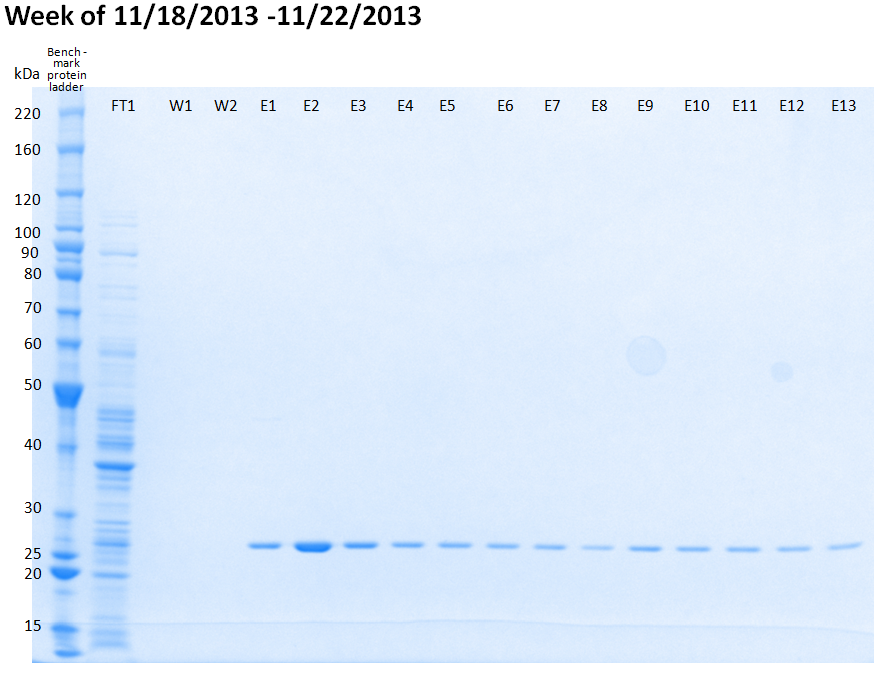
Progress Report Week of Nov. 18, 2013

(PL and XG)

**Protein expression and purification (XG)**

* To improve the yield of Elution step, GST Fusion Protein Purification method from GenScript was used. The recovery of target protein has been increased significantly. 3ml for E1, 2ml for E2, 1ml for E3-E8, and 0.5 ml for E9-E13.These will reduced the time and cost of purification.
* 
* 3.5-5 kDa Float-A-Lyzer dialysis tube has been ordered to obtain pure GST-tagged pGEX-6P3-PNCA protein. GST-tag will be cleaved from purified product (GST-tagged pGEX-6P3-PNCA).
* To concentrate purified protein to desired concentration, Millipore UFC 501096 Amicon Ultra-0.5 Centifugal filter concentrator will be ordered.
* The next step is measurement of purified enzyme concentration and activity.
* Half way through addressing experimental questions from referee reports and making relative change in the main manuscript (with tracking).

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

Continue the dockings from last week, other than docking to SIRT3 apo-enzyme and SIRT3 with intermediate (both constructed from pdbID: 4BVG), I also docked them into SIRT3 with co-product AADRP (pdbID: 4BVH) in order to exam their ability to inhibit using the same mechanism as Ex-527. This information should help us make a better selections for hits.

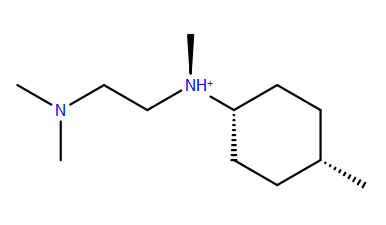
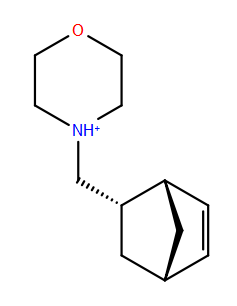
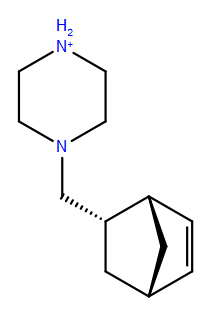
\* The first table lists the small molecules I examed on week 2.

