\* Calculated MM-GBSA values for top poses for selected small molecules (Week6)

\* The following table lists additional molecules I studied in week 6. Xiangying and I will provide a list of selected molecules next week.

|  |  |  |  |
| --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | SIRT3 (4BVG) with Interm | SIRT3 (4BVG) apo-enzyme | SIRT3(4BVH) with AADRP |
| 2,3,3-trichloro-2-propen-1-yl 6-(aminocarbonyl)-3-cyclohexene-1-carboxylate | -87.66 | -91.41 | -94.77 |
| 4-bicyclo[2.2.1]hept-2-ylmorpholine | -78.73 | -77.06 | -62.64 |
| N,N,N'-trimethyl-N'-(3-methylcyclohexyl)-1,2-ethanediamine | -77.82 | -74.62 | -63.02 |
| N-(3-cyclopropyl-2-propyn-1-yl)-N-methylcyclohexanamine | -76.96 | -72.05 | -75.24 |
| N'-bicyclo[2.2.1]hept-2-yl-N,N-dimethyl-1,3-propanediamine | -75.06 | -72.42 | -72.24 |
| N-(2-methoxy-1-methylethyl)bicyclo[2.2.1]heptan-2-amine | -74.26 | -73.65 | -57.91 |
| 4,10-dioxapentacyclo[6.3.1.0~2,7~.0~3,5~.0~9,11~]dodecane | -73.29 | -71.32 | -68.54 |
| N,N-dimethyl-N'-(4-methylcyclohexyl)-1,2-ethanediamine | -73.08 | -68.31 | -65.23 |
| N'-(4-ethylcyclohexyl)-N,N-dimethyl-1,2-ethanediamine | -72.81 | -72.14 | -56.67 |
| N-bicyclo[2.2.1]hept-2-yl-N,N',N'-trimethyl-1,2-ethanediamine | -72.46 | -63.94 | -67.84 |
| N-(2-methoxyethyl)bicyclo[2.2.1]heptan-2-amine | -71.00 | -67.41 | -63.75 |
| N-(3-methoxypropyl)bicyclo[2.2.1]heptan-2-amine | -70.45 | -73.22 | -69.21 |
| N,N-dimethyl-2-piperidin-4-ylethanamine | -70.13 | -51.44 | -56.46 |
| 4-ethynyl-1,3-dimethyl-4-piperidinol | -69.05 | -64.28 | -62.83 |
| 6-methoxy-3a,4,5,6,7,7a-hexahydro-1,3-benzothiazol-2-amine | -67.73 | -65.15 | -57.65 |
| N-(cyclopropylmethyl)cyclohexanamine | -67.19 | -65.68 | -57.40 |
| 4-[(3-methylcyclopentyl)amino]cyclohexanol | -67.15 | -69.68 | -67.43 |
| 2-hexanoylcyclohexanone | -67.13 | -65.67 | -58.78 |
| 3-(3,4-dichlorophenyl)-2,2-oxiranedicarboxamide | -66.93 | -61.16 | -72.79 |
| N-(3-pyridinylmethyl)cyclohexanamine | -66.65 | -63.25 | -68.86 |
| decahydro-7-quinolinol hydrochloride | -66.05 | -63.51 | -54.46 |
| N-(3-furylmethyl)-N-methylcyclohexanamine | -66.00 | -63.69 | -57.21 |
| 2,3,3-trichloro-1-methyl-2-propen-1-yl 6-(aminocarbonyl)-3-cyclohexene-1-carboxylate | -65.55 | -76.63 | -76.70 |
| 4-(4-ethylcyclohexyl)morpholine | -65.11 | -70.33 | -65.01 |
| 2-[3-(aminomethyl)piperidin-1-yl]ethanol | -65.10 | -53.39 | -58.43 |
| N-methyl-2-(2-methylpiperidin-1-yl)ethanamine | -64.84 | -60.72 | -54.11 |
| 2-[(cyclohexylmethyl)amino]ethanol hydrochloride | -64.80 | -54.07 | -58.75 |
| N-(4-pyridinylmethyl)cyclohexanamine | -64.52 | -57.64 | -63.05 |
| 3-propoxypiperidine | -64.51 | -52.24 | -60.21 |
| 4-(4-methylcyclohexyl)morpholine | -64.28 | -69.31 | -63.10 |
| 2-[(3-methylcyclohexyl)(propyl)amino]ethanol | -64.26 | -61.27 | -44.32 |
| hexahydro-1,4-benzoxathiin-2(3H)-one | -63.95 | -53.80 | -53.83 |
| N-methyl-2-(4-methylpiperidin-1-yl)ethanamine | -63.91 | -60.47 | -55.25 |
| 2-methyl-1-piperidin-4-ylpropan-1-ol | -63.70 | -53.78 | -55.15 |
| 2-isobutylcyclohexanol | -63.48 | -62.31 | -63.62 |
| N-(cyclohexylmethyl)propan-2-amine hydrochloride | -63.30 | -59.98 | -57.85 |
| N-propyltetrahydro-2H-pyran-4-amine | -62.80 | -62.33 | -50.05 |
| N-(2-pyridinylmethyl)cyclohexanamine | -62.45 | -57.85 | -74.15 |
| 4-(cyclohexylmethyl)morpholine | -62.42 | -64.02 | -71.35 |
| 4-allylpiperidin-4-ol | -61.97 | -55.58 | -63.44 |
| 2-methyl-3-(1-piperidinyl)-1-propanol | -61.92 | -60.86 | -60.06 |
| 3-piperidin-2-ylpropan-1-ol | -61.50 | -58.36 | -56.05 |
