

Figure S1. Two-dimensional image of interaction pattern of B(a)P against active of Oxysterols receptor LXR-beta (1P8D) using Protein Ligand Interaction Profiler (PLIP)

Table S2. The nature of the interactions of B(a)P/1P8D complex

Hydrophobic Interactions							
Index	Residue	AA	Distance	Ligand Atom	Protein Atom		
1	243A	PHE	3.29	2031	242		
2	271A	PHE	3.76	2038	462		
3	271A	PHE	3.76	2035	460		
4	274A	LEU	3.19	2029	487		
5	316A	THR	3.80	2028	815		
6	329A	PHE	3.88	2034	929		
7	329A	PHE	3.67	2025	923		
8	340A	PHE	3.82	2037	1024		
π-Stacking							
Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	329A	PHE	3.67	3.37	0.96	P	2019, 2020, 2021, 2024, 2028, 2030
2	329A	PHE	3.76	3.42	1.38	P	2019, 2021, 2022, 2023, 2026, 2027
3	329A	PHE	4.09	3.41	1.99	P	2019, 2020, 2022, 2025, 2029, 2031

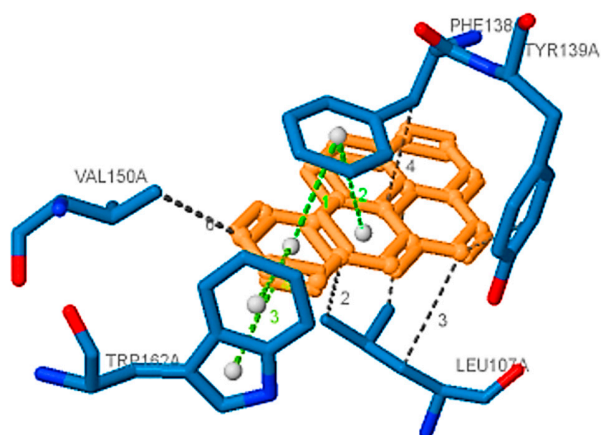


Figure S2. Two-dimensional image of interaction pattern of B(a)P against active of Heat shock protein HSP 90-beta (3NMQ) using Protein Ligand Interaction Profiler (PLIP)

Table S3. The nature of the interactions of B(a)P/3NMQ complex

Hydrophobic Interactions							
Index	Residue	AA	Distance	Ligand Atom	Protein Atom		
1	107A	LEU	3.90	1687	748		
2	107A	LEU	3.60	1693	747		
3	107A	LEU	3.85	1696	745		
4	138A	PHE	3.97	1686	958		
5	139A	TYR	3.79	1696	974		
6	150A	VAL	3.39	1704	1058		
π -Stacking							
Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	138A	PHE	3.68	5.73	0.54	P	1690, 1693, 1701, 1702, 1704, 1705
2	138A	PHE	4.16	5.71	1.71	P	1686, 1688, 1689, 1690, 1693, 1694
3	162A	TRP	4.90	82.83	1.42	T	1690, 1693, 1701, 1702, 1704, 1705
4	162A	TRP	4.79	81.43	0.81	T	1690, 1693, 1701, 1702, 1704, 1705

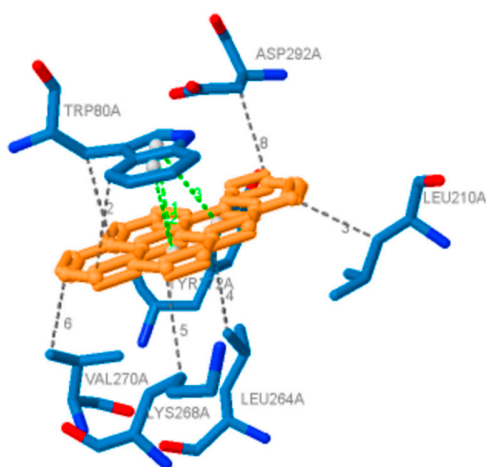


Figure S3. Two-dimensional image of interaction pattern of B(a)P against active of RAC-alpha serine/threonine-protein kinase (3O96) Using Protein Ligand Interaction Profiler (PLIP)