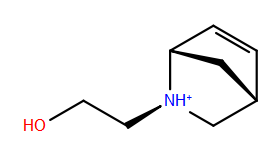
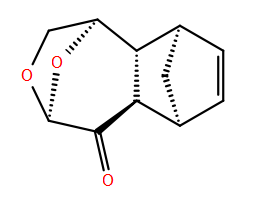
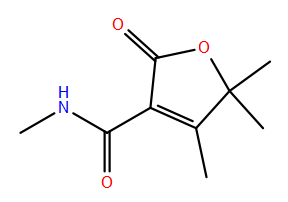
|  |  |  |  |
| --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | SIRT3 (4BVG) with Interm | SIRT3 (4BVG) apo-enzyme | SIRT3(4BVH) with AADRP |
| N,N,N'-trimethyl-N'-(4-methylcyclohexyl)-1,2-ethanediamine | -76.92 | -73.60 | -65.19 |
| 4-(bicyclo[2.2.1]hept-5-en-2-ylmethyl)morpholine | -76.87 | -72.03 | -76.46 |
| 1-(bicyclo[2.2.1]hept-5-en-2-ylmethyl)piperazine | -71.45 | -68.38 | -69.17 |
| 2-(2-azabicyclo[2.2.1]hept-5-en-2-yl)ethanol | -63.96 | -58.68 | -58.52 |
| 10,12-dioxatetracyclo[7.2.1.1~3,6~.0~2,7~]tridec-4-en-8-one | -58.21 | -57.11 | -41.52 |
| N,4,5,5-tetramethyl-2-oxo-2,5-dihydro-3-furancarboxamide | -57.74 | -54.69 | -65.48 |
| 3,4,4-trimethyl-3b,4,4a,5-tetrahydro-1H-cyclopropa[3,4]cyclopenta[1,2-c]pyrazole | -54.40 | -53.36 | -53.09 |
| 1',3'-dihydrospiro[cyclohexane-1,2'-imidazo[4,5-b]pyridine] | -53.04 | -51.90 | -39.14 |
| 4-[2-(2,4-cyclohexadien-1-yl)vinyl]aniline | -52.66 | -58.07 | -72.21 |
| 1-(2-cyclopenten-1-yl)-4-methoxybenzene | -52.44 | -51.95 | -67.63 |
| 5-methyl-4,5,6,7-tetrahydro-2,1-benzisoxazol-3-amine | -49.82 | -48.18 | -49.53 |
| 1-ethylbicyclo[2.2.1]heptan-2-one | -49.80 | -49.39 | -51.89 |
| 5,6,7,8-tetrahydro-3(2H)-cinnolinone | -49.66 | -48.72 | -50.88 |
| 3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one | -49.34 | -44.36 | -64.23 |
| 8-hydroxy-2,4-dimethyl-7H-chromen-7-one | -47.67 | -50.00 | -51.08 |
| 2-(1-aminoethylidene)-5,5-dimethyl-1,3-cyclohexanedione | -47.58 | -50.36 | -58.00 |
| 1-ethylbicyclo[2.2.1]heptan-2-one oxime | -47.39 | -44.01 | -53.29 |
| 3-(4,4-dimethyl-2,6-dioxocyclohexyl)propanenitrile | -47.26 | -46.89 | - |
| 3-pentyl-4,5,6,7-tetrahydro-2H-indazole | -47.19 | -57.32 | -79.23 |
| 7-chloro-2,1,3-benzothiadiazol-4-amine | -46.45 | -50.19 | -55.54 |
| 4-(methoxyimino)-3,6,6-trimethylbicyclo[3.1.0]hex-2-ene-2-carbonitrile | -46.42 | -46.94 | -35.54 |
| N'-2,1,3-benzoxadiazol-5-yl-N,N-dimethylimidoformamide | -46.37 | -45.92 | -47.54 |
| N-2,1,3-benzothiadiazol-4-ylacetamide | -46.12 | -46.15 | -55.34 |
| 7-methyl-8H-imidazo[4,5-e][2,1,3]benzothiadiazole | -45.94 | -48.57 | -50.27 |
| 5-chloro-2,1,3-benzoxadiazole 1-oxide | -45.91 | -45.01 | -41.06 |
| 7,8-dihydro-6H-cyclopenta[e][1,2,4]triazolo[1,5-a]pyrimidine | -45.84 | -45.84 | -46.00 |
| 5,5-dimethyl-4-phenyl-2(5H)-furanone | -45.44 | -50.21 | -58.85 |
| 4-(dichloromethyl)-4-methyl-2,5-cyclohexadien-1-one | -44.87 | -52.00 | -65.59 |
| 1,4,5,6-tetrahydrocyclopenta[c]pyrazole-3-carbohydrazide | -44.73 | -43.71 | -53.40 |
| 2-[3-(dimethylamino)-2-propen-1-ylidene]-1,3-cyclohexanedione | -44.55 | -58.40 | -65.84 |
| 4-(hydroxyimino)-3,6,6-trimethylbicyclo[3.1.0]hex-2-ene-2-carbonitrile | -44.21 | -50.18 | -54.58 |
| 6-methylfuro[3,4-c]pyridine-3,4(1H,5H)-dione | -44.11 | -44.43 | -48.55 |
| 2-methylbenzo-1,4-quinone 1-(O-acetyloxime) | -44.07 | -46.99 | -49.99 |
| 5-methyl-2,1,3-benzothiadiazol-4-amine | -43.98 | -44.95 | -56.68 |
| 2,2-dimethyl-2H-benzimidazol-4-amine 1-oxide | -43.79 | -45.80 | -56.52 |
| 5-methyl-1,4-dihydrocyclopenta[b]indol-3(2H)-one | -43.73 | -42.45 | -59.86 |
| 7-methyl-1,2,3,4-tetrahydrocyclopenta[b]indol-3-ol | -43.59 | -49.87 | -59.11 |
| 7-methyl-1,2,3,4-tetrahydrocyclopenta[b]indole-3-carboxamide | -43.58 | -45.12 | -73.79 |
| 4-chloro-2,1,3-benzoxadiazole | -43.29 | -40.05 | -45.33 |
| 1,3-dimethyl-6,7-dihydro-2-benzothiophen-4(5H)-one | -43.26 | -48.98 | -53.80 |
| 2,4-dimethyl-7H-chromen-7-one | -42.51 | -48.71 | -51.57 |
| 5,5-dimethyl-2-[(methylamino)methylene]-1,3-cyclohexanedione | -42.35 | -48.57 | -59.42 |
| 4,5,6,7-tetrahydro-2H-indazol-3-ol | -42.23 | -39.41 | -46.20 |
| 4-(2-cyclopenten-1-yl)phenol | -42.11 | -47.14 | -55.04 |
| N-(3,3-dimethyl-5-oxocyclohexylidene)glycine | -41.76 | -50.93 | -44.16 |
| 6,7-dihydro[1,4]dioxino[2,3-f][2,1,3]benzothiadiazole | -41.51 | -50.67 | -62.51 |
| 4,5,6,7-tetrahydro-2H-indazole-3-carboxamide | -41.45 | -48.74 | -56.50 |
| N-methyl-4-nitro-2,1,3-benzoxadiazol-5-amine | -41.40 | -50.01 | -45.77 |
| 2-aminocyclopent-1-ene-1-carbonitrile | -41.38 | -39.74 | -41.59 |
| 2,1,3-benzothiadiazole-4,5-diamine | -41.04 | -40.41 | -46.64 |
| 2,2-dimethyl-2,5,6,7-tetrahydro-4H-benzimidazol-4-one oxime 1-oxide | -40.92 | -41.58 | -54.42 |
| 1-methyl-1,4,5,6-tetrahydrocyclopenta[c]pyrazol-3-amine | -40.87 | -39.15 | -53.72 |
| 6,7-dihydro[1,4]dioxino[2,3-f][2,1,3]benzoxadiazole 1-oxide | -40.72 | -47.75 | -51.38 |
| 2,5-dimethyl-7,8-dihydro-6H-cyclopenta[e]pyrazolo[1,5-a]pyrimidine | -39.81 | -47.25 | -61.17 |
| 4-amino-6,6-dimethyl-6,7-dihydrocyclopenta[e][1,3]thiazin-2(5H)-one | -39.15 | -55.90 | -42.39 |
| 7-methyl-1,2,3,4-tetrahydrocyclopenta[b]indole-3-carbonitrile | -38.76 | -44.18 | -57.29 |
| 5,5-dimethyl-2-nitro-1,3-cyclohexanedione | -37.19 | -39.80 | -44.56 |
| 6,7-dihydro-2,1,3-benzoxadiazol-4(5H)-one O-2-propyn-1-yloxime | -37.08 | -48.95 | -61.77 |
| 2-methyl-7,8-dihydro-6H-cyclopenta[e][1,2,4]triazolo[1,5-a]pyrimidine | -37.07 | -51.00 | -54.19 |
| N-2,1,3-benzoxadiazol-4-ylacetamide | -36.80 | -41.26 | -51.45 |
| N,N-dimethyl-2,1,3-benzoxadiazole-4,7-diamine | -36.42 | -36.34 | -48.26 |
| 1-methyl-10-oxa-4-azatricyclo[5.2.1.0~2,6~]dec-8-ene-3,5-dione | -36.41 | -38.42 | -38.77 |
| 5-nitro-2,1,3-benzoxadiazol-4-amine | -35.95 | -34.97 | -45.51 |
| 5,6-difluoro-2,1,3-benzoxadiazole 1-oxide | -35.53 | -38.92 | -31.54 |
| 6,7-dihydro-2,1,3-benzoxadiazol-4(5H)-one hydrazone 1-oxide | -35.29 | -38.70 | -45.34 |
| 2-methyl-2H-indazol-6-amine | -34.72 | -40.04 | -46.91 |
| 2,1,3-benzoxadiazol-4-ylformamide | -34.55 | -37.63 | -44.48 |
| 6,6-dimethyl-2-methylenebicyclo[3.1.1]heptan-3-one oxime | -34.47 | -40.56 | -54.89 |
| 7-methylfuro[3,2-e][2,1,3]benzoxadiazole | -34.01 | -42.21 | -46.75 |
| 1-(hydroxymethyl)-10-oxa-4-azatricyclo[5.2.1.0~2,6~]dec-8-ene-3,5-dione | -33.78 | -35.14 | -40.66 |
| 1,7,7-trimethylbicyclo[2.2.1]heptan-2-one oxime | -33.70 | -23.10 | -49.99 |
| 2-(1-amino-2,2,2-trifluoroethylidene)cyclohexanone | -33.40 | -32.93 | -34.43 |
| 7-methyl-1,4-dihydrocyclopenta[b]indol-3(2H)-one | -32.85 | -37.73 | -55.50 |
| 10-oxa-4-azatricyclo[5.2.1.0~2,6~]dec-8-ene-3,5-dione | -32.57 | -34.43 | -33.62 |
| 6,7-dimethyl-6H-[1,2,5]oxadiazolo[3,4-e]indole | -30.79 | -48.20 | -58.08 |
| N-[(4-methylcyclohexyl)carbonyl]glycine | -29.36 | -50.77 | -31.07 |
| 1,7-dimethyl-10-oxa-4-azatricyclo[5.2.1.0~2,6~]dec-8-ene-3,5-dione | -28.13 | -32.43 | -40.85 |
| 2-[(dimethylamino)methylene]-5,5-dimethyl-1,3-cyclohexanedione | -26.98 | -44.83 | -66.91 |
| 1-bicyclo[2.2.1]hept-5-en-2-yl-1H-tetrazole-5-thiol | -24.18 | -36.52 | -36.27 |
| 5-phenyl-1,3-cyclohexanedione | -24.08 | -39.05 | -32.93 |
| 2-methyl-4,5,6,7-tetrahydro-8H-cyclopenta[d][1,2,4]triazolo[1,5-a]pyrimidin-8-one | -23.21 | -53.35 | -58.75 |
| [1,2,3]triazolo[4,5-f][1,2,3]benzotriazol-2(5H)-amine | -21.07 | -36.97 | -33.52 |
| 3-(4,5,6,7-tetrahydro-2H-indazol-3-yl)propanoic acid | -19.73 | -54.54 | -48.22 |
| 2-methyl-4,5,6,7-tetrahydro-2H-indazole-3-carboxylic acid | -16.52 | -31.66 | -36.91 |
| 7,9,10,12-tetraazatricyclo[4.3.3.0~1,6~]dodecane-8,11-dione | -16.18 | -27.73 | -31.43 |
| 2-oxo-2,5,6,7-tetrahydro-1H-cyclopenta[b]pyridine-3-carboxylic acid | -16.08 | -34.18 | -27.87 |
| 5-methyl-4,5,6,7-tetrahydro-2H-indazole-3-carboxylic acid | -13.92 | -30.77 | -45.04 |
| 7,7-dimethyl-2,3-dioxobicyclo[2.2.1]heptane-1-carboxylic acid | -13.69 | -16.03 | -45.00 |
| 4,5,6,7-tetrahydro-8H-cyclopenta[d][1,2,4]triazolo[1,5-a]pyrimidin-8-one | -9.45 | -28.68 | -30.78 |
| 2-tert-butyl-3-hydroxy-5-methylbenzo-1,4-quinone | -5.34 | -49.49 | -52.44 |
| 6,7,8,9-tetrahydro[1,2,4]triazolo[4,3-b]cinnolin-10-ol | -3.96 | -26.58 | -33.15 |
| 2-amino-4,5,6,7-tetrahydro-8H-cyclopenta[d][1,2,4]triazolo[1,5-a]pyrimidin-8-one | 15.14 | -30.03 | -32.48 |
| [1,2,3]triazolo[4,5-f][1,2,3]benzotriazole-4,8(1H,5H)-dione | 17.13 | -15.19 | 20.31 |
| 2H-1,2,3-benzotriazol-2-ylacetic acid | - | -45.92 | -38.30 |
| N'-(3-cyano-5,6-dihydro-4H-cyclopenta[b]thien-2-yl)imidoformamide | - | -48.71 | -64.09 |
|  | | |  |