| N-methyl-1-(1-methylpiperidin-3-yl)methanamine | -61.42 | -58.01 | -47.27 |
| 3-(4-methyl-1-piperidinyl)propanenitrile | -61.11 | -50.48 | -53.92 |
| N-methyl-2-(4-piperidinyl)acetamide | -60.39 | -56.47 | -59.56 |
| decahydro-4-quinolinol hydrochloride | -60.25 | -59.16 | -57.69 |
| N-bicyclo[2.2.1]hept-2-yl-4-morpholinamine | -60.19 | -57.50 | -67.34 |
| 2-methyloctahydro-4H-thiochromen-4-one | -60.08 | -58.12 | -63.57 |
| 4-butylcyclohexanecarbohydrazide | -59.04 | -57.59 | -61.64 |
| N-bicyclo[2.2.1]hept-2-yl-2-methylpropanamide | -58.97 | -51.19 | -72.11 |
| 3-(1-pyrrolidinyl)piperidine | -58.77 | -58.87 | -57.41 |
| N-(7-methylenebicyclo[3.3.1]non-2-en-3-yl)acetamide | -58.48 | -56.80 | -72.18 |
| 2-methyl-1-thia-4-azaspiro[4.5]decan-3-one | -58.32 | -57.36 | -53.65 |
| 3-[(2-hydroxycyclohexyl)methyl]dihydro-2(3H)-furanone | -58.05 | -58.44 | -67.40 |
| methyl 3-[2-(hydroxyimino)cyclohexyl]propanoate | -58.05 | -58.32 | -63.26 |
| 4-(1,1-dimethylpropyl)cyclohexanamine | -57.71 | -60.10 | -31.81 |
| 3-cyclohexyltetrahydro-2H-thiopyran | -57.58 | -55.95 | -68.58 |
| 2-methyloctahydro-2H-thiochromen-4-ol | -57.58 | -55.74 | -71.42 |
| 4-(2-aminoethyl)-1-methylpiperidin-4-ol | -57.25 | -54.17 | -56.21 |
| N~1~-(3,4-dichlorophenyl)-1,4-piperidinedicarboxamide | -57.25 | -69.25 | -55.22 |
| 2-methyl-N-(2-methylcyclohexyl)cyclopropanecarboxamide | -57.09 | -59.14 | -69.60 |
| N-cyclohexyltetrahydro-2H-pyran-4-amine | -57.00 | -52.86 | -62.95 |
| N-(tert-butyl)bicyclo[4.1.0]heptane-7-carboxamide | -56.99 | -53.14 | -60.21 |
| 3-(4-methylpiperidin-1-yl)propan-1-ol | -56.76 | -66.34 | -61.54 |
| N-bicyclo[2.2.1]hept-2-ylpropanamide | -56.46 | -48.32 | -65.57 |
| 7-(hydroxymethyl)bicyclo[3.3.1]nonan-3-ol | -55.98 | -53.44 | -56.03 |
| 2-piperidin-4-ylpropan-2-ol | -55.93 | -47.02 | -50.31 |
| 3-(1H-pyrazol-5-yl)piperidine | -55.48 | -52.35 | -60.29 |
| 4-cyclohexyl-1,3-thiazol-2-amine | -55.34 | -56.72 | -67.56 |
| 2-[(cyclohexylmethyl)(propyl)amino]ethanol | -55.15 | -65.25 | -67.62 |
| methyl 3-(2-oxocyclohexyl)propanoate | -54.90 | -54.75 | -63.95 |
| 5,6,7,8-tetrahydro-2(1H)-quinolinone | -53.99 | -54.20 | -51.04 |
| bicyclo[2.2.1]hept-2-ylamine | -53.74 | -49.98 | -51.80 |
| 4-ethynyl-2,2-dimethyltetrahydro-2H-pyran-4-ol | -53.72 | -51.48 | -51.38 |
| 6-methyl-2-(methylthio)-4-pyrimidinol | -53.58 | -52.86 | -47.68 |
| 2-methylquinolin-5-amine | -53.18 | -56.85 | -50.27 |
| ethyl 3-amino-3-oxo-2-(2-pyridinyl)propanoate | -53.13 | -46.66 | -60.97 |
| 4-amino-2-ethyl-6-methyl-3-pyridinol | -53.06 | -55.87 | -38.13 |
| 3',5',6',7'-tetrahydrospiro[cyclohexane-1,4'-imidazo[4,5-c]pyridine] | -53.05 | -55.18 | -31.00 |
| 2-pyrrolidin-2-ylpyridine | -53.02 | -50.34 | -59.45 |
| 4,5,6,7-tetrahydro-1,2-benzisoxazol-3-ylmethanol | -52.89 | -44.81 | -57.40 |
| N-cyclohexylcyclopropanecarboxamide | -52.82 | -52.47 | -57.07 |
| methyl 2-oxopiperidine-3-carboxylate | -52.76 | -50.46 | -53.46 |
| N-methyltetrahydro-2H-pyran-4-amine hydrochloride | -52.74 | -49.93 | -45.46 |
| 3,4,4-trimethyl-3b,4,4a,5-tetrahydrocyclopropa[4,5]cyclopenta[1,2-d]isoxazol-5a(3aH)-ol | -52.58 | -50.09 | -53.43 |
| pentacyclo[6.3.0.0~2,6~.0~3,10~.0~5,9~]undecan-4-one | -52.41 | -47.97 | -59.64 |
| 3-(chloromethylene)-1-methyl-2-piperidinone | -52.31 | -51.42 | -60.29 |
| 3-chloro-5-cyclohexyl-1H-1,2,4-triazole | -52.14 | -51.06 | -57.84 |
| bicyclo[3.3.1]nonane-2,6-diol | -51.65 | -51.66 | -50.39 |
| methyl 4-{[3-(aminocarbonyl)-1-piperidinyl]methyl}benzoate | -51.43 | -65.84 | -28.57 |
