

**Supplementary Table-8:** GOLD fitness scores for top-5 compounds for each cavity of Acetate kinase (ack) protein.

Cavity No	Inhibitors	Fitness Score	S (hb_ext)	S (vdw_ext)	S (hb_int)	S (int)	H bond and short contacts
1	Ceftiofur	59.39	3.60	47.33	0.00	-9.29	17
	Penicillin	55.02	6.42	37.20	0.00	-2.55	5
	Dihydropiperonaline	51.77	0.00	43.76	0.00	-8.40	5
	Guineensine	49.45	0.00	44.83	0.00	-12.18	1
	Piperdardine	47.65	1.11	42.74	0.00	-12.23	5
2	Ceftiofur	69.85	7.20	51.52	0.00	-8.19	11
	Piperdardine	54.40	3.44	44.34	0.00	-10.01	11
	Guineensine	54.56	2.53	46.21	0.00	-11.51	10
	Pipperolein B	51.84	5.44	42.00	0.00	-11.35	16
	Penicilline	51.20	5.59	33.97	0.00	-1.10	8
4	Dehydropiperonaline	57.69	9.75	43.05	0.00	-11.25	27
	Penicillin	57.06	0.90	42.58	0.00	-2.38	18
	Piperdardine	53.76	9.48	42.44	0.00	-14.07	23
	Trimethoprim sulphamethoxazole	51.26	8.48	38.93	0.00	-10.75	17
	Eugenyl acetate	51.12	5.86	36.86	0.00	-5.42	8
5	Ceftiofur	55.07	0.00	46.50	0.00	-8.87	14
	Guineensine	45.39	1.55	54.09	0.00	-9.87	3
	Pinoresinol	53.77	4.55	40.94	0.00	-7.08	14
	Penicilline	45.77	4.28	30.80	0.00	-0.85	10
	Piperdardine	44.40	6.00	34.37	0.00	-8.86	4