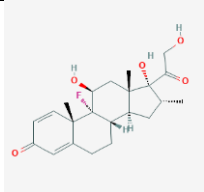
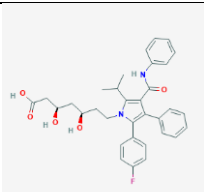
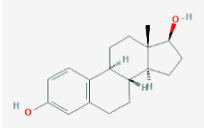
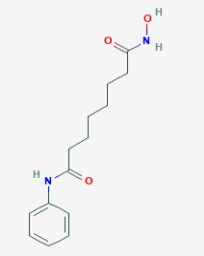
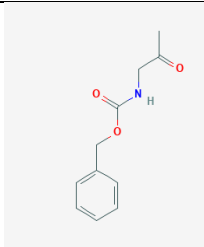
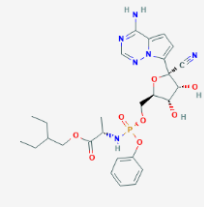
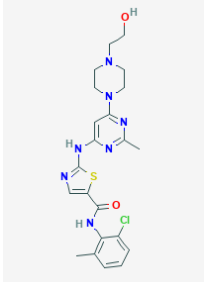
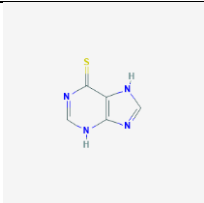
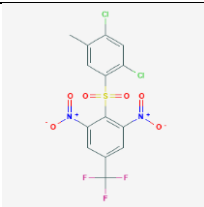
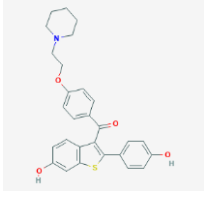
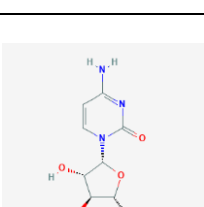
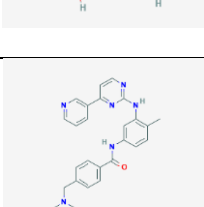
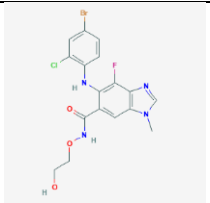
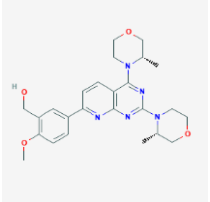
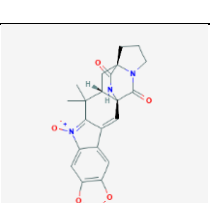
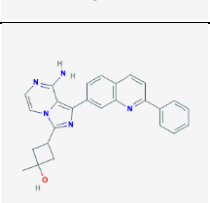
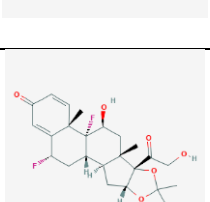
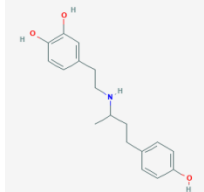
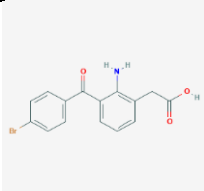
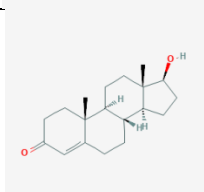
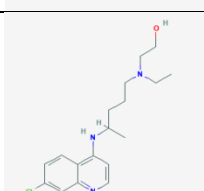


No.	COMPOUND	Max Norm. Rank	List ID	2D STRUCTURE	FORMULA	SMILE	MW	LogP/LogS	CLASSIFICATION	Drugs in clinical trials
1	Dexamethasone	1.00	Tr1 - Series 1-7, TrC1 - Series 1-7, TrC2 - Series 15		C ₂₂ H ₂₉ FO ₅	CC1CC2C3CCC4=C(C(=O)C=CC4(C3(C(C2(C1(C(=O)CO)O)C)O)F)C	392.5	1.93/-3.89	<u>MeSH</u> : Anti-inflammatory; Corticosteroid <u>TBC</u> : Steroid Hormone Receptor Agonist <u>Chem</u> : Steroid	Clinical Trials: 26 NCTs: NCT04325061, NCT04513184, NCT04509973, NCT04499313, NCT04395105, NCT04347980, NCT04344730, NCT04360876, NCT04452565, NCT04519385, NCT04327401, NCT04445506, NCT04476979, NCT04528329, NCT04366115, NCT04468646, NCT04445337, NCT04475991, NCT04461925, NCT04425863, NCT04402840, NCT04492501, NCT04381936, NCT04380818, NCT04462367, NCT04278404
