

Supplementary Data

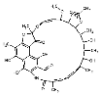
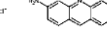
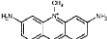
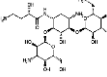
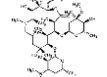
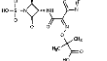
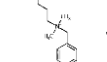
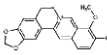
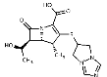
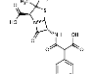
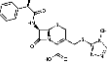
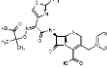
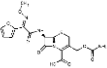
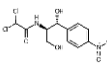
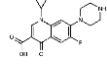
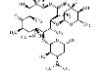
AcrAB–TolC, a major efflux pump in Gram negative bacteria: toward understanding its operation mechanism

















Soojin Jang*

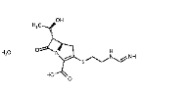
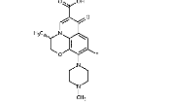
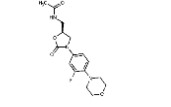
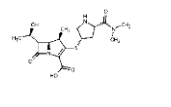
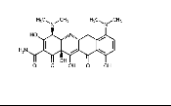
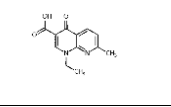
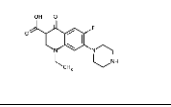
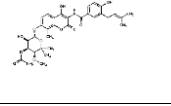
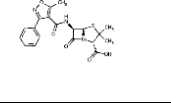
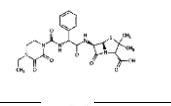
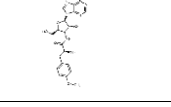
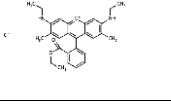
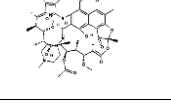
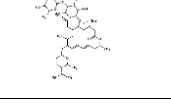
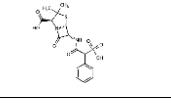
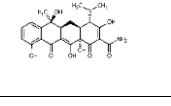
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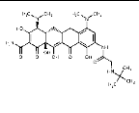
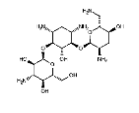
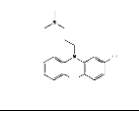
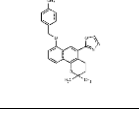
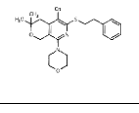
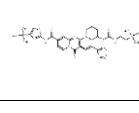
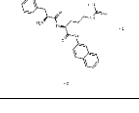
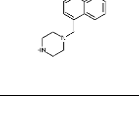
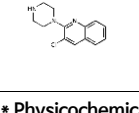
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Supplementary Table 1. Chemical structures and physicochemical properties of AcrAB-TolC substrates and inhibitors

Structure	Compound	Class	M. W. (g/mol)	HLB	logP	Topological polar surface area (Å ²)	Minimum projection area (Å ²)	Maximum projection area (Å ²)
	3-formyl-rifamycin	Ansamycin	725.788	17.243	5.187	218.38	91.81	159.13
	Acriflavine_1	Planar aromatic antiseptic & dye	244.7	5.614	1.848	64.93	25.75	74.57
	Acriflavine_2	Planar aromatic antiseptic & dye	224.286	2.885	-2.808	55.92	28.91	79.98
	Amikacin	Aminoglycoside	585.608	46.272	-8.584	331.94	76.66	141.69
	Azitromycin	Macrolide	748.996	21.354	2.183	180.08	116.17	169.25
	Azteronom	Anionic-beta lactam	435.43	22.599	-3.078	201.58	60.09	100.55
	Benzalkonium chloride	Planar aromatic cationic surfactant	227.78	11.395	-0.924	0	42.87	66.88
	Berberine	Planar aromatic quaternary ammonium	336.366	5.625	-1.283	40.8	43.16	101.85
	Biapenem	Carbapenam	351.4	16.865	-6.063	99.54	48.98	95.61
	Carbenicillin	Anionic-beta lactam	378.4	21.237	0.815	124.01	53.72	88.98
	Cefamandole	Beta lactam	462.5	23.013	0.027	150.54	56.82	95.06
	Ceftazidime	Beta lactam	547.58	25.735	-4.122	188.39	68.29	119.73
	Cefuroxime	Beta lactam	424.38	24.146	-0.903	173.76	60.77	95.84
	Chloramphenicol	Phenicol	323.13	18.319	0.879	112.7	39.36	77.63
	Ciprofloxacin	Fluoroquinolone	331.347	13.416	-0.88	72.88	43.14	96.57
	Clarithromycin	Macrolide	747.964	15.496	3.24	182.91	106.52	161.87

