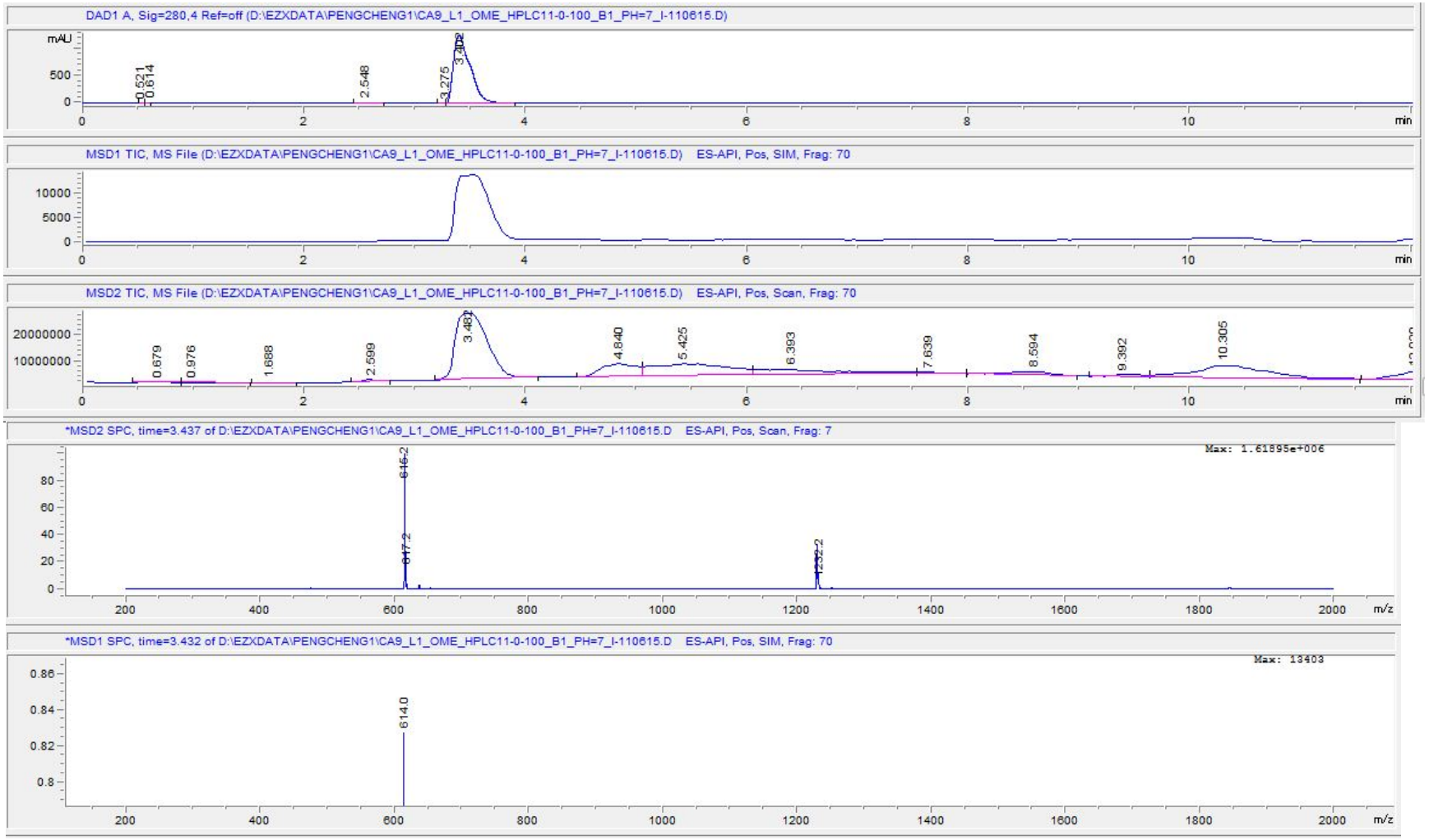
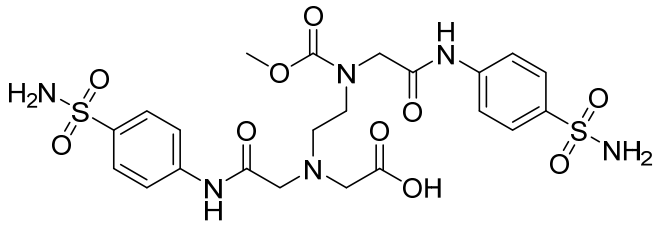
Evaluation of a Carbonic Anhydrase IX-Targeted Near-Infrared Dye for Fluorescence-Guided Surgery of Hypoxic Tumors