| N-cyclobutyl-N'-cyclohexylurea | -51.36 | -57.38 | -75.84 |
| 2-isopropyl-5-methyl-7-oxabicyclo[2.2.1]heptane-1,4-diol | -51.26 | -49.66 | -42.82 |
| 4-hydroxy-1-methyldecahydro-4-quinolinecarbonitrile | -50.85 | -57.39 | -44.84 |
| 2-methyl-3-(phenylethynyl)oxirane | -50.74 | -61.70 | -70.70 |
| 3-methyl-2-(methylthio)phenol | -50.63 | -49.30 | -57.60 |
| N-ethyl-1-phenylethanamine | -50.50 | -48.90 | -53.54 |
| 5-cyclohexyl-1,3,4-oxadiazol-2-amine | -50.40 | -46.44 | -53.97 |
| 7-azaspiro[4.5]decan-6-one | -50.40 | -48.79 | -58.39 |
| 3-(4-bromophenyl)-2,2-oxiranedicarboxamide | -50.38 | -52.33 | -65.47 |
| 5-amino-1-cyclohexyl-1H-pyrazol-3-ol | -50.31 | -47.44 | -51.46 |
| N-bicyclo[2.2.1]hept-2-ylmethanesulfonamide | -50.19 | -50.14 | -41.00 |
| 2-phenylazetidine | -49.94 | -44.49 | -48.14 |
| ethyl cyano(cyclohexylidene)acetate | -49.89 | -48.35 | -62.87 |
| 2-methylhexanamide | -49.75 | -51.30 | -55.14 |
| N-(4-methylcyclohexyl)-4-morpholinamine | -49.70 | -53.27 | -65.13 |
| 6-isopropyl-2-methyl-4-pyrimidinol | -49.64 | -43.57 | -42.47 |
| 2-methyl-6-propyl-4-pyrimidinol | -49.61 | -49.05 | -37.96 |
| 6-methyl-1,5,6,7-tetrahydro-4H-indazol-4-one | -49.61 | -48.46 | -47.34 |
| 4-hydroxy-1,3-dimethylpiperidine-4-carbonitrile | -49.59 | -41.32 | -47.59 |
| 4-(3-methyl-2-butenoyl)cyclohexanone | -49.54 | -56.70 | -64.07 |
| N-cyclohexyl-2-furamide | -49.41 | -52.10 | -72.96 |
| N-methyl-1-phenyl-1-propanamine | -49.32 | -38.74 | -57.92 |
| 8-methyl-1,2,3,4-tetrahydroquinoline | -49.20 | -46.92 | -50.12 |
| 3-amino-5-methyl-2-cyclohexen-1-one | -49.19 | -48.47 | -50.26 |
| N'-(3-methylcyclohexylidene)cyclopropanecarbohydrazide | -49.16 | -56.79 | -57.57 |
| 2-methyl-1,2,3,4-tetrahydroquinoline | -49.16 | -46.92 | -55.45 |
| N-(3-pyridinylmethyl)-2-propanamine | -49.14 | -39.56 | -51.47 |
| N-propylcyclohexanamine | -49.11 | -62.19 | -43.22 |
| 2-hydroxy-2-phenylpentanamide | -49.02 | -49.58 | -62.08 |
| 4-quinolinol | -48.95 | -47.85 | -44.31 |
| 3-(3-methylphenyl)-1-propanamine | -48.94 | -51.93 | -54.08 |
| hexahydro-1,3-benzodioxol-2-one | -48.79 | -47.91 | -46.18 |
| N-(2-methylcyclohexyl)cyclobutanecarboxamide | -48.75 | -56.49 | -71.11 |
| N-cyclohexyl-1-pyrrolidinecarboxamide | -48.67 | -54.70 | -71.03 |
| N~3~-cyclohexyl-beta-alaninamide | -48.38 | -53.77 | -59.03 |
| 2,5,6,8-tetrahydro-3H-pyrano[3,4-c]pyridazin-3-one | -47.78 | -47.17 | -43.03 |
| N-(1-propylcyclohexyl)acrylamide | -47.76 | -51.51 | -70.38 |
| N-(3-methylpyridin-4-yl)ethane-1,2-diamine | -47.74 | -47.42 | -37.02 |
| 5-oxo-1-propyl-3-pyrrolidinecarboxamide | -47.72 | -52.18 | -57.84 |
| N-(1-ethynylcyclohexyl)acetamide | -47.37 | -41.62 | -58.13 |
| 2-cyano-2-cyclohexylideneacetamide | -47.36 | -52.74 | -54.50 |
| 2-[(1-allylcyclohexyl)amino]ethanol | -47.31 | -57.09 | -43.70 |
| 2-methyl-3-phenylpropanamide | -47.25 | -40.78 | -59.10 |
| N-cyclohexyl-N-methylalanine | -47.24 | -46.44 | -38.12 |
| N-(2-methylcyclohexyl)-2-pyrimidinamine | -47.11 | -50.99 | -60.42 |
| 2-amino-2-(4-fluorophenyl)ethanol | -47.07 | -45.70 | -49.62 |
| N-bicyclo[2.2.1]hept-2-yl-2,2-dimethylpropanamide | -47.03 | -48.23 | -27.55 |
| 2-azabicyclo[2.2.1]heptane hydrochloride | -46.76 | -47.55 | -48.59 |
| bicyclo[3.3.1]nonan-2-one oxime | -46.72 | -44.15 | -52.00 |
| 2-ethyl-3-methyl-1H-indole | -46.62 | -36.65 | -54.52 |
| 3-methyl-2(1H)-quinolinone | -46.56 | -45.21 | -53.82 |
| piperidine-3-carbonitrile | -46.49 | -44.23 | -38.65 |
| 3-(4-oxo-1(4H)-pyridinyl)propanenitrile | -46.34 | -42.61 | -31.08 |