Table S4. The nature of the interactions of B(a)P/3O96 complex

Hydrophobic Interactions							
Index	Residue	AA	Distance	Ligand Atom	Protein Atom		
1	80A	TRP	3.91	3629	677		
2	80A	TRP	3.56	3620	671		
3	210A	LEU	3.34	3631	1801		
4	264A	LEU	3.85	3618	2254		
5	268A	LYS	3.69	3627	2285		
6	270A	VAL	3.39	3632	2302		
7	272A	TYR	3.66	3630	2319		
8	292A	ASP	3.55	3633	2483		
π-Stacking							
Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	80A	TRP	3.68	1.19	0.66	P	3615, 3616, 3618, 3621, 3625, 3627
2	80A	TRP	3.95	1.19	1.54	P	3615, 3616, 3618, 3621, 3625, 3627
3	80A	TRP	4.07	1.19	1.84	P	3615, 3617, 3618, 3619, 3622, 3623

π -Stacking

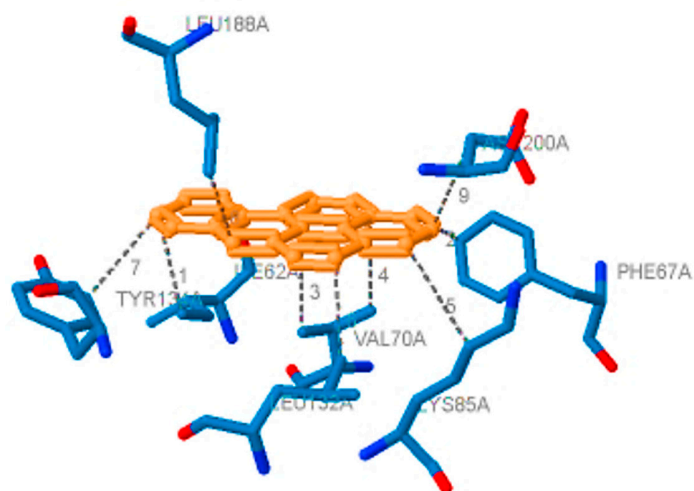


Figure S4. Two-dimensional image of interaction pattern of B(a)P against active of Glycogen synthase kinase-3 beta (4ACG) using Protein Ligand Interaction Profiler (PLIP).

Table S5. The nature of the interactions of B(a)P/4ACG complex

Hydrophobic Interactions					
Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	62A	ILE	3.53	2826	208
2	67A	PHE	3.52	2820	241
3	70A	VAL	3.79	2807	258
4	70A	VAL	3.47	2812	259
5	85A	LYS	3.93	2821	370
6	132A	LEU	3.57	2819	782
7	134A	TYR	3.74	2826	800
8	188A	LEU	3.56	2815	1261
9	200A	ASP	3.92	2824	1348

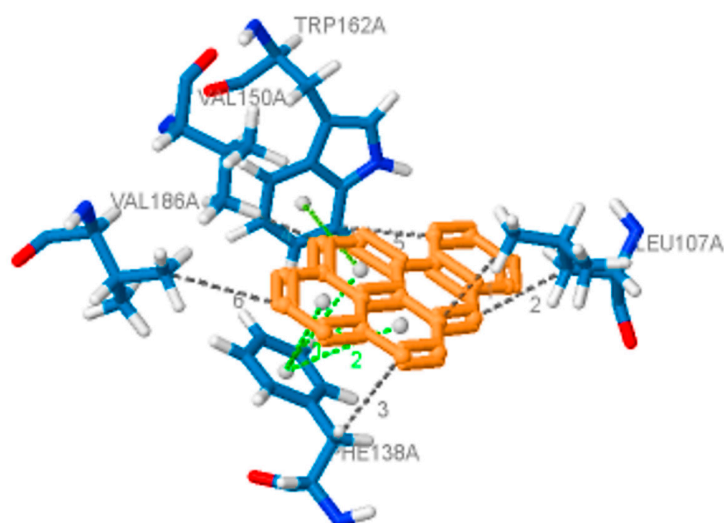


Figure S5. Two-dimensional image of interaction pattern of B(a)P against active of Heat shock protein HSP 90-alpha (5J20) using Protein Ligand Interaction Profiler (PLIP)

