Marine-Derived Compounds as Potential Inhibitors of Hsp90 for Anticancer and Antimicrobial Drug Development: A Comprehensive In Silico Study
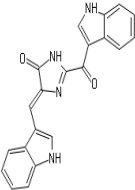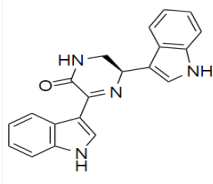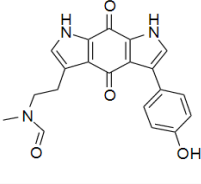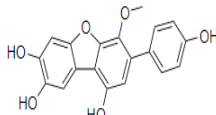
Mebarka Ouassaf, Lotfi Bourougaa, Samiah Hamad Al-Mijalli, Emad M. Abdallah, Ajmal R. Bhat, Sarkar M. A. Kawsar

Table S1. Properties and Definitions of Selected Marine-Derived Compounds as Potent Inhibitors of Hsp90 Protein.

| CMNPD	22591	9335	10015	360799	15115	20988
Structure						
Canonical SMILES	c1cc(ccc1O)C2=C([C@](OC C)(NC2=O)C(OC)=O)c3ccc(O)cc3	C1(=O)NC(=O)C(c2c[nH]c(cccc3)c23)=C1c4[nH]cnc4	C1=CC=C2C(=C1)C(=CN2)C(=O)C3=N C(=C(N3)C=C4C=NC5=CC=CC=C54)O	c12c(cccc1)[nH]cc2[C@@H]3CNC(=O)C(c4c[nH]c(c4ccc5)c5)=N3	CN(CCC1=CNC2=C1C(=O)C3=C(C2=O)NC=C3C4=CC=C(C=C4)O)C=O	COC1=C2C(=C(C=C1C3=CC=C(C=C3)O)O)C4=CC(=C(C=C4O2)O)O
PubChem CID	162904707	398493	136691197	16104844	11717517	53262759
Molecular formula	C20H15NO6	C15H10N4O2	C21H14N4O2	C20H16N4O	C20H17N3O4	C19H14O6
IUPAC name	methyl (2R)-2-ethoxy-3,4-bis(4-hydroxyphenyl)-5-oxo-1H-pyrrole-2-carboxylate	3-(1H-imidazol-5-yl)-4-(1H-indol-3-yl)pyrrole-2,5-dione	[4-hydroxy-5-(indol-3-ylidenemethyl)-1H-imidazol-2-yl]-(1H-indol-3-yl)methanone	((3R)-3,5-bis(1H-indol-3-yl)-2,3-dihydro-1H-pyrazin-6-one	N-[2-[3-(4-hydroxyphenyl)-4,8-dioxo-1,7-dihydropyrrolo[3,2-f]indol-5-yl]ethyl]-N-methylformamide	3-(4-hydroxyphenyl)-4-methoxydibenzofuran-1,7,8-triol
Synonym	Ianthellidone B	Didemnimide A	Rhopaladins D	(R)-6'-debromohamacanthin B	Zyzzyanone D	3''-deoxy-6'-O-desmethylcandidusin B
Resource	Demospongiae	Didemnum granulatum	tunicate Rhopalaea sp	Spongosorites	Zyzzya fuliginosa	Penicillium chermesinum

Classy fire subclass	Stilbenes	Indoles	Indoles	Indoles	Pyrroloindoles	Phenylbenzofurans

Table S2. Result Of Enrichment Study.

Pharmacophore model	AUC	RIE	ROC	BedROC160.9	Total active	Number of ranked actives
DDRRR	0.84	7.18	0.78	0.58	35	29

Table S3. Organ and End Points Toxicity for Top Leads Compound.