| tetrahydro-2H-pyran-4-carboxamide | -46.30 | -43.32 | -48.36 |
| 5-methyl-8-quinolinol | -46.26 | -39.16 | -54.15 |
| methyl 3-(1-hydroxycyclohexyl)-2-propynoate | -46.26 | -51.67 | -66.34 |
| 5-chloro-1H-indazole | -46.16 | -40.47 | -40.34 |
| N~1~-methyl-1,4-piperidinedicarboxamide | -46.16 | -46.19 | -53.51 |
| NoName | -46.10 | -44.81 | -42.24 |
| 4-cyclohexyl-2-methylphenol | -46.09 | -47.26 | -60.34 |
| 2-phenyl-2-(2-pyridinyl)acetamide | -45.77 | -46.80 | -37.85 |
| 2-amino-6-ethyl-5-methyl-4-pyrimidinol | -45.75 | -45.19 | -40.12 |
| 2-[benzylidene(oxido)amino]-2-methylpropanamide | -45.66 | -44.63 | -43.71 |
| 3-(4-fluorophenyl)-2,2-oxiranedicarboxamide | -45.66 | -52.43 | -53.19 |
| 2-ethyl-1H-benzimidazole | -45.39 | -44.50 | -46.99 |
| 2-amino-5-ethyl-6-methyl-4-pyrimidinol | -45.37 | -44.68 | -38.48 |
| 4-anilino-1,5-dihydro-2H-pyrrol-2-one | -45.27 | -44.01 | -53.58 |
| 2-amino-6-isopropyl-4-pyrimidinol | -45.19 | -42.79 | -39.15 |
| N-(cyclohexylmethyl)-2,2-dimethylpropanamide | -45.08 | -60.40 | -73.04 |
| 4-azatricyclo[4.3.1.1~3,8~]undecane hydrochloride | -45.04 | -47.60 | -60.53 |
| 4-(aminomethyl)benzamide | -44.88 | -43.30 | -42.78 |
| 4-methoxy-1-oxaspiro[4.5]dec-3-en-2-one | -44.77 | -52.50 | -51.42 |
| 4-ethoxy-6-methyl-2-pyrimidinamine | -44.77 | -42.00 | -43.21 |
| 4-(chloromethyl)benzonitrile | -44.68 | -36.35 | -45.05 |
| 2-oxopiperidine-3-carbohydrazide | -44.68 | -40.01 | -52.56 |
| 2-amino-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-ol | -44.53 | -43.98 | -43.92 |
| bicyclo[2.2.1]heptan-2-one oxime | -44.43 | -44.12 | -49.15 |
| tetrahydro-2H-pyran-4-amine hydrochloride | -44.05 | -41.26 | -44.63 |
| 3-methyl-N-nitropyridin-2-amine | -44.04 | -44.48 | -38.79 |
| 4-methoxy-N,6-dimethyl-2-pyrimidinamine | -44.02 | -45.90 | -53.29 |
| 6-fluoro-1,3-benzoxazol-2(3H)-one | -43.99 | -44.13 | -34.12 |
| 3-(4-methylphenyl)propan-1-amine | -43.86 | -41.11 | -60.40 |
| 3,11-dioxatetracyclo[6.3.0.0~2,6~.0~5,9~]undecane-4,10-dione | -43.75 | -44.04 | -52.82 |
| 2-amino-4-isopropylphenol | -43.73 | -44.53 | -39.43 |
| 4-amino-3-methylbenzamide | -43.69 | -42.78 | -46.42 |
| 3-ethyl-4-methylene-1-oxa-3-azaspiro[4.5]decan-2-one | -43.63 | -54.24 | -61.98 |
| 7-methyl-1,2,3,4-tetrahydrocyclopenta[b]indole-3-carboxamide | -43.58 | -45.12 | -73.79 |
| 2-methyl-4-phenyl-1H-imidazole | -43.36 | -50.73 | -43.75 |
| 4-amino-1-(cyclohexylmethyl)pyrrolidin-2-one | -43.24 | -56.49 | -60.23 |
| 2-azaspiro[5.5]undecan-1-one | -43.12 | -44.36 | -58.77 |
| 2,2-diphenylacetamide | -43.06 | -40.85 | -28.49 |
| N-methyl-1-(3-methylpyridin-2-yl)methanamine | -42.90 | -39.46 | -45.55 |
| N-(2-pyridinylmethyl)ethanamine | -42.85 | -38.74 | -48.07 |
| 3-cyclohexyl-1H-1,2,4-triazole-5-thiol | -42.81 | -43.72 | -44.63 |
| N-[(2-methylcyclohexyl)carbonyl]glycine | -42.68 | -49.79 | -40.91 |
| N-3-pyridinylpropanamide | -42.62 | -43.46 | -49.41 |
| N'-cyclohexylidenemethanesulfonohydrazide | -42.61 | -48.10 | -50.91 |
| 4-methyl-2(1H)-quinolinone | -42.60 | -41.50 | -52.95 |
| N-(3-pyridinylmethyl)ethanamine | -42.30 | -40.96 | -47.58 |
| 6-methyl-4-quinazolinamine | -42.16 | -43.71 | -46.38 |
| 5-cyclohexyl-1,3,4-thiadiazol-2-amine | -42.14 | -56.44 | -60.93 |
| 3-cyclohexyl-1H-pyrazole-4-carboxamide | -41.92 | -53.82 | -58.49 |
| 3,4-dihydro-2(1H)-quinoxalinone | -41.81 | -39.67 | -45.67 |
| 2-cyanobenzamide | -41.50 | -40.92 | -39.67 |
| 4-pentylcyclohexanecarboxylic acid | -41.44 | -48.09 | -43.73 |