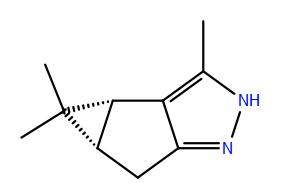
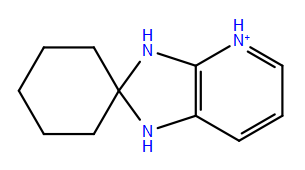
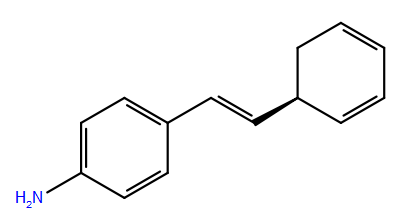
\*\*\* Note: without intermediate or AADRP, ligands don’t always bound to C-pockets

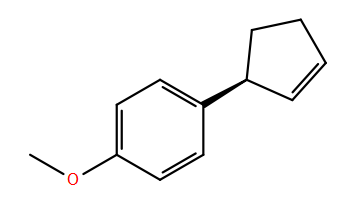
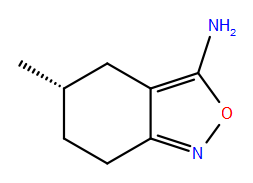
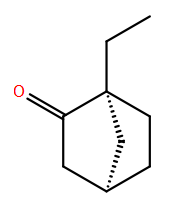
\*\*\* Note 2: Only deprotonated form of acids were considered in the above table, the acids in neutral (protonated) form were studied separately, only one isomer is selected for each compound.

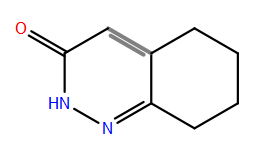
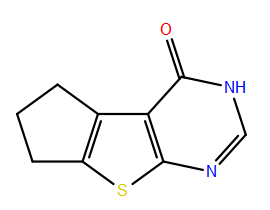
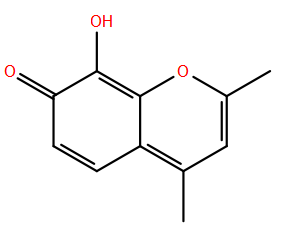
The top 15 ranked compound (docked to SIRT3 with intermediate) structures are list below.

1:2:3: 

4:5:6: 

7: 8: 9: 

10: 11: 12: 

13: 14: 15: 

\* For Comparison, we redocked most of the small molecules we studied earlier to the SIRT3 with O-AADRP receptor. And here are the results. Note that Ex527 increase its binding affinity in 4BVH signicantly, as Ex527 was bound in the original crystal structure.

|  |  |  |  |
| --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | SIRT3 (4BVG) with Interm | SIRT3 (4BVG) apo-enzyme | SIRT3(4BVH) with AADRP |
| NAM | -38.55 | -39.81 | -33.07 |
| Iso-NAM | -32.36 | -34.68 | -31.62 |
| Nicotinic Acid | -36.73 | -36.59 | -31.88 |
| Pyridine, 1-oxide | -27.34 | -26.74 | -27.46 |
| N(1)-methylnicotinamide | -44.51 | -48.04 | -43.26 |
| Nicotinic Acid, 1-oxide | -34.16 | -33.06 | -33.22 |
| Ex527 | -37.88 | -55.25 | -82.63 |
| ligand 1 | -36.72 | -34.77 | -33.05 |
| ligand 2 | -37.65 | -36.28 | -37.85 |
| ligand 3 | -30.47 | -36.43 | -43.88 |
| ligand 4 | -41.22 | -56.15 | -59.25 |
| ligand 5 | -49.04 | -50.26 | -50.24 |
| ligand 6 | -48.95 | -46.47 | -52.96 |
| ligand 7 | -45.74 | -46.08 | -45.43 |
| ligand 8 | -47.73 | -46.45 | -48.21 |
| ligand 9 | -50.94 | -50.61 | -51.38 |
| ligand 10 | -47.30 | -46.89 | -49.42 |
| ligand 11 | -49.19 | -48.03 | -53.05 |
| ligand 12 | -47.10 | -49.96 | -47.50 |
| ligand 13 | -52.42 | -48.80 | -57.51 |
| ligand 14 | -46.32 | -49.23 | -56.20 |
| ligand 15 | -57.88 | -52.63 | -60.07 |
| ligand 16 | -48.60 | -49.14 | -49.84 |

\* The following table lists the molecules we studied in week 3.

