

Figure S1. HS-549: **Top panel**) QC-HPLC: 250 X 4.6 mm Phenomenex 5  $\mu$  Luna C18 column, Mobile phase: A-0.1% TFA in water; B-0.1% TFA in acetonitrile. Gradient: 10% B for 0-2 min and 10% B to 70%B in 2-25 min (linear), flow rate 1mL/min. UV 220 nm. **Middle panel**)  $^1\text{H}$ -NMR spectrum (500 MHz,  $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ ) and **Bottom panel**)  $^{13}\text{C}$ -NMR spectrum (125 MHz,  $\text{CD}_3\text{C N}/\text{D}_2\text{O}$ ).

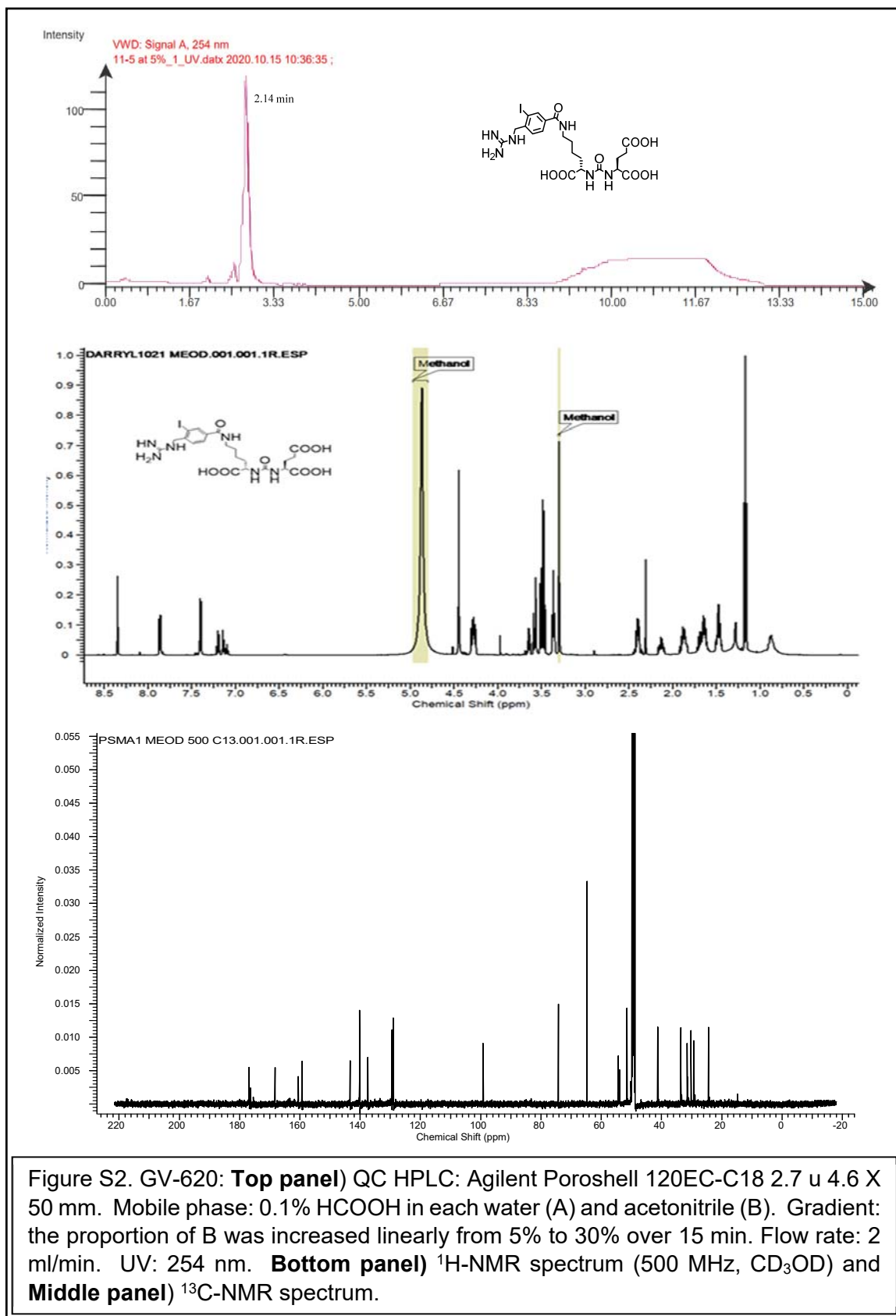