Supporting Information

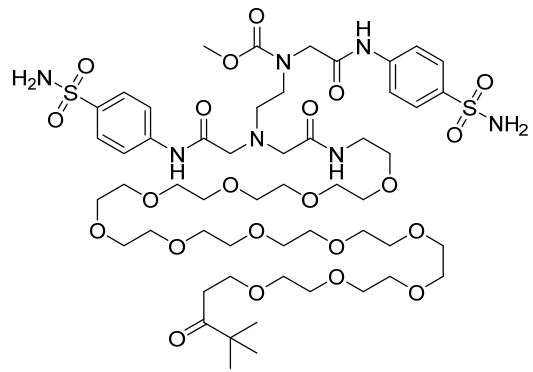


Chemical formula: $C_{22}H_{28}N_6O_{10}S_2$
Exact Mass: 600.13
Molecular Weight: 600.62



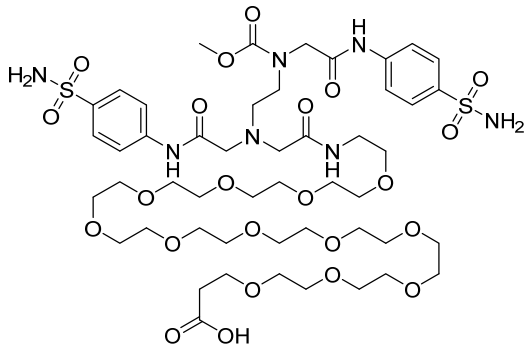
SI Figure 1. LC-MS characterization of methylated CA IX inhibitor.

Chemical formula:	$C_{53}H_{89}N_7O_{22}S_2$
Exact Mass:	1239.55
Molecular Weight:	1240.44

