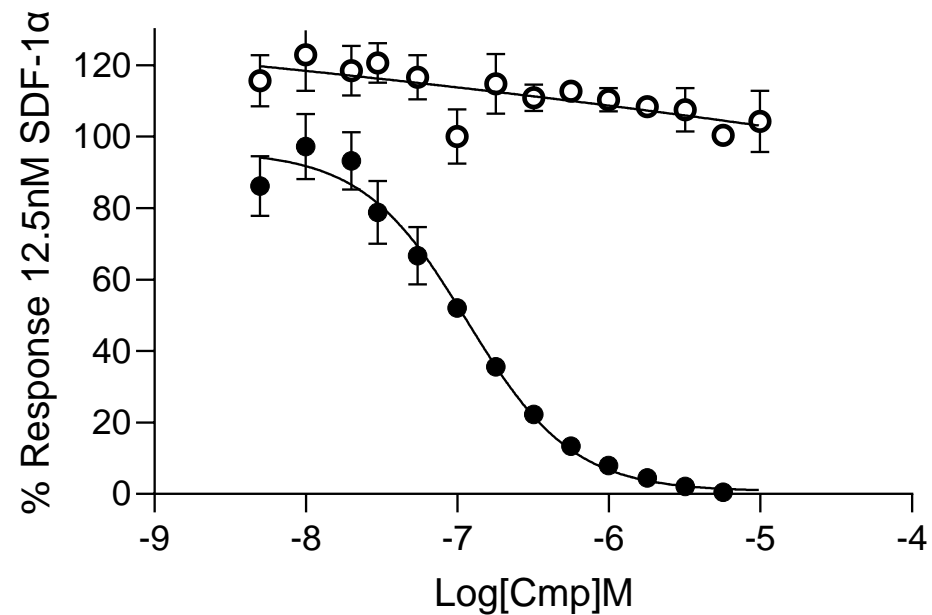
**Figure S4.** Mass Spectrometry of UCUF-728. Chemical Formula:  $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_5\text{S}$   
Calculated  $[\text{M}+\text{H}]$ : 401.12



**Figure S5.** Dose-dependent  $\beta$ -arrestin recruitment in U2OS-CXCR4 $bla$  cells of SDF-1 $\alpha$  purchased from A) R&D Systems (Log EC<sub>50</sub> =  $-7.33 \pm 0.06$ ) and B) Peprtech (Log EC<sub>50</sub> =  $-7.78 \pm 0.05$ ).



**Figure S6.** Percent Migration of Lymphoblasts Antagonized by AMD 3100. AMD3100 dose-dependently inhibited migration in CEM lymphoblasts with  $\log\text{IC}_{50} = -7.5 \pm 0.6$ . Data is normalized to media only (low control) and 6nM SDF-1 $\alpha$  (high control). Data is average of duplicate experiments performed n triplicate.



**Figure S7.** Antagonism of SDF-1 $\alpha$  binding to CXCR4 Receptor. SDF-1 $\alpha$  binding was validated using the Tag-Lite CXCR4 system (CisBio) according to manufacturer protocol. AMD3100 dose-dependently displaced SDF-1 $\alpha$  saturation binding (closed circles) and UCUF-728 did not displace SDF-1 $\alpha$  saturation binding (open circles).