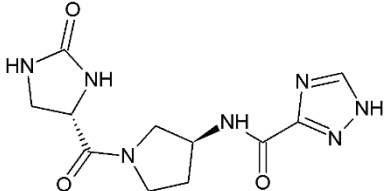
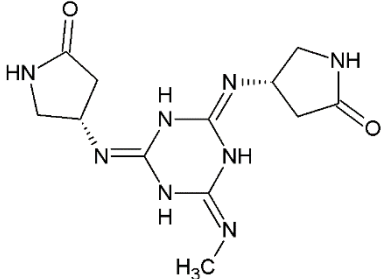
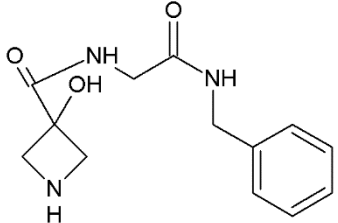
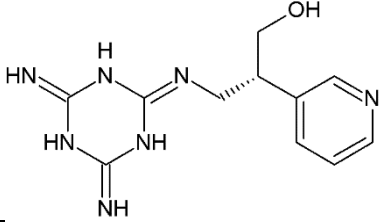
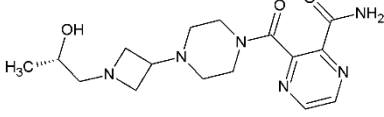
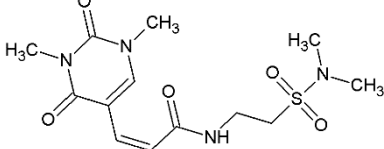
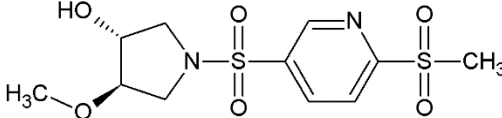
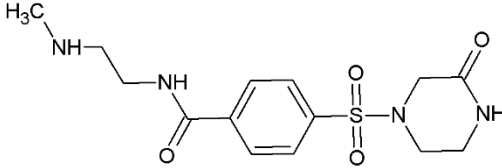
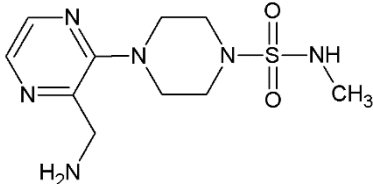
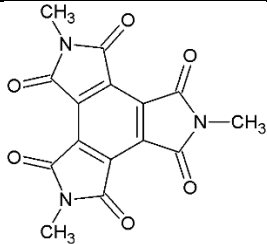
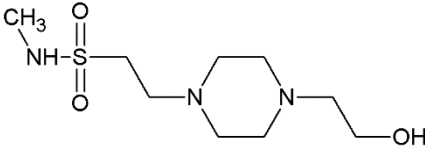
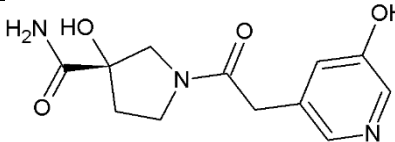
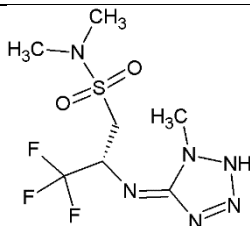
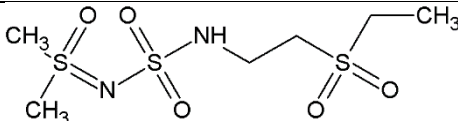
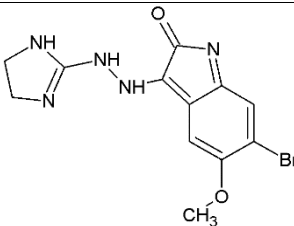
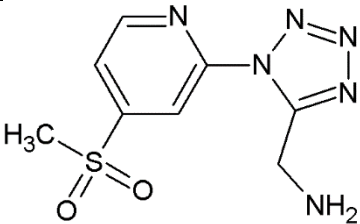


Table S1. Structures of the compounds selected for virtual screening.

