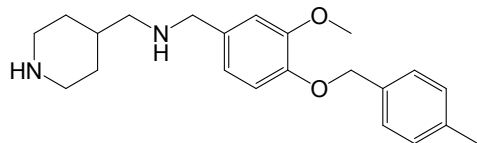


Sr.No	ROCK1		NOX2	
	Fitness	tanimoto combo	Fitness	tanimoto combo
1	0.956	0.666	1.487	0.734
2	1.521	0.632	1.231	0.696
3	1.321	0.705	1.925	0.738
4	1.452	0.694	1.651	0.643
5	1.621	0.653	1.561	0.658
6	0.921	0.738	1.521	0.594
7	1.06	0.688	1.32	0.522
8	1.02	0.696	1.683	0.468
9	1.018	0.751	1.681	0.503
10	1.226	0.708	1.926	0.518
11	0.854	0.718	1.554	0.522
12	0.864	0.593	1.621	0.552
13	1.054	0.643	1.91	0.517
14	1.54	0.634	1.597	0.539
15	1.375	0.636	1.977	0.522
16	1.228	0.709	1.628	0.643
17	1.131	0.632	1.531	0.658
18	1.158	0.691	1.884	0.634

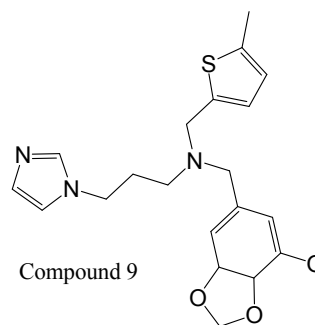
Table-3: Designed 18 molecules Fit values for both E-pharmacophore and shape.

Sr.No	NOX2 (LPS stimulated HUVEC)				Rhokinase				HEK Cell lines	IMR32 (MeHg 10uM)	SI (CC50/GIC50)
	H bond	Glide g score	Docking score	X-ROS IC50(μM)	H bond	Glide g score	Docking score	ROCK IC50(μM)	CC50(μM)	GIC50(uM)	
8	4	-8.152	-8.152	7.562	3	-7.43	-7.43	0.002042	1.607	59.650	0.0269
9	3	-9.319	-9.062	19.12	1	-6.79	-7.047	0.001632	1.15	33.470	0.0344
10	4	-11.614	-10.103	84.21	9	-7.91	-9.421	0.002129	2.232	64.46	0.0346
11	3	-7.687	-7.618	52.36	0	-8.422	-8.49	0.003273	1.257	1.987	0.6326
12	1	-7.358	-7.358	9.124	1	-8.014	-8.014	0.009287	0.5258	1.019	0.5160
13	5	-8.18	-8.18	11.65	1	-5.241	-5.241	0.01555	0.5308	7.571	0.0701
14	2	-9.603	-8.962	10.87	4	-8.013	-8.654	0.008751	0.4465	5.793	0.0771
15	5	-10.894	-10.829	19.25	6	-9.525	-9.59	0.001143	0.6616	35.42	0.0187
16	2	-8.497	-8.187	65.32	0	-5.861	-6.171	0.009488	0.1251	5.092	0.0246
17	2	-8.923	-9.255	123.6	3	-7.824	-8.156	0.007622	0.6146	0.8596	0.7150
18	9	-8.738	-10.229	56.14	8	-10.164	-11.656	0.007555	0.4455	2.073	0.2149

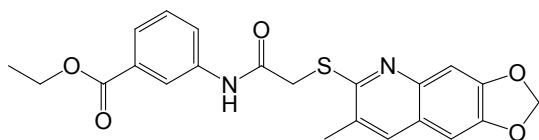
Table-4: 11 molecules docking score and invitro assay results.



