\* Calculated MM-GBSA values for top poses for selected small molecules (Week7)

|  |  |  |  |
| --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | SIRT3 (4BVG) with Interm | SIRT3 (4BVG) apo-enzyme | SIRT3(4BVH) with AADRP |
| (1-isobutylpiperidin-3-yl)methanol | -110.50 | -57.79 | -71.04 |
| 1,3'-bipiperidin-4-ylmethanol | -76.69 | -73.12 | -71.59 |
| 1-(2-methyl-2-buten-1-yl)-3-piperidinol | -74.50 | -72.75 | -70.29 |
| 1-(tetrahydro-3-thienyl)-4-piperidinol | -73.83 | -71.43 | -71.76 |
| 1-methyl-N-(tetrahydro-2-furanylmethyl)-4-piperidinamine | -72.98 | -75.90 | -81.49 |
| 1-(3-cyclopropyl-2-propyn-1-yl)piperidine | -72.75 | -71.67 | -68.63 |
| 1-(3-cyclohexen-1-ylmethyl)-4-piperidinol | -71.77 | -68.32 | -79.13 |
| 2-(1-cyclopentylpiperidin-4-yl)ethanamine | -71.54 | -69.47 | -71.36 |
| 1-[3-(2-furyl)-2-propen-1-yl]piperidine | -70.96 | -65.02 | -73.47 |
| (1-isobutylpiperidin-4-yl)methanol | -70.38 | -66.98 | -67.85 |
| 1-(3-cyclohexen-1-ylmethyl)-3-piperidinol | -69.54 | -68.08 | -81.91 |
| [1-(3-methylcyclopentyl)-3-piperidinyl]methanol | -69.16 | -70.49 | -69.88 |
| 1-ethyl-N-(2-methoxyethyl)-4-piperidinamine | -68.05 | -72.74 | -63.05 |
| 1-(3-thienylmethyl)-4-piperidinol | -67.53 | -65.19 | -69.23 |
| 1-(2-methylpyridin-4-yl)piperazine | -67.31 | -66.58 | -46.51 |
| 1-(1-isopropylpiperidin-3-yl)-N-methylmethanamine | -67.15 | -56.81 | -61.56 |
| 1-(1-cyclopentylpiperidin-4-yl)methanamine | -66.83 | -63.85 | -64.30 |
| 1-(4-hydroxy-1,4-dimethyl-3-piperidinyl)ethanone | -66.00 | -63.32 | -59.01 |
| (1R,9aR)-octahydro-2H-quinolizin-1-ylmethanol | -65.90 | -61.05 | -66.66 |
| 1-[1-(cyclopropylcarbonyl)piperidin-3-yl]methanamine | -65.78 | -54.78 | -68.82 |
| 1-(2-thienylmethyl)-4-piperidinol | -65.67 | -61.60 | -73.34 |
| 2,2,4,6-tetramethyl-3-oxabicyclo[3.3.1]non-6-ene | -65.28 | -62.64 | -47.29 |
| 1-acetyl-N-methyl-N-2-propyn-1-yl-4-piperidinamine | -65.28 | -58.75 | -60.91 |
| 2-(pyrrolidin-1-ylmethyl)piperidine | -65.27 | -61.32 | -59.59 |
| 1-(5-chloropyridin-2-yl)piperazine | -65.17 | -63.52 | -74.84 |
| 1-(3-thienylmethyl)-3-piperidinol | -64.89 | -57.69 | -72.30 |
| 1-(3-pyridinylmethyl)-4-piperidinol | -63.99 | -59.07 | -62.82 |
| 1-(1-isobutyrylpiperidin-4-yl)methanamine | -63.97 | -52.22 | -63.09 |
| [1-(2-furylmethyl)-2-piperidinyl]methanol | -63.69 | -55.13 | -70.97 |
| (3-pyridinylmethyl)tetrahydro-2H-pyran-4-ylamine | -63.63 | -54.90 | -63.18 |
| 2-methyl-N-propyl-1-piperidinecarboxamide | -63.46 | -63.35 | -80.75 |
| 1-cyclopentyl-3-piperidinamine | -63.40 | -61.12 | -66.45 |
| 2-(1-cyclopentylpiperidin-2-yl)ethanamine | -63.27 | -66.70 | -59.04 |
| 1-[2-(3-methyl-1H-1,2,4-triazol-5-yl)ethyl]piperidine | -62.70 | -56.69 | -63.24 |
| 1-(3-pyridinylmethyl)-3-piperidinol | -62.55 | -54.55 | -63.01 |
| 1-methyl-4-(2-methylprop-2-en-1-yl)piperidin-4-ol | -62.48 | -49.47 | -60.67 |
| 1-methyl-4-phenyl-4-piperidinol | -62.41 | -55.51 | -68.88 |
| 1-(2-pyridinyl)-4-piperidinol | -61.96 | -61.85 | -46.70 |
| 1-(2,2-dimethyltetrahydro-2H-pyran-4-yl)-1-pentanone | -61.52 | -62.55 | -73.55 |
