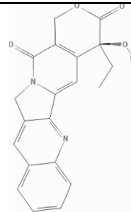
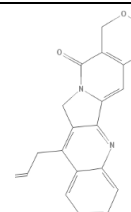
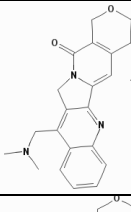
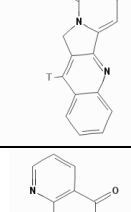
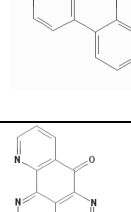
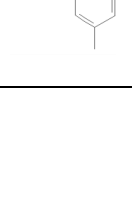
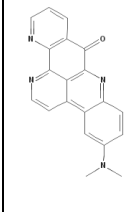
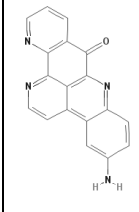
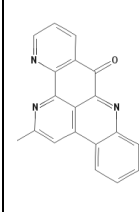
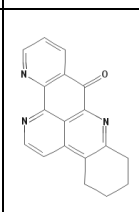
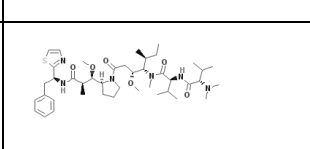
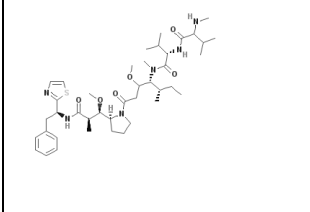
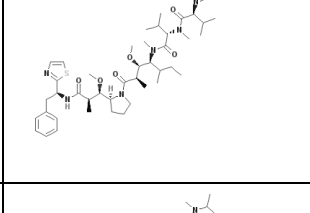
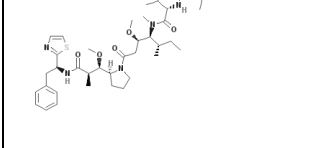
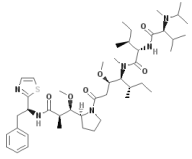
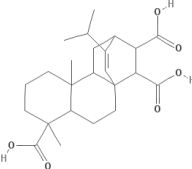
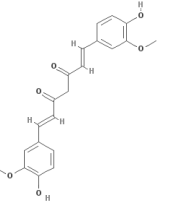
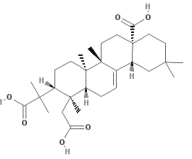
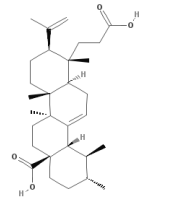
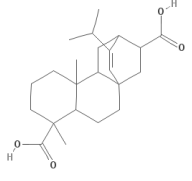


Supplementary Table: Chemical and Structural features of compounds used in Pharmacophore generation.

S.No	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Hydrogen Bond		Structure
				Donor	Acceptor	
1	Camptothecin	C ₂₀ H ₁₆ N ₂ O ₄	348.35	1	5	
2	SureCN4551967	C ₂₃ H ₂₀ N ₂ O ₄	388.41	1	5	
3	SureCN13529242	C ₂₃ H ₂₃ N ₃ O ₄	405.44	1	6	
4	CID59072382	C ₁₉ H ₁₄ N ₂ O ₄	336.33	1	5	
5	Ascididemin	C ₁₈ H ₉ N ₃ O	283.28	0	4	
6	SureCN6846666	C ₁₉ H ₁₁ N ₃ O	297.31	0	4	

7	SureCN6846896	$C_{20}H_{14}N_4O$	326.35	0	5	
8	SureCN6845707	$C_{18}H_{10}N_4O$	298.28	1	5	
9	AC1N8MW1	$C_{19}H_{11}N_3O$	297.31	0	4	
10	NSC702616.	$C_{18}H_{13}N_3O$	287.31	0	4	
11	Dolostatin 10	$C_{42}H_{68}N_6O_6S$	785.09	2	9	
12	SureCN14586604	$C_{41}H_{66}N_6O_6S$	771.06	3	9	
13	SureCN8231407	$C_{44}H_{72}N_6O_6S$	813.14	1	9	
14	SureCn12972230	$C_{44}H_{72}N_6O_6S$	813.14	2	9	

