

Supplementary Files

Identification of Efflux Pump Responsible for Antibiotic Resistance in *Pseudomonas aeruginosa* from Clinical Samples and In Silico Drug Designing

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Table S1. Dynamut result of mexA and mexB.

Gene	delta_vibrational _entropy	ddg_prediction	delta_stability_ encom	Mcsm	mutation	sdm	duet
MEX							
A	0.065	0.075	-0.052	0.032	E178K	0	0.363
	0.503	-0.242	-0.403	-0.371	S32P	-1.18	-0.479
	0.521	-0.11	-0.417	-0.31	K54G	0.74	0.059
	0.177	-0.377	-0.142	-0.301	T55V	0.83	0.132
	-0.141	0.255	0.113	-0.003	T59D	-0.36	0.183
	0.026	0.15	-0.021	-1.091	A110Y	0	-0.933
	-0.053	0.38	0.042	-0.377	S33Q	0.28	0.006
	0.04	-0.415	-0.032	-0.773	G44K	-2.62	-1.043
	0.571	-0.788	-0.457	-0.561	K69N	-0.91	-0.44
	-0.353	0.123	0.282	-0.454	G100I	-2.36	-0.817
	-0.06	-0.569	0.048	-0.146	I94Q	-1.29	-0.03
	0.488	-1.075	-0.39	-1.583	L57S	-2.49	-1.76
	0.017	0.372	-0.013	-0.013	N71I	1.51	0.559
MEX							
B	-0.036	0.279	0.029	-0.579	N28T	-0.27	-0.401
	0.427	-0.597	-0.342	-1.31	W4T	-0.28	-1.084
	-1.542	1.62	1.233	-1.691	A83K	-3.23	-1.906
	-0.027	0.6	0.021	0.134	Q30L	1.19	0.644
	0.013	-0.447	-0.01	-0.311	G74N	-1.44	-0.369
	-0.059	-0.001	0.047	-0.537	P40I	-0.03	-0.218
	-0.33	0.365	0.264	-0.849	P7F	0.98	-0.381
	0.032	0.781	-0.026	-0.978	S101W	1.5	-0.331
	-0.131	0.656	0.105	0.67	Q62M	0.54	0.971
	0.074	-0.146	-0.059	-0.233	Q58T	0.34	0.167
	-0.088	-0.031	0.07	-0.264	N43T	0.2	0.039
	0.116	-0.944	-0.093	-1.066	K80S	-1.6	-1.179
	0.893	0.157	-0.714	-0.742	R78P	-1.91	-1.187

-0.137	0.037	0.11	-0.064	Q97S	-0.91	0.155
0.003	-0.01	-0.002	-0.294	S22N	0.42	0.162
-0.109	1.418	0.087	-0.239	S75I	2.08	0.451
1.336	-2.441	-1.069	-2.853	L68S	-3.89	-3.204
0	0.273	0	0.431	Y106K	-0.03	0.715
-0.31	0.557	0.248	-0.418	D6T	-0.22	-0.246
0.934	-0.319	-0.747	-0.79	Y92G	0.3	-0.514
-0.115	0.232	0.092	-0.281	Q109S	-0.57	-0.087
-0.022	-0.005	0.018	0.38	H46V	0.01	0.425
-0.278	0.821	0.223	-0.198	T50L	0.99	0.232
-0.059	-0.313	0.048	0.309	D73S	-1.04	0.292
-0.156	-0.144	0.125	-0.23	L47K	-0.47	0.078
-0.026	-0.382	0.021	-0.379	V104P	-2.7	-0.696
-0.077	0.429	0.062	0.453	R107L	0.56	0.639
-0.765	0.717	0.612	-0.542	G37R	-1.14	-0.593
-0.283	-0.097	0.226	-0.678	G89Q	-1.25	-0.572
0.487	0.154	-0.39	0.433	H90V	0.14	0.46
0.054	0.033	-0.043	0.126	Q14D	-0.01	0.391
-0.06	0.035	0.048	-0.131	N11T	0.01	0.303
0.133	-0.252	-0.106	-0.742	N65E	-0.09	-0.525
0.393	-0.08	-0.315	-0.142	L87D	-0.62	0.128
0.086	-2.027	-0.069	-2.513	V77D	-4.38	-3.011
-0.426	0.502	0.341	-0.118	A96R	0.26	0.295
-0.2	1.607	0.16	-0.252	P102L	2.12	0.615
-0.048	-0.074	0.039	0.134	N99R	0.6	0.444
0.483	0.213	-0.387	-0.042	R56V	0.64	0.235
-0.144	0.412	0.115	-0.215	P72V	0.69	0.166
-0.156	-0.108	0.125	-0.273	I31L	-0.78	-0.128