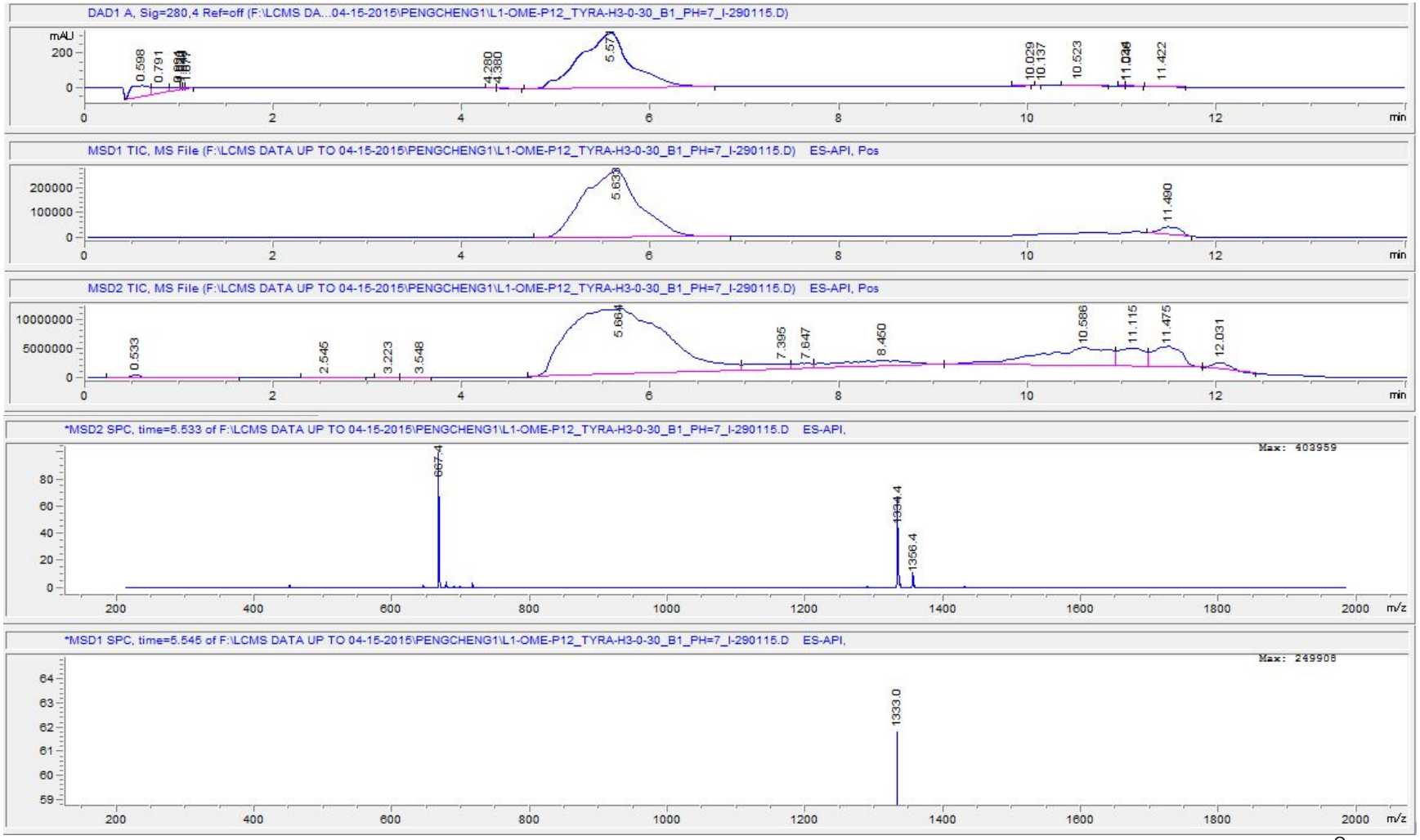


SI Figure 2. LC-MS characterization of protected PEGylated CA IX inhibitor.

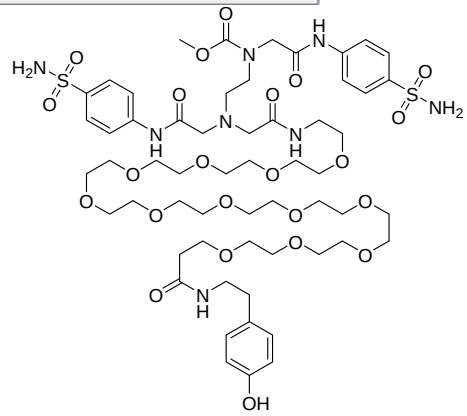
Chemical formula: $C_{49}H_{81}N_7O_{23}S_2$
Exact Mass: 1199.48
Molecular Weight: 1200.33



