

Supplementary data:

Table S1. Comprehensive library of 110 cannabinoid derivatives evaluated in the study.

Type	No	Compound	Pubchem ID (CID)	Molecular formula
Cannabichromene (CBC)	1	Cannabichromene	30219	C ₂₁ H ₃₀ O ₂
	2	Nor-Cannabichromene	158435095	C ₂₁ H ₂₈ O ₄
Cannabichromenic Acid (CBCA)	3	Cannabichromenic Acid	3084339	C ₂₂ H ₃₀ O ₄
	4	Cannabichromenate	54740355	C ₂₂ H ₂₉ O ₄ ⁻
Cannabidiol (CBD)	5	Cannabidiol	644019	C ₂₁ H ₃₀ O ₂
	6	Cannabidiol Hydroxyquinone	11393311	C ₂₁ H ₂₈ O ₃
	7	Cannabidiol-3-Monomethyl Ether	164905	C ₂₂ H ₃₂ O ₂
	8	Cannabidiol Dimethyl Ether	3081957	C ₂₃ H ₃₄ O ₂
	9	(+)-Cannabidiol	36688143	C ₂₁ H ₃₀ O ₂
	10	6beta-Hydroxycannabidiol	53357351	C ₂₁ H ₃₀ O ₃
	11	Abnormal Cannabidiol	89949	C ₂₁ H ₃₀ O ₂
	12	Cannabidiolic Acid	160570	C ₂₂ H ₃₀ O ₄
	13	2-[3-Methyl-6-(Prop-1-En-2-Yl) Cyclohex-2-En-1-Yl]-5-Pentylbenzene-1,3-Diol	521372	C ₂₁ H ₃₀ O ₂
	14	Pre-Cannabidiol Phenethyl Ester	25019755	C ₃₀ H ₃₈ O ₄
	15	Cannabidiol-Aldehyde Diacetate	3044489	C ₂₅ H ₃₂ O ₅
	16	6alpha-HydroxyCannabidiol	53357350	C ₂₁ H ₃₀ O ₃
	17	1''-HydroxyCannabidiol	121596213	C ₂₁ H ₃₀ O ₃
	18	5-(1,1-Dimethylheptyl) Cannabidiol	126670	C ₂₅ H ₃₈ O ₂
	19	7-Hydroxycannabidiol	11301963	C ₂₁ H ₃₀ O ₃
	20	2''-Hydroxycannabidiol	121596214	C ₂₁ H ₃₀ O ₃
	21	4''-HydroxyCannabidiol	53357352	C ₂₁ H ₃₀ O ₃
	22	5''-HydroxyCannabidiol	101621543	C ₂₁ H ₃₀ O ₃
	23	1-Hydroxy-3-N-Pentyl-Cannabidiol	3060519	C ₂₁ H ₃₀ O ₂
	24	Delta6-Cannabidiol	60209648	C ₂₁ H ₃₀ O ₂
	25	1S,2R-Epoxy-Cannabidiol-2',6'-Diacetate	148695	C ₂₅ H ₃₄ O ₅
	26	3''-HydroxyCannabidiol	121596215	C ₂₁ H ₃₀ O ₃
	27	O, O-Dimethyl Cannabidiol	91740340	C ₂₃ H ₃₄ O ₂
	28	7-Carboxycannabidiol	146592489	C ₂₁ H ₂₈ O ₄
	29	Cannabidibutol	59444413	C ₂₀ H ₂₈ O ₂
	30	10-(Diisopropylamino)Cannabidiol Diacetate	24845987	C ₃₁ H ₄₇ NO ₄
	31	10-((4-Aminobutyryl) Amino) Cannabidiol	44149593	C ₂₅ H ₃₈ N ₂ O ₃
	32	Cannabidiol Ethyl	129210056	C ₁₈ H ₂₄ O ₂
	33	Cannabidiol-D9	71314488	C ₂₁ H ₃₀ O ₂
	34	Abnormal Cannabidiol-D3	71684591	C ₂₁ H ₃₀ O ₂
	35	Cannabidiol Glycolate	86627027	C ₂₃ H ₃₃ O ₅ ⁻
	36	Cannabidiol? -D-Glucuronide	163285562	C ₂₇ H ₃₈ O ₈
	37	Cannabidiol-D9 -D-Glucuronide	163285718	C ₂₇ H ₃₈ O ₈
Cannabidiolic Acid (CBDA)	38	Cannabidiolic Acid	160570	C ₂₂ H ₃₀ O ₄
	39	Cannabidiolic Acid, Phenyl-Boronate	91750641	C ₂₈ H ₃₃ BO ₄
	40	Cannabidiolic Acid Methyl Ester	145996527	C ₂₃ H ₃₂ O ₄