| 3-(allyloxy)-2-pyridinamine | -41.29 | -43.14 | -56.68 |
| 3-phenylcyclobutanone | -41.21 | -40.45 | -44.69 |
| 4-hydrazino-3-nitropyridine | -41.10 | -40.75 | -31.79 |
| 2-amino-6-ethyl-4-pyrimidinol | -41.03 | -40.25 | -41.11 |
| 4-isopropyl-3,5,6,7,8,8a-hexahydro-2(1H)-quinazolinone | -41.01 | -48.27 | -66.94 |
| 4-chloro-1H-indazole | -40.99 | -37.06 | -41.96 |
| 5-[(methylamino)methyl]-2-pyrimidinamine | -40.87 | -38.51 | -37.30 |
| 3-(allyloxy)aniline | -40.81 | -45.13 | -49.49 |
| N-methyl-3-piperidin-1-ylpropan-1-amine | -40.78 | -48.11 | -52.13 |
| 5,6,7,8-tetrahydronaphthalen-2-amine | -40.76 | -41.37 | -55.29 |
| N,4-dimethyl-N-nitrosoaniline | -40.46 | -34.49 | -52.07 |
| N-methyl-2-nitroaniline | -40.36 | -39.26 | -41.22 |
| piperidine-4-carbonitrile | -40.21 | -40.52 | -38.20 |
| 3-(4-chlorophenyl)-2,2-dicyanocyclopropanecarboxamide | -40.13 | -52.37 | -62.22 |
| 2-ethyl-5-methylphenol | -40.10 | -38.07 | -55.31 |
| 2-cyano-2-cyclohexylideneethanethioamide | -39.82 | -45.62 | -47.79 |
| ethyl 3-amino-2-(2-hydroxy-3-oxo-5-phenyl-2,3-dihydro-2-furanyl)-3-oxopropanoate (non-preferred name) | -39.82 | -67.75 | -64.59 |
| 7,8-dihydro-5H-pyrano[4,3-d]pyrimidin-2-amine | -39.76 | -43.65 | -48.35 |
| 3-methyl-1-benzofuran | -39.75 | -38.26 | -44.71 |
| N-2-pyrimidinylurea | -39.68 | -39.96 | -38.88 |
| 4-[(acetylamino)methyl]cyclohexanecarboxylic acid | -39.67 | -43.38 | -34.14 |
| N-3-pyridinylacetamide | -39.65 | -38.90 | -43.79 |
| 2,3-dimethylpyridin-4-amine | -39.59 | -49.09 | -32.94 |
| 3-cyclohexyl-1H-1,2,4-triazol-5-amine | -39.52 | -39.01 | -51.12 |
| 2,3-dimethyl-4a,5,6,7,8,8a-hexahydroquinoxaline 1,4-dioxide | -39.44 | -56.28 | -54.90 |
| 3-phenyl-1H-pyrazole | -39.44 | -38.90 | -47.46 |
| 3-(4,5-dihydro-1,3-oxazol-2-yl)pyridine | -39.40 | -45.10 | -46.91 |
| 2,4-dioxo-3-chromanecarboxamide | -39.27 | -52.41 | -57.46 |
| 3-(1H-pyrazol-4-yl)pyridine | -39.09 | -39.11 | -47.35 |
| 2-chloronicotinonitrile | -38.98 | -36.54 | -42.58 |
| 3-(5-pyrimidinyl)-2-propyn-1-ol | -38.88 | -42.31 | -43.68 |
| piperidin-2-ylacetic acid | -38.88 | -33.64 | -44.25 |
| 2-methoxy-3-pyridinol | -38.70 | -37.29 | -38.16 |
| 2-oxo-2,3-dihydro-1H-benzimidazole-5-carbonitrile | -38.65 | -39.82 | -30.91 |
| 3-methyl-1H-indazol-7-amine | -38.64 | -37.31 | -43.79 |
| 3-methylbenzohydrazide | -38.60 | -37.71 | -45.64 |
| 6-chloro-2-pyridinecarboxamide | -38.58 | -45.72 | -45.74 |
| N-cyclohexylpropanamide | -38.55 | -37.09 | -51.64 |
| 5-methyl-1H-indole-3-carbaldehyde | -38.41 | -33.91 | -49.39 |
| N-(3-hydroxy-2-pyridinyl)acetamide | -38.41 | -38.62 | -47.21 |
| 2-pyridin-4-ylacetohydrazide | -38.13 | -39.38 | -47.30 |
| 3-amino-2-methylbenzamide | -38.06 | -37.30 | -39.66 |
| 2-azido-N-cyclohexylacetamide | -37.87 | -48.28 | -60.73 |
| N-nitro-2-pyridinamine | -37.87 | -38.17 | -28.18 |
| 3-amino-4-fluorobenzamide | -37.85 | -36.45 | -42.68 |
| N-hydroxy-4-pyridinecarboximidamide | -37.81 | -37.53 | -21.57 |
| 5-amino-1,3-benzoxazol-2(3H)-one | -37.67 | -36.24 | -33.81 |
| 3-methyl-4-phenyl-4H-1,2,4-triazole | -37.64 | -39.88 | -41.51 |
| 3-(1H-pyrazol-5-yl)aniline | -37.51 | -30.46 | -50.10 |
| 5-chloro-6-methyl-2-pyridinamine | -37.47 | -41.82 | -48.00 |
| 6-quinoxalinamine | -37.35 | -40.82 | -44.99 |
| 4-methyl-5,6-dihydrofuro[2,3-d]pyrimidin-2-amine | -37.26 | -46.69 | -52.56 |
| 6-amino-2-benzofuran-1(3H)-one | -37.17 | -39.77 | -43.06 |
| N-cyclohexyl-2,2-dimethylpropanamide | -37.12 | -41.00 | -63.87 |
| 2-methyl-1H-indole-3-carbonitrile | -36.89 | -37.00 | -41.99 |