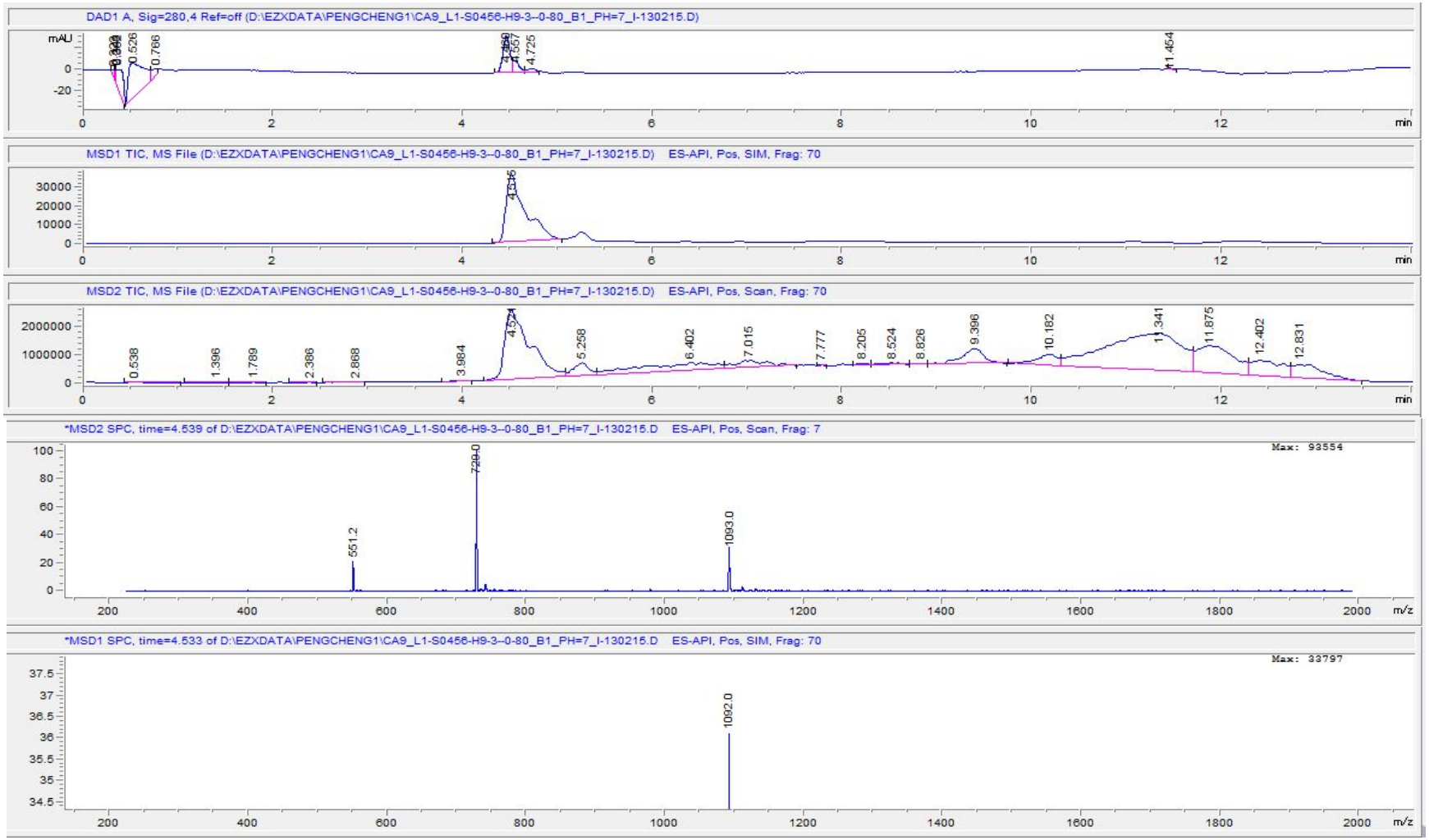
SI Figure 3. LC-MS characterization of deprotected PEGylated CA IX inhibitor.



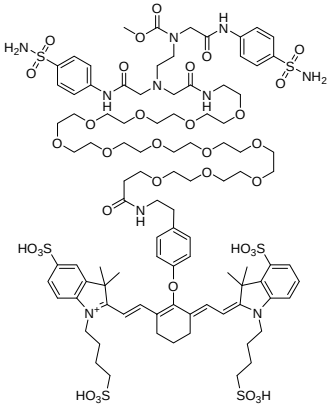
Chemical formula: $C_{57}H_{90}N_8O_{23}S_2$
Exact Mass: 1318.56
Molecular Weight: 1319.50



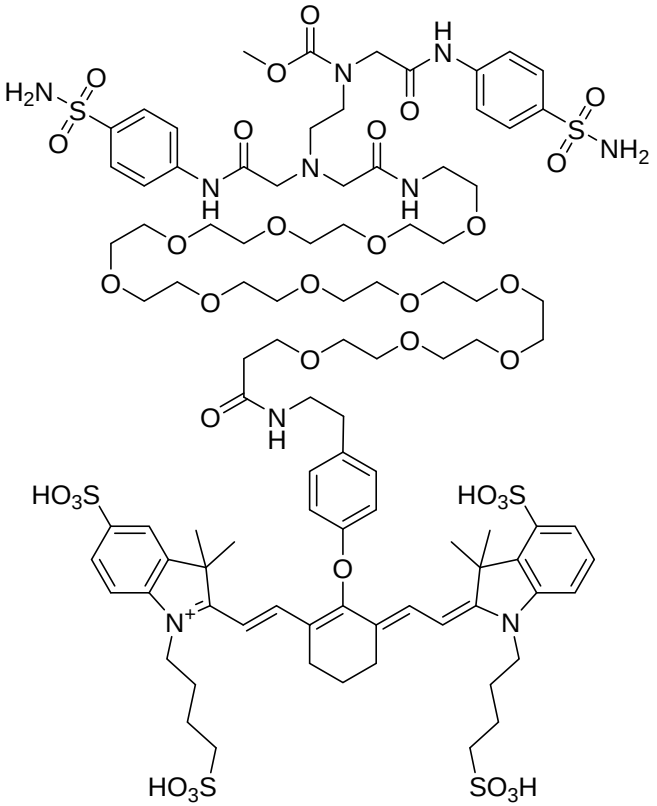
SI Figure 4. LC-MS characterization of tyramine-PEG-CA IX inhibitor.



