Supporting Information
Identification of the Naphthoquinone derivatives inhibitors binding site in Heat shock protein 90. An Induced-fit docking, Molecular Dynamics and 3D-QSAR study.

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TABLE S1: Experimental and theoretical data for all compounds of this study. (XP Score values in kcal/mol)

		pIC_{50}		XP Score				IF XP Score	
	IC_{50} (μM) Her2	Exp.	Calc.	Site 1	Site 2	Site3	Site 4	Site 1	Site 3
1	3.3 ± 1.0	5.481	5.481	-6.991	-2.626	-6.275	-4.288	-10.98	-8.13
2	6.6 ± 09	5.180	5.180	-6.487	-3.419	-5.578	-3.935	-9.43	-7.63
3	30.1 ± 1.1	4.521	4.521	-6.988	-1.668	-4.963	-3.196	-8.52	-8.32
4	3.2 ± 2.0	5.494	5.494	-6.414	-3.145	-4.897	-4.387	-10.44	-8.16
5	2.5 ± 1.4	5.602	5.602	-4.554	-3.117	-5.234	-4.881	-11.54	-8.48
6	4.8 ± 1.4	5.318	5.318	-5.602	-3.581	-6.755	-4.927	-10.09	-7.63
7	2.2 ± 0.1	5.657	5.657	-5.602	-3.581	-6.755	-4.927	-11.52	-7.06
8	2.3 ± 0.2	5.638	5.638	-3.299	-3.363	-5.133	-4.724	-12.09	-8.72
9	2.0 ± 0.2	5.698	5.698	-5.966	-3.302	-5.279	-4.088	-12.09	-8.05
10	5.3 ± 0.2	5.275	5.275	-4.583	-2.832	-4.959	-4.615	-10.27	-8.26
11	13.3 ± 2.6	4.876	4.876	-5.266	-2.434	-5.017	-4.952	-9.34	-8.65
12	24.6 ± 1.5	4.609	4.609	-2.975	-2.599	-5.293	-2.711	-9.59	-8.70
13	3.8 ± 0.6	5.420	5.420	-5.245	-2.657	-5.400	-3.025	-11.02	-9.30
14	3.0 ± 1.4	5.522	5.522	-4.597	-3.155	-5.096	-3.895	-11.24	-8.45
15	2.7 ± 0.7	5.568	5.568	-5.505	-2.959	-4.996	-3.041	-11.78	-8.82
16	2.8 ± 0.9	5.552	5.552	-5.593	-2.573	-4.648	-2.92	-10.92	-8.36
17	1.8 ± 0.4	5.744	5.744	-4.686	-3.465	-3.809	-1.083	-12.57	-8.90
18	6.3 ± 1.5	5.200	5.200	-5.422	-2.713	-4.557	-2.658	-10.93	-8.36
19	1.8 ± 0.5	5.744	5.744	-3.361	-1.89	-4.534	-2.334	-12.15	-8.95
20	2.0 ± 0.06	5.698	5.698	-6.698	-2.781	-5.021	-3.721	-12.53	-8.93
21	12.9 ± 0.4	4.889	4.889	-5.711	-2.379	-5.016	-3.424	-10.58	-7.92
22	3.0 ± 0.2	5.522	5.522	-2.167	-2.939	-5.082	-1.644	-11.27	-9.59
23	5.8 ± 0.8	5.236	5.236	-4.158	-1.285	-5.169	-3.947	-11.50	-7.43
24	44.2 ± 4.0	4.354	4.354	-6.678	-3.316	-5.936	-1.925	-8.56	-8.53
25	2.4 ± 0.08	5.619	5.619	-5.153	-2.432	-4.915	-2.874	-11.58	-7.47
26	9.9 ± 0.9	5.004	5.004	-5.830	-2.282	-5.719	-2.291	-11.20	-7.77
27	2.5 ± 1.2	5.602	5.602	-6.641	-2.469	-4.810	-3.164	-11.39	-7.25