| 2,3-dimethyl-6,7-dihydro-5H-cyclopenta[b]pyridin-4-amine hydrochloride | -60.71 | -67.82 | -60.77 |
| 1-benzyl-3-piperidinol | -60.65 | -53.97 | -63.35 |
| 10-azabicyclo[4.3.1]decane hydrochloride | -60.32 | -58.76 | -52.88 |
| 2-(methoxymethyl)piperidine hydrochloride | -60.32 | -53.60 | -53.91 |
| 2-[propyl(2-pyridinylmethyl)amino]ethanol | -60.19 | -49.93 | -71.31 |
| 1-ethyl-4-piperidin-4-ylpiperazine | -60.18 | -57.92 | -72.03 |
| 1-(1H-pyrrol-2-ylmethyl)-4-piperidinol | -60.17 | -56.79 | -61.23 |
| 1-(2-pyridinyl)azepane | -59.82 | -59.39 | -38.34 |
| 2-{[2-(4-pyridinyl)ethyl]thio}ethanol | -59.76 | -56.25 | -64.43 |
| 1-[1-(cyclopropylcarbonyl)piperidin-4-yl]methanamine | -59.76 | -49.48 | -62.20 |
| 2-(2-methyl-2,8-diazaspiro[4.5]dec-8-yl)ethanamine | -59.31 | -55.90 | -43.44 |
| 2-(1-isopropylpiperidin-2-yl)ethanamine | -58.97 | -51.79 | -52.44 |
| 2-methyl-2,8-diazaspiro[5.5]undecane | -58.90 | -55.06 | -49.10 |
| 2-tert-butyl-4-(hydroxymethyl)-6-methyl-3-pyridinol | -58.59 | -59.82 | -40.32 |
| 1-(2-pyridinylmethyl)-3-piperidinamine | -58.35 | -51.15 | -62.38 |
| 2-(tetrahydro-2H-pyran-4-yl)-1,3-thiazol-4-amine | -58.28 | -50.11 | -64.97 |
| 2,2-dimethyl-3-oxaspiro[5.5]undec-7-en-9-one | -58.28 | -56.36 | -44.24 |
| 10,12-dioxatetracyclo[7.2.1.1~3,6~.0~2,7~]tridec-4-en-8-one | -58.21 | -57.11 | -43.11 |
| 1-(piperidin-3-ylmethyl)pyrrolidin-2-one | -58.20 | -56.86 | -71.98 |
| 1-(3-pyridinylmethyl)azepane | -58.20 | -50.30 | -67.17 |
| 1-(2-pyridinyl)-3-piperidinol | -58.18 | -58.80 | -52.34 |
| 2-(2,7-diazaspiro[4.5]dec-7-yl)-2-oxoethanol | -58.16 | -56.01 | -66.69 |
| 1-propyl-4-(1-pyrrolidinyl)piperidine | -57.79 | -62.09 | -73.21 |
| 1-[(3-methylpyridin-2-yl)methyl]piperazine | -57.75 | -48.68 | -56.91 |
| 1-methyl-4-(3-pyridinylmethyl)piperazine | -57.72 | -52.73 | -66.54 |
| 1-(3-methylpyridin-4-yl)-1,4-diazepane | -57.40 | -54.72 | -49.35 |
| 1,4'-bipiperidin-4-ol | -57.18 | -55.19 | -66.07 |
| [1-(1-methyl-4-piperidinyl)-2-pyrrolidinyl]methanol | -57.04 | -58.90 | -67.61 |
| 1-(1-piperidinyl)-2-heptyn-4-ol | -56.98 | -65.54 | -72.35 |
| 1-(4-hydroxy-1,2,5-trimethyl-4-piperidinyl)ethanone | -56.83 | -59.48 | -48.06 |
| 2-benzylpiperidine | -56.72 | -54.04 | -60.04 |
| (4-methylphenyl)tetrahydro-2H-pyran-4-ylamine | -56.57 | -48.56 | -66.73 |
| (5-methyl-2-furyl)(pyridin-3-yl)methanol | -56.41 | -49.44 | -55.19 |
| 2-chloro-N-propylnicotinamide | -56.25 | -58.93 | -58.54 |
| 2-(2-methyltetrahydro-2H-pyran-4-yl)-1,3-thiazol-4-amine | -56.14 | -57.51 | -63.40 |
| 2,2-dimethyl-N-(1-methyl-4-piperidinyl)propanamide | -55.97 | -57.73 | -56.44 |
| 1-ethyl-4-(2-pyridinyl)piperazine | -55.87 | -56.75 | -60.01 |
| 1',4-dimethyl-1,4'-bipiperidine | -55.77 | -56.85 | -68.45 |
| (4,6-dimethyl-3-oxabicyclo[3.3.1]non-6-en-1-yl)methanol | -55.77 | -53.17 | -54.30 |
| 1-acetyloctahydro-1H-cyclopenta[b]pyridin-4-ol | -55.54 | -54.16 | -56.19 |
| 2-(5-methyl-3-isoxazolyl)piperidine | -55.43 | -46.82 | -65.62 |
| (3-isobutylpiperidin-3-yl)methanol | -55.36 | -55.17 | -55.61 |
