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MTT Raw data

| · · · · · · · · · · · · · · · · · · · | 0.0.00 | | | | | | | | |
|---------------------------------------|--|---|--|---|--|---|--|-----------|-----------|
| HepG2 48h | l | | | | | | | | |
| | С | 100 | 200 | 300 | 400 | 500 | | | |
| | 0.6814 | 0.6029 | 0.5159 | 0.4792 | 0.3538 | 0.2831 | | | |
| | 0.778 | 0.6603 | 0.512 | 0.4754 | 0. 4538 | 0. 2982 | | | |
| | 0.7074 | 0.5293 | 0.4611 | 0. 4398 | 0.3995 | 0.303 | | | |
| | 0.1014 | 0.0230 | 0. 4011 | 0. 1000 | 0.0000 | 0.000 | | | |
| | 1 | 0.884796 | 0.757118 | 0.703258 | 0.519225 | 0. 415468 | | | |
| | 1 | 0.848715 | 0.658098 | 0.611054 | 0.58329 | 0.38329 | | | |
| | 1 | 0.748233 | 0.651824 | 0.621713 | 0.564744 | 0.428329 | | AVERAGE | STDEV.S |
| | | | | | | | IC50 | | |
| | | | 75, 71177 | | | | 435. 219 | | |
| | | | 65. 80977 | | | | | 436. 543 | 25, 8934 |
| | 100 | 74. 8233 | 65.18236 | 62.17133 | 56. 47441 | 42.83291 | 463.073 | | |
| SKOV-3 4 | 8h | | | | | | | | |
| | С | 100 | 200 | 300 | 400 | 500 | | | |
| | 0.6725 | 0.5523 | 0.4783 | 0.3567 | 0.3016 | 0.2021 | | | |
| | 0.7855 | 0.639 | 0.5442 | 0.3998 | 0.2884 | 0.2142 | | | |
| | 0.6789 | 0.5866 | 0.4801 | 0.3685 | 0.2693 | 0.2311 | | | |
| | 1 | 0.001064 | 0.711227 | 0 520400 | 0 449476 | 0.20052 | | | |
| | 1 | | 0.692807 | | | | | | |
| | 1 | | 0.092807 | | | | | AVERAGE | ס מפתדים |
| | 1 | 0.804043 | 0.707173 | 0.04279 | 0.390071 | 0.340404 | IC50 | AVERAGE | SIDEV.S |
| | 100 | 82, 12639 | 71.12268 | 53, 04089 | 44, 84758 | 30, 05204 | 322, 851 | | |
| | 100 | | 69. 28071 | | | | | 313.8687 | 19, 34814 |
| | 100 | | 70.71734 | | | | 327.093 | | |
| A2780 48h | | | | | | | | | |
| 12100 1011 | C | 100 | 200 | 300 | 400 | 500 | | | |
| | 1.0226 | 0.906 | 0.7782 | 0.5607 | 0. 4291 | 0.3524 | | | |
| | 1.0641 | 0.9069 | 0.8958 | 0.6028 | 0.4344 | 0.3529 | | | |
| | 0.9995 | 0.8848 | 0.8764 | 0.6075 | 0. 4449 | 0.3123 | | | |
| | | | | | | | | | |
| | 1 | 0.885977 | 0.761001 | 0.548308 | 0.419617 | 0.344612 | | | |
| | 1 | 0.85227 | 0.841838 | 0.566488 | 0.408232 | 0.331642 | | | |
| | 1 | 0.885243 | 0.876838 | 0.607804 | 0.445123 | 0.312456 | | AVERAGE | STDEV.S |
| | | | | | | | IC50 | | |
| | 1.00 | | | | | | | | |
| | | | | | | 34. 46118 | 344. 271 | | |
| | 100 | 85, 22695 | 84. 18382 | 56.64881 | 40.82323 | 33.16418 | 344. 271 351. 444 | 354. 6067 | 12, 2277 |
| | 100 | 85, 22695 | 84. 18382 | 56.64881 | 40.82323 | | 344. 271 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 | 85, 22695 | 84. 18382 87. 68384 | 56.64881 | 40. 82323 44. 51226 | 33.16418 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C | 85. 22695 88. 52426 50 | 84. 18382 87. 68384 | 56. 64881 60. 78039 | 40. 82323 44. 51226 200 | 33.16418 31.24562 250 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C 0. 9701 | 85. 22695 88. 52426 50 0. 8275 | 84. 18382 87. 68384 100 0. 7391 | 56. 64881 60. 78039 150 0. 6365 | 40. 82323 44. 51226 200 0. 3304 | 33. 16418 31. 24562 250 0. 144 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C 0.9701 0.8862 | 85. 22695 88. 52426 50 0. 8275 0. 7892 | 84. 18382 87. 68384 100 0. 7391 0. 6866 | 56. 64881 60. 78039 150 0. 6365 0. 5087 | 40. 82323 44. 51226 200 0. 3304 0. 3098 | 33. 16418 31. 24562 250 0. 144 0. 1141 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C 0. 9701 | 85. 22695 88. 