Table S6. The nature of the interactions of B(a)P/5j20 complex

Hydrophobic Interactions							
Index	Residue	AA	Distance	Ligand Atom	Protein Atom		
1	107A	LEU	4.00	3267	1448		
2	107A	LEU	3.47	3272	1446		
3	138A	PHE	3.88	3276	1878		
4	150A	VAL	3.29	3275	2075		
5	162A	TRP	3.61	3279	2269		
6	186A	VAL	3.68	3281	2601		
π-Stacking							
Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	138A	PHE	3.89	16.76	1.11	P	3265, 3269, 3270, 3277, 3278, 3281
2	138A	PHE	4.49	16.82	1.92	P	3264, 3265, 3267, 3270, 3274, 3276
3	138A	PHE	4.00	16.81	0.63	P	3264, 3265, 3266, 3269, 3273, 3275
4	162A	TRP	4.83	72.72	0.48	T	3264, 3265, 3266, 3269, 3273, 3275

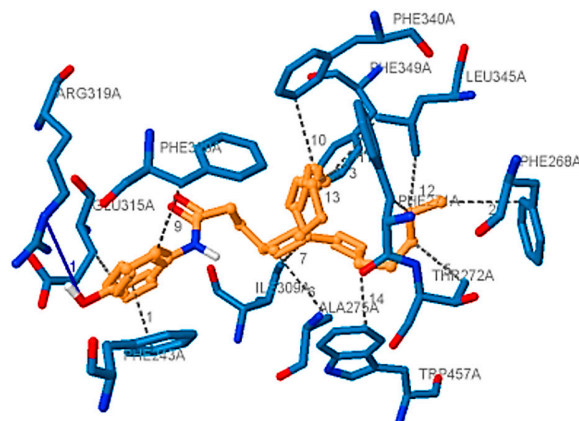


Figure S6. Two-dimensional image of interaction pattern of AM404 against active site of Oxysterols receptor LXR-beta (1P8D) using Protein Ligand Interaction Profiler (PLIP)

Table S7 The nature of the interactions of AM404/1P8D complex

Hydrophobic Interactions									
Index	Residue	AA	Distance		Ligand Atom		Protein Atom		
1	243A	PHE	3.83		2045		241		
2	268A	PHE	3.59		2040		437		
3	271A	PHE	3.35		2028		462		
4	271A	PHE	3.52		2039		460		
5	272A	THR	3.85		2038		473		
6	275A	ALA	3.79		2025		495		
7	309A	ILE	3.57		2033		758		
8	315A	GLU	3.86		2043		804		
9	329A	PHE	3.83		2046		923		
10	340A	PHE	3.44		2029		1024		
11	345A	LEU	3.73		2030		1063		
12	345A	LEU	3.65		2039		1064		
13	349A	PHE	3.92		2032		1099		
14	457A	TRP	3.58		2035		1985		
Hydrogen Bonds									
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	319A	ARG	3.19	4.00	140.15			2047 [O3]	839 [Ng+]

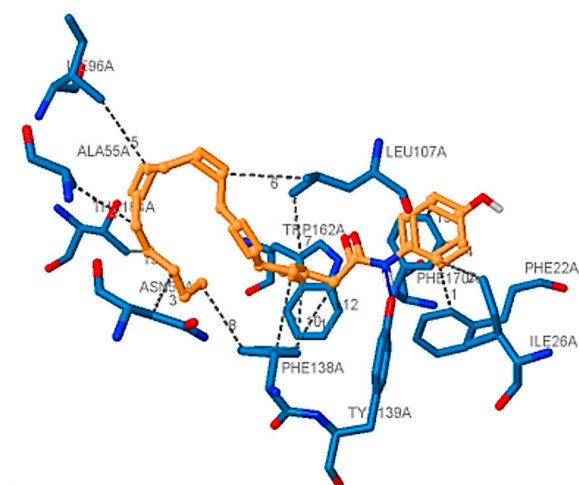


Figure S7. Two-dimensional image of interaction pattern of AM404 against active site of Heat shock protein HSP 90-beta (3NMQ) using Protein Ligand Interaction Profiler (PLIP)