15	SureCN12836708	$C_{45}H_{74}N_6O_6S$	827.17	2	9	
16	NSC15520	$C_{24}H_{34}O_6$	418.52	3	6	
17	Curcumin	$C_{21}H_{20}O_6$	368.37	2	6	
18	CHEMBL573822	$C_{30}H_{46}O_6$	502.68	3	6	
19	CHEMBL595750	$C_{30}H_{46}O_4$	470.68	2	4	
20	SureCN10820369	$C_{23}H_{34}O_4$	374.51	2	4	

Supplementary Figure 1: Statistics of Training set after clustering.

	Active	Name	Type	Feature Pattern	# Confs	Cluster ID	Pharmacophore-R1	AdMly
1	☑	CNC(C)CC2(C)CC1N(C)C(C)C3CCNC3CN	Training	■ ■ ■ ■ ■ ■ ■ ■	1	7	53.6000	1.0
2	☑	CNC(C)C(O)N(C)C(O)N(C)C(C)C(O)N(C)CC	Test	■ ■ ■ ■ ■ ■ ■ ■	13	10	50.9400	1.0
3	☑	CC1C2NC3CC0C9C3CNC(C32)C2NC0CC	Training	■ ■ ■ ■ ■ ■ ■ ■	1	6	49.7200	1.0
4	☑	CC1C2NC3CC0C9C3CNC(C32)C2NC0CC	Training	■ ■ ■ ■ ■ ■ ■ ■	1	6	49.7200	1.0
5	☑	CO(C)C2C(C)C4NC5CC0C0C04CNC(C)C	Training	■ ■ ■ ■ ■ ■ ■ ■	1	8	49.5800	1.0
6	☑	CC(C)C1C2C3C4NC5CC0C0C04CNC(C)C	Training	■ ■ ■ ■ ■ ■ ■ ■	1	8	49.5800	1.0
7	☑	CNC(C)C1C2C3C4NC5CC0C0C04CNC(C)C	Training	■ ■ ■ ■ ■ ■ ■ ■	1	11	49.5700	1.0
8	☑	CC0C1C2C3C4NC5CC0C0C04CNC(C)C	Training	■ ■ ■ ■ ■ ■ ■ ■	1	11	49.5700	1.0
9	☑	CNC(C)C(O)N(C)C(C)C(O)N(C)C(C)C(O)N(C)C	Test	■ ■ ■ ■ ■ ■ ■ ■	3	10	48.7500	1.0
10	☑	CC(C)C2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	2	48.4400	1.0
11	☑	CC1CC2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	9	47.7000	1.0
12	☑	CC1CC2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	8	47.6000	1.0
13	☑	CC(C)C(C)C(O)N(C)C(C)C(O)N(C)C(C)C(O)N(C)C	Test	■ ■ ■ ■ ■ ■ ■ ■	1	10	46.5400	1.0
14	☑	CNC(C)C(O)N(C)C(C)C(O)N(C)C(C)C(O)N(C)C	Test	■ ■ ■ ■ ■ ■ ■ ■	10	10	44.6400	1.0
15	☑	NC1CC2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	7	44.1800	1.0
16	☑	CO(C)C1C2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	4	43.6800	1.0
17	☑	CO(C)C1C2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	9	43.6800	1.0
18	☑	CO(C)C1C2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	25	5	43.6300	1.0
19	☑	CO(C)C1C2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Test	■ ■ ■ ■ ■ ■ ■ ■	4	10	42.7800	1.0
20	☑	CO(C)C1C2C3C4C5C6C7C8C9C0C1C2C3C4C5C6C7C8C9C0	Training	■ ■ ■ ■ ■ ■ ■ ■	1	1	42.6400	1.0

Supplementary Figure 2: Pharmacophore score values

Name	S...
Modelrad9-1	0.6759
Modelrad9-2	0.6757
Modelrad9-3	0.6757
Modelrad9-4	0.6730
Modelrad9-5	0.6726
Modelrad9-6	0.6725
Modelrad9-7	0.6708
Modelrad9-8	0.6703
Modelrad9-9	0.6545