| 1-(2,2-dimethyltetrahydro-2H-pyran-4-yl)propan-1-one | -55.29 | -54.95 | -58.54 |
| [(1-acetyl-3-piperidinyl)methyl]amine hydrochloride | -55.12 | -52.37 | -62.86 |
| 2-(1-piperidinylmethyl)phenol | -54.93 | -50.07 | -66.35 |
| 2-(1-piperidinyl)-4H-1,3,4-thiadiazin-5(6H)-one | -54.82 | -50.01 | -61.13 |
| 1-(2-furylmethyl)piperidin-4-one | -54.23 | -55.94 | -54.75 |
| 2-(1,3-thiazol-2-yl)piperidine | -54.11 | -48.27 | -61.62 |
| (4-fluorophenyl)tetrahydro-2H-pyran-4-ylamine | -53.59 | -41.67 | -54.18 |
| 2-(2-piperidin-2-ylethyl)pyridine | -53.52 | -60.25 | -68.11 |
| 2-[(6-methyl-2-propyl-4-pyrimidinyl)amino]ethanol | -53.46 | -57.69 | -38.57 |
| 1,4'-bipiperidin-3-ol | -53.46 | -50.63 | -65.30 |
| 1-(pyridin-3-ylmethyl)piperidin-4-amine | -53.36 | -47.37 | -53.82 |
| 2,6-dimethyl-2-(4-methyl-3-penten-1-yl)tetrahydro-2H-pyran | -53.18 | -64.07 | -71.73 |
| (4-methylphenyl)(3-pyridinylmethyl)amine | -52.75 | -47.35 | -59.53 |
| 1-acetyl-N-methyl-N-propyl-4-piperidinamine | -52.60 | -60.64 | -62.90 |
| 1-(pyridin-4-ylmethyl)piperidin-4-amine | -52.25 | -43.48 | -62.38 |
| 2-(4-ethyl-1-piperazinyl)pyrimidine | -52.21 | -51.73 | -61.36 |
| 1'-methyl-1,4'-bipiperidin-3-ol | -52.15 | -61.02 | -71.15 |
| 1-(2-piperidin-2-ylethyl)pyrrolidin-2-one | -51.95 | -62.44 | -74.95 |
| 1-cycloheptyl-3-piperidinamine | -51.83 | -48.94 | -62.98 |
| 1-(2,6-dimethylpyridin-4-yl)piperazine | -51.65 | -66.07 | -40.27 |
| 2-methyl-5-(1-piperidinyl)-3-pentyn-2-ol | -51.58 | -69.95 | -70.46 |
| 2,4-dimethyl-2,3-dihydrofuro[3,2-c]quinoline | -51.54 | -75.40 | -53.53 |
| 1'-ethyl-1,4'-bipiperidine | -51.22 | -56.97 | -52.98 |
| 2-methyl-6-piperidin-4-ylpyrimidin-4(3H)-one | -51.16 | -50.59 | -59.34 |
| 2-furyl(1-piperidinyl)acetonitrile | -51.13 | -49.08 | -60.68 |
| 1-oxa-3,8-diazaspiro[4.5]decan-2-one hydrochloride | -50.94 | -40.27 | -51.00 |
| 2-chloro-N,N-dimethylnicotinamide | -50.14 | -44.21 | -55.47 |
| 1-propionyl-4-piperidinamine hydrochloride | -50.02 | -40.48 | -56.72 |
| 2,5-dichloro-4-methoxypyridin-3-amine | -50.00 | -48.95 | -55.65 |
| 1-(2-pyrazinyl)-4-piperidinol | -49.82 | -48.92 | -60.25 |
| 1-(2-pyrimidinyl)-3-piperidinamine | -49.82 | -45.88 | -61.74 |
| (4-methylphenyl)(4-pyridinylmethyl)amine | -49.80 | -50.59 | -53.05 |
| 2-piperidin-2-ylpyridine | -49.79 | -44.53 | -61.66 |
| 1-(piperidin-4-ylmethyl)pyrrolidin-2-one | -49.71 | -52.29 | -72.70 |
| 1'-methyl-1,4'-bipiperidine | -49.50 | -51.75 | -55.64 |
| 1-(3-methylpyridin-2-yl)piperazine | -49.31 | -47.72 | -66.06 |
| 2-[(2-ethyl-6-methyl-3-pyridinyl)oxy]acetamide | -49.28 | -50.53 | -53.44 |
| 1-(3-methylpyridin-4-yl)piperazine | -49.08 | -60.59 | -45.94 |
| 2-(4-fluorophenyl)piperidine | -49.00 | -45.46 | -56.62 |
| (4,6,8-trimethyl-3-oxabicyclo[3.3.1]non-6-en-1-yl)methanol | -48.89 | -44.90 | -48.82 |
| 1-acetyl-3-piperidinecarbohydrazide | -48.82 | -46.89 | -59.93 |
| 2,2,5-trimethyl-3-piperidinone hydrochloride | -48.26 | -47.18 | -46.63 |
| 2-[(5-amino-6-chloropyrimidin-4-yl)amino]ethanol | -48.07 | -37.08 | -47.44 |
