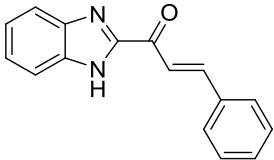
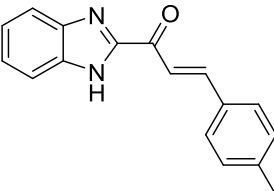
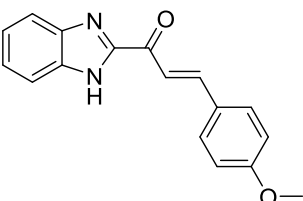
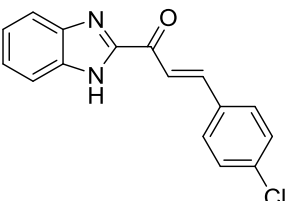
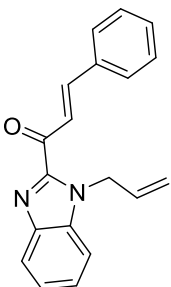
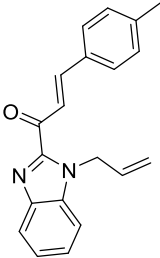
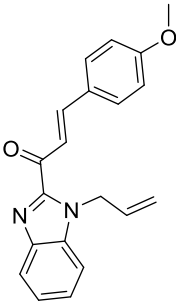
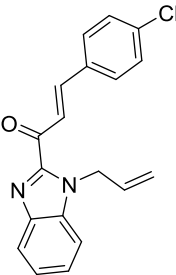
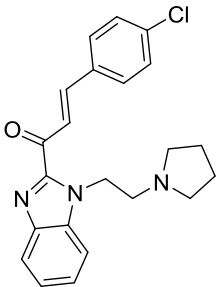
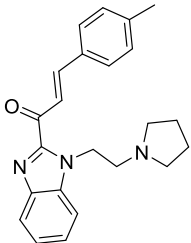


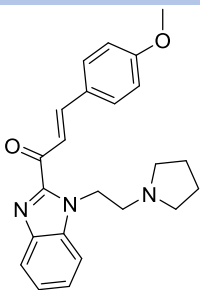
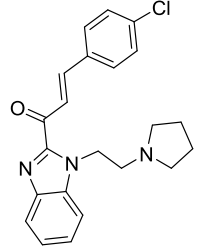
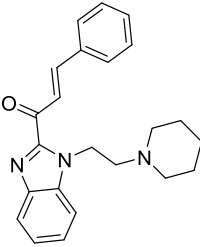
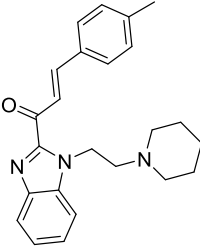
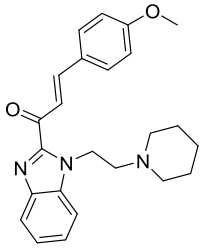
Supplementary File

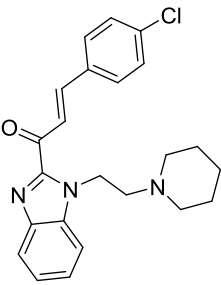
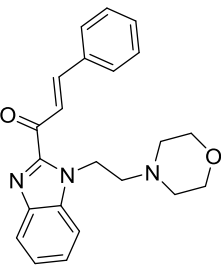
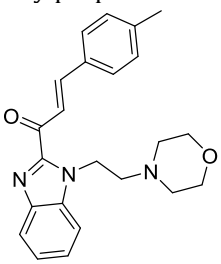
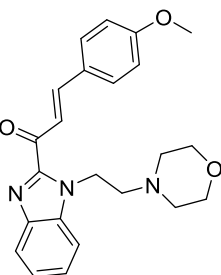
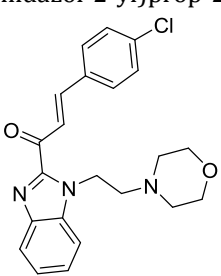
Supporting Information: ‘Theoretical Investigation and Design of Novel Anti-proliferative Agents against Hepatocellular Carcinoma from Benzimidazole-Chalcone derivatives’