Table S8. The nature of the interactions of AM404/3NMQ complex

Hydrophobic Interactions									
Index	Residue	AA	Distance		Ligand Atom		Protein Atom		
1	22A	PHE	3.03		1709		77		
2	26A	ILE	3.68		1709		112		
3	51A	ASN	3.68		1705		316		
4	55A	ALA	3.72		1703		343		
5	96A	ILE	3.82		1701		666		
6	107A	LEU	3.69		1698		748		
7	107A	LEU	3.63		1692		747		
8	138A	PHE	3.62		1707		960		
9	138A	PHE	3.75		1693		958		
10	138A	PHE	3.62		1692		961		
11	138A	PHE	3.66		1689		963		
12	162A	TRP	3.59		1689		1163		
13	170A	PHE	3.63		1712		1216		
14	170A	PHE	3.90		1710		1215		
15	184A	THR	3.70		1704		1318		
Hydrogen Bonds									
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	139A	TYR	1.92	2.80	142.08			1687 [Nam]	976 [O3]

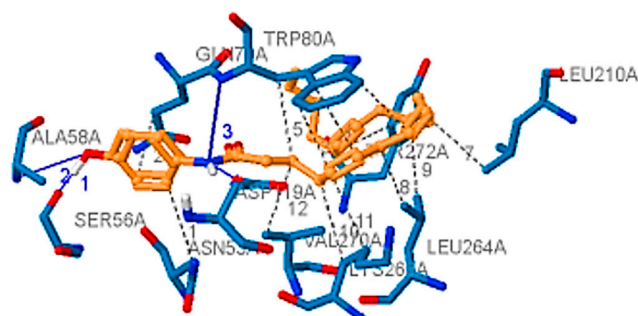


Figure S8. Two-dimensional image of interaction pattern of AM404 against active site of RAC-alpha serine/threonine-protein kinase (3O96) Using Protein Ligand Interaction Profiler (PLIP)

Table S9. The nature of the interactions of AM404/3O96 complex

Hydrophobic Interactions									
Index	Residue	AA	Distance		Ligand Atom		Protein Atom		
1	53A	ASN	3.79		3638		449		
2	79A	GLN	3.83		3639		663		
3	80A	TRP	3.74		3621		677		
4	80A	TRP	3.64		3622		674		
5	80A	TRP	3.67		3619		671		
6	80A	TRP	3.90		3624		678		
7	210A	LEU	3.52		3627		1803		
8	264A	LEU	3.79		3623		2254		
9	264A	LEU	3.64		3628		2253		
10	268A	LYS	3.81		3620		2284		
11	268A	LYS	3.69		3621		2285		
12	270A	VAL	3.92		3619		2302		
13	272A	TYR	3.54		3632		2317		
Hydrogen Bonds									
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	56A	SER	2.64	3.03	103.73			3643 [O3]	475 [O2]
2	58A	ALA	2.75	3.32	117.48			485 [Nam]	3643 [O3]
3	80A	TRP	2.93	3.72	137.14			667 [Nam]	3616 [Nam]
4	119A	ASP	1.92	2.88	155.12			3616 [Nam]	1009 [O.co2]

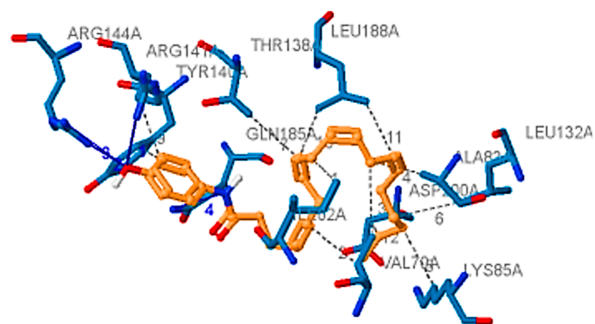


Figure S9. Two-dimensional image of interaction pattern of AM404 against active site of Glycogen synthase kinase-3 beta (4ACG) using Protein Ligand Interaction Profiler (PLIP).