2	Atorvastatin	1.00	Tr2 - Series 15		C ₃₃ H ₃₅ FN ₂ O ₅	CC(C)C1=C(C(=C(N1CCC(CC(CC(=O)O)O)O)C2=CC=C(C=C2)F)C3=CC=CC=C3)C(=O)NC4=CC=C(C=C4	558.6	4.24/-5.95	<u>MeSH</u> : Anticholesteremic <u>TBC</u> : Cholesterol synthesis Inhibitor <u>Chem</u> : Pyrrole	Clinical Trials: 4 NCTs: NCT04380402, NCT04486508, NCT04466241, NCT04333407
3	Beta-estradiol	1.00	TrC4 - PBMC		C ₁₈ H ₂₄ O ₂	CC12CCC3C(C1CC2O)CCC4=C3C=C(C(=C4)O	272.4	3.57/-4.11	<u>MeSH</u> : Estrogen (MeSH) <u>TBC</u> : Estrogen receptor agonist <u>Chem</u> : Steroid	Clinical Trial: 1 NCTs: NCT04359329
4	Vorinostat	1.00	Tr3 - BALF		C ₁₄ H ₂₀ N ₂ O ₃	C1=CC=C(C=C1)NC(=O)CCCCC(=O)NO	264.32	1.88/-3.57	<u>MeSH</u> : Antineoplastic <u>TBC</u> : Histone deacetylase inhibitor <u>Chem</u> : Anilide	

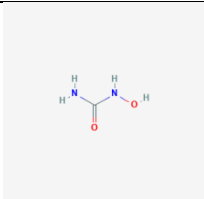
10	Benzyl (2-oxopropyl) carbamate	1.00	HPAV, TaxAV		C ₁₁ H ₁₃ NO ₃	CC(=O)CNC(=O)OC1=CC=CC=C1	207.23	0.89/-2.72	<i>MeSH</i> : - <i>TBC</i> : SARS-CoV replicase polyprotein 1ab inhibitor; 3 clpro protease inhibitor <i>Chem</i> : Benzyloxycarbonyl; Ketone	
11	Remdesivir	1.00	TaxAV, HPAV		C ₂₇ H ₃₅ N ₆ O ₈ P	CCC(CC)COC(=O)C(C)NP(=O)(OCC1C(C(C(O1)(C#N)C2=CC=C3N2N=CN=C3N)O)OC4=CC=CC=C4	602.6	2.20/-3.25	<i>MeSH</i> : Antiviral <i>TBC</i> : Adenine nucleotide analogue <i>Chem</i> : Aromatic amine	Clinical Trials: 48 NCTs: NCT04365725, NCT04431453, NCT04410354, NCT04252664, NCT04292899, NCT04292730, NCT04409262, NCT04501952, NCT04257656, NCT04345419, NCT04323761, NCT04401579, NCT04492475, NCT04280705, NCT04330690, NCT04321616, NCT04488081, NCT04492501, NCT04302766, NCT04315948, NCT04501978, NCT04519424, NCT04405310, NCT04370262, NCT04523831, NCT04359095, NCT04373044, NCT04482699