| 2-chloro-N-methylnicotinamide | -47.87 | -47.01 | -49.20 |
| 1-azabicyclo[2.2.2]oct-3-ylmethanol hydrochloride | -47.82 | -42.14 | -55.00 |
| 2-(3-fluorophenyl)piperidine | -47.57 | -42.22 | -56.60 |
| 2-phenylpiperidine | -47.55 | -43.66 | -59.74 |
| 1-(cyclobutylcarbonyl)-4-piperidinone | -47.46 | -56.59 | -60.52 |
| 2-methyl-N-(3-pyridinylmethyl)-2-propanamine | -47.39 | -48.47 | -54.82 |
| 1-ethyl-2-piperidinecarboxylic acid hydrochloride | -47.36 | -44.54 | -47.31 |
| 2-(3-methylpiperidin-1-yl)propanoic acid | -47.25 | -44.17 | -38.69 |
| 1-(2-piperidin-4-ylethyl)pyrrolidin-2-one | -47.22 | -62.83 | -72.01 |
| (4-chloro-2-pyridinyl)methanol hydrochloride | -47.11 | -46.93 | -50.11 |
| 2-chloro-4-(methoxymethyl)-6-methylnicotinonitrile | -46.98 | -52.62 | -39.89 |
| (2-ethyl-1-piperidinyl)acetic acid | -46.72 | -42.47 | -46.06 |
| 2-ethyl-6-methyl-4-nitro-3-pyridinol | -46.60 | -56.85 | -21.36 |
| 1-[(1-methyl-1H-pyrazol-5-yl)carbonyl]piperidine | -46.52 | -51.88 | -54.70 |
| 1-{[(2-amino-5-pyrimidinyl)methyl]amino}-2-propanol | -46.40 | -53.25 | -52.62 |
| 2-methyl-4-(2-pyridinyl)-3-butyn-2-ol | -46.39 | -56.29 | -67.13 |
| (4-methylphenyl)(4-pyridinylmethylene)amine | -46.21 | -45.65 | -48.32 |
| 1-(4-methylphenyl)piperidin-4-one | -46.11 | -46.03 | -62.94 |
| 2-nitro-1-pyridin-4-ylethanol | -46.10 | -47.76 | -43.92 |
| 1-phenyl-2-(3-pyridinyl)ethanol | -46.10 | -54.49 | -57.56 |
| 1-(cyclopropylcarbonyl)-4-piperidinone | -46.06 | -49.05 | -52.91 |
| 2-(bromomethyl)-3-methylpyridine | -45.97 | -41.69 | -55.18 |
| 2-(4-methyl-1-piperidinyl)aniline | -45.76 | -43.28 | -56.32 |
| 2-chloro-4-(dimethylamino)nicotinonitrile | -45.73 | -45.17 | -50.60 |
| 2-amino-7,7-dimethyl-7,8-dihydro-5(6H)-quinazolinone | -45.69 | -49.60 | -55.62 |
| 1-(4-fluorophenyl)piperidin-4-one | -45.65 | -47.18 | -50.00 |
| 2,6-dichloro-4-methylnicotinonitrile | -45.57 | -48.61 | -50.38 |
| 2-hydroxy-N'-(4-pyridinylmethylene)propanohydrazide | -45.53 | -49.83 | -46.24 |
| 1-(4-pyridinyl)indoline | -45.47 | -49.55 | -57.49 |
| 2-chloro-4,6-dimethylnicotinamide | -45.39 | -51.74 | -59.66 |
| [1-(2-pyrimidinyl)-3-piperidinyl]methanol | -45.35 | -49.88 | -67.10 |
| 1-(4-fluorophenyl)-3-oxabicyclo[3.1.0]hexan-2-one | -45.16 | -52.54 | -62.01 |
| 1-(pyridin-3-ylmethyl)-1H-pyrazol-5-amine | -45.13 | -47.15 | -57.90 |
| 2-(3-methoxyphenyl)-6-methylpyridine | -45.11 | -47.10 | -58.63 |
| 2-(pyridin-3-yloxy)aniline | -44.91 | -49.29 | -55.32 |
| 2-amino-5,6,7,8-tetrahydro-4-quinazolinol | -44.84 | -44.28 | -48.96 |
| 1-[2-amino-2-(hydroxyimino)ethyl]pyridinium chloride | -44.83 | -43.31 | -39.44 |
| 1-ethyl-3-piperidinecarboxylic acid hydrochloride | -44.81 | -45.34 | -45.60 |
| 2-(4,5-dihydro-1H-imidazol-2-yl)pyridine hydrochloride | -44.60 | -44.77 | -47.90 |
| 2-(methylthio)-6,7-dihydro-5H-cyclopenta[b]pyridine-3-carbonitrile | -44.38 | -51.90 | -72.48 |
| 2-chloro-8-quinolinol | -44.31 | -50.18 | -58.51 |
| 2-propylisonicotinamide | -44.26 | -50.06 | -54.25 |
