4-Acetyl-Antroquinonol B Suppresses SOD2-Enhanced Cancer Stem Cell-Like Phenotypes and Chemoresistance of Colorectal Cancer Cells by Inducing hsa-miR-324 re-Expression

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Figure S1. Bioinformatics-based systemic pharmacoanalyses reveal health effects of 4-AAQB. Predicted values of the health benefits of 4-AAQB are shown in several human systems, with the highest (~99%) health effects in the gastrointestinal system, which includes the colon and rectum, using the ACD/Labs 2.0 v5.0.0.184 platform.

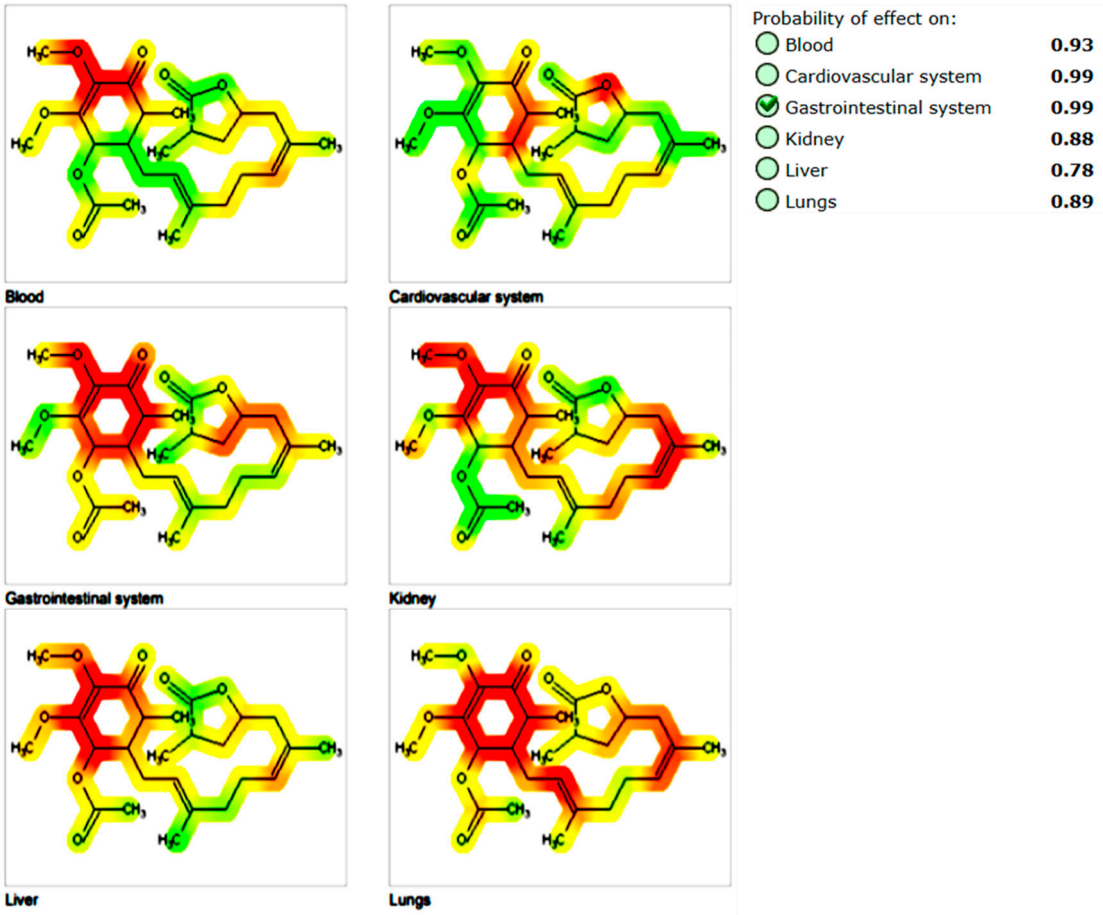

Figure S2. 4-AAQB dose determination and ADMET analyses for in vivo assays. (**A**) Bioinformatic computation of the physicochemical descriptors and prediction of ADME parameters, pharmacokinetic properties, drug-like nature and medicinal chemistry friendliness of 4-AAQB using the SwissADME platform. (**B**) Data showing the results of in silico drug safety/toxicity analysis on the pkCSM platform. Charts showing (**C**) the administration route and bioinformatics-based predicted lethality dose, LD in different species, and (**D**) Predicted values for oral acute toxicity hazard categories, OECD ranges, using the ACD/Labs 2.0 v5.0.0.184. ADMET: absorption, distribution, metabolism, excretion, and toxicity; OECD: Organisation for Economic Cooperation and Development; Cat.: category.