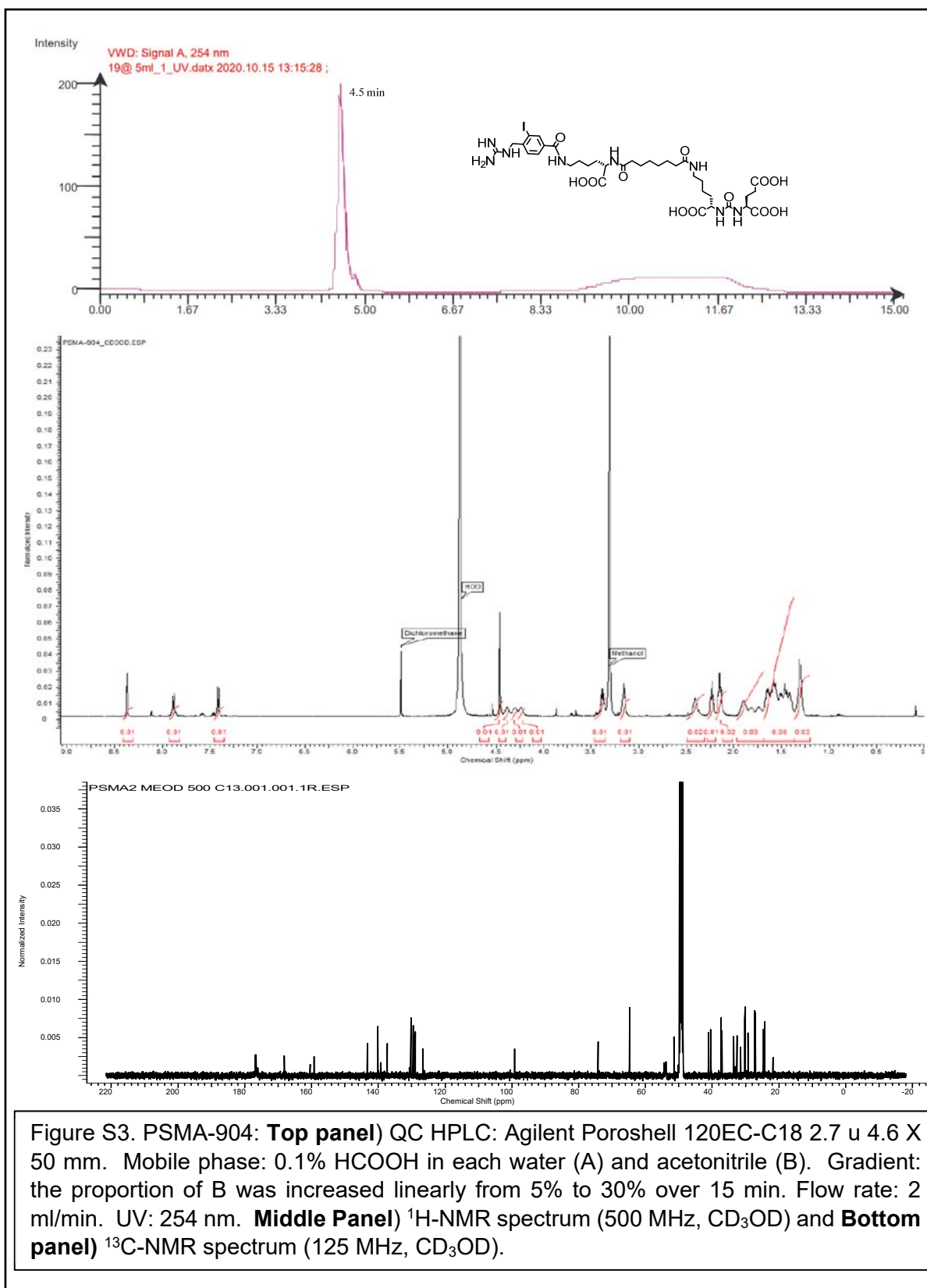
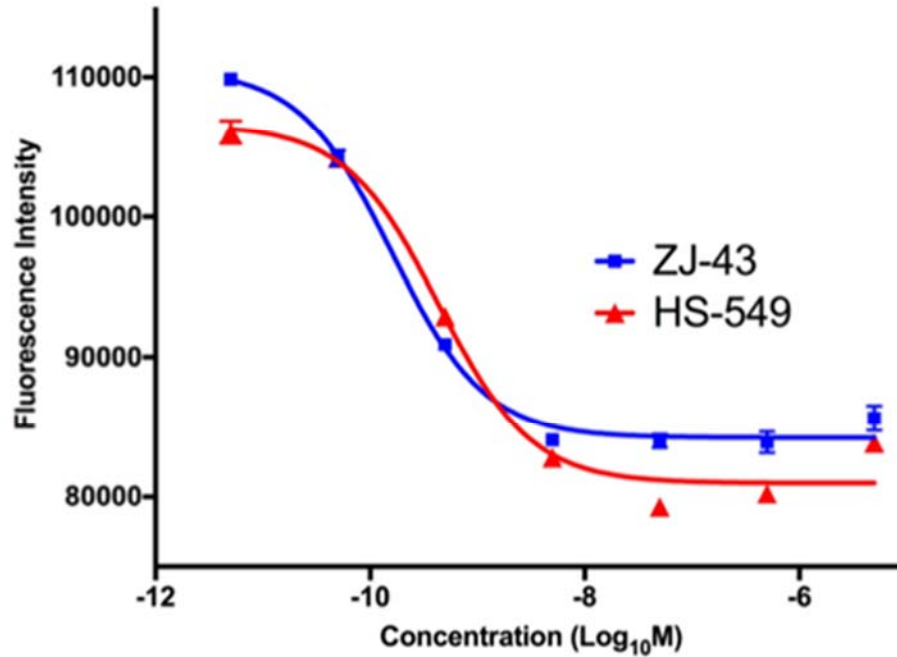


Figure S2. GV-620: **Top panel)** QC HPLC: Agilent Poroshell 120EC-C18 2.7 u 4.6 X 50 mm. Mobile phase: 0.1% HCOOH in each water (A) and acetonitrile (B). Gradient: the proportion of B was increased linearly from 5% to 30% over 15 min. Flow rate: 2 ml/min. UV: 254 nm. **Bottom panel)**  $^1\text{H-NMR}$  spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) and **Middle panel)**  $^{13}\text{C-NMR}$  spectrum.