52426 50 0. 8275 | 84. 18382 87. 68384 100 0. 7391 | 56. 64881 60. 78039 150 0. 6365 | 40. 82323 44. 51226 200 0. 3304 | 33. 16418 31. 24562 250 0. 144 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C 0. 9701 0. 8862 0. 9495 | 85. 22695 88. 52426 50 0. 8275 0. 7892 0. 796 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 | 150 0.6365 0.5087 0.5284 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 | 33. 16418 31. 24562 250 0. 144 0. 1141 0. 1062 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C 0. 9701 0. 8862 0. 9495 | 85, 22695 88, 52426 50 0, 8275 0, 7892 0, 796 0, 853005 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 0. 76188 | 56. 64881 60. 78039 150 0. 6365 0. 5087 0. 5284 0. 656118 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 0. 340583 | 33.16418 31.24562 250 0.144 0.1141 0.1062 0.148438 | 344. 271 351. 444 | 354. 6067 | 12. 2277 |
| MCF-7 48h | 100 100 C 0.9701 0.8862 0.9495 | 85. 22695 88. 52426 50 0. 8275 0. 7892 0. 796 0. 853005 0. 890544 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 0. 76188 0. 774769 | 56. 64881 60. 78039 150 0. 6365 0. 5087 0. 5284 0. 656118 0. 574024 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 0. 340583 0. 349582 | 33. 16418 31. 24562 250 0. 144 0. 1141 0. 1062 0. 148438 0. 128752 | 344. 271 351. 444 | | |
| MCF-7 48h | 100 100 C 0. 9701 0. 8862 0. 9495 | 85. 22695 88. 52426 50 0. 8275 0. 7892 0. 796 0. 853005 0. 890544 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 0. 76188 | 56. 64881 60. 78039 150 0. 6365 0. 5087 0. 5284 0. 656118 0. 574024 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 0. 340583 0. 349582 | 33. 16418 31. 24562 250 0. 144 0. 1141 0. 1062 0. 148438 0. 128752 | 344, 271 351, 444 368, 105 | 354. 6067 | |
| MCF-7 48h | 100 100 C 0.9701 0.8862 0.9495 | 85. 22695 88. 52426 50 0. 8275 0. 7892 0. 796 0. 853005 0. 890544 0. 838336 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 0. 76188 0. 774769 0. 771775 | 56. 64881 60. 78039 150 0. 6365 0. 5087 0. 5284 0. 656118 0. 574024 0. 556503 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 0. 340583 0. 349582 0. 29247 | 33. 16418 31. 24562 250 0. 144 0. 1141 0. 1062 0. 148438 0. 128752 0. 111848 | 344, 271 351, 444 368, 105 | | |
| MCF-7 48h | 100 100 C 0.9701 0.8862 0.9495 | 85. 22695 88. 52426 50 0. 8275 0. 7892 0. 796 0. 853005 0. 890544 0. 838336 85. 30048 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 0. 76188 0. 774769 0. 771775 | 56. 64881 60. 78039 150 0. 6365 0. 5087 0. 5284 0. 656118 0. 574024 0. 556503 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 0. 340583 0. 349582 0. 29247 34. 05834 | 33. 16418 31. 24562 250 0. 144 0. 1141 0. 1062 0. 148438 0. 128752 0. 111848 14. 84383 | 344. 271 351. 444 368. 105 IC50 152. 946 | AVERAGE | STDEV.S |
| MCF-7 48h | 100 100 C 0.9701 0.8862 0.9495 1 1 1 | 85. 22695 88. 52426 50 0. 8275 0. 7892 0. 796 0. 853005 0. 890544 0. 838336 85. 30048 89. 05439 | 84. 18382 87. 68384 100 0. 7391 0. 6866 0. 7328 0. 76188 0. 774769 0. 771775 76. 18802 77. 47687 | 56. 64881 60. 78039 150 0. 6365 0. 5087 0. 5284 0. 656118 0. 574024 0. 556503 65. 61179 57. 40239 | 40. 82323 44. 51226 200 0. 3304 0. 3098 0. 2777 0. 340583 0. 349582 0. 29247 34. 05834 34. 95825 | 33. 16418 31. 24562 250 0. 144 0. 1141 0. 1062 0. 148438 0. 128752 0. 111848 14. 84383 | 344. 271 351. 444 368. 105 IC50 152. 946 | | STDEV.S |