| 2-ethyl-2-methyltetrahydro-2H-pyran-4-carbothioamide | -44.23 | -49.54 | -41.67 |
| 1-(2-pyrimidinyl)-3-piperidinol | -44.22 | -48.72 | -62.26 |
| 1-ethyl-4-piperidinecarboxylic acid hydrochloride | -44.20 | -42.25 | -45.86 |
| 1-(6-methyl-2-pyridinyl)-2,5-pyrrolidinedione | -44.18 | -48.43 | -53.76 |
| (6,8,9-trimethyl-3-oxabicyclo[3.3.1]non-6-en-1-yl)methanol | -44.17 | -40.81 | -54.28 |
| 1-(2-furylmethyl)-2,6-piperidinedione | -44.08 | -49.61 | -45.90 |
| 1,4-dihydropyrido[2,3-b]pyrazine-2,3-dione | -44.02 | -43.66 | -38.83 |
| 2-(1-piperidinyl)propanoic acid hydrochloride | -43.82 | -44.73 | -34.92 |
| [2-(dimethylamino)-3-pyridinyl]methanol hydrochloride | -43.58 | -62.25 | -46.93 |
| 2-amino-6-(difluoromethoxy)-5-methyl-4-pyrimidinol | -43.25 | -40.08 | -42.38 |
| 1H-pyrrolo[2,3-f]quinoline | -43.25 | -42.36 | -52.40 |
| 2-cyano-2-(2,2-dimethyltetrahydro-4H-pyran-4-ylidene)acetamide | -43.15 | -50.28 | -43.01 |
| 2-azaspiro[5.5]undecan-1-one | -43.12 | -44.36 | -58.77 |
| 1-(2-pyridin-4-ylethyl)piperazine | -43.10 | -54.31 | -65.12 |
| 1-(4,6-dimethoxy-5-pyrimidinyl)ethanone | -43.08 | -46.16 | -46.53 |
| 2-(2-phenylethyl)-3-pyridinol | -42.98 | -55.23 | -55.66 |
| 2-amino-5-nitronicotinamide | -42.71 | -48.84 | -41.06 |
| 2-(4-pyridinyl)-1H-imidazo[4,5-c]pyridine | -42.68 | -41.06 | -47.36 |
| 1-phenyl-2-(4-pyrimidinyl)ethanone | -42.43 | -50.37 | -62.95 |
| 2-(2-pyridinylamino)ethanol hydrochloride | -42.34 | -50.48 | -48.72 |
| 1-(2-fluorophenyl)piperidin-4-one | -42.13 | -43.85 | -57.43 |
| 2,4-dichloro-5-fluoropyrimidine | -42.02 | -42.83 | -42.46 |
| 1-(cyclobutylcarbonyl)-4-methylpiperidine | -41.62 | -46.30 | -66.57 |
| 1-benzoylpiperidine | -41.55 | -35.22 | -63.75 |
| 2',6'-dimethyl-2,3'-bipyridin-6-amine | -41.12 | -46.57 | -60.01 |
| 2-[(pyridin-4-ylmethyl)amino]-2-thioxoacetamide | -41.04 | -49.69 | -46.43 |
| 2-chloro-5,6-dimethylnicotinonitrile | -40.83 | -45.31 | -54.09 |
| 2-[(4-methylpyridin-2-yl)amino]-2-thioxoacetamide | -40.66 | -50.82 | -53.66 |
| 2,4-dimethylfuro[3,2-c]quinoline | -40.54 | -49.81 | -48.47 |
| [6-(dimethylamino)-3-pyridinyl]methanol hydrochloride | -40.42 | -60.61 | -55.63 |
| 2-phenyl-1H-imidazo[4,5-c]pyridine | -40.35 | -40.04 | -51.60 |
| 1-methyl-2-piperidinecarboxylic acid hydrochloride | -40.23 | -37.31 | -42.87 |
| 1-(methylsulfonyl)-4-piperidinone | -40.13 | -40.14 | -38.60 |
| 2-(4-morpholinyl)-4,6-pyrimidinediamine | -39.96 | -39.43 | -48.87 |
| 1-(2-pyridin-2-ylethyl)pyrrolidin-2-one | -39.93 | -49.82 | -62.28 |
| 2,2'-(1,2-ethenediyl)dipyridine | -39.75 | -51.66 | -61.25 |
| 2-(4-morpholinyl)nicotinonitrile | -39.73 | -51.32 | -49.74 |
| 1,4-dimethyl-4-piperidinecarboxylic acid hydrochloride | -39.69 | -37.65 | -47.48 |
| 2-(4-pyridinyl)-1H-benzimidazole | -39.64 | -34.92 | -49.92 |
| 1-(cyclopropylcarbonyl)-2-piperidinecarboxylic acid | -39.58 | -40.35 | -45.55 |
| 1-(1H-tetrazol-5-ylmethyl)piperidine | -39.49 | -39.54 | -44.57 |
| 2-(4-piperidinyl)propanoic acid hydrochloride | -39.36 | -36.46 | -45.50 |