, NCT04365764, NCT04356417, NCT04401475, NCT04386447, NCT04359901, NCT04403477, NCT04359667, NCT04395170, NCT04429529, NCT04361461, NCT04480333, NCT04345614, NCT04349410, NCT04374071, NCT04335123, NCT04404608, NCT04351503, NCT04514627, NCT04334460, NCT04278404
12	Dasatinib	0.95	Tr1 - Series 1-7, Tr3 - BALF		C ₂₂ H ₂₆ ClN ₇ O ₂ S	CC1=C(C(=CC=C1)Cl)NC(=O)C2=CN=C(S2)NC3=CC(=NC(=N3)C)N4CCN(CC4)CCO	488	2.77/-4.58	<i>MeSH</i> : Antineoplastic <i>TBC</i> : Src Tyrosine kinase inhibitor <i>Chem</i> : Aromatic amine; Thiazoles, aminopyrimidine	

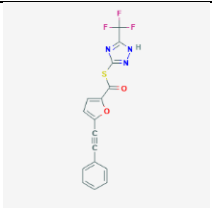
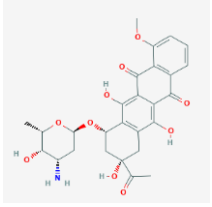
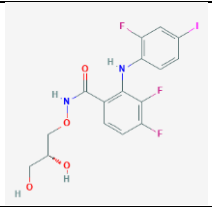
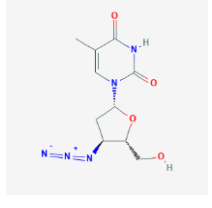
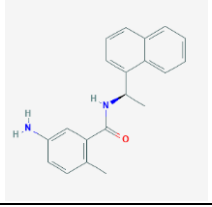
13	Mercaptopurine	0.95	Tr4 - PBMC, GW		C ₅ H ₄ N ₄ S	C1=NC2=C(N1)C(=S)N=CN2	152.18	-0.13/-2.32	<i>MeSH</i> :Antineoplastic;Immunomodulatory agent;Antimetabolite <i>TBC</i> :Purine analogue;Enzyme inhibitor <i>Chem</i> :Sulfhydryl compound;Aryl thiol;Purine analogue	
14	D3F	0.95	HPAV, TaxAV		C ₁₄ H ₇ Cl ₂ F ₃ N ₂ O ₆ S	CC1=CC(=C(C=C1C)Cl)S(=O)(=O)C2=C(C=C(C=C2[N+](=O)[O-]))C(F)(F)F)[N+](=O)[O-]	459.2	3.43/-6.24	<i>MeSH</i> :Enzyme inhibitor <i>TBC</i> : SARS replicase polyprotein 1a inhibitor <i>Chem</i> :Nitrobenzene; Toluene;Trifluoromethylbenzene;	
15	Raloxifene	0.95	TrC1 - Series 1-7		C ₂₈ H ₂₇ NO ₄ S	C1CCN(CC1)CCOC2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)O	473.6	5.45/-5.97	<i>MeSH</i> :Antineoplastic; Bone Density Conservation agent <i>TBC</i> :Hormone;Selective estrogen receptor modulator; Estrogen antagonist <i>Chem</i> : Aromatic cyclic amino compound; Benzylidene.	