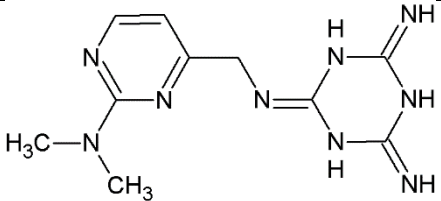
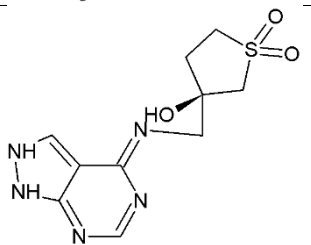
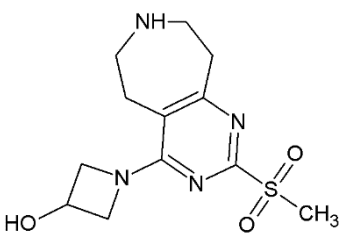
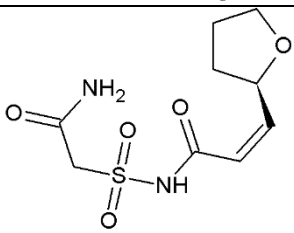
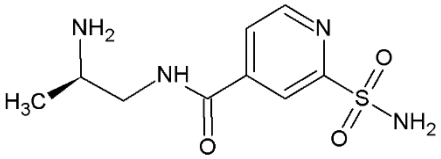
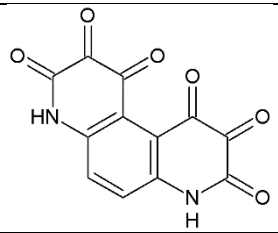
ZINC ID	Name	Structure
ZINC000000033762	4-(1,2-dimethyl-3,5-dioxo-1,2,4-triazolidin-4-yl)benzenesulfonamide	
ZINC000001663005	(1 <i>R</i> ,2 <i>S</i> ,3 <i>R</i>)-1-(1,2,4-benzotriazin-3-yl)butane-1,2,3,4-tetrol	
ZINC000019594727	1,4,7,10,13,16-hexazacyclooctadecane	
ZINC000039404119	methyl 3-[bis(methylsulfonyl)amino]propanoate	
ZINC000090475824	1,2,4,5-Tetrazine, 3,6-bis(ethylsulfonyl)-	
ZINC000863703032	<i>N</i> -{(2 <i>R</i>)-1-[methoxy(methyl)amino]-1-oxopropan-2-yl}-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3- <i>d</i>]pyrimidine-7-carboxamide	
ZINC001156694532	(4 <i>R</i>)-4-[[3-(piperazin-1-ylcarbonyl)pyridin-2-yl]amino]isoxazolidin-3-one	

ZINC000938450483	<i>N</i> -[(3 <i>S</i>)-1-[(4 <i>S</i>)-2-oxoimidazolidin-4-yl]carbonyl]pyrrolidin-3-yl]-1 <i>H</i> -1,2,4-triazole-3-carboxamide	
ZINC000362648055	(4 <i>S</i> ,4' <i>S</i>)-4,4'-[[6-(methylimino)-1,3,5-triazinane-2,4-diylidene]dinitrilo]dipyrrolidin-2-one	
ZINC000852816657	<i>N</i> -[2-(benzylamino)-2-oxoethyl]-3-hydroxyazetidine-3-carboxamide	
ZINC000624224393	(2 <i>R</i>)-3-[(4,6-diimino-1,3,5-triazinan-2-ylidene)amino]-2-(pyridin-3-yl)propan-1-ol	
ZINC000941661806	3-[(4-{1-[(2 <i>S</i>)-2-hydroxypropyl]azetidin-3-yl}piperazin-1-yl)carbonyl]pyrazine-2-carboxamide	
ZINC000493041505	(2 <i>Z</i>)-3-(1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)- <i>N</i> -[2-(dimethylsulfamoyl)ethyl]prop-2-enamide	
ZINC000576768709	(3 <i>R</i> ,4 <i>R</i>)-4-methoxy-1-[[6-(methylsulfonyl)pyridin-3-yl]sulfonyl]pyrrolidin-3-ol	
ZINC000262531716	<i>N</i> -[2-(Methylamino)ethyl]-4-(3-oxopiperazin-1-yl)sulfonylbenzamide	

ZINC001158970356	(2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>S</i> ,6 <i>R</i>)-6-(hydroxymethyl)-3-[(4-methoxypyridin-2-yl)amino]tetrahydro-2 <i>H</i> -pyran-2,4,5-triol	
ZINC000353827182	<i>N</i> -methyl- <i>N'</i> -[(3 <i>E</i>)-2-methyl-1,2-dihydro-3 <i>H</i> -1,2,4-triazol-3-ylidene]benzene-1,3-disulfonamide	
ZINC000583151023	<i>N</i> -{2-[(dimethylsulfamoyl)amino]ethyl}-1,3-dioxo-2,3-dihydro-1 <i>H</i> -isoindole-5-carboxamide	
ZINC000623936890	<i>N</i> -(4,6-diimino-1,3,5-triazinan-2-ylidene)-1-[2-(morpholin-4-yl)ethyl]-1 <i>H</i> -pyrazol-4-amine	
ZINC001116751280	2-[[[6-bromo-5-methoxypyridin-3-yl)carbonyl]amino]propanediamide	
ZINC001259045039	<i>N</i> -(2-amino-2-oxoethyl)-2-[[2-(4,5-trifluorophenyl)sulfonyl]amino]acetamide	
ZINC000517234699	2-amino- <i>N</i> -(2-[[2-(dimethylamino)pyrimidin-5-yl]amino]-2-oxoethyl)acetamide	
ZINC001219697045	(3 <i>aR</i> ,9 <i>bS</i>)- <i>N</i> -[2-(3-hydroxyazetidin-3-yl)ethyl]-5-oxo-2,3,3 <i>a</i> ,4,5,9 <i>b</i> -hexahydro-1 <i>H</i> -pyrrolo[3,4- <i>c</i>]isoquinoline-8-carboxamide	