Chemical formula: $C_{95}H_{137}N_{10}O_{35}S_6^+$
Exact Mass: 2169.76
Molecular Weight: 2171.54



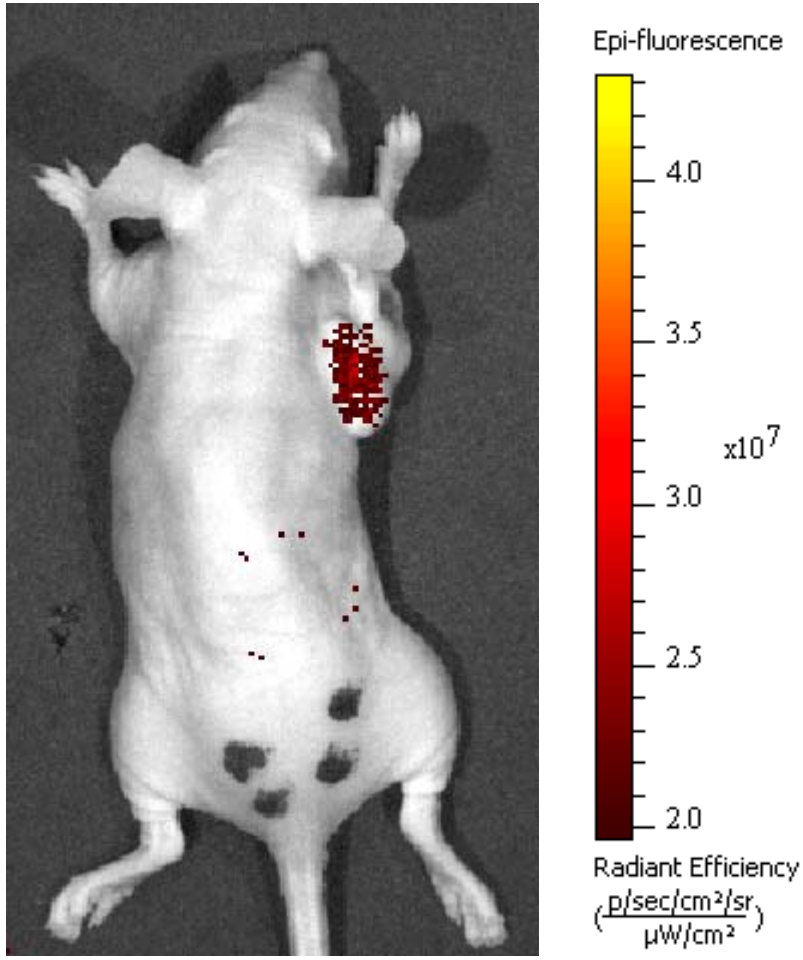
SI Figure 5. LC-MS characterization of Hypoxyfluor.



Hypoxyfluor physical properties:

Chemical formula $C_{95}H_{137}N_{10}O_{35}S_6^+$
Exact Mass: 2169.76
Molecular Weight: 2171.54
Elemental Analysis: 52.55% C, 6.36% H, 6.45% N, 25.79% O, 8.86% S
Physical appearance: Green colored solid
Water solubility: highly water soluble
Stability: stable for >3 months when protected from light at 0 ^oC

SI Figure 6. Chemical structure and physical properties of Hypoxyfluor.



SI Figure 7. Representative images of Hypoxyfluor treated HT-29 tumor bearing mice. Mice bearing HT-29 tumors were injected via tail vein with 13 nmol Hypoxyfluor. Fluorescence images were acquired 8 hours post injection.