

MTT Raw data

HepG2 48h									
	C	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			
	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		
	100	88.4796	75.71177	70.3258	51.92251	41.54682	435.219		
	100	84.87147	65.80977	61.1054	58.32905	38.32905	411.337	436.543	25.8934
	100	74.8233	65.18236	62.17133	56.47441	42.83291	463.073		
SKOV-3 48h									
	C	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	0.821264	0.711227	0.530409	0.448476	0.30052			
	1	0.813495	0.692807	0.508975	0.367155	0.272693			
	1	0.864045	0.707173	0.54279	0.396671	0.340404			
								AVERAGE	STDEV. S
							IC50		
	100	82.12639	71.12268	53.04089	44.84758	30.05204	322.851		
	100	81.34946	69.28071	50.89752	36.71547	27.26926	291.662	313.8687	19.34814
	100	86.40448	70.71734	54.27898	39.66711	34.04036	327.093		
A2780 48h									
	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		
	100	88.59769	76.10014	54.83082	41.96167	34.46118	344.271		
	100	85.22695	84.18382	56.64881	40.82323	33.16418	351.444	354.6067	12.2277
	100	88.52426	87.68384	60.78039	44.51226	31.24562	368.105		
MCF-7 48h									
	C	50	100	150	200	250			
	0.9701	0.8275	0.7391	0.6365	0.3304	0.144			
	0.8862	0.7892	0.6866	0.5087	0.3098	0.1141			
	0.9495	0.796	0.7328	0.5284	0.2777	0.1062			
	1	0.853005	0.76188	0.656118	0.340583	0.148438			
	1	0.890544	0.774769	0.574024	0.349582	0.128752			
	1	0.838336	0.771775	0.556503	0.29247	0.111848			
								AVERAGE	STDEV. S
							IC50		
	100	85.30048	76.18802	65.61179	34.05834	14.84383	152.946		
	100	89.05439	77.47687	57.40239	34.95825	12.8752	149.913	147.5873	6.825431
	100	83.8336	77.17746	55.65034	29.24697	11.18483	139.903		

RT-PCR Raw data

		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	0.983789
300	1	1.183827	0.938198	0.672292
0		1	1	1
200		0.969964	0.923968	0.890571
300		0.920699	0.744243	0.60859
0		100	100	100
200		96.99636	92.39677	89.05708
300		92.06995	74.42429	60.85897
		2		
	GADPH	VEGF	MMP9	Bcl-2
0	16.597	21.599	19.8289	21.03039
200	16.258	20.015	17.49089	17.88341
300	15.59	18.098	13.44504	11.47748
0	1	1.30138	1.194728	1.26712
200	1	1.231086	1.075833	1.099976
300	1	1.160872	0.862414	0.736208
0		1	1	1
200		0.945985	0.900484	0.868091
300		0.892032	0.72185	0.581009
0		100	100	100
200		94.59854	90.04835	86.80915
300		89.2032	72.185	58.10088
		3		
	GADPH	VEGF	MMP9	Bcl-2
0	17.2579	21.8269	21.5297	19.80413
200	17.4149	20.8691	19.1938	17.43541
300	16.9874	19.1891	15.2704	11.5258
0	1	1.264748	1.247527	1.14754
200	1	1.198347	1.102148	1.001178
300	1	1.129608	0.898925	0.678491
0		1	1	1
200		0.947499	0.883466	0.872456
300		0.893148	0.720566	0.591257
0		100	100	100
200		94.74987	88.34662	87.24556
300		89.31483	72.05655	59.12571

Scratch Raw data

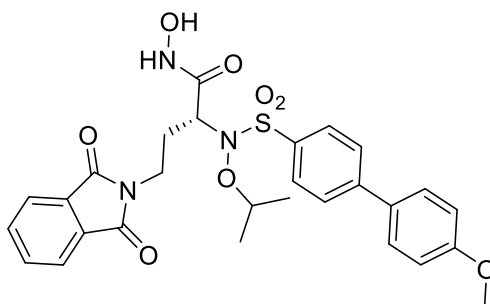
Apopotosis Raw data

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

CCCCCOC(=O)CC(S(=O)(=O)[O-])[Na+]

SNH

EN140 Structural



EN140

Interaction and energy of SNH and MMP9

ForcefieldBase	TopHits	-CDOCKER_ENERGY	-CDOCKER_INTERACTION_ENERGY	POSE_NUMBER
CHARMm				
	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	Forcefield	Interaction Energy (kcal/mol)	VDW Interaction Energy (kcal/mol)	Electrostatic Interaction Energy (kcal/mol)
4WZV_prep	4WZV_prep-CHARMm	-90.6301423	-44.2597691	-46.3703732

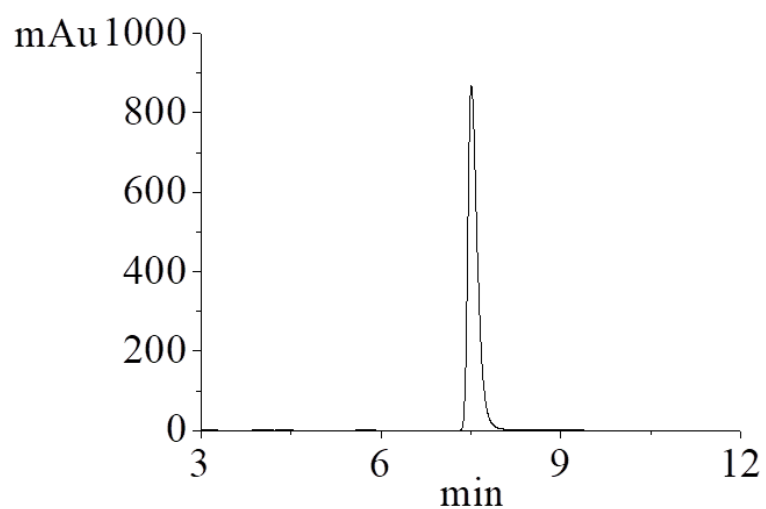
Report-SNH Calculate Interaction Energy

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

Report-SNH Calculate Binding Energy

Ligand Name	Binding Energy (kcal/mol)	Ligand Energy (kcal/mol)	Protein Energy (kcal/mol)	Complex Energy (kcal/mol)	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
		(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