| 4H-[1,2,4]triazolo[1,5-a]benzimidazole | -36.81 | -38.74 | -45.62 |
| 5-quinolinylmethanol | -36.67 | -44.93 | -46.32 |
| 2-methyl-4-nitropyridine 1-oxide | -36.45 | -37.66 | -39.43 |
| 6-amino-1,3-benzoxazol-2(3H)-one | -36.43 | -35.50 | -35.20 |
| 4-methoxy-3-nitropyridine | -36.34 | -34.24 | -38.36 |
| 2,4,6-trimethyl-5-pyrimidinol | -36.30 | -37.43 | -36.59 |
| 2-adamantanamine | -36.23 | -34.39 | -51.00 |
| 4-oxo-1-adamantanecarboxamide | -36.17 | -36.54 | -52.21 |
| 4-methyl-3-nitro-2-pyridinamine | -36.14 | -35.55 | -43.51 |
| 2-oxo-1-adamantanecarboxamide | -36.07 | -36.28 | -50.51 |
| N-cyclohexyl-2-methylpropanamide | -36.06 | -46.73 | -65.15 |
| 2,1-benzoxaborol-1(3H)-ol | -35.78 | -37.13 | -37.69 |
| 2,4,4,6-tetramethyl-1,4-dihydro-3,5-pyridinedicarbonitrile | -35.75 | -45.87 | -42.80 |
| 4-amino-N-methylbenzamide | -35.64 | -34.09 | -41.02 |
| 4-phenyl-1H-1,2,3-triazole | -35.56 | -35.14 | -43.05 |
| 5-fluoro-1,3-benzoxazol-2-amine | -35.47 | -27.99 | -34.25 |
| 6-quinolinamine | -35.39 | -35.47 | -41.62 |
| N-3-isoxazolylcyclohexanecarboxamide | -35.39 | -50.92 | -67.24 |
| 3-(3-pyridinyl)-2,2-oxiranedicarboxamide | -35.20 | -55.05 | -51.37 |
| 3-(2-chlorophenyl)-2,2-dicyanocyclopropanecarboxamide | -34.97 | -55.29 | -60.13 |
| quinolin-8-amine | -34.88 | -36.33 | -47.55 |
| N-(cyclohexylmethyl)methanesulfonamide | -34.84 | -41.53 | -49.29 |
| 5-bromobicyclo[3.3.1]nonane-1-carboxamide | -34.50 | -37.79 | -55.13 |
| N-cyanobenzamide | -34.46 | -33.67 | -41.58 |
| 5-amino-2-fluorobenzamide | -34.42 | -34.30 | -42.01 |
| 2-cyclohexylpropanoic acid | -34.25 | -36.70 | -31.45 |
| 2-methyl-1,3-benzoxazol-6-amine | -34.14 | -36.59 | -45.24 |
| 4-hydroxyphthalonitrile | -34.05 | -33.40 | -44.05 |
| 2-cyano-2-(2-naphthyl)acetamide | -34.01 | -48.33 | -55.62 |
| 5-quinolinamine | -33.87 | -33.91 | -41.70 |
| 8-quinolinylmethanol | -33.87 | -41.67 | -49.28 |
| 2-methyl-1,3-benzoxazol-6-ol | -33.47 | -41.77 | -50.40 |
| tricyclo[3.2.1.0~2,4~]octane-3-carboxylic acid | -33.43 | -35.23 | -40.33 |
| 4-oxatricyclo[4.3.1.1~3,8~]undecan-5-one | -33.43 | -33.72 | -54.56 |
| isoquinoline-1-carbonitrile | -33.40 | -34.08 | -39.25 |
| methyl 2-aminoisonicotinate | -33.18 | -39.07 | -38.45 |
| 8-methyl-5-quinolinamine | -32.77 | -35.36 | -41.35 |
| 2-hydrazino-1H-benzimidazole | -32.70 | -32.39 | -35.03 |
| 2,3-diphenyl-2-cyclopropene-1-carboxamide | -32.66 | -35.13 | - |
| 4,6-dimethyl-2-pyrimidinecarbonitrile | -32.63 | -36.95 | -38.16 |
| 4-oxo-4-phenylbutanenitrile | -32.41 | -43.78 | -51.24 |
| nicotinaldehyde hydrazone | -31.89 | -23.70 | -32.63 |
| 2-adamantanone oxime | -31.71 | -17.34 | -48.18 |
| bicyclo[3.3.1]nonan-2-one semicarbazone | -31.66 | -42.19 | -49.44 |
| ethyl 3-(aminocarbonyl)-1,4'-bipiperidine-1'-carboxylate | -31.57 | -73.41 | -20.11 |
| 2-pyridinecarbothioamide | -31.48 | -32.33 | -35.59 |
| 2-fluorobenzenecarbothioamide | -31.23 | -29.30 | -34.53 |
| 2-aminonicotinaldehyde | -31.22 | -33.26 | -38.14 |
| 2,2-dicyano-3-phenylcyclopropanecarboxamide | -31.02 | -44.06 | -54.81 |
| 2-cyano-N'-cyclohexylideneacetohydrazide | -30.94 | -47.14 | -46.24 |
| 7-methyl-1,8-naphthyridin-2-amine | -30.81 | -45.90 | -55.04 |
| 2-methyl-1H-benzimidazole-5-carbonitrile | -30.60 | -35.50 | -41.42 |
| 3-amino-4-phenyl-1H-pyrrole-2,5-dione | -30.56 | -45.73 | -51.22 |
| 4-(3,4-dimethoxyphenyl)tetrahydro-2H-pyran-4-carboxamide | -30.28 | -58.73 | -55.75 |
| 6-methyl-1H-pyrazolo[3,4-b]pyridin-3-amine | -30.13 | -33.90 | -40.88 |