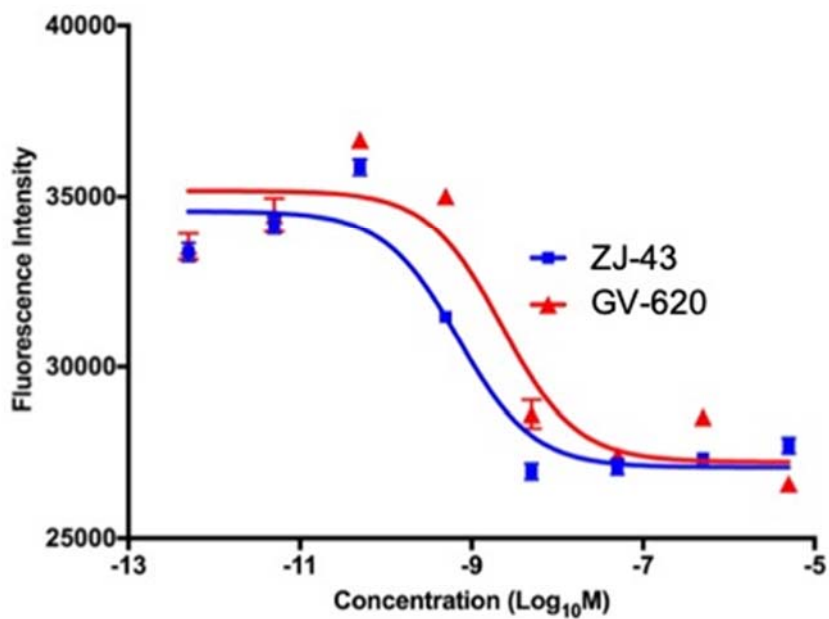
# HS-549



Compound	$\text{IC}_{50}$ (nM)	$\text{IC}_{50}$ 95% Confidence Interval (nM)	$\text{K}_i$ (nM)	$\text{K}_i$ 95% Confidence Interval (nM)
HS-549	0.43	0.31 – 0.60	0.09	0.06 – 0.12
ZJ-43	0.16	0.12 – 0.21	0.03	0.02 – 0.04

Figure S4. Amplex assay data for HS-549.

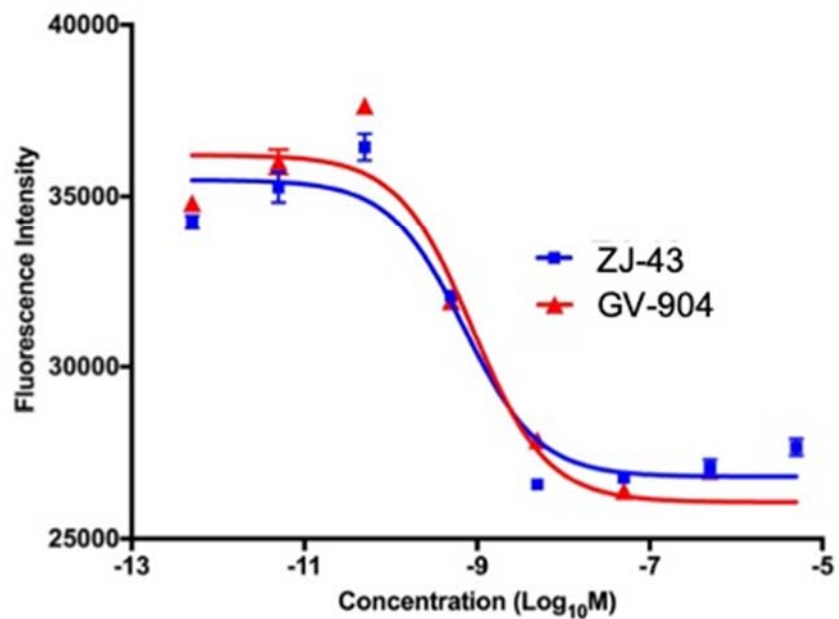
# GV-620



Compound	$\text{IC}_{50}$ (nM)	$\text{IC}_{50}$ 95% Confidence Interval (nM)	$\text{K}_i$ (nM)	$\text{K}_i$ 95% Confidence Interval (nM)
GV-620	2.24	0.89 – 5.64	0.45	0.18 – 1.13
ZJ-43	0.70	0.34 – 1.43	0.14	0.07 – 0.29