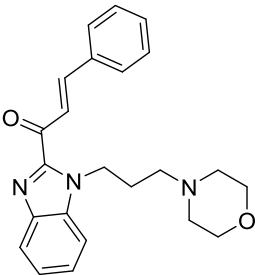
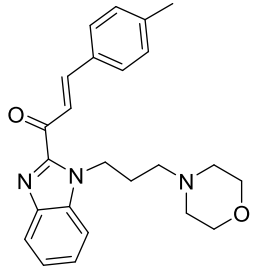
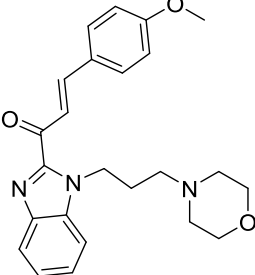
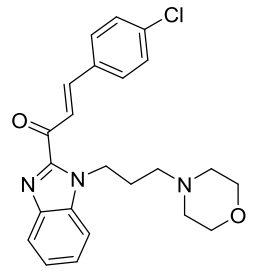
Table S1. Structures, IUPAC Nomenclatures, and Anti-cancer activities of the studied compounds against HepG2 Cell line

Entry	Structure	pIC ₅₀ (μM)
1	 (E)-1-(1H-benzo[d]imidazol-2-yl)-3-phenylprop-2-en-1-one	-1.38
2	 (E)-1-(1H-benzo[d]imidazol-2-yl)-3-(p-tolyl)prop-2-en-1-one	-1.77
3	 (E)-1-(1H-benzo[d]imidazol-2-yl)-3-(4-methoxyphenyl)prop-2-en-1-one	-2.15
4	 (E)-1-(1H-benzo[d]imidazol-2-yl)-3-(4-chlorophenyl)prop-2-en-1-one	-1.56
5	 (E)-1-(1-allyl-1H-benzo[d]imidazol-2-yl)-3-phenylprop-2-en-1-one	-1.19

Entry	Structure	pIC ₅₀ (μ M)
6	 (E)-1-(1-allyl-1H-benzo[d]imidazol-2-yl)-3-(p-tolyl)prop-2-en-1-one	-2.07
7	 (E)-1-(1-allyl-1H-benzo[d]imidazol-2-yl)-3-(4-methoxyphenyl)prop-2-en-1-one	-2.50
8	 (E)-1-(1-allyl-1H-benzo[d]imidazol-2-yl)-3-(4-chlorophenyl)prop-2-en-1-one	-1.25
9	 (E)-3-(4-chlorophenyl)-1-(1-(2-(pyrrolidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.01
10	 (E)-1-(1-(2-(pyrrolidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)-3-(p-tolyl)prop-2-en-1-one	-1.81

Entry	Structure	pIC ₅₀ (μM)
11	 (E)-3-(4-methoxyphenyl)-1-(1-(2-(pyrrolidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.56
12	 (E)-3-(4-chlorophenyl)-1-(1-(2-(pyrrolidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.19
13	 (E)-3-phenyl-1-(1-(2-(piperidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.01
14	 (E)-1-(1-(2-(piperidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)-3-(p-tolyl)prop-2-en-1-one	-1.51
15	 (E)-3-(4-methoxyphenyl)-1-(1-(2-(piperidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.77

Entry	Structure	pIC ₅₀ (μM)
16	 (E)-3-(4-chlorophenyl)-1-(1-(2-(piperidin-1-yl)ethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.75
17	 (E)-1-(1-(2-morpholinoethyl)-1H-benzo[d]imidazol-2-yl)-3-phenylprop-2-en-1-one	-1.56
18	 (E)-1-(1-(2-morpholinoethyl)-1H-benzo[d]imidazol-2-yl)-3-(p-tolyl)prop-2-en-1-one	-1.62
19	 (E)-3-(4-methoxyphenyl)-1-(1-(2-morpholinoethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.71
20	 (E)-3-(4-chlorophenyl)-1-(1-(2-morpholinoethyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.33

Entry	Structure	pIC ₅₀ (μM)
21	 (E)-1-(1-(3-morpholinopropyl)-1H-benzo[d]imidazol-2-yl)-3-phenylprop-2-en-1-one	-1.04
22	 (E)-1-(1-(3-morpholinopropyl)-1H-benzo[d]imidazol-2-yl)-3-(p-tolyl)prop-2-en-1-one	-1.68
23	 (E)-3-(4-methoxyphenyl)-1-(1-(3-morpholinopropyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.52
24	 (E)-3-(4-chlorophenyl)-1-(1-(3-morpholinopropyl)-1H-benzo[d]imidazol-2-yl)prop-2-en-1-one	-1.98