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Physicochemical properties of phenol and flavone derivatives correlated with their efficacy as inducers of a cancer-protective enzyme and as inhibitors of carcinogenesis in rodents

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Our investigations establish linear correlations between the ionization potential of exogenous phenol (P) and flavone (F) derivatives and their biological effects on induction of a powerful cancer-protective enzyme NAD(P)H:quinone reductase (NQO1) via the Nrf2-Keap1 pathway. They also show that the NQO1 activation involves (i) oxidation of the P and F inducers to oxidant species which are their quinone derivatives (Q) and (ii) oxidation by these quinones Q of two highly reactive thiol groups of a protein Keap1 activating transcription factor Nrf2. The linear correlations observed for beneficial cancer-protective pathways triggered by electrophiles Q *in vitro* explain the linear correlations which we observe *in vivo* (rodents) for the inhibition of chemically-induced carcinogenesis by P and F derivatives. Our *in silico* evaluation of biological activity of P and F derivatives should orient the rational design of new congeners with greater potency for cancer chemoprotection and might reduce the expensive use of *in vivo* and *in vitro* bioassays.

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