TABLE S2: Hydrogen bonding analysis for selected compounds

Compound 9					
Acceptor	Hydrogen	Donator	Frequency	Distance	Angle
9@O2	TRP_162@HE1	TRP_162@NE1	47.24%	2.87	159.65
ASN_51@OD1	**9**@H1	**9**@N1	23.94%	2.88	153.07
9@O3	GLY_108@H	GLY_108@N	4.57%	2.90	159.13
9@O1	ASN_51@HD21	ASN_51@ND2	1.18%	2.88	152.76
9@O1	GLY_108@H	GLY_108@N	0.83%	2.88	138.46
9@O3	ASN_106@HD21	ASN_106@ND2	0.57%	2.89	157.69
9@O1	SER_52@HG	SER_52@OG	0.14%	2.76	163.68
9@O3	ASN_106@HD22	ASN_106@ND2	0.13%	2.87	139.33
9@O2	ASN_51@HD21	ASN_51@ND2	0.05%	2.89	166.30
9@O1	LYS_58@HZ2	LYS_58@NZ	0.04%	2.90	148.62
9@N1	ASN_51@HD21	ASN_51@ND2	0.03%	2.94	129.92
9@O3	ASN_51@HD21	ASN_51@ND2	0.02%	2.90	145.17
9@O2	TYR_139@HH	TYR_139@OH	0.01%	2.88	128.32
9@O1	ASN_106@HD21	ASN_106@ND2	0.01%	2.89	140.14
9@O1	ASN_51@HD22	ASN_51@ND2	0.01%	2.93	140.65
9@N1	ASN_106@HD21	ASN_106@ND2	0.01%	2.96	121.19
Compound 17					
Acceptor	Hydrogen	Donator	Frequency	Distance	Angle
17@O1	ASN_106@HD21	ASN_106@ND2	37.58%	2.88	157.97
17@O3	ASN_106@HD21	ASN_106@ND2	2.53%	2.87	156.60
17@O1	ASN_51@HD21	ASN_51@ND2	1.15%	2.89	153.88
17@O2	TYR_139@HH	TYR_139@OH	0.15%	2.84	130.65
ASN_106@OD1	**17**@H1	**17**@N1	0.12%	2.90	127.60
17@N1	ASN_106@HD21	ASN_106@ND2	0.03%	2.96	127.19
17@O1	ASN_106@HD22	ASN_106@ND2	0.02%	2.91	146.88
17@O3	ASN_106@HD22	ASN_106@ND2	0.01%	2.94	124.73
Compound 19					
Acceptor	Hydrogen	Donator	Frequency	Distance	Angle
19@O2	PHE_138@H	PHE_138@N	13.02%	2.89	146.50
19@O1	THR_184@HG1	THR_184@OG1	8.95%	2.80	159.52
19@O3	ASN_51@HD22	ASN_51@ND2	0.75%	2.88	140.68
19@O3	THR_184@HG1	THR_184@OG1	0.23%	2.81	158.84
19@O3	ASN_51@HD21	ASN_51@ND2	0.12%	2.90	133.37
19@O1	ASN_51@HD21	ASN_51@ND2	0.06%	2.90	136.70
19@O2	GLY_137@H	GLY_137@N	0.03%	2.89	138.94

Compound 20					
Acceptor	Hydrogen	Donator	Frequency	Distance	Angle
20@O3	ASN_51@HD21	ASN_51@ND2	2.46%	2.87	144.54
20@O1	ASN_51@HD21	ASN_51@ND2	1.98%	2.90	154.74
20@O3	ASN_51@HD22	ASN_51@ND2	0.01%	2.83	121.11
20@O3	PHE_138@H	PHE_138@N	0.01%	2.96	154.24
GLY_97@O	**20**@H1	**20**@N1	0.01%	2.99	123.83