Supporting Information

Anti- metatype antibody screening, sandwich immunoassay development, and structural insights for β-lactams based on penicillin binding protein

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Buffers

The common buffer solutions used in the experiment are listed:

(1) Coating buffer (0.05 mol L^{-1} carbonate buffer, pH 9.6)

(2) Phosphate buffer solution (PBS buffer, 0.01 mol L^{-1}, pH 7.4)

(2) Blocking buffer (2% skim milk powder (w/v))

(3) Washing buffer (PBST, PBS buffer with 0.05% Tween-20 (v/v), pH 7.2)

(4) Boric acid buffer (0.02 mol L^{-1}, pH 9.0, containing 10% DMF)

(5) Stopping reagent (2 mol L^{-1} H_2SO_4)

Table S1 Identification of PBP2x*-drugs.

complex	OD values
PBP2x*-PNG	0.02
PBP2x*-AMP	0.06
PBP2x*-AMX	0.03
PBP2x*-CTX	0.02
PBP2x*-KF	0.05

Table S2. Molecular descriptors of β-lactams.

β-lactams	MW	SA	V_m	E	μ	MPI	PSA	Log P
PNG	334	349.91	383.72	-1421.77	6.56	15.28	227.32	0.84
AZL	461	456.26	506.79	-1889.07	4.38	17.17	307.44	-0.74
AMX	365	365.85	406.47	-1551.59	4.91	15.82	235.05	-0.58
AMP	349	359.57	397.55	-1476.76	5.57	14.89	231.54	-0.2
OXA	402	391.47	448.25	-1665.10	6.46	15.28	256.52	1.5
CLX	437	413.48	469.29	-2123.97	7.50	15.78	282.88	2.06
PIPC	518	513.33	574.90	-2079.76	6.77	17.27	353.25	-0.71
DCX	470	433.68	490.75	-2582.84	6.82	15.18	276.65	2.62
CFM	456	428.85	467.15	-2205.11	4.54	17.45	287.51	0.25
CFN	460	444.25	493.17	-2154.24	18.32	26.67	342.16	-8.29
CPZ	650	608.81	684.48	-2845.33	6.16	18.40	431.69	-0.56
CFAP	423	412.84	455.00	-2060.56	5.74	16.91	277.45	-3.68
CFP	484	462.94	524.20	-2228.60	15.75	25.66	346.09	-5.97
CTRX	558	506.00	562.11	-2843.24	6.15	19.10	349.09	0.02
KF	427	384.85	420.15	-1967.68	12.89	19.55	272.55	0.04
CFT	527	489.19	539.45	-2717.27	4.05	15.86	308.51	1.17
CTX	458	442.07	474.00	-2206.28	4.37	16.41	291.37	0.14
CFZ	463	423.66	46.73	-2465.01	8.86	19.57	308.16	-1.09

molecular weight, MW; van der Waals surface area, SA; molecular volume, Vm; energy, E; molecular dipole moment, μ; molecular polarity index, MPI; polar surface area, PSA; hydrophobic constant, Log P.

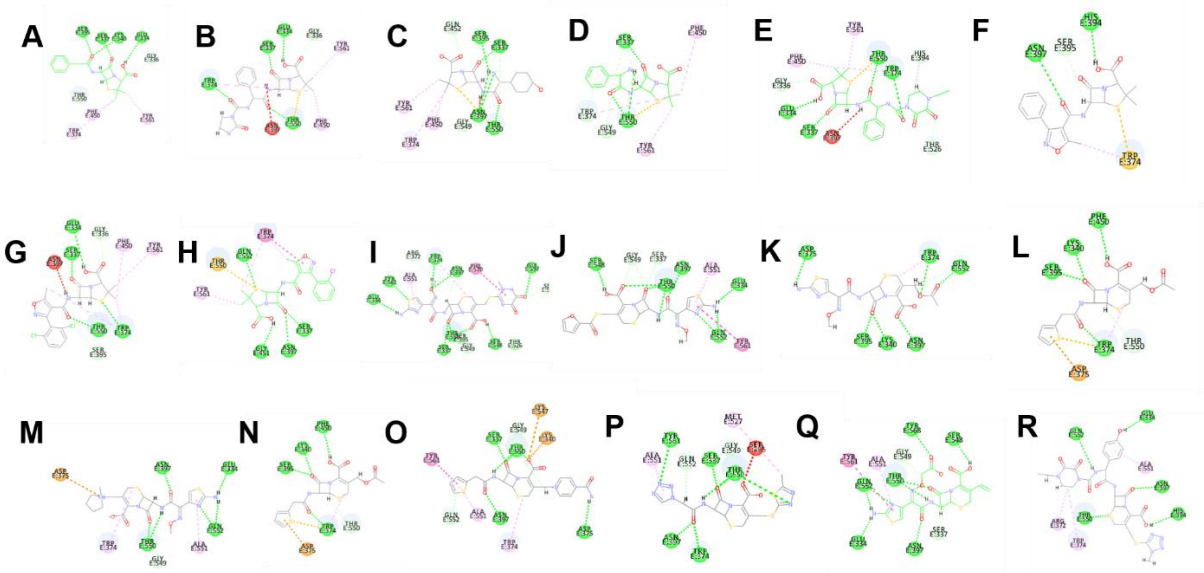

Figure S1. Two-dimensional schematic diagram of the interactions between PBP2x (PDB code: 2z2m) and (A) PNG; (B) AZL; (C) AMX; (D) AMP; (E) PIPC; (F) OXA; (G) DCX; (H) CLX; (I) CTRX; (J) CFT; (K) CTX; (L) CFAP; (M) CFP; (N) KF; (O) CFN; (P) CFZ; (Q) CFM; (R) CPZ. Hydrogen bonds are shown as green dashed lines, hydrophobic interactions are displayed as purple dashes, and the electrostatic force is expressed as orange dashes.