|			22591		9335		10015		360799		15115		20988		MEY	
			Probability	Prediction	Probability	Prediction	Probability	Prediction	Probability	Prediction	Probability	Prediction	Probability	Prediction	Probability	Prediction
Organ toxicity	Hepatotoxicity	dili	0.50	inactive	0.51	inactive	0.50	inactive	0.72	inactive	0.62	inactive	0.67	inactive	0.55	active
Toxicity end points	Carcinogenicity	carcino	0.58	inactive	0.51	active	0.55	active	0.56	inactive	0.59	active	0.62	active	0.71	inactive
	Immunotoxicity	immuno	0.95	inactive	0.73	inactive	0.7	inactive	0.98	inactive	0.79	inactive	0.8	inactive	0.54	inactive
	Mutagenicity	mutagen	0.67	inactive	0.61	inactive	0.6	active	0.67	inactive	0.54	inactive	0.55	inactive	0.78	inactive
	Cytotoxicity	cyto	0.66	inactive	0.7	inactive	0.74	inactive	0.77	inactive	0.55	inactive	0.95	inactive	0.64	inactive
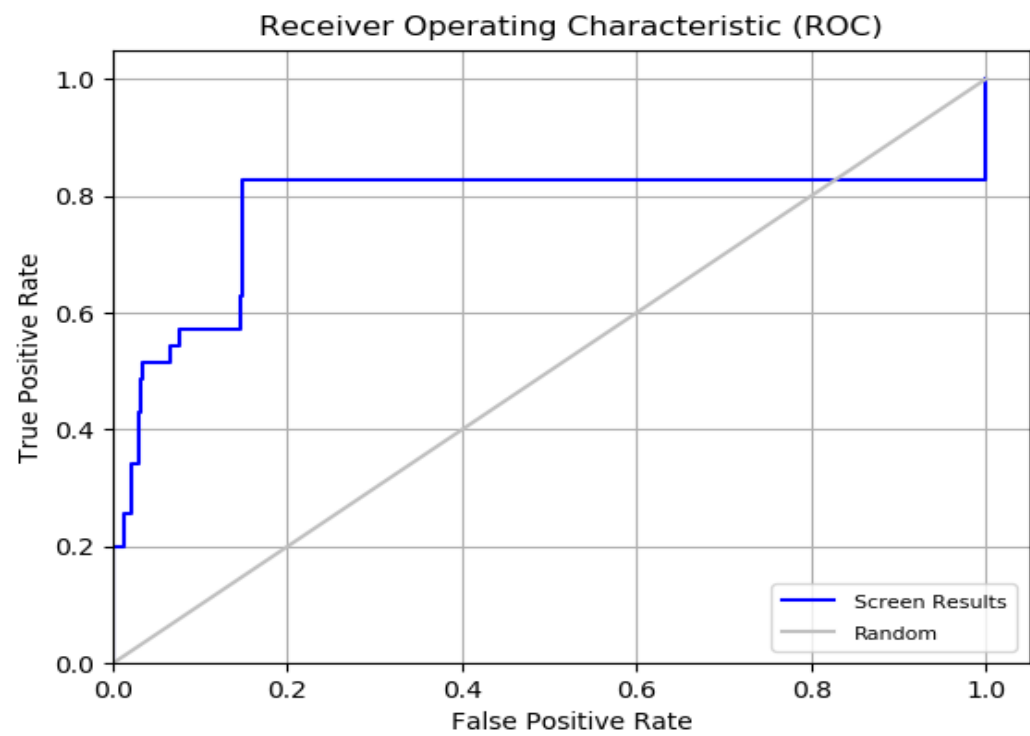
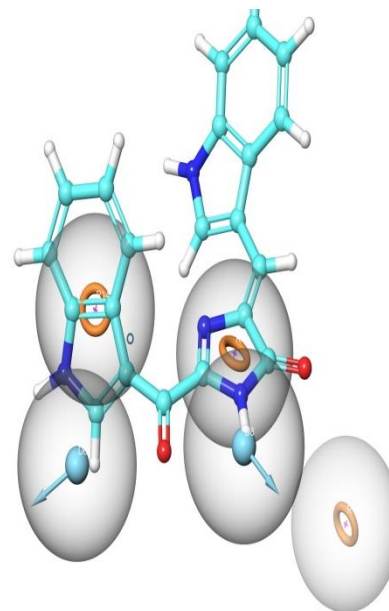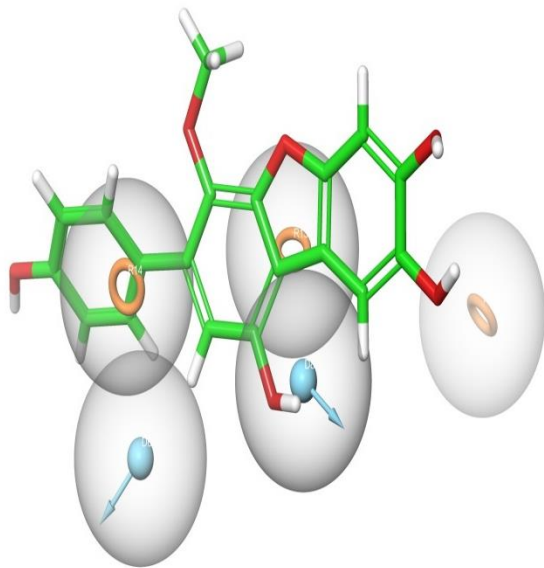**Figure S1.** ROC plot of the pharmacophore model.
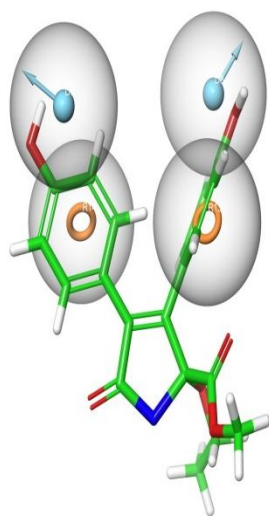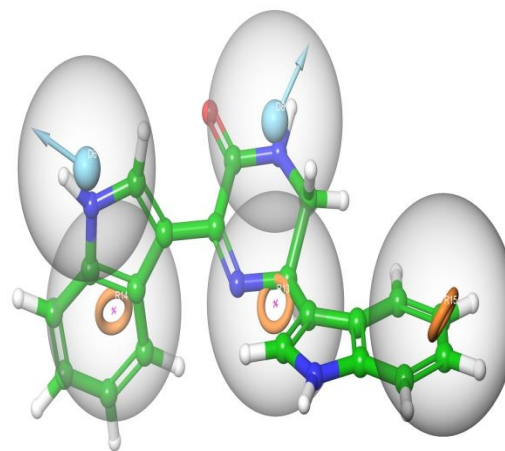
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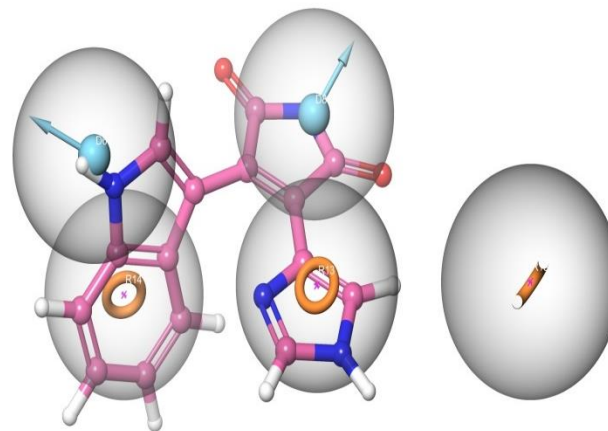
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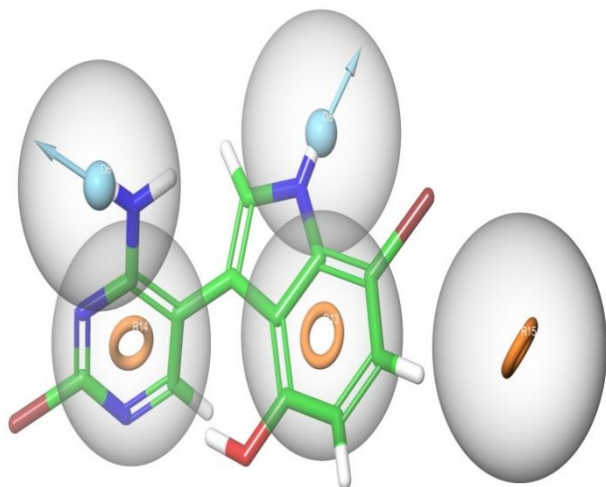
15115

10015

20988

360799

Figure S2. The model map onto top leads.