

Supporting Information to Accompany:

Binding-induced, turn-on fluorescence of the EGFR/ERBB kinase inhibitor, lapatinib

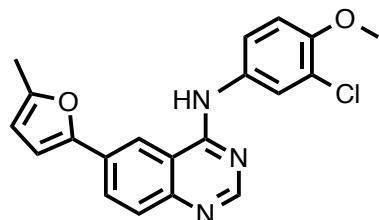
James N. Wilson,^a Wenjun Liu,^b Adrienne S. Brown^a and Ralf Landgraf^b

^a Department of Chemistry, University of Miami, 1301 Memorial Drive, Coral Gables, Florida 33124, United States

^b Department of Biochemistry and Molecular Biology, University of Miami, Miami, Florida 33101-6129, United States

Table S1. Atomic coordinates of lapatinib fragment from PDB ID 1XKK	S2
Figure S1. Lapatinib-treated cells costained for ERBB2	S3
Figure S2. 2-photon confocal microscope image of BT474 cells treated with lapatinib	S3

Table S1. Atomic coordinates of lapatinib fragment from PDB ID 1XKK.



Atom #	Atom	X	Y	Z
1	C	-4.888871	-4.07038	0.024331
2	C	-5.195525	-2.61766	0.115972
3	C	-6.342844	-1.90129	0.232618
4	C	-5.96931	-0.523617	0.22425
5	C	-4.613289	-0.488995	0.105711
6	O	-4.134419	-1.767523	0.03604
7	C	-3.636675	0.590012	0.045463
8	C	-4.06119	1.939779	0.156685
9	C	-3.167047	2.970651	0.077436
10	C	-1.788251	2.714838	-0.104888
11	N	-0.926615	3.76782	-0.20696
12	C	0.326618	3.454714	-0.388527
13	N	0.879579	2.22098	-0.443423
14	C	0.064858	1.196733	-0.332179
15	N	0.592033	-0.069665	-0.400714
16	C	2.00333	-0.300905	-0.37667
17	C	2.653631	-0.684991	-1.53744
18	C	4.01863	-0.955442	-1.526925
19	C	4.750473	-0.846056	-0.34728
20	O	6.072812	-1.086981	-0.247552
21	C	6.741931	-1.553561	-1.398891
22	C	4.08148	-0.45342	0.822176
23	Cl	4.977031	-0.308037	2.307392
24	C	2.727803	-0.181152	0.808341
25	C	-1.355176	1.37529	-0.187472
26	C	-2.293343	0.326484	-0.12789
27	H	-3.888264	-4.268475	0.415095
28	H	-5.60703	-4.655313	0.603113
29	H	-7.341358	-2.30471	0.314352
30	H	-6.631882	0.32567	0.300441
31	H	-5.115266	2.15215	0.298712
32	H	-3.481561	4.005583	0.147322
33	H	1.030002	4.277291	-0.486835
34	H	0.028405	-0.793627	0.019793
35	H	2.086358	-0.770958	-2.457022
36	H	4.510978	-1.249416	-2.445115
37	H	7.783011	-1.684035	-1.106841
38	H	6.332399	-2.513554	-1.732556
39	H	2.237098	0.13555	1.720957
40	H	-1.979621	-0.703987	-0.245492
41	H	6.683637	-0.830613	-2.220594
42	H	-4.921959	-4.429036	-1.010165

Figure S1. Methanol fixed MCF7 cells stained with mouse anti-ERBB2 and labeled with goat anti-mouse Alexa 546 (red channel) then exposed to lapatinib (green channel). The two channels are spatially segregated with virtually no overlap observed.

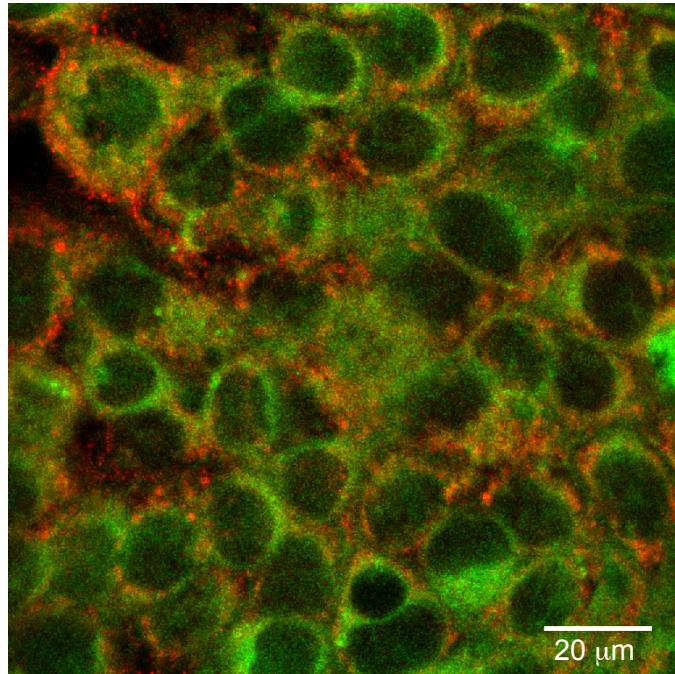


Figure S2. Two-photon (765 nm excitation) confocal microscopy of BT474 cells treated with lapatinib; only a perinuclear, cytosolic pool is observed.

