

## Supporting Information

### **Evaluating mAbs Binding Abilities to Omicron Subvariant RBDs: Implications for Selecting Effective mAb Therapies**

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Table S1  $\Delta\Delta G_{\text{ASIE}}$  calculated through ASIE method for LY-COV1404/RBDs systems, all values are in kcal/mol.

<b>WT</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>BA.2</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>BA.5</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>BF.7</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>XBB.1.5</b>	$\Delta\Delta G_{\text{ASIE}}$
T345	0.04	T345	0.59	T345	0.06	T345	0.03	T345	0.39
R346	-0.57	R346	0.77	R346	-0.22	T346	-0.01	T346	0.08
N439	-0.61	N439	0.09	N439	0.30	N439	0.17	N439	-0.09
N440	-1.10	K440	-1.94	K440	0.01	K440	-1.97	K440	-1.89
L441	0.71	L441	0.56	L441	1.04	L441	0.02	L441	0.98
S443	0.37	S443	0.27	S443	0.28	S443	0.96	S443	0.61
K444	2.50	K444	3.44	K444	3.14	K444	3.67	K444	1.20
V445	4.08	V445	3.49	V445	4.39	V445	4.42	P445	3.12
N448	0.90	N448	1.54	N448	1.84	N448	0.78	N448	0.53
Y449	0.60	Y449	0.93	Y449	0.90	Y449	0.69	Y449	0.08
N450	-2.78	N450	-5.34	N450	-5.28	N450	-2.33	N450	-0.90
Y451	0.49	Y451	0.96	Y451	0.79	Y451	0.36	Y451	0.26
Q498	2.22	R498	0.03	R498	1.45	R498	-0.96	R498	1.28
P499	1.48	P499	1.62	P499	1.92	P499	2.37	P499	2.12
T500	2.42	T500	2.01	T500	2.30	T500	2.51	T500	3.76
Q506	0.21	Q506	0.12	Q506	0.09	Q506	0.16	Q506	0.54
R509	0.24	R509	-0.54	R509	0.72	R509	0.32	R509	0.30

Table S2  $\Delta\Delta G_{ASIE}$  calculated through ASIE method for REGN-10933/RBDs systems, all values are in kcal/mol.

WT	$\Delta\Delta G_{ASIE}$	BA. 2	$\Delta\Delta G_{ASIE}$	BA. 5	$\Delta\Delta G_{ASIE}$	BF.7	$\Delta\Delta G_{ASIE}$	XBB.1. 5	$\Delta\Delta G_{ASIE}$
R40 3	0.01	R40 3	-3.32	R40 3	-0.54	R40 3	-1.38	R403	-3.75
D40 5	1.08	N40 5	-0.13	N40 5	-0.21	N40 5	0.75	N405	-0.16
E40 6	0.37	E40 6	0.47	E40 6	-0.06	E40 6	-0.98	E406	-0.10
Q40 9	-0.02	Q40 9	0.10	Q40 9	-0.04	Q40 9	1.21	Q409	0.02
K41 7	-1.73	N41 7	0.13	N41 7	-0.63	N41 7	1.57	N417	0.01
I418	0.01	I418	0.11	I418	0.01	I418	0.71	I418	0.07
D42 0	0.12	D42 0	-2.95	D42 0	-0.10	D42 0	-0.04	D420	0.05
Y43 1	0.02	Y43 1	2.31	Y43 1	0.19	Y43 1	0.33	Y431	1.02
Y45 3	0.10	Y45 3	1.42	Y45 3	-0.05	Y45 3	0.63	Y453	-0.51
L45 5	0.67	L45 5	0.96	L45 5	0.20	L45 5	1.29	L455	3.23
F456	-0.12	F456	0.35	F456	1.83	F456	0.90	F456	2.54
K45 8	-0.05	K45 8	-0.18	K45 8	-1.19	K45 8	0.04	K458	0.08
I472	0.00	I472	0.09	I472	1.77	I472	0.01	I472	0.00
Y47 3	1.17	Y47 3	0.55	Y47 3	0.59	Y47 3	0.06	Y473	2.41
Q47 4	-0.10	Q47 4	-1.10	Q47 4	-0.35	Q47 4	-0.04	Q474	0.10
S477	0.38	N47 7	-0.03	N47 7	-3.37	N47 7	-0.79	N477	-3.69
T47 8	0.86	K47 8	-0.18	K47 8	-3.46	K47 8	-0.35	K478	1.61
C48 0	0.04	C48 0	-0.02	C48 0	0.05	C48 0	1.07	C480	-0.06
N48 1	-0.40	N48 1	-0.25	N48 1	-0.35	N48 1	-0.72	N481	0.26
F486	-0.43	F486	6.84	V48 6	0.88	V48 6	0.49	P486	0.38