|  |  |  |  |
| --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | SIRT3 (4BVG) with Interm | SIRT3 (4BVG) apo-enzyme | SIRT3(4BVH) with AADRP |
| (3-ethoxypropyl)(4-methylcyclohexyl)amine | -85.06 | -80.79 | -64.74 |
| (4-methylcyclohexyl)(tetrahydro-2-furanylmethyl)amine | -84.73 | -81.59 | -85.12 |
| 1-(2,6-dimethyl-5-hepten-1-yl)-3-piperidinecarboxamide | -82.08 | -86.76 | -43.80 |
| (2-methoxyethyl)(4-methylcyclohexyl)amine | -78.45 | -75.03 | -66.24 |
| 1-(2,6-dimethyl-5-hepten-1-yl)-4-piperidinecarboxamide | -78.43 | -78.74 | -38.96 |
| (4-ethylcyclohexyl)(2-methoxyethyl)amine | -76.67 | -68.96 | -61.07 |
| (3-methoxypropyl)(3-methylcyclohexyl)amine | -75.84 | -67.68 | -67.20 |
| (4-ethylcyclohexyl)(3-methoxypropyl)amine | -75.72 | -67.92 | -56.89 |
| (1-cyclohexyl-3-pyrrolidinyl)methanol | -71.85 | -69.14 | -69.31 |
| 1-(1-methyl-3-phenylpropyl)-4-piperidinecarboxamide | -68.99 | -72.06 | -35.06 |
| (1R,2R)-2-(propylamino)cyclohexanol | -68.75 | -67.85 | -63.08 |
| (2-furylmethyl)(4-methylcyclohexyl)amine | -68.03 | -61.15 | -68.93 |
| (1-bicyclo[2.2.1]hept-2-yl-2-pyrrolidinyl)methanol | -67.54 | -65.40 | -64.54 |
| (2-furylmethyl)(2-methylcyclohexyl)amine | -67.26 | -66.18 | -68.92 |
| 1-(2,6-dichlorobenzyl)-4-piperidinecarboxamide | -66.60 | -62.37 | -52.68 |
| 1-(1-propylpiperidin-3-yl)methanamine | -66.43 | -63.71 | -60.68 |
| (1,1-dimethyl-2-piperidin-1-ylethyl)amine | -62.57 | -59.18 | -50.03 |
| (1-isopropylpiperidin-3-yl)methanol | -62.34 | -59.51 | -61.70 |
| {4-[(methylamino)methyl]tetrahydro-2H-pyran-4-yl}methanol | -62.18 | -61.93 | -61.21 |
| 1-(1-ethylpiperidin-3-yl)methanamine | -61.99 | -58.64 | -53.90 |
| [1-(4-methylcyclohexyl)-2-pyrrolidinyl]methanol | -61.90 | -64.22 | -64.66 |
| 1-(1,2,3,4-tetrahydro-2-naphthalenyl)-3-piperidinecarboxamide | -61.03 | -65.38 | -53.47 |
| (1-ethylpiperidin-3-yl)methanol | -61.00 | -54.97 | -55.55 |
| 1-(2,3-dichlorobenzyl)-4-piperidinecarboxamide | -60.98 | -71.17 | -61.04 |
| 1-(1-ethylpiperidin-2-yl)methanamine | -60.90 | -44.57 | -55.42 |
| (3-propylpiperidin-3-yl)methanol | -60.77 | -56.62 | -63.90 |
| (3-methyl-1,5-dioxaspiro[5.5]undec-3-yl)amine | -60.49 | -57.78 | -10.93 |
| 1-(2-aminoethyl)piperidin-4-ol | -60.18 | -56.73 | -43.04 |
| (1-methylpiperidin-4-yl)methanol | -59.23 | -56.97 | -50.37 |
| (1,3-dimethylpiperidin-3-yl)methanol | -58.67 | -52.82 | -58.12 |
| 1-(2,4-dichlorobenzyl)-3-piperidinecarboxamide | -58.49 | -65.73 | -70.61 |
| [1-(cyclohexylmethyl)-2-pyrrolidinyl]methanol | -58.22 | -63.50 | -69.07 |
| 1-(2,4-dichlorobenzyl)-4-piperidinecarboxamide | -58.08 | -71.32 | -72.87 |
| 1-(2-aminoethyl)piperidin-3-ol | -57.21 | -54.09 | -46.75 |
| 1-(2,6-dichlorobenzyl)-3-piperidinecarboxamide | -55.76 | -60.89 | -66.12 |
| (1-methylbicyclo[2.2.1]hept-2-yl)amine hydrochloride | -55.01 | -51.56 | -55.77 |
| (1-ethyltricyclo[2.2.1.0~2,6~]hept-3-yl)amine hydrochloride | -54.42 | -56.67 | -59.78 |
| 1-(1-ethylpropyl)-5-oxo-3-pyrrolidinecarboxamide | -54.14 | -53.16 | -41.39 |
| 1-(2,3-dichlorobenzyl)-3-piperidinecarboxamide | -53.35 | -64.91 | -60.70 |
| (cyclohexylmethyl)[2-(dimethylamino)ethyl]methylamine | -52.54 | -56.01 | -67.39 |
| [1-(2-aminoethyl)piperidin-2-yl]methanol | -52.04 | -54.41 | -50.61 |
| (3-ethylpiperidin-3-yl)methanol | -52.02 | -47.83 | -58.10 |
| (tetrahydro-2H-pyran-4-ylmethyl)amine hydrochloride | -51.91 | -48.94 | -52.14 |
| (1-benzylpropyl)amine | -51.88 | -51.45 | -56.55 |
| 1-(1-piperidinyl)acetone oxime | -51.80 | -49.09 | -50.02 |
| 1-(1-methyl-2,5-dioxo-3-pyrrolidinyl)-4-piperidinecarboxamide | -51.02 | -64.29 | -64.56 |
| 1-(2,5-dimethylbenzyl)-3-piperidinecarboxamide | -50.86 | -60.11 | -72.36 |
| 1-(2,5-dimethylbenzyl)-4-piperidinecarboxamide | -50.67 | -50.69 | -72.06 |
| 1-(2,4-difluorobenzyl)-4-piperidinecarboxamide | -50.05 | -59.53 | -62.93 |
| 1-(2,6-difluorobenzyl)-4-piperidinecarboxamide | -49.39 | -48.49 | -66.21 |
| (5-chloro-2-methylphenyl)methylamine | -48.95 | -41.64 | -51.49 |
| 1-(2,4-difluorobenzyl)-3-piperidinecarboxamide | -48.84 | -59.75 | -64.44 |
| 1-(1-acetylpiperidin-4-yl)methanamine | -48.61 | -49.60 | -54.41 |
| 1-(1-adamantyl)propan-1-one | -48.37 | -28.94 | -44.91 |
| (1-pyridin-4-ylpropyl)amine | -48.34 | -42.19 | -43.99 |
| (4-methylpiperidin-1-yl)acetic acid | -48.01 | -45.30 | -39.51 |
| (1-cyclohexyl-1H-imidazol-5-yl)methanol | -47.47 | -59.00 | -47.04 |
| (4-fluorobenzyl)methylamine | -47.13 | -44.13 | -41.73 |
| (2-phenylpropyl)amine | -47.13 | -44.92 | -53.68 |
| (3-amino-2-oxatricyclo[3.3.1.1~3,7~]dec-1-yl)methanol | -46.95 | -44.00 | -52.89 |