| 2-(3-methoxyphenyl)pyridine | -39.30 | -43.39 | -64.74 |
| 2,5-dimethyl-8-quinolinol | -39.12 | -43.85 | -62.41 |
| 2,6-dimethyl-4-quinolinamine | -39.11 | -60.68 | -44.03 |
| 1-phenyl-2-(2-pyridinyl)ethanone | -38.72 | -50.90 | -67.79 |
| 2-hydroxy-6-phenylnicotinonitrile | -38.55 | -47.10 | -45.51 |
| 2-(2-pyridinyl)-1H-imidazo[4,5-b]pyridine | -38.52 | -51.80 | -55.94 |
| 1-[(2-methyl-1,3-oxazol-4-yl)carbonyl]piperidine | -38.32 | -53.78 | -67.15 |
| 2-(1-pyrrolidinyl)-4,6-pyrimidinediamine | -38.24 | -48.67 | -49.79 |
| 2-hydrazino-6-(methoxymethyl)-4-methylnicotinonitrile | -38.14 | -44.86 | -50.89 |
| (4,6-dimethyl-2-pyrimidinyl)methylcyanamide | -37.97 | -41.27 | -33.32 |
| 2-amino-7-methyl-7,8-dihydro-5(6H)-quinazolinone | -37.68 | -50.14 | -53.79 |
| 2-methoxy-8-quinolinol | -37.49 | -42.65 | -56.69 |
| (pyrimidin-4-ylmethyl)amine dihydrochloride | -37.28 | -33.92 | -31.14 |
| 2-[2-(2-pyridinyl)ethyl]aniline | -37.27 | -43.95 | -55.40 |
| 2-methoxy-4,6-dimethylnicotinonitrile | -37.27 | -36.11 | -33.49 |
| 1-(1H-imidazol-1-yl)isoquinoline | -37.17 | -43.46 | -44.89 |
| 2-(4-methylpyrimidin-2-yl)benzonitrile | -37.07 | -43.26 | -55.36 |
| {[2-(4-pyridinyl)ethyl]thio}acetic acid | -36.93 | -51.01 | -41.27 |
| 2,6-dimethoxy-4-methylnicotinamide | -36.87 | -50.01 | -52.28 |
| 2-furaldehyde 2-pyridinylhydrazone | -36.79 | -38.91 | -57.95 |
| 2-methylpyrido[2,3-d]pyrimidin-4(3H)-one | -36.74 | -38.58 | -47.14 |
| 1-(pyridin-4-ylmethyl)-1H-pyrazol-5-amine | -36.59 | -32.95 | -50.42 |
| 2-(difluoromethoxy)-4,6-dimethylnicotinonitrile | -36.53 | -37.24 | -26.82 |
| 2-amino-4-(methylamino)-5-nitronicotinonitrile | -36.53 | -40.69 | -36.24 |
| 1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-one | -35.97 | -30.53 | -48.26 |
| 2-(1-piperidinyl)-4,6-pyrimidinediamine | -35.69 | -49.90 | -48.50 |
| 2-[(3-pyridinylmethylene)amino]phenol | -35.67 | -43.57 | -50.37 |
| 2-(methylamino)-8-quinolinol | -35.62 | -47.32 | -57.81 |
| 2-hydrazino-4-(methoxymethyl)-6-methylnicotinonitrile | -35.61 | -47.27 | -49.61 |
| (2-amino-6-chloro-4-pyrimidinyl)cyanamide | -35.59 | -32.51 | -39.67 |
| 2-(2-pyridin-4-ylethyl)aniline | -35.50 | -43.93 | -51.36 |
| 1-ethyl-3,6-diazatricyclo[4.3.1.1~3,8~]undecan-9-one | -35.41 | -26.50 | -33.41 |
| 2,6-dimethoxy-4-methylnicotinonitrile | -35.14 | -37.61 | -42.56 |
| 2-(4-hydroxyphenyl)-3-pyridinol | -34.85 | -48.30 | -52.13 |
| 1-(4-amino-2,6-dimethyl-5-pyrimidinyl)ethanone | -34.60 | -45.86 | -49.20 |
| 2-methyl-1,2-dihydro-3H-pyrazolo[4,3-c]quinolin-3-one | -34.56 | -48.24 | -54.51 |
| {[2-(2-pyridinyl)ethyl]thio}acetic acid | -34.19 | -60.93 | -41.45 |
| 1-piperidinylacetic acid hydrate | -34.08 | -38.60 | -30.51 |
| 1-methyl-4-(1-methyl-4-piperidinyl)piperazine | -34.02 | -52.15 | -69.74 |
| 2,3,4,6-tetrahydro-1H-pyrido[1,2-a]quinazoline | -33.90 | -64.54 | -49.50 |
| 1,3,5-trimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol | -33.87 | -31.22 | -61.55 |
| 1-(2-pyridinylamino)-2,5-pyrrolidinedione | -33.86 | -48.96 | -49.29 |
| 2-(dimethylamino)nicotinic acid | -33.27 | -35.41 | -22.20 |