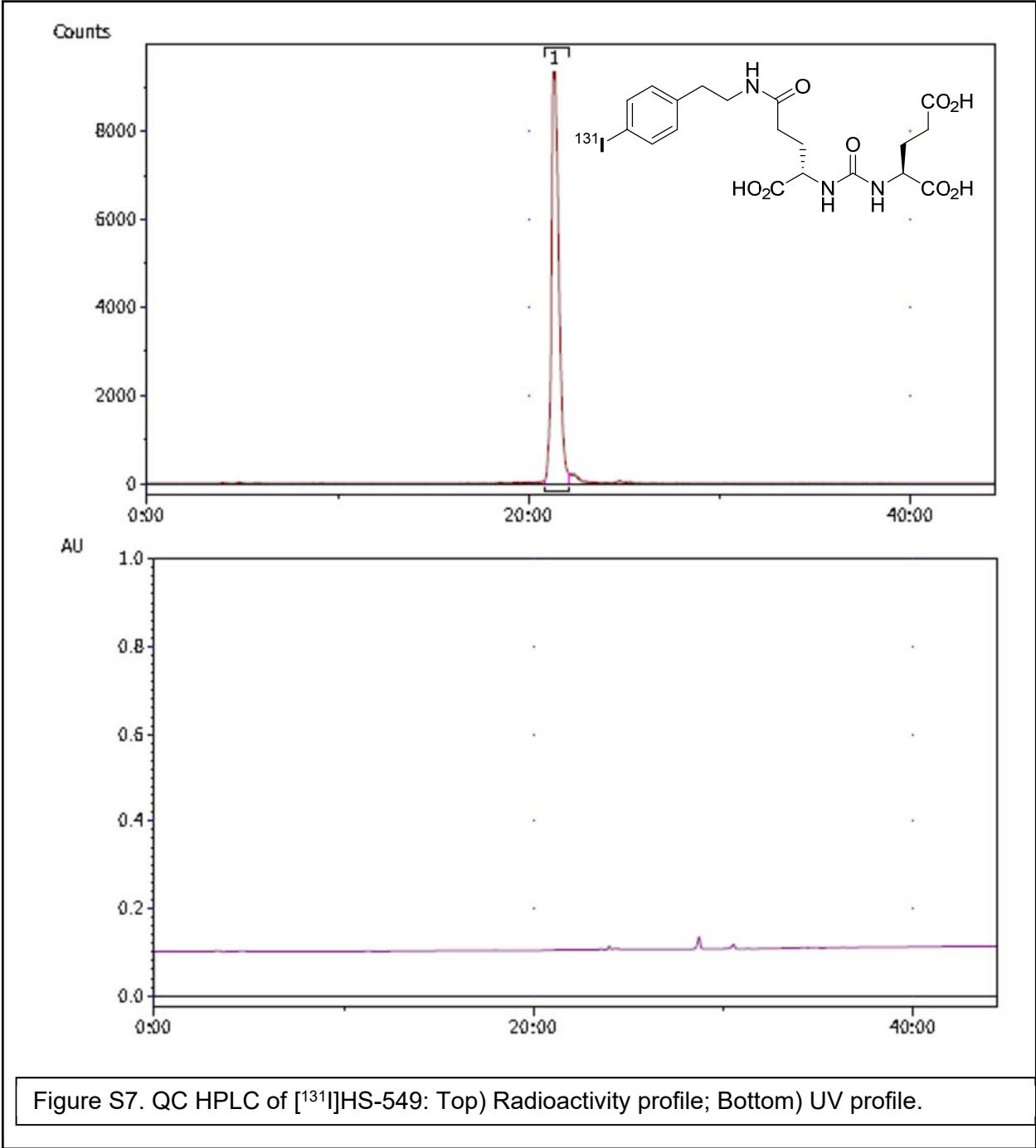
Figure S5. Amplex assay data for GV-620.