| (1-methyl-2-pyridin-2-ylethyl)amine | -46.62 | -39.96 | -52.72 |
| (1-methylpiperidin-2-yl)acetic acid | -45.32 | -42.65 | -43.35 |
| (2-chloro-3-methoxyphenyl)amine | -44.46 | -37.06 | -47.79 |
| 1-(2,6-difluorobenzyl)-3-piperidinecarboxamide | -44.26 | -51.51 | -71.37 |
| 1-(2,5-difluorobenzyl)-3-piperidinecarboxamide | -43.72 | -53.73 | -74.16 |
| 1-(1-hydroxycyclohexyl)ethanoneoxime | -43.39 | -43.98 | -52.67 |
| (1H-benzimidazol-2-ylmethyl)amine | -43.13 | -41.48 | -46.32 |
| 1-(1,2,3,4-tetrahydro-2-naphthalenyl)-4-piperidinecarboxamide | -42.78 | -59.62 | -46.59 |
| 1-(2,3-dihydro-1,4-benzodioxin-6-ylsulfonyl)-4-piperidinecarboxamide | -42.58 | -52.27 | -32.28 |
| 1-(2,3-dimethoxybenzyl)-3-piperidinecarboxamide | -41.81 | -65.64 | -52.75 |
| (2-isopropoxyphenyl)amine | -41.71 | -41.96 | -58.42 |
| (2-methylpiperidin-1-yl)acetic acid | -41.40 | -40.05 | -43.13 |
| 1-(2,5-dimethoxybenzyl)-4-piperidinecarboxamide | -41.26 | -55.93 | -32.14 |
| (2-cyclopropylphenyl)amine | -41.03 | -43.14 | -52.07 |
| (1-phenylethyl)formamide | -40.77 | -42.26 | -49.96 |
| (3-methylpiperidin-1-yl)acetic acid | -38.99 | -39.66 | -41.92 |
| (1H-indol-4-ylmethyl)amine | -38.45 | -31.83 | -42.78 |
| (6-methyl-2-pyridinyl)cyanamide | -37.98 | -36.28 | -36.33 |
| (2-aminophenyl)methanol | -37.76 | -34.83 | -37.42 |
| [2-(2-fluorophenyl)ethyl]hydrazine | -37.52 | -39.04 | -46.44 |
| 1-(1-methylcyclohexyl)-1-ethanone semicarbazone | -37.47 | -53.06 | -34.54 |
| 1-(1-piperidin-1-ylcyclohexyl)methanamine | -36.54 | -39.76 | -57.45 |
| 1-(1-hydroxycyclohexyl)-1-ethanone semicarbazone | -36.02 | -55.07 | -50.21 |
| [(2-hydroxycyclohexyl)thio]acetic acid | -35.08 | -55.72 | -47.80 |
| (1-methylpiperidin-4-ylidene)acetic acid | -34.12 | -45.71 | -40.28 |
| (3-methyl-1-adamantyl)formamide | -33.95 | -19.27 | -31.84 |
| 1-(1-naphthylmethyl)-3-piperidinecarboxamide | -33.06 | -62.60 | -58.71 |
| (1S,2S,4S)-bicyclo[2.2.1]hept-5-en-2-ylacetic acid | -32.85 | -44.74 | -42.35 |
| (hydroxyimino)(phenyl)acetonitrile | -30.67 | -30.39 | -34.52 |
| (2-amino-4-methylphenyl)dimethylamine | -30.51 | -31.88 | -48.77 |
| (3-cyano-2-pyridinyl)cyanamide | -30.36 | -33.82 | -35.62 |
| (5-hydroxytricyclo[3.3.1.1~3,7~]dec-2-ylidene)acetonitrile | -29.81 | -30.32 | -56.22 |
| (4-oxocyclohexyl)acetic acid | -26.98 | -34.85 | -31.57 |
| (2-oxopiperidin-1-yl)acetic acid | -25.59 | -37.32 | -37.97 |
| (1-adamantylamino)acetonitrile | -23.73 | -17.00 | -17.00 |
| 1-(2,2-diphenylethyl)-3-piperidinecarboxamide | -23.39 | -58.19 | -58.19 |
| (4,6-dimethyl-2-pyrimidinyl)cyanamide | -20.31 | -31.10 | -23.75 |
| 1-(2,3-dimethoxybenzyl)-4-piperidinecarboxamide | -17.76 | -61.07 | -48.51 |
| [1,3]oxazolo[4,5-c]pyridine-2-thiol | -7.70 | -30.41 | -32.06 |
| 1-(1H-tetrazol-1-yl)cyclohexanecarboxylic acid | -6.80 | -31.27 | -27.71 |
| 1-(2-{[4-(6-methyl-1,3-benzothiazol-2-yl)phenyl]amino}-2-oxoethyl)-4-piperidinecarboxamide | - | -86.68 | -65.25 |
| 1-({3-[(3,4-dimethylphenoxy)methyl]-4-methyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazol-1-yl}methyl)-4-piperidinecarboxamide | - | -80.44 | -80.44 |
| 1-({5-[(3-fluorobenzoyl)amino]-1-phenyl-1H-pyrazol-4-yl}carbonyl)-4-piperidinecarboxamide | - | -77.44 | -77.44 |
| 1-({5-[(4-methylbenzoyl)amino]-1-phenyl-1H-pyrazol-4-yl}carbonyl)-4-piperidinecarboxamide | - | -75.21 | -75.21 |
| 1-({5-[(2-fluorobenzoyl)amino]-1-phenyl-1H-pyrazol-4-yl}carbonyl)-4-piperidinecarboxamide | - | -71.77 | -71.77 |
| 1-({2-[(4-methylbenzoyl)amino]-4,5,6,7-tetrahydro-1-benzothien-3-yl}carbonyl)-4-piperidinecarboxamide | - | -71.56 | -71.56 |
| 1-(2,5-dioxo-1-phenyl-3-pyrrolidinyl)-4-piperidinecarboxamide | - | -71.50 | -71.50 |
| 1-(2,4-dimethoxy-3-methylbenzyl)-4-piperidinecarboxamide | - | -67.38 | -17.00 |
| 1-(2,4,5-trimethoxybenzyl)-4-piperidinecarboxamide | - | -65.83 | -7.16 |
| 1-(2,3,4-trimethoxybenzyl)-4-piperidinecarboxamide | - | -65.81 | -65.81 |
| (1-ethylpiperidin-4-yl)methanol | - | -62.11 | -51.99 |
| 1-(1,1-dioxido-1,2-benzisothiazol-3-yl)-4-piperidinecarboxamide | - | -55.84 | -55.84 |
| (1-isopropylpiperidin-4-yl)methanol | - | -53.36 | -61.20 |
| (1-methyl-2-pyridin-3-ylethyl)amine | - | -50.41 | -48.21 |
| 1-(1-naphthoyl)-4-piperidinecarboxamide | - | -43.63 | -51.04 |
| 1-(10H-phenothiazin-10-ylcarbonyl)-4-piperidinecarboxamide | - | -42.96 | -42.96 |
| 1-(2,2-diphenylethyl)-4-piperidinecarboxamide | - | -33.18 | -33.18 |
| (1H-indol-5-ylmethyl)amine | - | -29.33 | -43.92 |
| 1-(2-adamantyl)-3-piperidinecarboxamide | - | -24.69 | -24.69 |

