

Supplementary Data File 1. Summary of NPD8790 analog bioactivity. Chemical structures, molecular properties, and a summary of bioactivity for 51/84 NPD8790 analogs identified in benzimidazole analog screen. Dose response (LC_{50}) data is provided for *C. elegans* KCN survival assays, *C. elegans* wild-type and *ben-1* development and viability assays, and HEK293 viability assays. Dose response (IC_{50}) data is also provided for *in vitro* complex I activity assays from wild-type *C. elegans* and *B. taurus* heart mitochondria. IC_{50} and LC_{50} values were estimated from fitted dose-response curves; all dose response data are the mean of at least two biological replicates. “-“ indicate values that were not determined.

Supplementary Data File 2. Class A, B, and C benzimidazole structure-activity relationships.

Chemical structures and summary of bioactivity for 27 NPD8790 analogs belonging to class A, B, and C benzimidazoles. For each compound, the core structure, and the positions of R₁, R₂, R₃, and R₄ groups are indicated. Dose response (LC₅₀) data is provided for *C. elegans* KCN survival assays, *C. elegans* wild-type and *ben-1* development and viability assays, and HEK293 viability assays. Dose response (IC₅₀) data is provided for *in vitro* complex I activity assays from wild-type *C. elegans* and *B. taurus* heart mitochondria. IC₅₀ and LC₅₀ values were estimated from fitted dose-response curves; all dose response data are the mean of at least two biological replicates. “-“ indicate values that were not determined.