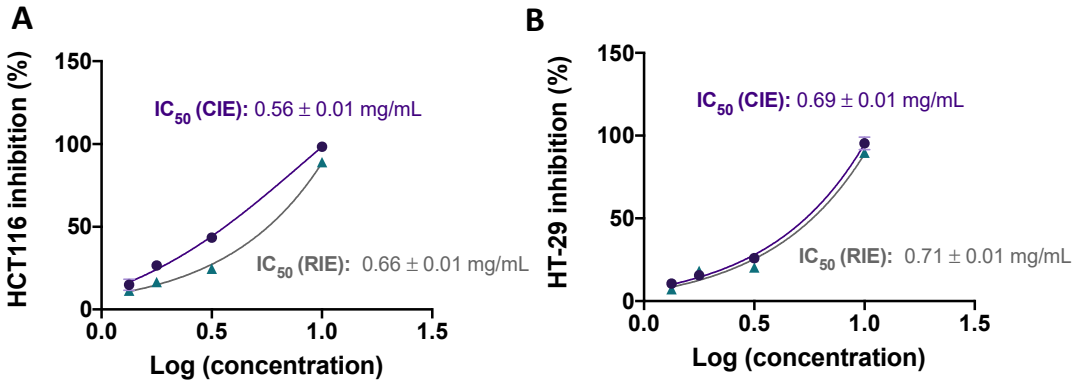
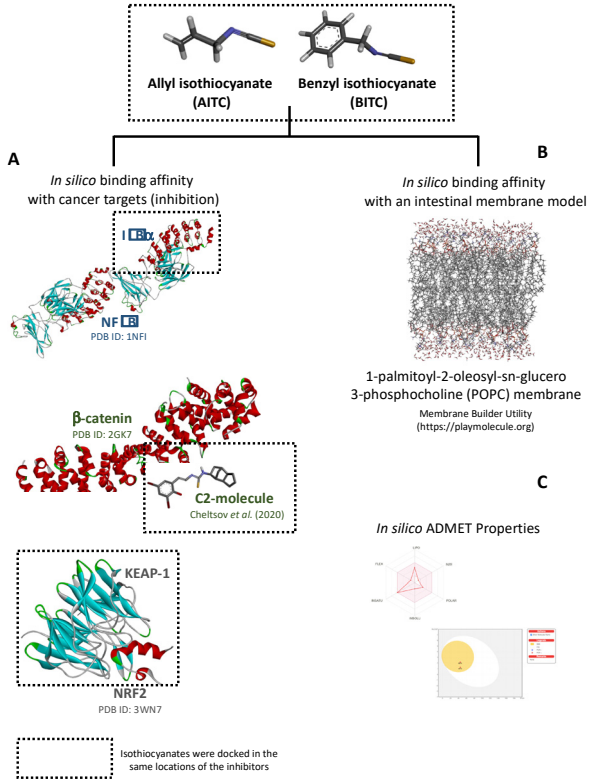
*Supplementary File*




**Supplementary Figure S1.** Three parameters dose-response curves of CIE and RIE treatments for: **(A)** HCT116 and **(B)** HT29 cells.




**Supplementary Figure S2.** Overall scheme of the *in silico* docking procedure.

Isothiocyanates (Allyl isothiocyanate of AITC; benzyl isothiocyanate of BITC) were downloaded from PubChem Database (AITC PubChem CID: 5971; BITC PubChem CID: 2346) and used as ligands, that were prepared in Discovery Studio Visualizer. Then, two *in silico* approaches were used: (A) ligands were docked in the same position of inhibitors from the cancer target molecules: IκBα, C2-molecule, and KEAP-1, respectively for NFκB, β-catenin, and NRF2; (B) Ligands were docked in a simulation of intestinal permeation using a generated 1-palmitoyl-2-oleosyl-sn-glycero-3-phosphocholine (POPC) membrane, that was generated in the Membrane Builder utility from https://playmolecule.org (accessed on 18 September 2022); (C) The verification of the *in silico* ADMET properties of

the ligands was screened through bioinformatic utilities (admetSAR 2.0 and SwissADME online software).

**Supplementary Table S1.** Validation of HPLC method using for the identification and quantification of isothiocyanates.

| Standard Name | Detection Wavelength (nm) | RT (min) | Linearity Range (µg/mL) | Regression Coefficient ($R^2$) | LOD (µg/mL) | LOQ (µg/mL) |
|---|---|---|---|---|---|---|
| AITC | 240 | 21.51 | 0-100 | 0.991 | 2.05 | 2.24 |
| BITC | 240 | 37.85 | 0-100 | 0.996 | 2.10 | 2.38 |

AITC: Allyl isothiocyanate; BITC: benzyl isothiocyanate; RT: retention time; LOD: Limit of detection; LOQ: limit of quantification.

**Supplementary Table S2.** Results from the recovery test of isothiocyanates.

| Standard Name | Amount Tested | Initial Amount (µg/ml) | Found Amount (µg/mL) | Recovery (%) | Average Recovery (%) | RSD (%) |
|---|---|---|---|---|---|---|
| AITC | Low | 15.20 | 14.89 | 97.96 | 98.69 | 0.79 |
| | Medium | 35.71 | 35.21 | 98.59 | | |
| | High | 60.22 | 59.93 | 99.52 | | |
| BITC | Low | 14.90 | 14.88 | 99.87 | 99.27 | 0.64 |
| | Medium | 40.23 | 39.67 | 98.61 | | |
| | High | 62.14 | 61.72 | 99.32 | | |

AITC: Allyl isothiocyanate; BITC: benzyl isothiocyanate; RSD: Relative standard deviation.