\* The following table lists some additional molecules I studied in week 4.

|  |  |  |  |
| --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | SIRT3 (4BVG) with Interm | SIRT3 (4BVG) apo-enzyme | SIRT3(4BVH) with AADPR |
| 1-(3-phenyl-2-propen-1-yl)-4-piperidinecarboxamide | -77.62 | -77.01 | -51.55 |
| 1-(3,4-dichlorobenzyl)-4-piperidinecarboxamide | -75.75 | -71.20 | -73.72 |
| 1-(3-phenylpropyl)-4-piperidinecarboxamide | -72.54 | -71.13 | -45.62 |
| 1-(4-hydroxy-3-iodo-5-methoxybenzyl)-4-piperidinecarboxamide | -72.20 | -69.20 | -42.53 |
| 1-(3-anilino-3-oxopropyl)-4-piperidinecarboxamide | -71.85 | -70.42 | -42.83 |
| 1-(3,7-dimethyl-6-octen-1-yl)-4-piperidinecarboxamide | -71.28 | -81.11 | -22.70 |
| 1-(3-phenyl-2-propen-1-yl)-3-piperidinecarboxamide | -70.98 | -77.84 | -64.51 |
| 1-(bicyclo[2.2.1]hept-5-en-2-ylmethyl)-4-piperidinecarboxamide | -70.96 | -69.33 | -56.61 |
| 1-(2-methyl-3-phenyl-2-propen-1-yl)-3-piperidinecarboxamide | -70.08 | -76.67 | -37.92 |
| 1-(3-chlorobenzyl)-4-piperidinecarboxamide | -69.50 | -63.29 | -76.14 |
| 1-(3-phenylbutyl)-4-piperidinecarboxamide | -69.31 | -67.35 | -43.55 |
| 1-(tetrahydro-3-thienyl)-4-piperidinecarboxamide | -69.15 | -66.87 | -76.50 |
| 1-(3-bromobenzyl)-4-piperidinecarboxamide | -68.97 | -66.43 | -75.97 |
| 1-(3-phenylpropyl)-3-piperidinecarboxamide | -68.52 | -74.09 | -40.59 |
| 1-(2-anilino-2-oxoethyl)-4-piperidinecarboxamide hydrochloride | -67.47 | -64.74 | -50.19 |
| 1-(3,7-dimethyl-2,6-octadien-1-yl)-3-piperidinecarboxamide | -67.35 | -80.91 | -27.83 |
| 1-(4-chlorobenzyl)-4-piperidinecarboxamide | -65.91 | -66.78 | -59.07 |
| 1-(2-methyl-2-buten-1-yl)-3-piperidinecarboxamide | -65.55 | -66.61 | -70.97 |
| 1-(2-phenylethyl)-4-piperidinecarboxamide | -65.39 | -63.80 | -58.54 |
| 1-(4-bromobenzyl)-4-piperidinecarboxamide | -65.03 | -67.90 | -47.89 |
| 1-(2-methyl-2-buten-1-yl)-4-piperidinecarboxamide | -64.24 | -72.01 | -64.97 |
| 1-(3-aminopropyl)piperidin-4-ol | -64.22 | -62.15 | -56.33 |
| 1-(3-pyridinylmethyl)-4-piperidinecarboxamide | -63.07 | -59.40 | -63.13 |
| 1-(3-methylcyclopentyl)-3-piperidinecarboxamide | -63.06 | -63.90 | -69.16 |
| 1-(tetrahydro-3-thienyl)-3-piperidinecarboxamide | -62.93 | -70.55 | -73.26 |
| 1-(2-methyl-3-phenyl-2-propen-1-yl)-4-piperidinecarboxamide | -62.36 | -70.83 | -44.29 |
| 1-(2-hydroxybicyclo[2.2.1]hept-7-yl)-2,2-dimethyl-1-propanone | -62.32 | -61.81 | -17.98 |
| 1-(2-chlorobenzyl)-4-piperidinecarboxamide | -62.02 | -63.06 | -77.61 |
| 1-(bicyclo[2.2.1]hept-5-en-2-ylmethyl)-3-piperidinecarboxamide | -61.99 | -76.79 | -65.62 |
| 1-(3-methylcyclopentyl)-4-piperidinecarboxamide | -61.54 | -67.38 | -70.89 |
| 1-(3-aminopropyl)-4-piperidinecarboxamide | -61.49 | -59.56 | -59.23 |
| 1-(2-aminoethyl)piperidine-3-carboxamide | -61.46 | -57.67 | -55.69 |
| 1-(3,4-dichlorobenzyl)-3-piperidinecarboxamide | -61.35 | -77.70 | -70.90 |
| 1-(4-nitrobenzyl)-4-piperidinecarboxamide | -61.32 | -58.95 | -38.43 |
| 1-(3-cyclohexen-1-ylmethyl)-3-piperidinecarboxamide | -61.21 | -69.87 | -86.65 |
| 1-(3-fluorobenzyl)-4-piperidinecarboxamide | -60.97 | -60.68 | -63.90 |
| 1,3,5-trimethylpiperidin-4-one | -60.82 | -55.04 | -49.10 |
| 1-(3-bromobenzyl)-3-piperidinecarboxamide | -60.66 | -70.05 | -72.58 |
| 1-(2-bromobenzyl)-4-piperidinecarboxamide | -60.44 | -62.73 | -80.02 |
| 1-(2-thienylmethyl)-3-piperidinecarboxamide | -60.38 | -56.28 | -75.71 |
| 1,2,2,5-tetramethylpiperidin-4-ol | -60.26 | -57.11 | -55.28 |
| 1-(4-fluorobenzyl)-4-piperidinecarboxamide | -60.23 | -59.85 | -57.83 |
| 1-(2-phenylpropyl)-3-piperidinecarboxamide | -60.21 | -64.24 | -59.67 |
| 1-(3-phenylbutyl)-3-piperidinecarboxamide | -60.20 | -77.68 | -49.59 |
| 1-(3-bromo-4-hydroxy-5-methoxybenzyl)-3-piperidinecarboxamide | -59.86 | -70.00 | -40.35 |
| 1-(3-bromo-4-fluorobenzyl)-4-piperidinecarboxamide | -59.52 | -66.21 | -70.25 |
| 1-(3-methylcyclohexyl)-4-piperidinecarboxamide | -58.85 | -62.97 | -70.73 |
| 1-(2-chloro-6-fluorobenzyl)-4-piperidinecarboxamide | -57.13 | -57.55 | -66.78 |
| 1-(phenylacetyl)-4-piperidinecarboxamide | -57.05 | -58.39 | -42.84 |
| 1-(3-chlorobenzyl)-3-piperidinecarboxamide | -56.88 | -59.74 | -75.03 |
| 1-(3-bromo-4-fluorobenzyl)-3-piperidinecarboxamide | -56.79 | -72.99 | -65.60 |
| 1-(2-phenylpropyl)-4-piperidinecarboxamide | -56.54 | -61.84 | -45.11 |
| 1-(3-iodobenzoyl)-4-piperidinecarboxamide | -56.07 | -62.05 | -45.58 |
| 1-(4-bromobenzyl)-3-piperidinecarboxamide | -55.57 | -66.00 | -60.91 |
| 1-(2-phenylethyl)-3-piperidinecarboxamide | -55.30 | -68.84 | -64.50 |
| 1-(4-chlorobenzyl)-3-piperidinecarboxamide | -55.16 | -63.62 | -66.46 |
| 1,2,5-trimethyl-4-piperidinone oxime | -54.89 | -52.13 | -45.18 |
| 1-(4-methylcyclohexyl)-4-piperidinecarboxamide | -54.88 | -66.18 | -60.45 |
| 1-(4-isopropylbenzyl)-3-piperidinecarboxamide | -54.70 | -66.12 | -22.22 |
| 1-(4-methoxybenzyl)-3-piperidinecarboxamide | -54.58 | -63.97 | -47.27 |