Cannabigerol (CBG)	41	Cannabigerol	5315659	C ₂₁ H ₃₂ O ₂
	42	Cannabigerol-D9	137699827	C ₂₁ H ₃₂ O ₂
	43	Cannabigerol-C4	131973883	C ₂₀ H ₃₀ O ₂
	44	Cannabigerol (CBG)	160109	C ₂₁ H ₃₂ O ₂
	45	O-Methylcannabigerol	13864080	C ₂₂ H ₃₄ O ₂
	46	Pre-Cannabigerol Phenethyl Ester	25015884	C ₃₀ H ₄₀ O ₄
	47	Cannabigerol Quinone Acid	148268014	C ₂₂ H ₃₀ O ₅
Cannabigerolic acid (CBGA)	48	Cannabigerolic Acid	6449999	C ₂₂ H ₃₂ O ₄
	49	Cannabigerolic Acid Monomethyl Ether	24739091	C ₂₃ H ₃₄ O ₄
Cannabinol (CBN)	50	Cannabinol	2543	C ₂₁ H ₂₆ O ₂
	51	Cannabinol Methyl Ether	628150	C ₂₂ H ₂₈ O ₂
	52	Dronabinol	16078	C ₂₁ H ₃₀ O ₂
	53	Delta-8-Tetrahydrocannabinol	638026	C ₂₁ H ₃₀ O ₂
	54	Delta.6-Tetrahydrocannabinol	2977	C ₂₁ H ₃₀ O ₂
	55	Delta.1- Tetrahydrocannabinol	2978	C ₂₁ H ₃₀ O ₂
	56	Ajulemic acid	3083542	C ₂₅ H ₃₆ O ₄
	57	8-Hydroxy-Delta (9)-Tetrahydrocannabinol	169652	C ₂₁ H ₃₀ O ₃
	58	Cannabiorcol	59444404	C ₁₇ H ₁₈ O ₂
	59	11-Hydroxytetrahydrocannabinol	644022	C ₂₁ H ₃₀ O ₃
	60	Cannabinol, Pentafluoropropionate	91745387	C ₂₄ H ₂₅ F ₅ O ₃
	61	Cannabinol, Tetrahydro-	3034462	C ₂₁ H ₃₀ O ₂
	62	Cannabinol-C2	59444399	C ₁₈ H ₂₀ O ₂
	63	Cannabinol, Acetate	90473109	C ₂₃ H ₂₈ O ₃
	64	Cannabinol, Trifluoroacetate	91744577	C ₂₃ H ₂₅ F ₃ O ₃
	65	Cannabinol, Heptafluorobutyrate	91745794	C ₂₅ H ₂₅ F ₇ O ₃
	66	Cannabinol-C4	59444392	C ₂₀ H ₂₄ O ₂
	67	Delta4-Isotetrahydrocannabinol	186077	C ₂₁ H ₃₀ O ₂
	68	(-)-11-9-Tetrahydro Cannabinol-9-Methanol-D9	71752421	C ₂₁ H ₃₀ O ₃
	69	11-Nor-9-Tetrahydro Cannabinol-9-Carboxylic-D5 Acid	102320329	C ₁₉ H ₂₄ O ₄
	70	11-Acetoxy-9-Tetrahydro Cannabinol	14263538	C ₂₃ H ₃₂ O ₄
	71	11-9-Tetrahydro Cannabinol-9-Carboxylic Acid-D-Glucuronide	163285415	C ₂₇ H ₃₆ O ₁₀
	72	11-Nor-9-Tetrahydro Cannabinol-9-Carboxylate Acyl -D-Glucuronide	163285414	C ₂₇ H ₃₆ O ₁₀
Delta-9-tetrahydrocannabinol (Delta-9-THC)	73	Delta9-Tetrahydrocannabinol; Dronabinol	16078	C ₂₁ H ₃₀ O ₂
	74	Butyl-Delta (9)-Tetrahydrocannabinol	6453891	C ₂₀ H ₂₈ O ₂
	75	8-Hydroxy-Delta (9)-Tetrahydrocannabinol	169652	C ₂₁ H ₃₀ O ₃
	76	1-Nor-9-Carboxy-Delta-9-Tetrahydrocannabinol	108207	C ₂₁ H ₂₈ O ₄
	77	11-Hydroxytetrahydrocannabinol	644022	C ₂₁ H ₃₀ O ₃
	78	Delta-9-11-Carboxytetrahydrocannabinol	107885	C ₂₁ H ₂₈ O ₄
	79	1-Trans- Delta.9-Tetrahydrocannabinol	2978	C ₂₁ H ₃₀ O ₂
	80	Tetrahydrocannabinol Acetate	198013	C ₂₃ H ₃₂ O ₃
	81	N-Hexyl-Delta-9-Tetrahydrocannabinol	161906	C ₂₂ H ₃₂ O ₂