| 3-amino-2,6-difluorobenzonitrile | -30.08 | -30.05 | -33.88 |
| 4-(1H-pyrazol-5-yl)aniline | -30.01 | -30.11 | -47.95 |
| 2,3-dihydroxybenzaldehyde oxime | -30.00 | -32.49 | -45.61 |
| 3-oxo-3-phenylpropanenitrile | -29.88 | -31.62 | -45.01 |
| N-(2,6-dimethyl-4-oxo-1(4H)-pyridinyl)thiourea | -29.81 | -34.28 | -35.18 |
| 4-(1H-pyrazol-4-yl)aniline | -29.61 | -28.06 | -46.22 |
| N-hydroxy-2-pyridinecarboximidamide | -29.56 | -31.88 | -36.62 |
| quinuclidine-3-carboxylic acid | -29.49 | -29.81 | -47.49 |
| 2,6-difluoro-4-pyrimidinamine | -29.23 | -31.15 | -30.38 |
| 4-fluoro-1H-indazol-3-amine | -28.92 | -34.57 | -40.93 |
| tetrahydro-2H-pyran-2-ylacetic acid | -28.36 | -43.90 | -33.08 |
| 6-methyl-3-quinolinol | -28.07 | -47.15 | -24.76 |
| 2,4-diaminopyrimidine-5-carbonitrile | -28.05 | -32.70 | -30.71 |
| 2-amino-4,6-pyrimidinediol | -27.78 | -35.74 | -25.42 |
| 5-methyl-3-phenyl-1H-pyrazole | -27.49 | -36.14 | -57.04 |
| 9-oxobicyclo[3.3.1]nonane-3-carboxylic acid | -27.43 | -17.41 | -37.69 |
| 2,2-dimethyltetrahydro-2H-pyran-4-carboxylic acid | -27.29 | -35.95 | -36.19 |
| 3-(1-hydroxycyclohexyl)prop-2-ynoic acid | -26.80 | -41.82 | -42.55 |
| 6-fluoro-1,3-benzoxazol-2-amine | -26.69 | -36.88 | -43.42 |
| spiro[cyclopropane-1,9'-fluorene]-2-carboxamide | -26.60 | -50.63 | -31.74 |
| 3-(2-oxocyclohexyl)propanoic acid | -26.33 | -53.09 | -37.21 |
| 3-quinolinol | -25.85 | -36.12 | -28.31 |
| 2-amino-N-methylbenzamide | -25.78 | -37.10 | -51.00 |
| 2,5,6-triamino-4-pyrimidinol | -25.52 | -21.93 | -28.88 |
| 3-hydroxy-4-methoxybenzonitrile | -25.18 | -36.28 | -45.46 |
| bicyclo[4.1.0]heptane-7-carboxylic acid | -24.94 | -41.38 | -39.50 |
| 3H-imidazo[4,5-b]pyridin-2-ylacetonitrile | -24.90 | -42.95 | -42.31 |
| 3H-[1,2,3]triazolo[4,5-d]pyrimidine-5,7-diamine | -24.36 | -36.19 | -34.04 |
| N-hydroxybicyclo[3.3.1]nonane-1-carboxamide | -24.18 | -40.78 | -54.25 |
| 5-phenyl-1,3-cyclohexanedione | -24.08 | -39.05 | -32.93 |
| N-2H-tetrazol-5-ylcyclohexanecarboxamide | -23.33 | -42.31 | -42.18 |
| 3,5-dimethyl-7-oxo-6-oxabicyclo[3.2.1]octane-2-carboxylic acid | -22.91 | -35.76 | -30.96 |
| 5-hydroxyadamantan-2-one | -22.07 | -33.41 | -46.71 |
| spiro[oxirane-2,2'-tricyclo[3.3.1.1~3,7~]decane]-3,3-dicarboxamide | -21.43 | -33.84 | - |
| tetrahydro-2H-pyran-4-carboxylic acid | -21.38 | -22.35 | -29.05 |
| 4-hydroxy-1-oxaspiro[4.5]dec-3-en-2-one | -21.29 | -30.07 | -39.31 |
| 2-oxo-4-phenyl-1,2,3,4,5,6,7,8-octahydro-3-quinolinecarboxamide | -21.28 | -49.44 | - |
| 4-propylbicyclo[2.2.2]octane-1-carboxylic acid | -20.84 | -29.69 | - |
| 3-(3,4-dimethyl-2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)propanoic acid | -19.97 | -51.09 | -43.37 |
| 4-(cyclohexyloxy)-4-oxo-2-butenoic acid | -19.96 | -52.88 | -53.54 |
| 2-adamantanecarbohydrazide | -19.94 | -17.07 | -27.79 |
| 3-pyridin-2-ylpropanoic acid | -19.37 | -45.60 | -30.32 |
| 3-pyridin-4-ylpropanoic acid | -19.01 | -38.41 | -30.63 |
| 5-fluoro-2-hydrazino-4-pyrimidinamine | -18.87 | -20.76 | 6.69 |
| tricyclo[4.3.1.1~3,8~]undecan-4-one | -18.76 | -33.76 | -47.30 |
| 6-methylpyridine-2-carboxylic acid 1-oxide | -18.17 | -24.49 | -26.18 |
| 3-chlorobenzoic acid | -17.88 | -27.63 | -28.14 |
| 6,9-dimethyl-2,3,4,9-tetrahydro-1H-carbazole-1-carboxamide | -15.61 | -49.58 | -71.55 |
| N-2-pyrimidinylglycine | -14.98 | -40.29 | -25.27 |
| 3-(3-nitro-1H-1,2,4-triazol-1-yl)-1-adamantanecarboxamide | -14.87 | -43.16 | -29.85 |
| 6-chloro-2-pyridinecarboxylic acid | -13.35 | -34.77 | -29.58 |
| 2,6-dimethylisonicotinic acid | -13.26 | -26.32 | -20.78 |