| | | 1 | | |
|-----|----------|-----------|------------|---|
| | GADPH | VEGF | MMP9 | Bcl-2 |
| 0 | 16.757 | 21.546 | 21.124 | 18.511 |
| 200 | 16.964 | 21.157 | 19.759 | 16.689 |
| 300 | 16.472 | 19.5 | 15. 454 | 11.074 |
| | | | | |
| 0 | 1 | 1.285791 | 1.260608 | 1.104673 |
| 200 | 1 | 1.24717 | 1.164761 | |
| 300 | 1 | 1.183827 | | 0.672292 |
| | _ | | | *************************************** |
| 0 | | 1 | 1 | 1 |
| 200 | | | 0.923968 | |
| 300 | | 0. 920699 | | 0.60859 |
| 000 | | 0.020000 | V. 111210 | 0.0000 |
| 0 | | 100 | 100 | 100 |
| 200 | | | 92.39677 | |
| 300 | | 92.06995 | | |
| 300 | | 52.00555 | 14. 42423 | 00.00001 |
| | | 2 | | |
| | GADPH | VEGF | MMP9 | Bcl-2 |
| 0 | 16.597 | | 19.8289 | |
| 200 | 16. 258 | 20.015 | | |
| 300 | 15.59 | 18.098 | 13. 44504 | 11. 47748 |
| 000 | 10.00 | 10.000 | 10. 11001 | 11. 11110 |
| 0 | 1 | 1 30138 | 1.194728 | 1.26712 |
| 200 | 1 | | 1.075833 | |
| 300 | 1 | | 0.862414 | |
| 300 | | 1.100072 | 0.002414 | 0. 130200 |
| 0 | | 1 | 1 | 1 |
| 200 | | 0.945985 | | |
| 300 | | 0.892032 | 0.72185 | |
| 300 | | 0.052052 | 0.12100 | 0.001000 |
| 0 | | 100 | 100 | 100 |
| 200 | | | 90.04835 | |
| 300 | | 89. 2032 | | |
| 300 | | 05. 2032 | 12.100 | 30.10000 |
| | | 3 | | |
| | GADPH | VEGF | MMP9 | Bcl-2 |
| 0 | 17. 2579 | 21.8269 | | |
| 200 | 17. 4149 | 20.8691 | | 17. 43541 |
| 300 | 16. 9874 | 19.1891 | 15. 2704 | 11.5258 |
| 000 | 10.0011 | 10.1001 | 10.2101 | 11.0200 |
| 0 | 1 | 1, 264748 | 1.247527 | 1.14754 |
| 200 | 1 | | 1.102148 | 1.001178 |
| 300 | 1 | | 0.898925 | |
| 500 | | 1.127000 | J. JJJJJZJ | J. 5104JI |
| 0 | | 1 | 1 | 1 |
| 200 | | | 0.883466 | |
| 300 | | 0.893148 | 0.720566 | 0.591257 |
| 300 | | 0.093140 | 0. 120000 | 0.031407 |
| 0 | | 100 | 100 | 100 |
| 200 | | 94. 74987 | | |
| | | | | |
| 300 | | 09. 31483 | 72.05655 | 59.12571 |