N48 7	1.07	N48 7	0.00	N48 7	-1.70	N48 7	3.61	N487	0.67
C48 8	-0.12	C48 8	1.10	C48 8	1.33	C48 8	0.13	C488	0.85
Y48 9	2.64	Y48 9	0.02	Y48 9	2.63	Y48 9	8.12	Y489	0.11
P491	0.03	P491	0.03	P491	0.37	P491	0.04	P491	0.50
Q49 3	0.11	R49 3	6.05	Q49 3	0.08	Q49 3	-0.13	Q493	0.10
Y50 5	-0.36	H50 5	0.27	H50 5	-0.19	H50 5	0.86	H505	0.28

Table S3  $\Delta\Delta G_{ASIE}$  calculated through ASIE method for REGN-10987/RBDs systems, all values are in kcal/mol.

<b>WT</b>	$\Delta\Delta G_{ASIE}$	<b>BA.2</b>	$\Delta\Delta G_{ASIE}$	<b>BA.5</b>	$\Delta\Delta G_{ASIE}$	<b>BF.7</b>	$\Delta\Delta G_{ASIE}$	<b>XBB.1.5</b>	$\Delta\Delta G_{ASIE}$
R346	-0.42	R346	-1.00	R346	-0.66	T346	0.00	T346	-0.02
N437	0.00	N437	0.05	N437	0.00	N437	0.00	N437	1.27
N439	0.02	N439	0.37	N439	-0.09	N439	0.01	N439	0.51
N440	-0.05	K440	-1.22	K440	-3.08	K440	-0.48	K440	0.26
D442	0.35	D442	0.85	D442	0.37	D442	0.50	D442	0.47
S443	-0.11	S443	-0.85	S443	0.06	S443	0.00	S443	0.16
K444	0.03	K444	1.36	K444	0.43	K444	-0.86	K444	-1.02
V445	2.51	V445	2.60	V445	2.17	V445	-0.08	P445	2.12
Y449	1.40	Y449	0.41	Y449	4.64	Y449	1.80	Y449	-0.44
N450	-0.54	N450	-0.11	N450	-0.08	N450	-0.17	N450	-0.05
L452	0.20	L452	0.03	R452	-0.41	R452	-0.99	L452	0.00
S494	1.06	S494	0.00	S494	0.15	S494	-0.31	S494	0.00
Q498	2.19	R498	-0.62	R498	1.17	R498	3.56	R498	2.30
P499	1.37	P499	0.56	P499	-0.76	P499	0.09	P499	1.07
T500	1.80	T500	0.38	T500	0.18	T500	-0.71	T500	4.79
N501	-0.46	Y501	0.10	Y501	0.15	Y501	3.80	Y501	0.54
V503	0.00	V503	0.00	V503	-0.01	V503	0.02	V503	0.93
Y505	0.30	H505	-0.01	H505	-0.01	H505	2.14	H505	0.04
Q506	0.04	Q506	0.22	Q506	0.00	Q506	0.08	Q506	1.97
Y508	0.03	Y508	0.06	Y508	0.02	Y508	0.04	Y508	0.99
R509	-0.42	R509	0.32	R509	-0.45	R509	-0.54	R509	-0.52

Table S4  $\Delta\Delta G_{\text{ASIE}}$  calculated through ASIE method for 002-S21F2/RBDs

systems, all values are in kcal/mol.

<b>WT</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>BA.2</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>BA.5</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>BF.7</b>	$\Delta\Delta G_{\text{ASIE}}$	<b>XBB.1.5</b>	$\Delta\Delta G_{\text{ASIE}}$
<b>E340</b>	-0.17	E340	-0.08	E340	-0.85	E340	0.47	E340	0.10
<b>N343</b>	0.49	N343	0.59	N343	0.31	N343	0.57	N343	1.14
T345	2.50	T345	3.03	T345	2.37	T345	1.56	T345	1.43
R346	5.13	R346	3.71	R346	6.54	T346	1.24	T346	0.04
K356	-0.62	K356	-0.20	K356	-0.88	K356	-0.41	K356	-0.23
N440	-0.75	K440	0.06	K440	-0.13	K440	0.62	K440	-0.64
L441	1.97	L441	1.82	L441	2.01	L441	1.60	L441	2.03
K444	-0.40	K444	-0.13	K444	2.44	K444	0.37	K444	-0.64
V445	0.95	V445	1.12	V445	0.30	V445	0.57	P445	0.64
N448	0.44	N448	0.29	N448	0.84	N448	0.27	N448	0.55
N450	-0.47	N450	-0.57	N450	-0.69	N450	-0.27	N450	-0.37
Y451	0.45	Y451	0.42	Y451	0.80	Y451	0.45	Y451	0.38
P499	0.56	P499	0.77	P499	0.15	P499	0.41	P499	0.46
R509	0.86	R509	1.11	R509	0.79	R509	0.48	R509	1.09

Table S5  $\Delta\Delta G_{ASIE}$  calculated through ASIE method for 1D1/RBDs

systems, all values are in kcal/mol.