| 2-oxo-1-adamantanecarboxylic acid | -12.76 | -13.87 | -31.21 |
| 3-(2H-tetrazol-5-yl)pyridine | -12.31 | -28.72 | -24.11 |
| 3,5-dimethyl-1-adamantanecarboxamide | -11.80 | -11.44 | -25.13 |
| 2-cyclohexylidene-N-nitrohydrazinecarboximidamide | -11.75 | -29.23 | -19.09 |
| 2-pyrimidinylcyanamide | -10.61 | -25.50 | -12.75 |
| 6-methoxynicotinic acid | -10.08 | -30.96 | -27.37 |
| 3-amino-2-hydroxybenzoic acid | -8.79 | -11.39 | -22.53 |
| 2-mercaptobenzoic acid | -8.23 | -23.39 | -29.77 |
| 3-(4-methoxyphenyl)acrylonitrile | -7.92 | -47.07 | -45.45 |
| 3-aminoisonicotinic acid | -7.26 | -23.21 | -22.38 |
| 3-(benzylthio)-3-(4-bromophenyl)-2-cyanopropanamide | -2.70 | -65.38 | - |
| 3-(1-adamantyl)-1-propanol | -1.89 | -26.76 | 2.51 |
| tricyclo[3.3.1.1~3,7~]dec-2-ylideneacetic acid | 14.75 | -16.45 | -35.21 |
| bicyclo[2.2.2]oct-5-ene-2,3-dicarboxylic acid | 16.57 | -5.77 | -12.91 |
| 2,6-dihydroxyisonicotinic acid | 22.86 | -8.77 | 6.01 |
| ethyl 4-{3-[4-(aminocarbonyl)-1-piperidinyl]-2,5-dioxo-1-pyrrolidinyl}benzoate | - | -83.95 | -48.83 |
| methyl 4-{3-[4-(aminocarbonyl)-1-piperidinyl]-2,5-dioxo-1-pyrrolidinyl}benzoate | - | -79.38 | -39.95 |
| ethyl 4-({[4'-(aminocarbonyl)-1,4'-bipiperidin-1'-yl]carbonothioyl}amino)benzoate | - | -72.85 | -63.62 |
| ethyl 3-amino-3-oxo-2-[3-(2-oxo-2-phenylethylidene)-3,4-dihydro-2-quinoxalinyl]propanoate | - | -70.60 | - |
| 3-phenyl-2-(4'H-spiro[cyclopentane-1,3'-isoquinolin]-1'-yl)propanamide | - | -69.46 | - |
| ethyl 4-(aminocarbonyl)-1,4'-bipiperidine-1'-carboxylate | - | -67.85 | 3.10 |
| 4-{3-[4-(aminocarbonyl)-1-piperidinyl]-2,5-dioxo-1-pyrrolidinyl}benzoic acid | - | -66.83 | -38.39 |
| 4'-propyl-1,1'-bi(cyclohexyl)-4-carboxamide | - | -66.54 | -22.72 |
| ethyl {[4-amino-1-(aminocarbonyl)-5-cyano-3-azaspiro[5.5]undeca-2,4-dien-2-yl]thio}acetate | - | -65.93 | - |
| ethyl 3-amino-2-(4,6-diphenyl-2-pyrimidinyl)-3-oxopropanoate | - | -62.86 | - |
| N~1~-cyclohexyl-1,4-piperidinedicarboxamide | - | -61.37 | -54.05 |
| ethyl 2-amino-5-{[3-(aminocarbonyl)-1-piperidinyl]carbonyl}-4-methyl-3-thiophenecarboxylate | - | -61.22 | -6.62 |
| 4-amino-5-cyano-2-{[2-(4-methylphenyl)-2-oxoethyl]thio}-3-azaspiro[5.5]undeca-2,4-diene-1-carboxamide | - | -58.69 | - |
| N~1~-[1-(3-isopropenylphenyl)-1-methylethyl]-1,4-piperidinedicarboxamide | - | -56.04 | -44.87 |
| 4-amino-2-[(2-anilino-2-oxoethyl)thio]-5-cyano-3-azaspiro[5.5]undeca-2,4-diene-1-carboxamide | - | -55.62 | -46.03 |
| 4-amino-5-cyano-2-thioxo-3-azaspiro[5.5]undec-4-ene-1-carboxamide | - | -52.85 | 2.47 |
| 2-cyano-3-[5-hydroxy-3-methyl-1-(4-phenyl-1,3-thiazol-2-yl)-1H-pyrazol-4-yl]-3-phenylpropanamide | - | -47.32 | -46.33 |
| 9-benzyl-2,3,4,9-tetrahydro-1H-carbazole-1-carboxamide | - | -45.51 | - |
| 4-amino-5-cyano-2-(methylthio)-3-azaspiro[5.5]undeca-2,4-diene-1-carboxamide | - | -40.52 | -0.77 |
| 2-methyl-N~1~-(2-methylphenyl)-4-thioxo-3-azaspiro[5.5]undec-1-ene-1,5-dicarboxamide | - | -32.42 | - |
| 2,3,3-triphenylpropanamide | - | -30.50 | - |
| 2-methyl-4-(methylthio)-N~1~-phenyl-3-azaspiro[5.5]undeca-1,3-diene-1,5-dicarboxamide | - | -30.34 | - |
| 2-methyl-N~1~-phenyl-4-thioxo-3-azaspiro[5.5]undec-1-ene-1,5-dicarboxamide | - | -17.70 | - |
| 5-cyano-4-oxo-2-thioxo-3-azaspiro[5.5]undecane-1-carboxamide | - | -15.23 | - |
| 3-hydroxy-1-adamantanecarboxylic acid | - | -14.02 | -35.61 |
| 4-oxo-1-adamantanecarboxylic acid | - | -12.28 | -39.02 |
| 2'-{[4-(aminocarbonyl)-1-piperidinyl]carbonyl}-2-biphenylcarboxylic acid | - | 3.40 | - |