	82	O-Methyl-Delta-9 Tetrahydrocannabinol	3082445	C ₂₂ H ₃₂ O ₂
	83	Ethyl-Delta-9-Tetrahydrocannabinol	195772	C ₁₈ H ₂₄ O ₂
	84	11-Nor-Delta (9)-Tetrahydrocannabinol-9-Carboxylic Acid	44814488	C ₂₁ H ₂₈ O ₄
	85	8-Hydroxy-Delta-9-THC	623131	C ₂₁ H ₃₀ O ₃
	86	Delta-9-THC- Trifluoroacetate	530244	C ₂₃ H ₂₉ F ₃ O ₃
	87	2'-Hydroxy-Delta (9)-THC	127844	C ₂₁ H ₃₀ O ₃
	88	3'-Hydroxy-THC	194062	C ₂₁ H ₃₀ O ₃
	89	6a,7,8,10a-Tetrahydro-1-Hydroxy-6,6-Dimethyl-3-(Pentyl-5,5,5-D3)-6H-Dibenzo (B, D) Pyran-9-Carboxylic Acid, (6aR,10aR)-	76969399	C ₂₁ H ₂₈ O ₄
	90	4'-Hydroxy-THC	6453619	C ₂₁ H ₃₀ O ₃
	91	8,11-Dihydroxy-Delta-9-Tetrahydrocannabinol	126961369	C ₂₁ H ₃₀ O ₄
	92	6-Hydroxymethyl-Delta (9)-Tetrahydrocannabinol	44151059	C ₂₁ H ₃₀ O ₃
	93	Delta-9-Tetrahydrocannabinol Dichloroethyl Carbamoyl Ester	133911	C ₂₆ H ₃₇ Cl ₂ NO ₃
	94	3',11- Dihydroxy-Delta (9)-Tetrahydrocannabinol	194083	C ₂₁ H ₃₀ O ₄
	95	THC-11-Oic Acid Glucuronide	173519	C ₂₇ H ₃₆ O ₁₀
	96	Methyl 1-Dehydroxy-1-Methoxy-11-Nor-. Delta. -9-Tetrahydrocannabinol-9-Carboxylate	628690	C ₂₃ H ₃₂ O ₄
	97	9-(Hydroxymethyl)-6,6-Dimethyl-3-Pentyl-6a,7,8,10a-Tetrahydrobenzo[C]Chromene-1,8-Diol	6420382	C ₂₁ H ₃₀ O ₄
	98	Methoxy-THC	53802961	C ₂₂ H ₃₂ O ₂
	99	Delta9-Tetrahydrocannabinol Hemisuccinate	162707	C ₂₅ H ₃₄ O ₅
	100	Di-Desoxy-Delta9-Tetrahydrocannabinol	50919315	C ₂₁ H ₃₀
	101	5-Desoxy-Delta9-Tetrahydrocannabinol	50919314	C ₂₁ H ₃₀ O
	102	1-Desoxy-Delta9-Tetrahydrocannabinol	50919316	C ₂₁ H ₃₀ O
	103	(+)-Delta9-Tetrahydrocannabinol	134740	C ₂₁ H ₃₀ O ₂
	104	8-Oxo-Delta9-Tetrahydrocannabinol	101152951	C ₂₁ H ₂₈ O ₃
	105	11-Nor-9-Carboxy-Delta9-Tetrahydrocannabinol Glucuronide	122401304	C ₂₇ H ₃₆ O ₁₀
	106	8beta,11-Dihydroxy-Delta (9)-THC	148024	C ₂₁ H ₃₀ O ₄
Delta-9-tetrahydrocannabinolic acid (Delta-9-THCA)	107	Delta-9-Tetrahydrocannabinolic Acid	98523	C ₂₂ H ₃₀ O ₄
	108	Delta-9- Tetrahydrocannabinolic Acid-C4 B	46889976	C ₂₂ H ₃₀ O ₄
	109	Delta-9-Tetrahydrocannabinolic Acid A	620758	C ₂₂ H ₃₀ O ₄
	110	Delta9-Tetrahydrocannabutolicacid	59444388	C ₂₁ H ₂₈ O ₄