ZINC001364199721	4-[3-(aminomethyl)pyrazin-2-yl]- <i>N</i> -methylpiperazine-1-sulfonamide	
ZINC000012322217	2,5,8-Trimethyl-1 <i>H</i> -dipyrrolo[3,4- <i>e</i> :3',4'- <i>g</i>]isoindole-1,3,4,6,7,9(2 <i>H</i> ,5 <i>H</i> ,8 <i>H</i>)-hexone	
ZINC001329482875	2-[4-(2-hydroxyethyl)piperazin-1-yl]- <i>N</i> -methylethanesulfonamide	
ZINC001346492570	(3 <i>S</i>)-3-hydroxy-1-[(5-hydroxypyridin-3-yl)acetyl]pyrrolidine-3-carboxamide	
ZINC000517602023	(2 <i>R</i>)-3,3,3-trifluoro- <i>N,N</i> -dimethyl-2-[[<i>(5E)</i> -1-methyl-1,2-dihydro-5 <i>H</i> -tetrazol-5-ylidene]amino]propane-1-sulfonamide	
ZINC001423678455	<i>N</i> -[dimethyl(oxido)-1 ⁶ -sulfanylidene]- <i>N'</i> -[2-(ethylsulfonyl)ethyl]sulfuric diamide	
ZINC000857210028	6-bromo-3-[2-(4,5-dihydro-1 <i>H</i> -imidazol-2-yl)hydrazinyl]-5-methoxy-2 <i>H</i> -indol-2-one	
ZINC001168918857	1-{1-[4-(methylsulfonyl)pyridin-2-yl]-1 <i>H</i> -tetrazol-5-yl}methanamine	

ZINC001167923698	2-[(2-chloro-6,7-dihydro-5H-pyrrolo[3,4- <i>d</i>]pyrimidin-4-yl)amino]-2-(hydroxymethyl)propane-1,3-diol	
ZINC000972896897	<i>N</i> -{ <i>trans</i> -3-[(pyridin-4-ylcarbonyl)amino]cyclobutyl}ethanediamide	
ZINC001364023987	<i>N</i> '-{[(3 <i>R</i> ,4 <i>R</i>)-4-hydroxytetrahydrofuran-3-yl]sulfamoyl}- <i>N,N</i> -dimethylmethanesulfonimidoamide	
ZINC000808047782	(2 <i>S</i>)-3-[[2-amino-6-(1 <i>H</i> -pyrazol-1-yl)pyrimidin-4-yl]amino]-2-hydroxy- <i>N</i> -methylpropanamide	
ZINC001363986270	3-[[[(dimethylamino)(methyl)oxido-1 ⁶ -sulfanylidene]sulfamoyl](methyl)amino]propanamide	
ZINC000547286627	(4 <i>E</i>)-4-[[2-(2 <i>S</i>)-2-sulfamoylpropyl]imino]-1,4-dihydropyridine-3-carboxamide	
ZINC001158867950	6-(6-methyl-2,6-diazaspiro[3.3]hept-2-yl)pyridazine-3-sulfonamide	
ZINC000425289994	(1 <i>R</i> ,2 <i>R</i> ,1' <i>R</i> ,2' <i>R</i>)-2,2'-[[6-(methylimino)-1,3,5-triazinane-2,4-diylidene]dinitrilo]dicyclobutanol	

ZINC000624085464	4-[[[(4,6-diimino-1,3,5-triazinan-2-ylidene)amino]methyl]- <i>N,N</i> -dimethylpyrimidin-2-amine	
ZINC001364169073	(3 <i>R</i>)-3-[[[(4 <i>Z</i>)-1,2-dihydro-4 <i>H</i> -pyrazolo[3,4- <i>d</i>]pyrimidin-4-ylideneamino]methyl]tetrahydrothiophene-3-ol 1,1-dioxide	
ZINC001166935835	1-[2-(methylsulfonyl)-6,7,8,9-tetrahydro-5 <i>H</i> -pyrimido[4,5- <i>d</i>]azepin-4-yl]azetidin-3-ol	
ZINC001118094695	(2 <i>Z</i>)- <i>N</i> -[(2-amino-2-oxoethyl)sulfonyl]-3-[(2 <i>R</i>)-tetrahydrofuran-2-yl]prop-2-enamide	
ZINC000648129059	<i>N</i> -[(2 <i>R</i>)-2-aminopropyl]-2-sulfamoylpyridine-4-carboxamide	
ZINC000005582647	4,7-dihydro-4,7-phenanthroline-1,2,3,8,9,10-hexone	
ZINC000002865127	1,5-dihydroxy-4,4,8,8-tetramethoxy-4 <i>H</i> ,8 <i>H</i> -[1,2,5]oxadiazolo[3,4- <i>f</i>][2,1,3]benzoxadiazole-1,5-dium	