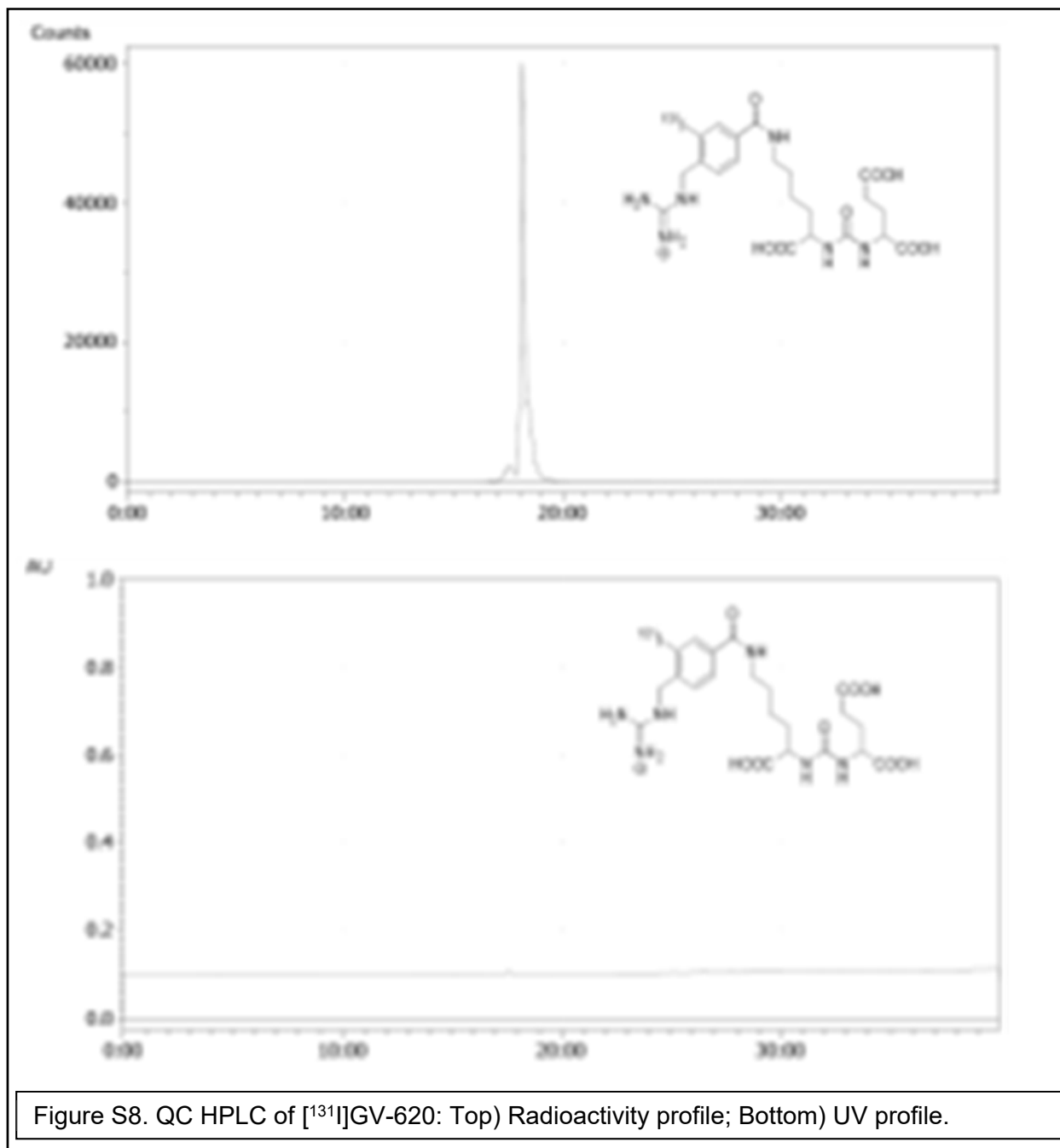
# GV-904



Compound	$\text{IC}_{50}$ (nM)	$\text{IC}_{50}$ 95% Confidence Interval (nM)	$\text{K}_i$ (nM)	$\text{K}_i$ 95% Confidence Interval (nM)
GV-904	0.88	0.47 – 1.63	0.18	0.09 – 0.32
ZJ-43	0.70	0.37 – 1.32	0.14	0.07 – 0.26

Figure S6. Amplex assay data for GV-904.







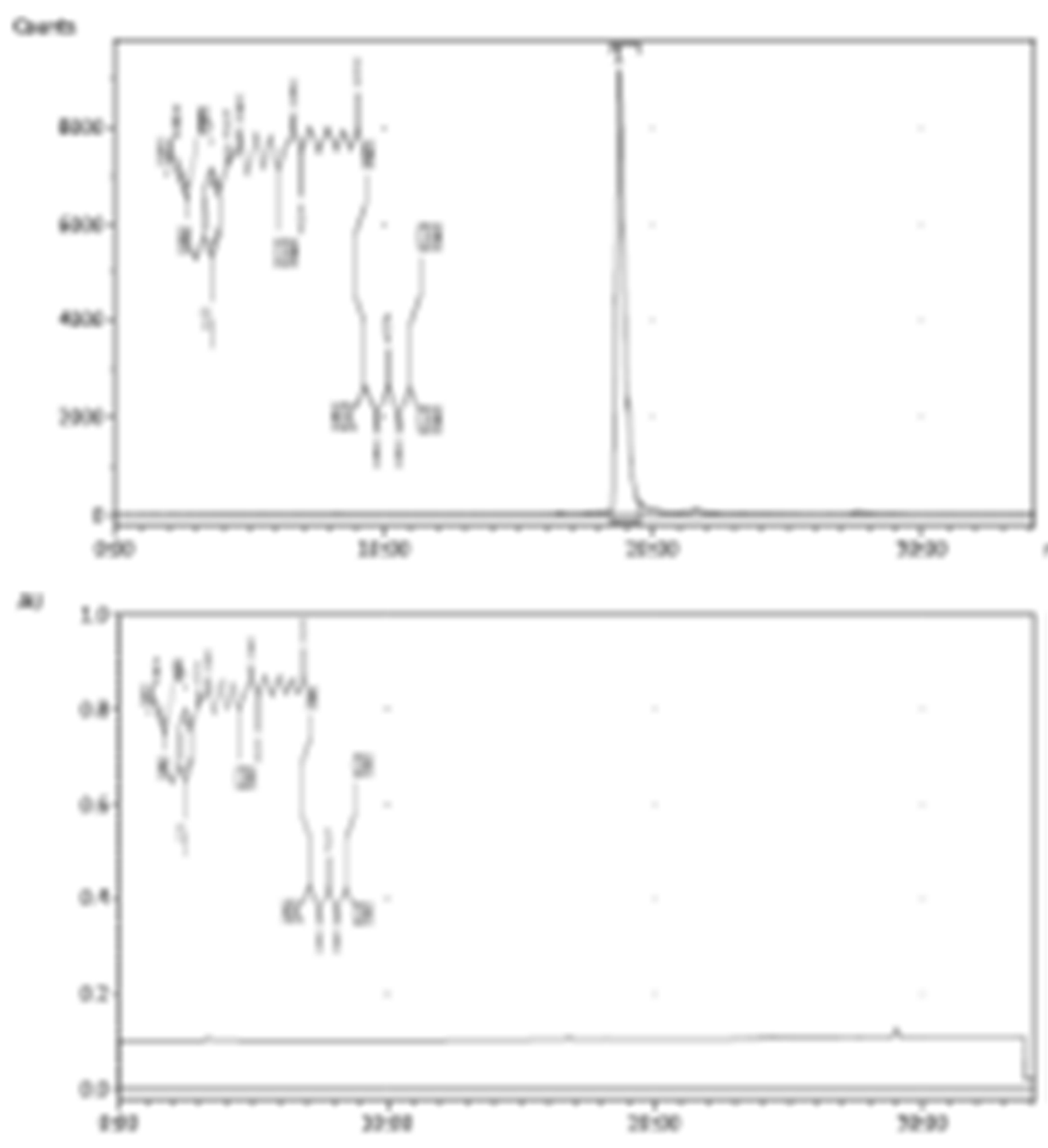


Figure S9. QC HPLC of [<sup>131</sup>I]GV-904: Top) Radioactivity profile; Bottom) UV profile.

