Synthesis of 4-substituted primary aliphatic aminoanthraquinones
and in silico studies

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Supporting Information File: The NMR and LC-MS for the synthesized compounds (Figures S 1 – S 20).
Figure S 1: LC/MS of 1-Amino-4-[(2-hydroxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (5).
Figure S 2: 100 MHz $^{13}$C NMR spectrum of 1-Amino-4-[(2-hydroxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (S).
Figure S 3: $^1$H NMR (400 MHz, DMSO) spectrum of 1-Amino-4-[(2-hydroxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (5).
Figure S 4: LC/MS of 1-Amino-4-[(2-hydroxyethyl)amino]-2-methylanthracene-9,10-dione (6).
Figure S 5: $^1$H NMR (400 MHz, DMSO-$d_6$) spectrum of 1-Amino-4-[(2-hydroxyethyl)amino]-2-methylantracene-9,10-dione (6).
Figure S 6: LC/MS of 1-Amino-4-[cyclopentane amine]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (7).
Figure S 7: LC/MS of 1-Amino-4-[(propan-2-yl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (8).
Figure S 8: $^1$H NMR (400 MHz, DMSO-d6) of 1-Amino-4-[(propan-2-yl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (8).
Figure S 9: LC/MS of 1-Amino-4-[(morpholin-2-yl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (10).
Figure S 10: $^1$H NMR (400 MHz, DMSO) of 1-Amino-4-[(morpholin-2-yl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (10).
**Figure S 11:** LC/MS of 1-Amino-4-(propylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (11).
Figure S 12: 100 MHz $^{13}$C NMR spectrum of 1-Amino-4-(propylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (11).
Figure S 13: LC/MS of 1-Amino-4-(butylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (12).
**Figure S 14:** 100 MHz $^{13}$C NMR spectrum of 1-Amino-4-(butylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (12).
Figure S 15: LC/MS of 1-[3,3-bis(2-hydroxyethyl)triaz-1-en-1-ol]-4-[(2-hydroxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate acid (14).
Figure S 16: $^1$H NMR (400 MHz, DMSO) spectrum of 1-[3,3-bis(2-hydroxyethyl)triaz-1-en-1-ol]-4-[2-hydroxyethyl]amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate acid (14).
Figure S 17: $^1$H NMR (400 MHz, DMSO) LC/MS spectrum of 4-[(2-hydroxyethyl)amino]-1-[(E)-(morpholin-4-ol)diazeny]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (15).
Figure S 18: LC/MS of 1-[3-(Benzoic acid)triaz-1-en-1-ol]-4-[(2-hydroxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (16).
Figure S 19: LC/MS of 1-[(3-(Benzoic acid)triaz-1-en-1-ol]-4-[(2-hydroxyethyl)amino]-9,10-dio xo-9,10-dihydroanthracene-2-sulfonic acid (16).
Figure S 20: $^1$H NMR (400 MHz, DMSO) LC/MS spectrum of 1-(3,3-diethyltriaz-1-en-1-ol)-4-[(2-hydroxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (17).