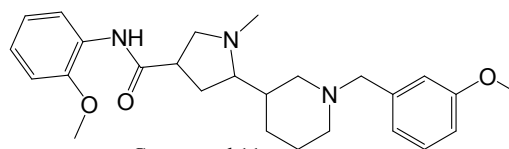
Compound 8



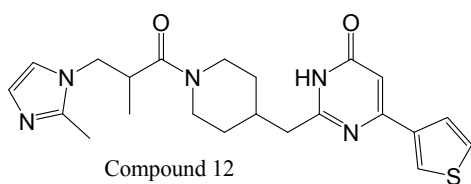
Compound 9



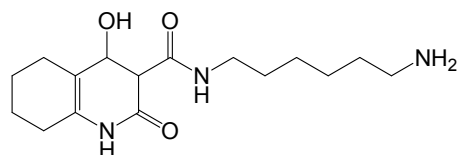
Compound 10



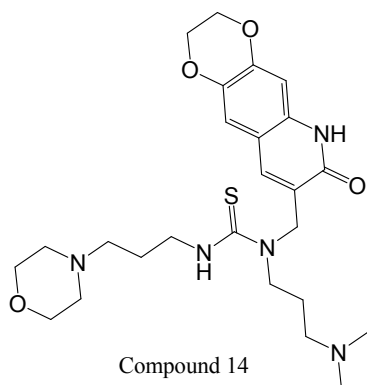
Compound 11



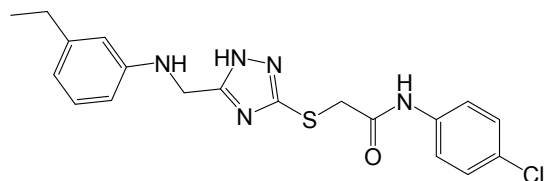
Compound 12



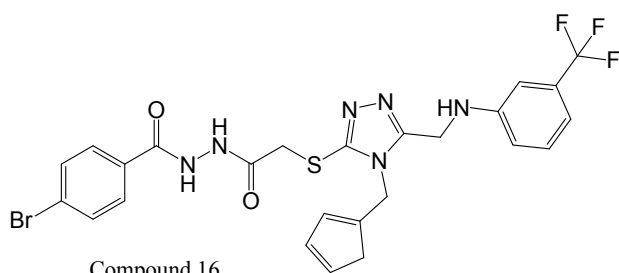
Compound 13



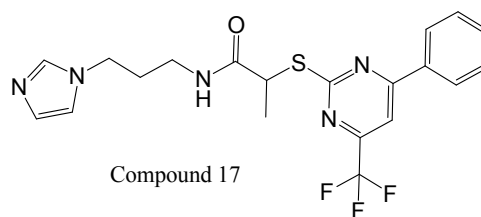
Compound 14



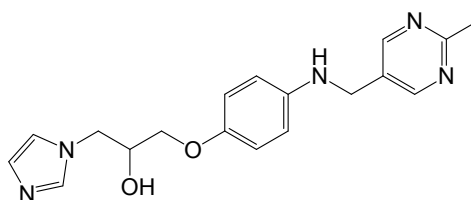
Compound 15



Compound 16



Compound 17



Compound 18

Figure S1: Excluded 11 compounds structures.

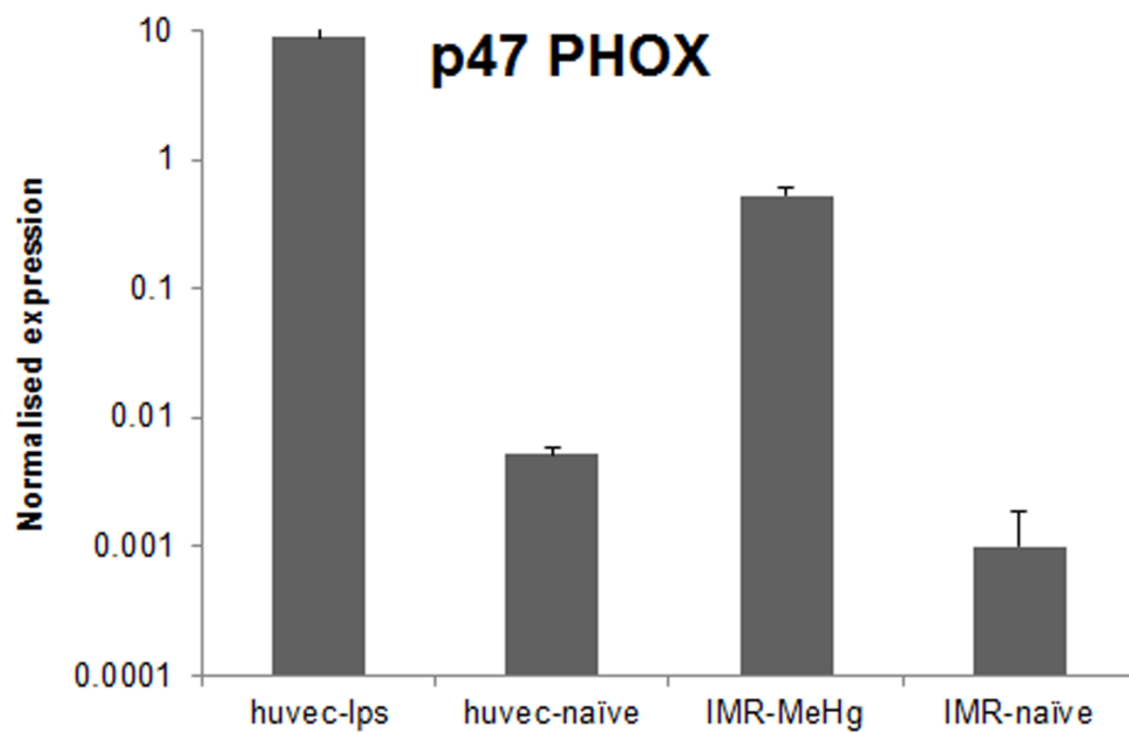


Figure S2: p47PHOX expression using RT-PCR in LPS treated U87MG cell lines and MeHg treated IMR-32 cell lines.

