

**Supplementary Table 1.** The IUPAC name of final hit compounds from Maybridge database

Hit compounds from maybridge database	IUPAC name
PD00533	2-({[2-(5-chloro-2-methoxyanilino)ethyl]imino} methyl)-6-methoxyphenol
CD01374	N3-{4-chloro-2-[(2-phenylhydrazino) carbonyl]phenyl}-2-phenoxy nicotinamide
CD04888	N1-(2,5-dichlorophenyl)-2-[2-(bicyclo[2.2.1] hept-5-en-2-ylamino)-4-oxo-4,5-dihydro-1,3-thiazol-5-yl]acetamide
CD01278	N1-(2,6-dimethylphenyl)-2-[2-(1,4,5,6-tetrahydro pyrimidin-2-yl)benzoyl]hydrazine-1-carbothioamide
S10124	1-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl] piperidine -4-carboxamide
HTS05738	N-{4-[(1,1-dioxo-1 lambda~6~,4-thiazinan-4-yl)methyl] phenyl}-5-methyl-3-isoxazolecarboxamide
BTB01629	N3-{4-chloro-2-[(2-phenylhydrazino)carbonyl]phenyl}-2-phenoxy nicotinamide