| | | | | | AVERAGE | STDEV. S |
|-------|-----|-----------|-----------|-----------|--------------|--------------|
| Bcl-2 | 0 | 100 | 100 | 100 | 100 | 0 |
| | 200 | 89.05708 | 86.80915 | 87. 24556 | 87. 70392936 | 1.192003811 |
| | 300 | 60.85897 | 58.10088 | 59.12571 | 59. 36185059 | 1.394125519 |
| | | | | | AVERAGE | STDEV. S |
| MMP9 | 0 | 100 | 100 | 100 | 100 | 0 |
| | 200 | 92.39677 | 90.04835 | 88.34662 | 90. 26391419 | 2. 033660486 |
| | 300 | 74. 42429 | 72.185 | 72.05655 | 72. 8886133 | 1.331484859 |
| | | | | | AVERAGE | STDEV.S |
| VEGF | 0 | 100 | 100 | 100 | 100 | 0 |
| | 200 | 96.99636 | 94. 59854 | 94. 74987 | 95. 44825615 | 1.342830789 |
| | 300 | 92.06995 | 89. 2032 | 89.31483 | 90.19599268 | 1.623854241 |

Scratch Raw data

| | | 1 | | | | 2 | | | | 3 | |
|-----|------|----------|----------|-----|------|----------|----------|-----|------|----------|----------|
| | 0 | 24 | 48 | | 0 | 24 | 48 | | 0 | 24 | 48 |
| | | | | | | | | | | | |
| 0 | 4580 | 3320 | 2413 | 0 | 4839 | 3628 | 2385 | 0 | 4769 | 3468 | 2465 |
| 100 | 5530 | 4258 | 3021 | 100 | 5624 | 4588 | 2730 | 100 | 5251 | 4171 | 2909 |
| 200 | 5390 | 4450 | 3454 | 200 | 5312 | 4419 | 3660 | 200 | 5585 | 4699 | 4096 |
| 300 | 6904 | 6582 | 6468 | 300 | 6935 | 6686 | 6441 | 300 | 7110 | 6902 | 6524 |
| 400 | 6462 | 6379 | 6381 | 400 | 6598 | 6563 | 6555 | 400 | 6499 | 6354 | 6389 |
| 0 | 1 | 0.275109 | 0.473144 | 0 | 1 | 0.250258 | 0.50713 | 0 | 1 | 0.272804 | 0.48312 |
| 100 | 1 | 0.230018 | 0.453707 | 100 | 1 | 0.184211 | 0.51458 | 100 | 1 | 0.205675 | 0.44601 |
| 200 | 1 | 0.174397 | 0.359184 | 200 | 1 | 0.16811 | 0.310994 | 200 | 1 | 0.158639 | 0.266607 |
| 300 | 1 | 0.04664 | 0.063152 | 300 | 1 | 0.035905 | 0.071233 | 300 | 1 | 0.029255 | 0.082419 |
| 400 | 1 | 0.012844 | 0.012535 | 400 | 1 | 0.005305 | 0.006517 | 400 | 1 | 0.022311 | 0.016926 |
| | 0 | 1 | 1 | | 0 | 1 | 1 | | 0 | 1 | 1 |
| | 100 | 0.836097 | 0.958919 | | 100 | 0.736082 | 1.014692 | | 100 | 0.753931 | 0.923187 |
| | 200 | 0.633919 | 0.759142 | | 200 | 0.671746 | 0.613244 | | 200 | 0.581515 | 0.551844 |
| | 300 | 0.169531 | 0.133473 | | 300 | 0.143471 | 0.140463 | | 300 | 0.107237 | 0.170598 |
| | 400 | 0.046688 | 0.026493 | | 400 | 0.021197 | 0.012851 | | 400 | 0.081785 | 0.035034 |
| | | | | | | | | | | | |
| | | 24 | 48 | | | 24 | 48 | | | 24 | 48 |
| | 0 | 100 | 100 | | 0 | 100 | 100 | | 0 | 100 | 100 |
| | 100 | 83.60975 | | | 100 | 73.60815 | 101.4692 | | 100 | 75.39313 | |
| | 200 | 63.39194 | 75.91422 | | 200 | 67.17457 | 61.32436 | | 200 | 58.15145 | |
| | 300 | | 13.34726 | | 300 | | 14.04629 | | 300 | 10.72368 | |
| | 400 | 4.668809 | 2.64926 | | 400 | 2.119665 | 1.285101 | | 400 | 8.178459 | 3.50341 |