| 1-(2-furylmethyl)-3-piperidinecarboxamide | -54.57 | -55.08 | -69.98 |
| 1-(2-fluorobenzyl)-4-piperidinecarboxamide | -54.21 | -49.64 | -69.37 |
| 1-(aminomethyl)-N-ethyl-N-methylcyclohexanamine | -54.16 | -49.05 | -58.46 |
| 1-(3-cyclohexen-1-ylmethyl)-4-piperidinecarboxamide | -53.98 | -65.20 | -75.67 |
| 1-(4-nitrobenzyl)-3-piperidinecarboxamide | -53.98 | -59.06 | -59.59 |
| 1-(4-methylcyclohexyl)-4-piperidinol | -53.51 | -55.09 | -59.36 |
| 1-(3-methylcyclohexyl)-3-piperidinol | -53.49 | -68.15 | -67.36 |
| 1-(cyclohexylmethyl)-4-methylpiperazine | -52.98 | -56.70 | -67.41 |
| 1-(3-fluorobenzyl)-3-piperidinecarboxamide | -52.59 | -57.95 | -67.35 |
| 1-(3-nitrobenzyl)-3-piperidinecarboxamide | -52.20 | -62.89 | -66.58 |
| 1-(3,4-dimethoxybenzyl)-3-piperidinecarboxamide | -52.06 | -65.48 | -49.66 |
| 1-(3-methylbenzyl)-3-piperidinecarboxamide | -51.90 | -57.57 | -71.09 |
| 1-(3-methylcyclohexyl)-3-piperidinecarboxamide | -51.48 | -71.88 | -65.99 |
| 1-(2-chlorobenzyl)-3-piperidinecarboxamide | -51.44 | -62.57 | -79.41 |
| 1-(2-furoyl)-4-piperidinecarboxamide | -51.12 | -48.34 | -61.95 |
| 1-(3,4-difluorobenzyl)-3-piperidinecarboxamide | -50.91 | -57.85 | -60.87 |
| 1,4-dimethyldecahydroquinolin-4-ol | -50.89 | -50.55 | -55.70 |
| 1-(4-methylbenzyl)-3-piperidinecarboxamide | -50.78 | -54.28 | -58.90 |
| 1,3-dimethyl-4-piperidinone oxime | -50.62 | -50.04 | -44.70 |
| 1,5,6,7-tetrahydro-4H-indol-4-one | -50.08 | -48.70 | -41.49 |
| 1-(4-iodobenzoyl)-4-piperidinecarboxamide | -49.84 | -65.04 | -59.60 |
| 1-(4-hydroxy-3-iodo-5-methoxybenzyl)-3-piperidinecarboxamide | -49.73 | -69.25 | -43.29 |
| 1-(2-naphthylmethyl)-3-piperidinecarboxamide | -49.22 | -58.12 | -50.55 |
| 1-(4-methoxy-3-methylbenzyl)-3-piperidinecarboxamide | -49.15 | -56.29 | -44.95 |
| 1-(4-fluorobenzyl)-3-piperidinecarboxamide | -48.66 | -60.09 | -60.96 |
| 1-(3,4-dichlorobenzoyl)-4-piperidinecarboxamide | -48.53 | -68.18 | -49.04 |
| 1-(4-methoxy-2,5-dimethylbenzyl)-3-piperidinecarboxamide | -47.72 | -57.08 | -34.13 |
| 1-(3-fluorobenzoyl)-4-piperidinecarboxamide | -47.52 | -52.76 | -56.55 |
| 1-(5-bromo-2-methoxybenzyl)-3-piperidinecarboxamide | -46.95 | -65.08 | -63.79 |
| 1-(3-methylbenzoyl)-4-piperidinecarboxamide | -46.93 | -54.25 | -55.12 |
| 1',3'-dihydrospiro[cyclohexane-1,2'-imidazo[4,5-b]pyridine] | -46.88 | -51.90 | -39.14 |
| 1,4-diazabicyclo[3.2.2]nonan-3-one | -46.67 | -45.96 | -47.84 |
| 1-(2-phenoxypropanoyl)-4-piperidinecarboxamide | -46.67 | -68.67 | -39.34 |
| 1-(cyclohexylmethyl)-3-piperidinecarboxamide | -46.39 | -67.86 | -79.47 |
| 1-(morpholin-4-ylmethyl)cyclohexanamine | -46.19 | -46.44 | -51.35 |
| 1,2-cyclopentanedicarboxamide | -46.12 | -48.49 | -58.14 |
| 1-(4-ethylphenyl)ethanamine | -46.09 | -34.10 | -59.11 |
| 1-(2-methoxybenzyl)-3-piperidinecarboxamide | -45.95 | -58.27 | -55.47 |
| 1-(4-methylcyclohexyl)-3-piperidinecarboxamide | -45.36 | -63.49 | -60.21 |
| 1-(5-bromo-2-methoxybenzyl)-4-piperidinecarboxamide | -45.34 | -73.18 | -43.48 |
| 1-(2-nitrobenzyl)-3-piperidinecarboxamide | -45.11 | -58.45 | -56.93 |
| 1-(3-methylbutyl)-5-oxo-3-pyrrolidinecarboxamide | -44.93 | -60.11 | -60.38 |
| 1-(cyanomethyl)piperidine-3-carboxamide | -44.81 | -43.30 | -51.83 |
| 1-(3-ethoxy-4-methoxybenzyl)-4-piperidinecarboxamide | -44.77 | -77.11 | -22.66 |
| 1-(3-phenylpropanoyl)-4-piperidinecarboxamide | -44.68 | -58.74 | -40.63 |
| 1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane-6,7-diol | -44.40 | -40.24 | -34.05 |
| 1,4-diazaspiro[5.5]undecan-5-one | -44.40 | -43.30 | -57.52 |
| 1,3-benzothiazol-2-amine | -44.01 | -42.00 | -49.12 |
| 1,2,6-trimethylpyridin-4(1H)-one | -43.93 | -39.97 | -45.25 |
| 1-(5-bromo-2,4-dimethoxybenzyl)-4-piperidinecarboxamide | -43.83 | -67.72 | -38.81 |
| 1-(4-fluorobenzoyl)-4-piperidinecarboxamide | -43.44 | -53.82 | -50.88 |
| 1-(2-furoyl)-2-phenylprolinamide | -42.31 | -34.17 | -17.74 |
| 1-(3-methylbenzyl)-4-piperidinecarboxamide | -41.69 | -64.61 | -72.63 |
| 1-(phenylsulfonyl)-4-piperidinecarboxamide | -41.42 | -38.26 | -41.28 |
| 1,3-dihydro-2-benzofuran-5-amine | -41.36 | -39.85 | -44.65 |
| 1,2-dimethyl-1H-indole | -40.30 | -39.08 | -48.28 |
| 1-(2-bromobenzoyl)-2-phenylprolinamide | -40.20 | -29.83 | -29.83 |
| 1-(4-ethylcyclohexyl)-3-piperidinecarboxamide | -40.10 | -64.73 | -61.94 |
| 1,4-dimethoxybenzene | -39.77 | -35.51 | -42.82 |
| 1-(2-hydroxyphenyl)-1H-pyrrole-2,5-dione | -39.37 | -44.59 | -59.00 |
| 1-(3-methylpyridin-4-yl)methanamine | -39.26 | -35.98 | -37.68 |
| 1-(piperidin-1-ylmethyl)cyclohexanamine | -39.08 | -39.71 | -55.71 |
| 1,1-cyclopropanedicarboxamide | -38.40 | -35.96 | -38.32 |
| 1-(3-hydroxy-1-adamantyl)ethanone | -37.97 | -36.94 | -52.92 |
| 1-(3-chlorobenzoyl)-4-piperidinecarboxamide | -37.39 | -59.33 | -58.31 |
| 1-(4-aminophenyl)ethanoneoxime | -36.31 | -29.29 | -40.70 |