<b>WT</b>	$\Delta\Delta G_{ASIE}$	<b>BA.2</b>	$\Delta\Delta G_{ASIE}$	<b>BA.5</b>	$\Delta\Delta G_{ASIE}$	<b>BF.7</b>	$\Delta\Delta G_{ASIE}$	<b>XBB.1.5</b>	$\Delta\Delta G_{ASIE}$
<b>R403</b>	-1.26	R403	-1.43	R403	-0.81	R403	-1.09	R403	-1.65
<b>D405</b>	-0.18	N405	-1.27	N405	-1.79	N405	-1.05	N405	-0.36
<b>T415</b>	0.83	T415	1.00	T415	0.71	T415	1.05	T415	0.99
<b>K417</b>	1.89	N417	0.30	N417	0.23	N417	0.37	N417	0.25
<b>D420</b>	-2.99	D420	-3.63	D420	-3.97	D420	-3.04	D420	-3.06
<b>Y421</b>	2.30	Y421	2.51	Y421	2.78	Y421	2.30	Y421	3.55
<b>Y453</b>	0.51	Y453	0.41	Y453	0.43	Y453	0.41	Y453	0.48
<b>L455</b>	2.44	L455	2.93	L455	2.27	L455	2.09	L455	2.79
<b>F456</b>	2.53	F456	2.60	F456	2.35	F456	2.31	F456	2.54
<b>K458</b>	0.62	K458	0.64	K458	0.37	K458	0.58	K458	1.14
<b>Y473</b>	1.39	Y473	1.43	Y473	1.34	Y473	1.51	Y473	1.27
<b>T478</b>	-0.07	K478	-0.98	K478	-0.61	K478	-0.58	K478	-0.42
<b>F486</b>	0.91	F486	0.38	V486	0.00	V486	-0.12	P486	0.41
<b>N487</b>	2.02	N487	1.51	N487	2.51	N487	0.90	N487	1.83
<b>Y489</b>	1.91	Y489	0.39	Y489	2.24	Y489	1.87	Y489	2.06
<b>Q498</b>	-0.65	R498	-0.19	R498	-0.10	R498	-0.21	R498	-0.13
<b>N501</b>	-0.54	Y501	1.50	Y501	1.37	Y501	1.39	Y501	1.53
<b>Y505</b>	5.06	H505	3.73	H505	3.18	H505	3.37	H505	3.63

Table S6  $\Delta\Delta G_{ASIE}$  calculated through ASIE method for 47D11/RBDs

systems, all values are in kcal/mol.

<b>WT</b>	$\Delta\Delta G_{ASIE}$	<b>BA.2</b>	$\Delta\Delta G_{ASIE}$	<b>BA.5</b>	$\Delta\Delta G_{ASIE}$	<b>BF.7</b>	$\Delta\Delta G_{ASIE}$	<b>XBB.1.5</b>	$\Delta\Delta G_{ASIE}$
<b>N334</b>	-0.05	N334	1.28	N334	0.25	N334	0.30	N334	0.60
<b>L335</b>	3.75	L335	4.11	L335	4.90	N334	0.30	L335	4.05
<b>P337</b>	0.77	P337	0.67	P337	1.01	L335	3.67	P337	0.84
<b>F338</b>	0.30	F338	1.14	F338	0.48	P337	0.55	F338	1.20
<b>D339</b>	0.00	D339	0.99	D339	1.45	F338	0.76	H339	5.85
<b>F342</b>	0.70	F342	0.86	F342	0.88	D339	1.24	F342	0.14
<b>N343</b>	0.57	N343	0.33	N343	0.97	N343	0.36	N343	0.45
<b>V362</b>	0.20	V362	0.18	V362	0.04	V362	0.13	V362	0.62
<b>D364</b>	0.47	D364	-1.66	D364	1.19	D364	1.17	D364	0.00
<b>Y365</b>	0.40	Y365	0.43	Y365	0.09	Y365	0.11	H365	0.88
<b>V367</b>	0.99	V367	0.84	V367	1.51	V367	1.15	V367	0.88
<b>L368</b>	0.80	L368	0.55	L368	1.04	L368	1.01	I368	1.66
<b>S371</b>	0.17	F371	-0.65	F371	2.89	F371	1.72	F371	0.45
<b>S373</b>	-0.07	P373	0.67	P373	0.33	P373	0.32	P373	0.47
<b>F374</b>	0.23	F374	0.77	F374	0.74	F374	0.50	F374	0.00
<b>N388</b>	0.04	N388	0.25	N388	-0.58	N388	-0.40	N388	0.20
<b>P527</b>	0.42	P527	0.46	P527	1.50	P527	1.32	P527	0.73