Table S2. Predicted active site amino acids for EGFR (1M17), VEGFR-1 (3HNG), and VEGFR-2 (3U6J) as identified by PrankWeb.

Protein	Predicted Active Sites	Chain Name & Residues Number
EGFR (PDB ID: 1M17)	Pocket 1	A_694 A_695 A_699 A_702 A_719 A_721 A_723 A_734 A_735 A_738 A_742 A_751 A_766 A_767 A_768 A_769 A_772 A_773 A_813 A_817 A_818 A_820 A_830 A_831 A_833 A_834 A_851 A_853
	Pocket 1	A_1013 A_1018 A_1019 A_1020 A_1021 A_1022 A_1038 A_1039 A_1040 A_1042 A_1043 A_1045 A_1047 A_1053 A_807 A_874 A_878 A_881 A_882 A_885 A_891 A_892
VEGFR-1 (PDB ID: 3HNG)	Pocket 2	A_1026 A_1029 A_1039 A_1040 A_1041 A_1044 A_1045 A_1050 A_833 A_834 A_841 A_859 A_861 A_878 A_882 A_892 A_907 A_909 A_910 A_911 A_912 A_913 A_915 A_916 A_919
	Pocket 3	A_1026 A_1052 A_1065 A_1091 A_1098 A_1099 A_918 A_922
	Pocket 4	A_1083 A_1100 A_1118 A_1137
VEGFR-2 (PDB ID: 3U6J)	Pocket 1	A_1019 A_1024 A_1025 A_1026 A_1027 A_1028 A_1044 A_1045 A_1046 A_1048 A_1049 A_1053 A_1059 A_1066 A_1067 A_1068 A_868 A_885 A_888 A_889 A_892 A_898 A_899
	Pocket 2	A_1035 A_1045 A_1046 A_1047 A_1050 A_1051 A_840 A_841 A_848 A_866 A_868 A_889 A_899 A_916 A_917 A_918 A_919 A_922 A_923