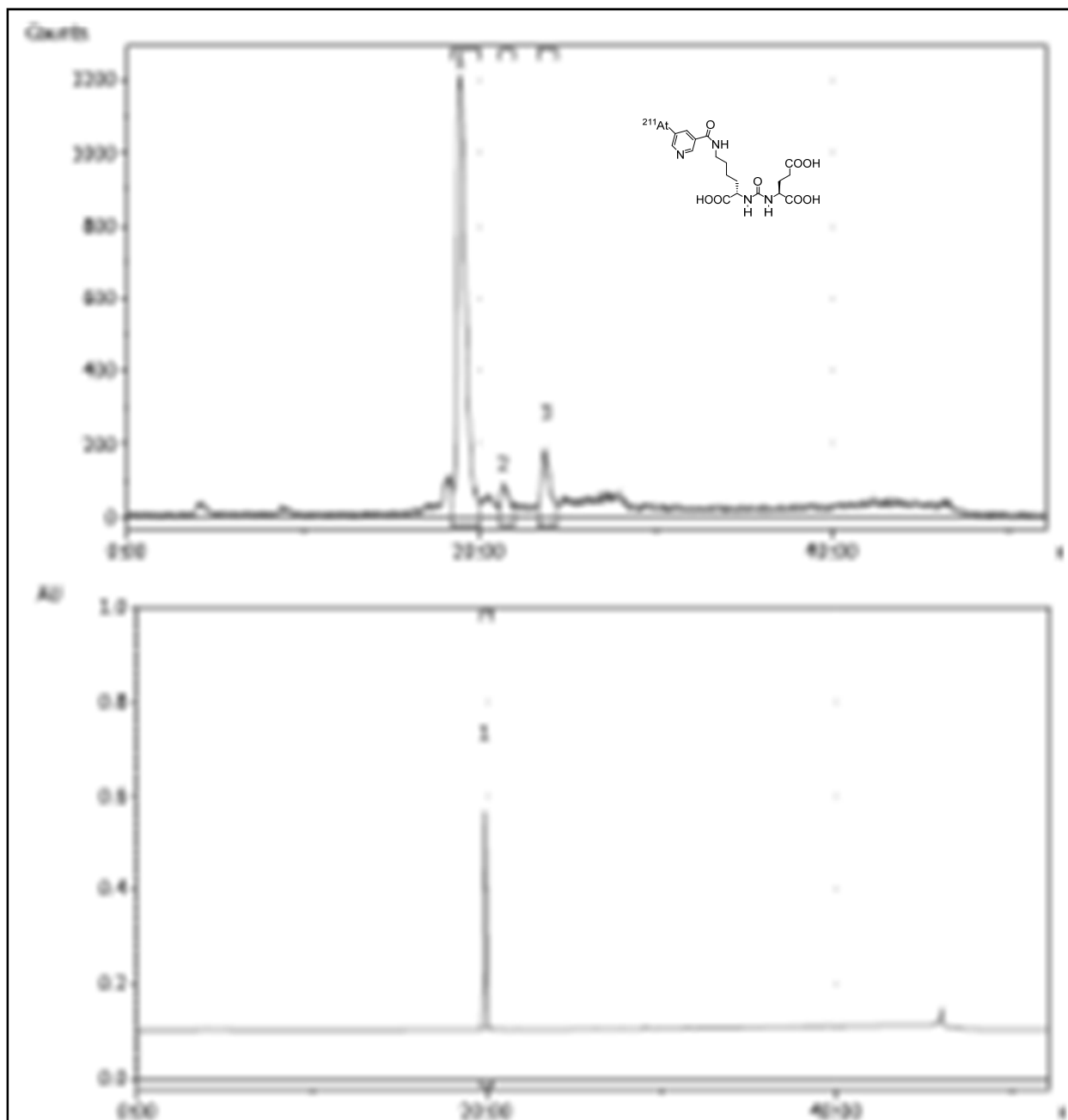
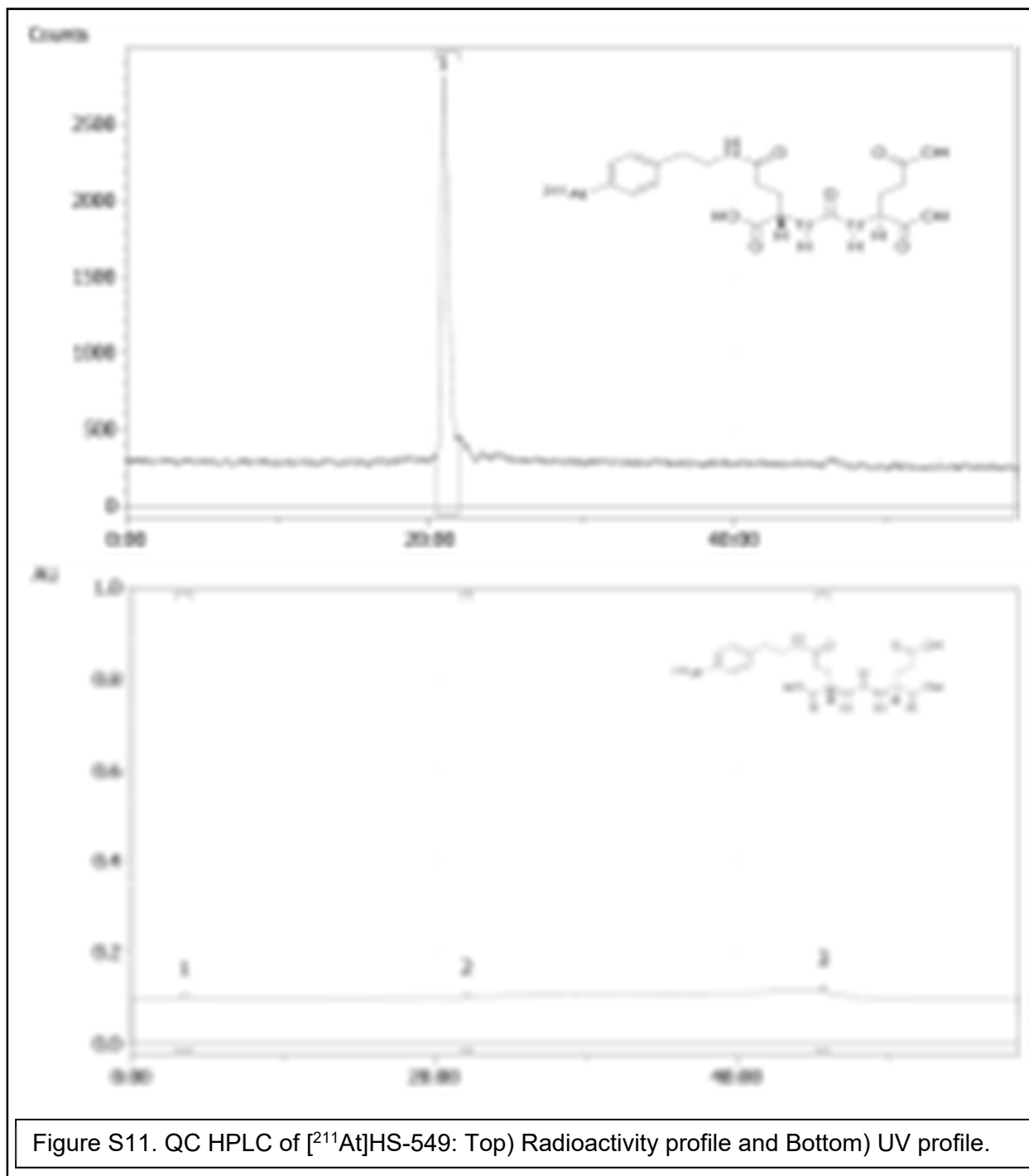