	Clindamycin	Lincomycin	424.98	21.345	1.038	102.26	72.48	103.94
	Cloxacillin	Beta lactam	435.88	19.139	2.302	112.74	68.26	88.31
	Crystal violet	Planar aromatic dye	407.99	2.89	1.396	9.49	69.24	115.51
	Dequalinium	Planar aromatic quaternary ammonium	456.677	1	-3.591	59.8	66.41	156.6
	Dicloxacillin	Beta lactam	470.32	18.968	2.906	112.74	67.56	89.07
	Dodecyl β -D-maltoside	Nonionic surfactant	510.621	14.368	0.82	178.53	65.87	149.03
	Doripenem	Carbapenam	420.5	27.832	-5.564	162.06	55.18	108.39
	Doxorubicin	Anthracycline	543.525	17.968	0.765	206.07	76.14	135.22
	Doxycycline	Tetracycline	444.44	21.623	-0.611	178.46	69.78	92.31
	Enoxacin	Fluoroquinolone	320.324	14.439	-1.028	85.77	42.61	94.61
	Ertapenem	Carbapenam	475.52	27.445	-3.21	156.27	73.49	117.16
	Erythromycin	Macrolide	733.937	16.089	2.596	193.91	107.16	147.81
	Ethidium bromide	Planar aromatic dye	394.316	0.73	-0.913	55.92	47.18	98.84
	Fusidic acid	protein synthesis inhibitor	516.719	4.566	4.422	104.06	76.47	136.59
	Gentamicin	Aminoglycoside	477.603	39.747	-3.137	199.73	73.63	117.98
	Hoechst 33342	Planar aromatic dye	452.562	10.274	4.75	73.07	56.31	127.76

	Imipenem	Carbapenam	317.36	23.541	-3.797	113.72	37.49	85.22
	Levofloxacin	Fluoroquinolone	361.373	14.683	-1.062	73.32	45.74	101.81
	Linezolid	Oxazolidinone	337.351	15.039	0.637	71.11	47.21	88.82
	Meropenem	Carbapenam	383.46	27.418	-4.354	110.18	55.31	99.51
	Minocycline	Tetracycline	457.483	21.941	-2.614	164.63	63.79	107.96
	Nalidixic acid	Antimicrobial naphthyridone	232.239	8.67	0.873	70.5	34.3	74.9
	Norfloxacin	Fluoroquinolone	319.336	13.939	-0.988	72.88	42.78	94.8
	Novobiocin	Aminocoumarin	612.632	17.74	3.409	196.1	61.67	168.77
	Oxacillin	Beta lactam	401.44	19.339	1.698	112.74	67.52	86.84
	Piperacillin	Beta lactam	517.56	30.769	-0.258	156.43	86.7	114.71
	Puromycin	Aminonucleoside	471.518	21.297	-0.299	160.88	67.09	127.06
	Rhodamine 6G	Planar aromatic dye	479.02	0.28	6.709	63.5	79.31	127.34
	Rifampicin	Ansamycin	822.9	28.744	2.833	220.15	121.44	167.71
	Spiramycin	Macrolide	843.065	21.867	2.496	195.38	109.86	196.22
	Sulbenicillin	Anionic-beta lactam	414.45	21.709	0.38	141.08	55.67	91.63
	Tetracycline	Tetracycline	444.44	23.048	-3.499	181.62	62.4	96.76

	Tigecycline	Tetracycline	585.658	31.848	-3.86	205.76	78.97	140.1
	Tobramycin	Aminoglycoside	467.52	43.61	-6.478	268.17	66.33	115.16
	Chlorpromazine	Phenothiazine antipsychotic, EPI	318.86	10.268	4.535	6.48	54.73	79.81
	2H- benzo [h] chromene WK2	EPI	400.478	3.76	5.073	57.38	53.96	123.92
	MBX2319	EPI	668.53	7.652	4.401	34.59	70.64	116.94
	D13-9001	EPI	694.79	22.67	-1.005	207.99	112.98	169.88
	PABN Phenylalanine- Arginine-β- Naphthylamide	EPI	519.47	26.164	1.726	146.12	62.89	126.78
	1-(1- naphthylmethyl)- piperazine	EPI	226.323	15.879	2.368	15.27	43.01	73.97
	BDM88855	EPI	247.73	11.553	2.902	28.16	38	74.09

* Physicochemical properties (molecular weight, hydrophilic-lipophilic Balance, logP, topological polar surface area, minimum projection area, maximum projection area obtained from the UCSF ChimeraX (93, 94)) of 57 molecules that have been tested as either substrates or inhibitors for AcrAB-TolC (57, 60, 62, 63, 66, 95-97).