

Supplementary Table 3

ErbB4	EGFR	ErbB2	Contact	Lapatinib atom
D836 (N)	D	D	H-bond	F34
F837 (N,O)	F	F	H-bond	F34
774M (N,O)	M	M	H-bond	N18
F837	F	F	VDW	F34, C32
M747	M	M	VDW	C33
L839	L	L	VDW	C35
L769	L	L	VDW	C28
T771	T	T	VDW	O27
T835	T	T	VDW	C25
V707	V	V	VDW	C23
L825	L	L	VDW	C21, C39
724A	A	A	VDW	C19, C38