16	Cytarabine	0.95	TrC3 - BALF		C ₉ H ₁₃ N ₃ O ₅	C1=CN(C(=O)N=C1N)C2C(C(C(O)C2)O)O	243.22	-2.18/-0.74	<i>MeSH</i> :Antineoplastic; Immunosuppressive; Antimetabolite; Antiviral <i>TBC</i> : Pyrimidine analogue; Tyrosine protein kinase Src inhibitor; protease inhibitor <i>Chem</i> : Heterocycle; Pyrimidine; Arabinonucleoside	
17	Imatinib	0.95	TrC4 - PBMC		C ₂₉ H ₃₁ N ₇ O	CC1=C(C=C(C=C1)NC(=O)C2=CC=C(C=C2)CN3CCN(CC3)C)NC4=NC=CC(=N4)C5=CN=CC=C5	493.6	3.47/-4.53	<i>MeSH</i> :Antineoplastic <i>TBC</i> :Tyrosine kinase inhibitor <i>Chem</i> :Benzamides; Aromatic amine	Clinical Trials: 5 NCTs: NCT04394416, NCT04422678, NCT04346147, NCT04357613, NCT04356495

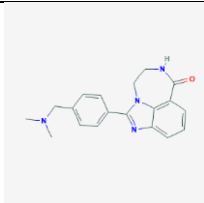
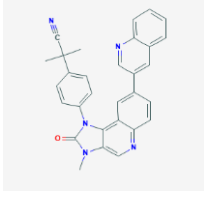
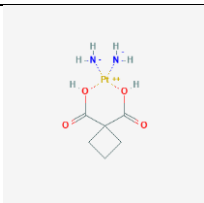
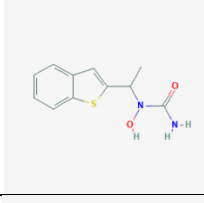
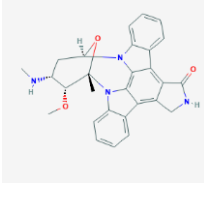
18	Selumetinib	0.89	Tr1 - Series 1-7		C ₁₇ H ₁₅ BrClFN ₄ O ₃	CN1C=NC2=C1C=C(C(=C2F)NC3=C(C=C(C=C3)Br)Cl)C(=O)NOCCO	457.7	3.24/-4.34	<u>MeSH</u> : -Anti-neurofibromatosis type 1 <u>TBC</u> :MAP kinase inhibitor; MEK inhibitor <u>Chem</u> :Secondary amino; Benzimidazole	
19	Azd-8055	0.89	Tr2 - Series 15		C ₂₅ H ₃₁ N ₅ O ₄	CC1COCCN1C2=N C(=NC3=C2C=CC(=N3)C4=CC(=C(C=C4)OC)CO)N5CCOC C5C	465.5	2.87/-3.29	<u>MeSH</u> : Experimental antiproliferative <u>TBC</u> :Phosphatidyl inositol 3' kinase-related kinase inhibitor; Voltage-gated potassium channel ligand; Rapamycin kinase inhibitor <u>Chem</u> : Oxazine; Morpholine	
20	Avrainvillamide-analog-3	0.89	Tr3 - BALF		C ₂₂ H ₂₁ N ₃ O ₅	CC1(C2CC34CCCN3C(=O)C2(C=C5C1=[N+](C6=CC7=C(C=C65)OCO7)[O-]))NC4=O)C	407.4	0.67/-2.79	<u>MeSH</u> :Experimental antiproliferative <u>TBC</u> :Nuclear chaperone nucleophosmin ligand <u>Chem</u> : Alkaloid	
21	Linsitinib	0.89	Tr4 - PBMC		C ₂₆ H ₂₃ N ₅ O	CC1(CC(C1)C2=NC(=C3N2C=CN=C3N)C4=CC5=C(C=C4)C=CC(=N5)C6=CC=CC=C6)O	421.5	4.32/-5.19	<u>MeSH</u> : Antineoplastic <u>TBC</u> : Insulin receptor inhibitor; Insulin-like growth factor-I receptor inhibitor; Type II Receptor tyrosine kinase inhibitor <u>Chem</u> :Pyrazines; Quinoline	
22	Fluocinoloneacetate	0.89	TrC2 - Series 15		C ₂₄ H ₃₀ F ₂ O ₆	CC1(OC2CC3C4CC(C5=CC(=O)C=CC5(C4(C(CC3(C2(O1)C(=O)CO)C)O)F)C)F)C	452.5	2.47/-3.92	<u>MeSH</u> : Anti-inflammatory <u>TBC</u> : Steroid Hormone Receptor Agonist <u>Chem</u> :Steroid; Alcohol; Ketone	Structurally similar in clinical trials: Budesonide