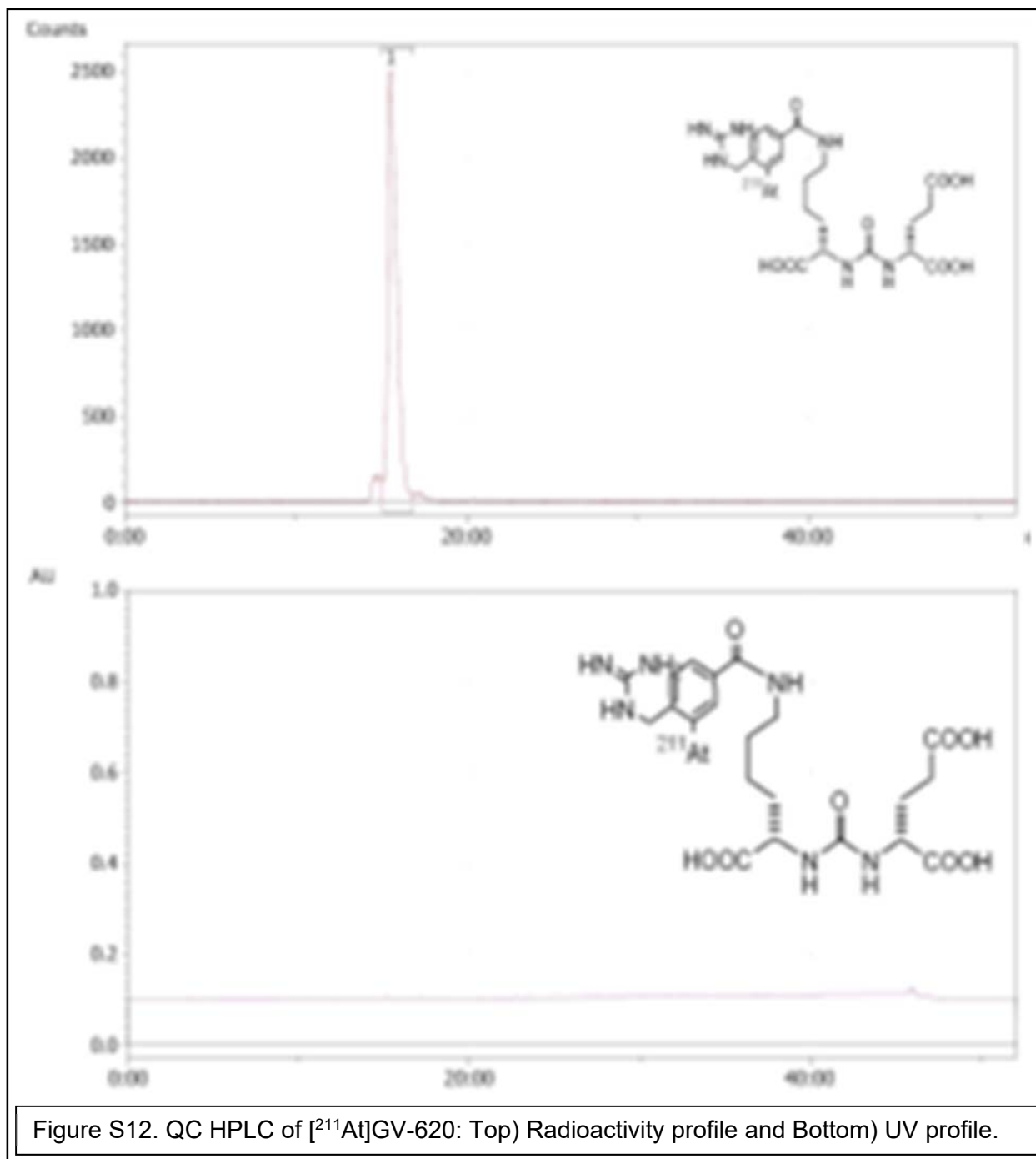