| 1-(6-methylpyridin-2-yl)methanamine | -36.16 | -32.89 | -40.49 |
| 1,3-benzodioxol-5-ylmethanol | -36.08 | -43.57 | -44.95 |
| 1-(3-bromobenzoyl)-4-piperidinecarboxamide | -35.96 | -59.94 | -54.53 |
| 1,3-benzoxazole-2-thiol | -35.33 | -35.64 | -41.64 |
| 1-(3-hydroxy-4-methoxybenzyl)-4-piperidinecarboxamide | -35.11 | -64.47 | -55.26 |
| 1-(3-phenoxybenzyl)-4-piperidinecarboxamide | -35.06 | -68.20 | -43.94 |
| 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid | -34.48 | -36.03 | -42.88 |
| 1-(4-methoxybenzoyl)-4-piperidinecarboxamide | -33.15 | -59.61 | -45.20 |
| 1-(2-bromobenzoyl)-4-piperidinecarboxamide | -32.30 | -51.96 | -36.10 |
| 1-(phenylsulfonyl)cyclopropanecarboxamide | -32.24 | -41.54 | -56.11 |
| 1-(4-nitrobenzoyl)-4-piperidinecarboxamide | -31.95 | -55.64 | -57.33 |
| 1-(2-fluorobenzoyl)-4-piperidinecarboxamide | -30.66 | -49.54 | -50.38 |
| 1-(4-methylphenyl)ethanoneoxime | -30.07 | -37.99 | -42.55 |
| 1-(2-methoxybenzyl)-4-piperidinecarboxamide | -29.77 | -50.44 | -57.19 |
| 1,5,6,7-tetrahydro-4H-indol-4-one oxime | -29.51 | -42.91 | -44.90 |
| 1-(3,4-dimethoxyphenyl)cyclopentanecarboxamide | -29.16 | -45.10 | -64.85 |
| 1-(cyclohexylmethyl)-4-piperidinecarboxamide | -29.14 | -65.79 | -68.69 |
| 1-(benzylsulfonyl)-4-piperidinecarboxamide | -28.10 | -55.79 | -20.82 |
| 1,6-dimethyl-2,3,4,9-tetrahydro-1H-carbazole-1-carboxamide | -27.62 | -41.57 | -81.11 |
| 1-(2-methylbenzoyl)-4-piperidinecarboxamide | -27.53 | -49.39 | -45.96 |
| 1-(4-morpholinyl)cyclohexanecarbonitrile | -27.46 | -38.53 | -47.14 |
| 1-(phenylsulfonyl)cyclohexanecarboxamide | -26.73 | -24.48 | -20.86 |
| 1-(anilinocarbonothioyl)-4-piperidinecarboxamide | -25.06 | -46.27 | -28.90 |
| 1,4,7-trimethyl-1H-indole | -24.75 | -36.29 | -50.66 |
| 1,7,7-trimethyl-3-[(methylimino)methyl]bicyclo[2.2.1]heptan-2-ol | -20.22 | -26.90 | -51.15 |
| 1-(phenoxyacetyl)-4-piperidinecarboxamide | -19.94 | -68.13 | -49.80 |
| 1,3-adamantanedicarboxamide | -19.84 | -17.82 | -26.65 |
| 1-(4-phenylcyclohexyl)-3-piperidinecarboxamide | -18.15 | -77.51 | -77.51 |
| 1-(2-chloro-4-methylbenzoyl)-4-piperidinecarboxamide | -10.79 | -58.38 | -55.07 |
| 1-(4-methylbenzoyl)-4-piperidinecarboxamide | -10.58 | -56.16 | -42.92 |
| 1,3-bis(hydroxyamino)adamantane | -9.36 | -7.94 | -33.90 |
| 1-(cyclohexylacetyl)-4-piperidinecarboxamide | -7.78 | -40.66 | -49.35 |
| 1-(4-methoxy-2,3-dimethylbenzyl)-4-piperidinecarboxamide | -4.38 | -59.54 | -34.13 |
| 1-(4-methoxy-3-methylbenzyl)-4-piperidinecarboxamide | -4.35 | -61.58 | -51.29 |
| 1-(3-chloro-4-methylbenzoyl)-4-piperidinecarboxamide | -3.59 | -57.95 | -51.90 |
| 1,3-dihydro-2H-imidazo[4,5-b]pyridine-2-thione | 2.96 | -15.32 | -20.64 |
| 1-(2-chloro-4-nitrobenzoyl)-4-piperidinecarboxamide | - | -60.69 | -46.23 |
| 1-(2-naphthoyl)-4-piperidinecarboxamide | - | -53.39 | -48.89 |
| 1-(2-naphthylsulfonyl)-4-piperidinecarboxamide | - | -48.49 | -31.06 |
| 1'-(2-phenylethyl)-1,4'-bipiperidine-3-carboxamide | - | -80.04 | -43.20 |
| 1-(3,4,5-trimethoxybenzoyl)-4-piperidinecarboxamide | - | -61.56 | -21.39 |
| 1-(3,4,5-trimethoxybenzyl)-4-piperidinecarboxamide | - | -64.26 | -44.33 |
| 1-(3,4-dimethoxybenzoyl)-4-piperidinecarboxamide | - | -60.67 | -31.41 |
| 1-(3,4-dimethoxybenzyl)-4-piperidinecarboxamide | - | -64.80 | -53.20 |
| 1-(3,5-dimethoxybenzyl)-4-piperidinecarboxamide | - | -56.02 | -40.71 |
| 1-(3,5-di-tert-butyl-4-hydroxybenzyl)-3-piperidinecarboxamide | - | -55.83 | -55.83 |
| 1-(3,5-di-tert-butyl-4-hydroxybenzyl)-4-piperidinecarboxamide | - | -52.22 | -52.22 |
| 1-(3-methyl-4-nitrobenzoyl)-4-piperidinecarboxamide | - | -55.02 | -37.77 |
| 1-(4,6-dianilino-1,3,5-triazin-2-yl)-4-piperidinecarboxamide | - | -79.23 | -79.23 |
| 1-(4-biphenylylmethyl)-4-piperidinecarboxamide | - | -59.58 | -59.58 |
| 1-(4-bromobenzoyl)-2-phenylprolinamide | - | -50.68 | -50.68 |
| 1-(4-chlorobenzoyl)-4-piperidinecarboxamide | - | -56.48 | -43.71 |
| 1-(4-ethylcyclohexyl)-4-piperidinecarboxamide | - | -58.75 | -49.17 |
| 1-(4-methoxyphenyl)-5-oxo-2-phenylprolinamide | - | -27.90 | -27.90 |
| 1-(4-methyl-3-nitrobenzoyl)-4-piperidinecarboxamide | - | -56.79 | -41.02 |
| 1-(4-methylphenyl)-5-oxo-2-phenylprolinamide | - | -43.62 | -43.62 |
| 1-(4-phenylcyclohexyl)-4-piperidinecarboxamide | - | -68.78 | -68.78 |
| 1-(4-tert-butylbenzoyl)-4-piperidinecarboxamide | - | -58.12 | -58.12 |
| 1-(4-tert-butylcyclohexyl)-3-piperidinecarboxamide | - | -52.92 | -25.12 |
| 1-(4-tert-butylcyclohexyl)-4-piperidinecarboxamide | - | -44.17 | -17.58 |
| 1-(9-anthrylmethyl)-3-piperidinecarboxamide | - | -63.60 | -63.60 |
| 1-(9-anthrylmethyl)-4-piperidinecarboxamide | - | -58.08 | -58.08 |
| 1-(9H-fluoren-2-ylmethyl)-3-piperidinecarboxamide | - | -68.26 | -68.26 |
| 1-(9H-fluoren-2-ylmethyl)-4-piperidinecarboxamide | - | -63.24 | -63.24 |
| 1-(mesitylsulfonyl)-4-piperidinecarboxamide | - | -13.64 | 10.58 |
| 1,4-cubanedicarboxylic acid | - | -16.17 | 0.29 |