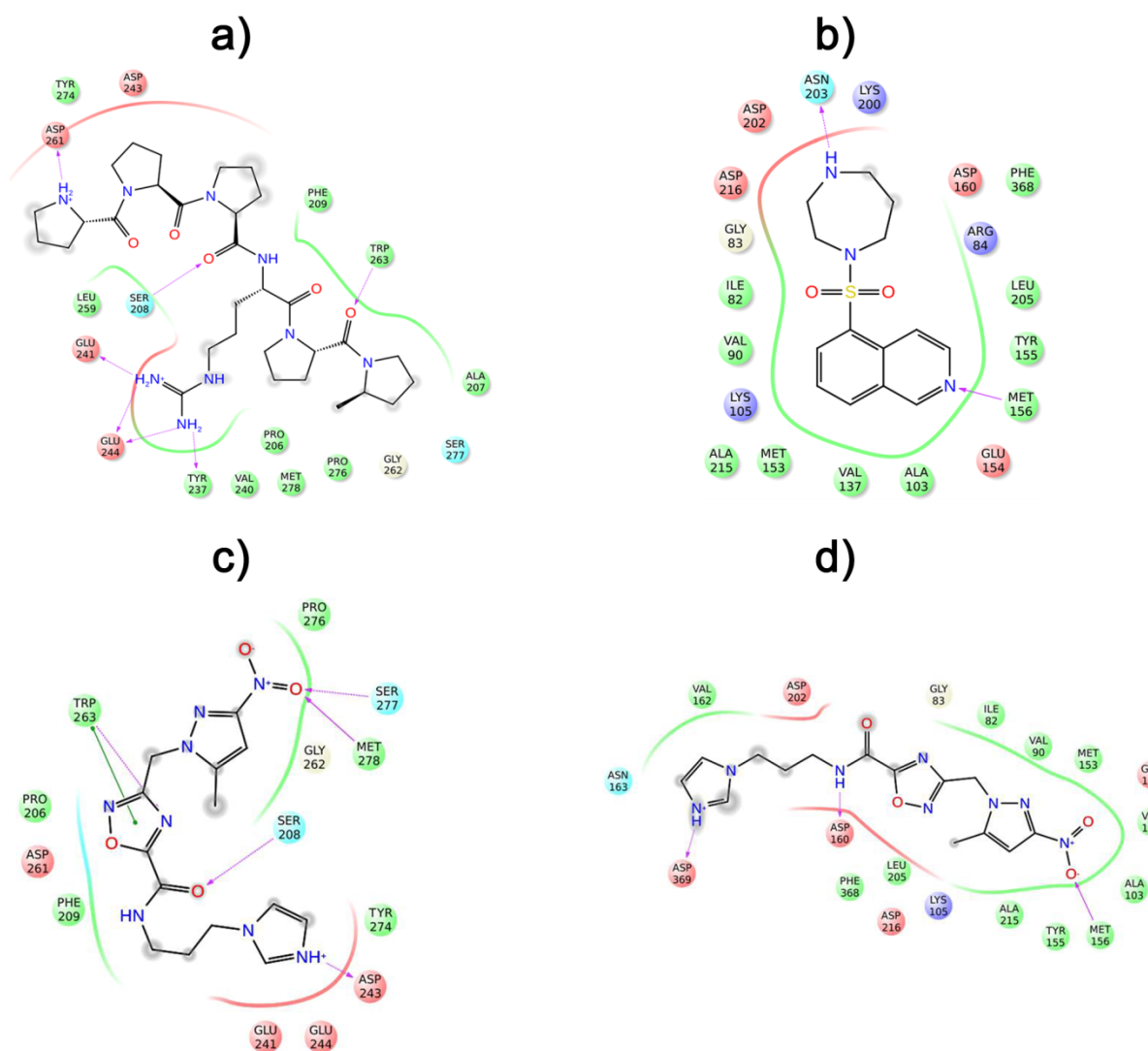


Figure S3: a) interaction picture of peptide5 in NOX2 (p47 phox), b) interaction picture of fasudil in NOX2. c) and d) compound3 interaction picture in NOX2 (p47 phox) and ROCK-I respectively.