0.36	-0.415	-0.288	-0.437	Q27A	1.02	0.148
0.141	0.074	-0.113	-0.129	D91F	0.01	-0.101
0.034	-0.439	-0.028	-0.725	G38Q	-1.24	-0.747
-0.071	-0.033	0.057	-0.17	D19Q	-0.18	0.164
-0.065	-0.463	0.052	-0.435	G34E	-2.35	-0.55
1.689	-3.385	-1.351	-3.319	F63T	-2.42	-3.432
0.112	0.054	-0.09	-1.07	I24L	0.28	-0.644
-0.084	0.008	0.067	-0.846	N9Q	0.09	-0.429
0.401	-0.874	-0.321	-1.124	A60G	-1.79	-1.244
0.048	0.252	-0.038	-0.405	S21Q	1.24	0.278
-0.7	0.767	0.56	-0.913	G88F	-0.07	-0.81
0.329	-0.517	-0.264	-0.27	Q45A	1.17	0.126
-0.016	-0.254	0.013	-0.254	E61S	-2.47	-0.441
0.536	-0.118	-0.429	-0.334	L36Q	-1.05	-0.308
-0.066	-0.105	0.053	0.156	H25Q	0.25	0.364
0.128	-0.036	-0.102	-0.996	L15I	0.86	-0.63
0.737	-2.546	-0.59	-2.865	I66D	-2.44	-3.139
0.554	0.023	-0.443	-0.078	Q35V	1.2	0.4
0.027	-0.146	-0.021	-0.837	A8E	0.42	-0.29
-0.713	0.623	0.57	-1.261	A23K	-1.29	-1.115
-0.158	0.34	0.127	0.189	D108N	0.06	0.426
-0.033	0.279	0.027	0.103	S12D	0.82	0.731
0.638	-0.125	-0.51	-0.798	R2T	-0.42	-0.627
-0.348	0.858	0.278	0.325	D81R	-0.13	0.528
-0.577	1.049	0.462	-0.386	G53V	0.29	-0.001
-0.282	-0.354	0.226	-0.963	V29P	-3.81	-1.545
0.047	-0.037	-0.038	-0.299	G18V	0.6	0.247
0.392	-0.251	-0.314	-0.982	L5V	0.87	-0.386

-0.096	-0.005	0.077	-0.338	T16A	-0.2	-0.247
-0.104	0.158	0.083	-0.409	A26L	-0.68	-0.176
0.187	-2.405	-0.149	-2.525	V82T	-2.61	-2.741
0.071	0.302	-0.057	-0.964	E64K	-0.46	-0.709
-0.065	0.531	0.052	-0.427	P17Q	1.61	0.277
-0.675	0.579	0.54	-0.602	N95Y	0.19	-0.507
-0.583	0.118	0.466	-0.731	G103D	-1.46	-0.581
-0.136	0.065	0.108	-0.369	I52V	-0.09	-0.069
0.19	0.167	-0.152	-0.714	D84G	1.49	-0.063
-0.258	0.454	0.206	-0.403	I51M	-0.76	-0.422
1.075	-1.103	-0.86	-1.544	Y13P	-0.65	-1.523
1.058	-3.308	-0.846	-2.928	L10G	-3.01	-3.441
-0.546	0.746	0.436	-0.331	F98M	-0.14	-0.309
-0.291	0.27	0.233	0.117	R105A	0.09	0.221
-0.443	0.532	0.354	-0.895	A49F	0.02	-0.765
-0.182	0.119	0.145	-0.509	L39G	-0.07	-0.197
-0.202	0.454	0.162	-0.679	V70Y	-1	-0.754