Figure S10. HPLC of  $[^{211}\text{At}]\text{YC-550}$  co-injected with YC-IV-550 standard: Top) Radioactivity profile and Bottom) UV profile.





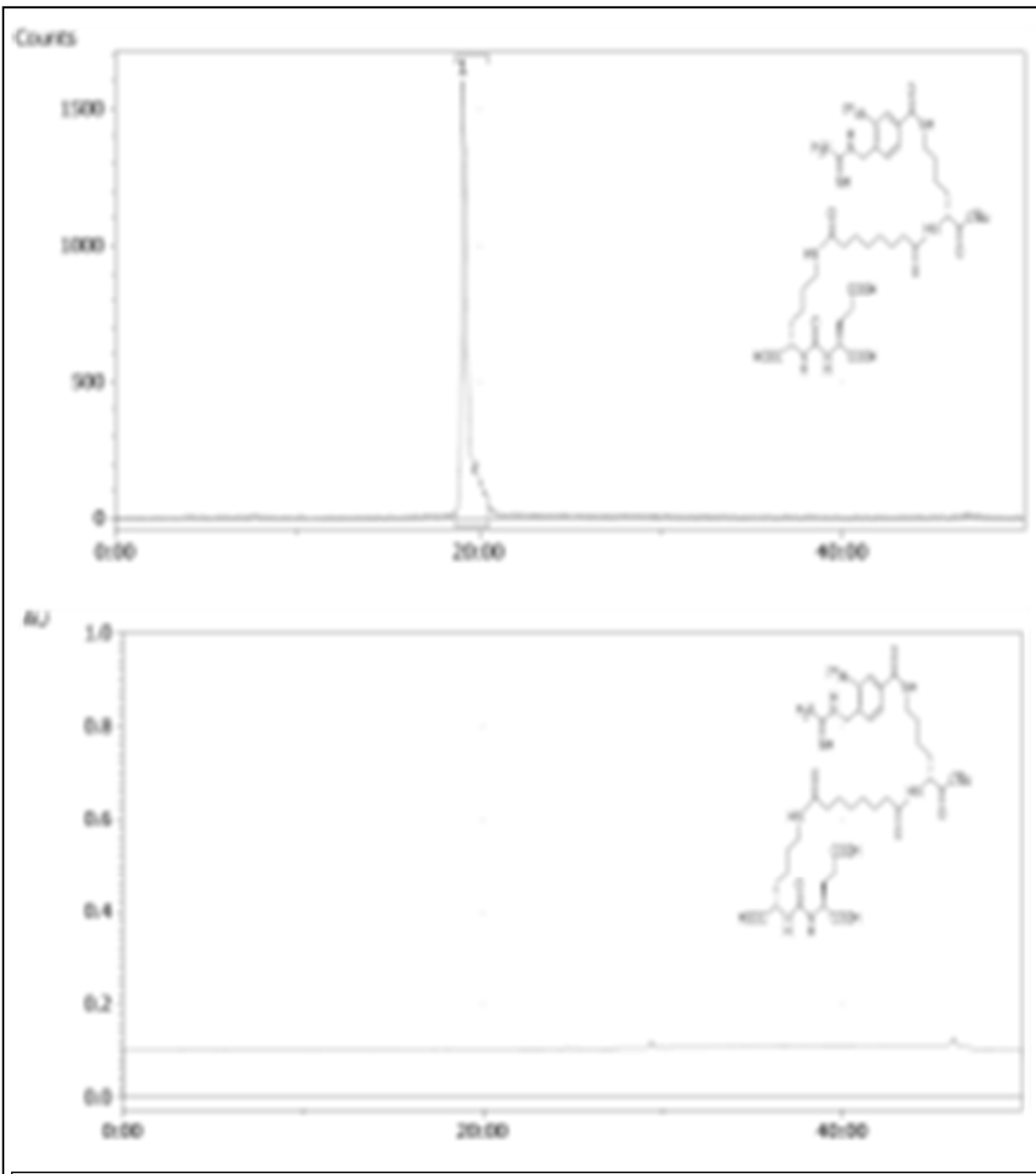


Figure S13. QC HPLC of  $[^{211}\text{At}]\text{GV-904}$ : Top) Radioactivity profile and Bottom) UV profile.