| [(2R,6S)-2,6-dimethylpiperidin-1-yl]acetic acid | -33.13 | -39.00 | -38.44 |
| 1-cyclopropyl-6-oxo-3-piperidinecarboxylic acid | -33.02 | -38.38 | -37.26 |
| 1-allyl-6-oxopiperidine-3-carboxylic acid | -32.80 | -38.63 | -42.97 |
| 1,3,4,6-tetramethyl-1H-pyrazolo[3,4-d]pyrimidine | -32.77 | -45.15 | -32.54 |
| 1-methyl-3,6-diazatricyclo[4.3.1.1~3,8~]undecan-9-one oxime | -32.66 | -29.68 | -54.86 |
| 1,7-dimethylpyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione | -32.53 | -41.79 | -45.60 |
| 2-chloro-6-hydrazino-9H-purine | -32.52 | -36.03 | -34.59 |
| 2-(pyridin-2-ylthio)propanoic acid | -32.51 | -55.46 | -49.90 |
| 1-pyrimidin-5-yl-1H-benzimidazole | -32.45 | -43.89 | -44.54 |
| 1-methyl-3,6-diazatricyclo[4.3.1.1~3,8~]undecan-9-one | -32.44 | -31.23 | -35.91 |
| 1-isobutyl-6-oxopiperidine-3-carboxylic acid | -32.39 | -39.90 | -42.63 |
| 2-(tert-butylsulfonyl)pyridine | -32.08 | -35.98 | -66.57 |
| 2-[(4-methyl-2-pyrimidinyl)thio]propanoic acid | -32.00 | -65.17 | -49.42 |
| 2-cyano-3-(3-pyridinyl)acrylamide | -31.98 | -52.77 | -49.38 |
| 2-chloro-N'-hydroxy-4,6-dimethylpyridine-3-carboximidamide | -31.89 | -47.27 | -59.98 |
| 2,3,5,6-tetrafluoro-4-pyridinamine | -31.86 | -30.85 | -28.10 |
| 2,3-dimethyl-6-phenylpyridine | -31.73 | -44.29 | -57.91 |
| 2-(9H-purin-6-ylamino)ethanol | -31.56 | -33.99 | -36.48 |
| 2-amino-3-quinolinecarboxamide | -31.51 | -43.79 | -54.07 |
| 2,8-dimethoxyquinoline | -31.48 | -44.36 | -59.96 |
| (5H-indeno[1,2-b]pyridin-5-ylidenemethyl)amine | -31.40 | -46.19 | -53.66 |
| 1H-pyrazolo[4,3-c]quinolin-3-amine | -31.19 | -41.02 | -52.68 |
| 2-pyridinecarbaldehyde 2-pyridinylhydrazone | -30.91 | -46.20 | -53.40 |
| 1-acetyl-N,N-dimethyl-4-piperidinecarboxamide | -30.79 | -51.98 | -60.32 |
| 1-[3-(3-pyridinyl)-1H-1,2,4-triazol-5-yl]methanamine | -30.59 | -39.85 | -35.07 |
| 1,4,6-trimethyl-1H-pyrazolo[3,4-b]pyridin-3-amine | -30.34 | -45.95 | -27.01 |
| 2-ethyl-4,6-dimethyl-3-pyridinyl acetate | -30.12 | -43.46 | -26.39 |
| 1-ethyl-6-oxopiperidine-3-carboxylic acid | -29.83 | -34.10 | -31.07 |
| 1-methyl-9H-beta-carbolin-3-ol | -29.69 | -43.99 | -58.93 |
| 1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol | -29.54 | -26.94 | -43.22 |
| 1-methyl-3-pyridin-3-yl-1H-pyrazol-5-amine | -28.60 | -40.83 | -51.04 |
| 1-methyl-3-pyridin-2-yl-1H-pyrazol-5-amine | -28.48 | -39.25 | -57.67 |
| 1,2,2,6,6-pentamethylpiperidin-4-ol | -28.07 | -22.16 | -54.45 |
| 1H-pyrazolo[3,4-b]quinolin-3-amine | -27.50 | -38.27 | -49.66 |
| 2-methyl-1,10-phenanthroline | -27.04 | -46.31 | -53.98 |
| 2-(4-methyl-1H-pyrazol-1-yl)nicotinonitrile | -26.97 | -39.30 | -55.43 |
| 2-methylquinoline-4-carbonitrile | -26.55 | -37.65 | -47.21 |
| 1-isobutyryl-4-piperidinecarboxylic acid | -26.33 | -39.62 | -38.59 |
| 1-isopropyl-6-oxopiperidine-3-carboxylic acid | -26.00 | -34.60 | -35.51 |
| 2-(3-methyl-1H-1,2,4-triazol-5-yl)pyridine | -25.87 | -41.21 | -51.83 |
| 1-(aminocarbonyl)-3-piperidinecarboxylic acid | -25.79 | -36.69 | -31.93 |