Table S10. The nature of the interactions of AM404/4ACG complex

Hydrophobic Interactions									
Index	Residue	AA	Distance	Ligand Atom	Protein Atom				
1	62A	ILE	3.61	2818	208				
2	70A	VAL	3.70	2814	257				
3	70A	VAL	3.97	2821	258				
4	83A	ALA	3.55	2821	355				
5	85A	LYS	3.55	2826	370				
6	132A	LEU	3.75	2825	782				
7	138A	THR	3.95	2817	833				
8	140A	TYR	3.51	2831	847				
9	141A	ARG	3.53	2831	858				
10	188A	LEU	3.63	2817	1262				
11	188A	LEU	3.67	2822	1261				
12	200A	ASP	3.71	2827	1348				
Hydrogen Bonds									
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	141A	ARG	3.00	3.97	166.96			862 [Ng+]	2835 [O3]
2	144A	ARG	1.97	2.94	167.86			885 [Ng+]	2835 [O3]
3	144A	ARG	3.29	3.95	126.25			886 [Ng+]	2835 [O3]
4	185A	GLN	3.05	3.85	139.50			1238 [Nam]	2808 [Nam]

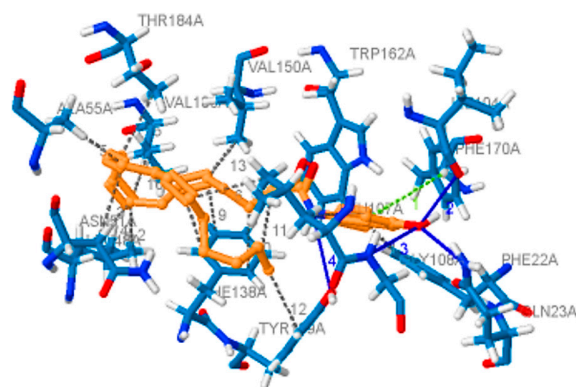


Figure S10. Two-dimensional image of interaction pattern of AM404 against active site of Heat shock protein HSP 90-alpha (5J20) using Protein Ligand Interaction Profiler (PLIP)

Table S11. The nature of the interactions of AM404/5j20 complex

Hydrophobic Interactions									
Index	Residue	AA	Distance		Ligand Atom		Protein Atom		
1	22A	PHE	3.49		3291		93		
2	48A	LEU	3.68		3273		532		
3	51A	ASN	3.86		3277		578		
4	51A	ASN	3.67		3273		578		
5	55A	ALA	3.88		3277		626		
6	107A	LEU	3.59		3280		1448		
7	107A	LEU	3.84		3287		1446		
8	138A	PHE	3.58		3271		1880		
9	138A	PHE	3.75		3270		1882		
10	138A	PHE	3.70		3268		1881		
11	138A	PHE	3.72		3267		1883		
12	139A	TYR	3.78		3285		1903		
13	150A	VAL	3.70		3270		2075		
14	162A	TRP	3.75		3291		2269		
15	184A	THR	3.65		3275		2565		
16	186A	VAL	3.79		3273		2601		
Hydrogen Bonds									
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	23A	GLN	2.15	3.05	145.55			113 [Nam]	3292 [O3]
2	104A	ILE	2.39	2.98	117.60			3292 [O3]	1398 [O2]
3	108A	GLY	3.12	3.80	124.88			1461 [Nam]	3292 [O3]
4	139A	TYR	3.13	3.77	122.24			3265 [Nam]	1905 [O3]
π -Stacking									
Index	Residue	AA	Distance		Angle	Offset	Stacking Type	Ligand Atoms	
1	170A	PHE	5.25		62.15	1.87	T	3286, 3287, 3288, 3289, 3290, 3291	