Apopotosis Raw data

| 0 | 100 | 200 | 300 | 400 | 500 |
|------|-------|-------|-------|------|------|
| 5.07 | 5.84 | 14.95 | 19.88 | 45.1 | 60.6 |
| 7.35 | 14.31 | 16.06 | 19.74 | 46 | 58.3 |
| 6.1 | 12.85 | 15.42 | 19.1 | 43.7 | 54.2 |

SNH Structural

SNH

EN140

Interaction and energy of SNH and MMP9

| | <u> </u> | | | |
|--------------------------|----------|-----------------|-----------------------------|-------------|
| ForcefieldBase CHARMm | TopHits | -CDOCKER_ENERGY | -CDOCKER_INTERACTION_ENERGY | POSE_NUMBER |
| | 6 | 55. 1987 | 53. 1878 | 1 |
| | 6 | 54.9668 | 54.9119 | 2 |
| | 6 | 52. 3698 | 54.3461 | 3 |
| | 6 | 51.3626 | 50. 4906 | 4 |
| | 6 | 51.1261 | 50. 0855 | 5 |
| | 6 | 50. 3972 | 47.6168 | 6 |

Analysis of the Interaction Bond between Posture 2 and MMP9. Molecule in the figure represents SNH molecule.

✓ ••• Molecule:Na21 - A:ASP185:OD2

✓ • • A:ALA191:HN - Molecule:O20

✓ • • A:HIS190:HA - Molecule:O20

✓ • • • Molecule:H24 - A:ALA189:O

✓ • • Molecule:H25 - A:GLU227:OE2

✓ • • Molecule:C19 - A:LEU222

✓ • • Molecule:C19 - A:LEU243

Report-EN140 Calculate Interaction Energy

| Name | | | Energy (kcal/mol) | Electrostatic Interaction Energy (kcal/mol) |
|-----------|------------------|-------------|-------------------|---|
| 4WZV_prep | 4WZV_prep-CHARMm | -90.6301423 | -44.2597691 | -46.3703732 |

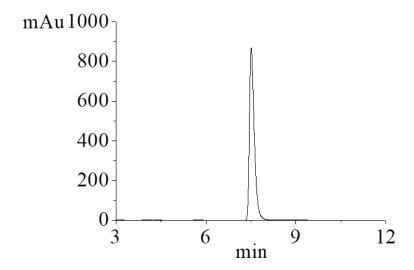
Report-SNH Calculate Interaction Energy

| Name | Forcefield | | VDW Interaction | |
|-------------|--------------------|-------------|-----------------|----------------------------------|
| | | 3, | 3, | Interaction Energy (kcal/mol) |
| SNH_model_1 | SNH_model_1-CHARMm | -83.2091424 | -40.6743099 | -42.5348325 |

Report-SNH Calculate Binding Energy

| _ | Binding Energy (kcal/mol) | | (kcal/mol) | Energy | Entropic Energy (kcal/mol) |
|----------|------------------------------|----------|------------|------------|----------------------------------|
| Molecule | -172.7831 | -12.1012 | -4723.1825 | -4908.0668 | 20.5935 |

High Performance Liquid Chromatography



In vivo experiment data

| n=5 | PBS group | SNH treated group | Cyclophosphamide treated group | |
|------------------------|------------|-------------------|--------------------------------|--|
| n=5 | 1 DS group | (300mg/kg) | (25mg/kg) | |
| 1 | 1. 545 | 0.718 | 0. 138 | |
| 2 | 1. 476 | 0.759 | 0. 374 | |
| 3 | 0. 953 | 0.401 | 0. 149 | |
| 4 | 0. 906 | 0.527 | 0. 157 | |
| 5 | 1. 427 | 0.699 | 0. 279 | |
| | 6. 307 | 3. 104 | 1. 097 | |
| | 1. 2614 | 0. 6208 | 0. 2194 | |
| Tumor inhibitory rates | | 0. 507848422 | 0. 826066276 | |