| 1,3-diazatricyclo[3.3.1.1~3,7~]decane-5,7-diamine | -25.67 | -22.45 | -33.13 |
| 2-(2,2,6,6-tetramethylpiperidin-4-yl)ethanol | -25.66 | -42.22 | -42.24 |
| 2-aminoquinoline-3-carbonitrile | -25.42 | -38.78 | -52.28 |
| 2-phenyl-5-pyrimidinamine | -25.10 | -36.57 | -50.29 |
| 1-acetyl-3-piperidinecarboxylic acid | -24.40 | -39.65 | -35.13 |
| 2-(methylthio)-5-pyrimidinecarboxylic acid | -24.19 | -27.50 | -32.31 |
| 2-(2,2,6,6-tetramethylpiperidin-4-yl)acetamide | -23.67 | 1.88 | -35.95 |
| 2-cyano-N'-(3-pyridinylmethylene)acetohydrazide | -23.42 | -42.80 | -48.60 |
| (4,6-dimethyl-2-pyrimidinyl)ethylcyanamide | -22.92 | -45.06 | -46.53 |
| [4-(3-pyridinyl)-2-pyrimidinyl]cyanamide | -22.57 | -41.19 | -26.95 |
| 2-(dimethylamino)-8-quinolinol | -22.54 | -38.17 | -61.24 |
| 1-propionyl-4-piperidinecarboxylic acid | -22.01 | -37.53 | -42.11 |
| 1-(2-quinolinyl)acetone | -21.96 | -51.49 | -65.85 |
| [4-(2-pyridinyl)-2-pyrimidinyl]cyanamide | -21.86 | -42.73 | -33.85 |
| (2-hydroxypyridin-3-yl)(oxo)acetic acid | -21.76 | -31.48 | -33.51 |
| 1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-one oxime | -20.88 | -20.52 | -51.68 |
| 2-amino-4-(2-furyl)-6-methylnicotinonitrile | -20.78 | -39.60 | - |
| 1-propionyl-3-piperidinecarboxylic acid | -20.66 | -45.46 | -42.41 |
| 2-hydroxy-4-quinolinecarboxylic acid | -20.48 | -26.81 | -36.42 |
| [4-(4-pyridinyl)-2-pyrimidinyl]cyanamide | -20.38 | -39.05 | -13.15 |
| 2-(4H-1,2,4-triazol-4-yl)isonicotinic acid | -20.33 | -17.35 | -14.46 |
| 2,2,6,6-tetramethyl-4-nitropiperidine | -20.19 |  | -35.03 |
| 2,6,8-trimethyl-4-quinolinamine | -20.10 | -64.27 | -36.37 |
| 2-pyrimidin-2-ylbenzonitrile | -19.49 | -40.71 | -53.24 |
| 2-aminoisonicotinic acid hydrochloride | -19.01 | -25.62 | -17.50 |
| 2-propylisonicotinic acid | -18.82 | -30.22 | -32.76 |
| 1,8-dimethyl-3,6-diazatricyclo[4.3.1.1~3,8~]undecan-9-one | -17.72 | -23.18 | -34.07 |
| [4-(2-furyl)-2-pyrimidinyl]cyanamide | -17.28 | -42.13 | -25.21 |
| 2-(1-piperidinyl)-5-pyrimidinecarbonitrile | -15.51 | -41.92 | -49.96 |
| (4-phenyl-2-pyrimidinyl)cyanamide | -15.16 | -39.20 | -27.23 |
| 2-oxo-1,2-dihydropyrido[1,2-a]pyrimidin-5-ium-4-olate | -12.56 | -27.03 | -32.58 |
| 2,6-dimethoxy-4-methylnicotinic acid | -11.67 | -34.34 | -21.91 |
| 2-amino[1,3]thiazolo[4,5-d]pyrimidine-5,7-diol | -11.48 | -24.98 | -29.82 |
| 2,4-dioxo-3-azabicyclo[3.1.0]hexane-1,5-dicarbonitrile | -9.83 | -18.86 | -12.38 |
| 2-methyl-8-quinolinol 1-oxide | -9.82 | -34.91 | -31.61 |
| 1,3,5,7-tetramethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol | -8.10 | -23.42 | -50.88 |
| 1-pyridin-3-yl-1H-tetrazole-5-thiol | -8.05 | -17.03 | -12.49 |
| 2-methyl-4-quinolinecarboxylic acid | -7.86 | -15.51 | -23.79 |
| 2-mercapto-6-(trifluoromethyl)-4-pyrimidinol | -6.75 | -18.77 | -12.83 |
| 2-quinolinecarboxylic acid | -4.93 | -35.24 | -37.90 |
| 2-mercapto-4-(methoxymethyl)-6-methylnicotinonitrile | 3.68 | -28.27 | -5.38 |
| 2,7-naphthyridine-1,3,6,8-tetrol | 28.99 | -4.62 | 7.18 |
| 2,5,7-trimethyl-8-quinolinol | - | -40.29 | -57.92 |