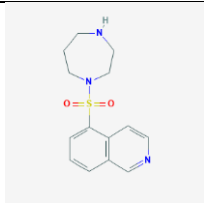
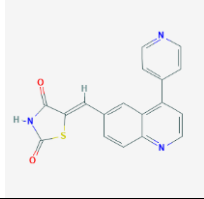
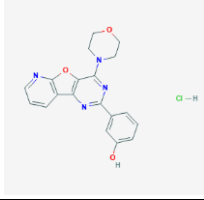
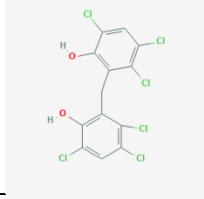
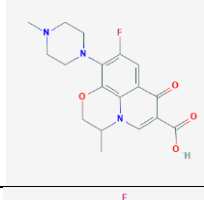
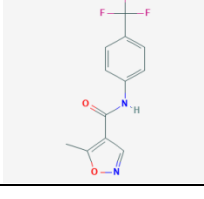
23	Dobutamine	0.89	TrC3 - BALF		C ₁₈ H ₂₃ NO ₃	CC(CCC1=CC=C(C=C1)O)NCCC2=CC(=C(C=C2)O)O	301.4	2.97/-4.34	<i>MeSH</i> : Sympathomimetic; Cardiac stimulant <i>TBC</i> : Adrenergic beta-1 Receptor Agonist <i>Chem</i> : Catecholamine; secondary amine	
24	Bromfenac	0.89	TrC4 - PBMC		C ₁₅ H ₁₂ BrNO ₃	C1=CC(=C(C=C1)C(=O)C2=CC=C(C=C2)Br)N)CC(=O)O	334.16	3.00/-4.42	<i>MeSH</i> : NSAID <i>TBC</i> : COX inhibitor <i>Chem</i> : Ketone; Benzophenones; Aromatic amine; Anilines;	
25	Testosterone	0.89	GW		C ₁₉ H ₂₈ O ₂	CC12CCC3C(C1CC2O)CCC4=CC(=O)CCC34C	288.4	2.99/-3.94	<i>MeSH</i> : Hormone, Androgen, Anabolic <i>TBC</i> : Sex hormone receptor agonist <i>Chem</i> : Steroid; Androgen	Structurally similar in clinical trials: Hydrocortisone
26	Hydroxychloroquine	0.89	HPH		C ₁₈ H ₂₆ ClN ₃ O	CCN(CCCC(C)NC1=C2C=CC(=CC2=N1)C)CCO	335.9	3.87/-4.11	<i>MeSH</i> : Antiparasitic agent, Antimalarial, Antirheumatic agent <i>TBC</i> : Enzyme inhibitor, heme polymerase inhibitor, endosomes modulator, toll-like receptors inhibitor <i>Chem</i> : Aromatic amine; Aminoquinoline	Clinical Trials: 250 NCTs: NCT04328272, NCT04382625, NCT04364815, NCT04358081, NCT04355026, NCT04340544, NCT04365231, NCT04329832, NCT04363866, NCT04361318, NCT04351620, NCT04429867, NCT04329611, NCT04345692, NCT04466540, NCT04385264, NCT04371406, NCT04307693, NCT04333225, NCT04334382, NCT04477083, NCT04349592, NCT04387760, NCT04342221, NCT04331834, NCT04353271, NCT04336332, NCT04374903, NCT04372017, NCT04348474, NCT04394442, NCT04359537, NCT04405921, NCT04315896, NCT04359953, NCT04362332, NCT04347889, NCT04435808, NCT04369742, NCT04323631, NCT04391127, NCT04370782, NCT04522466, NCT04397328, NCT04330586, NCT04329572, NCT04371926, NCT04329923, NCT04392128, NCT04377646, NCT04389359, NCT04341870, NCT04466280, NCT04358068,

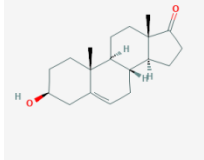
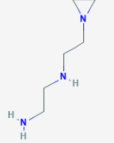
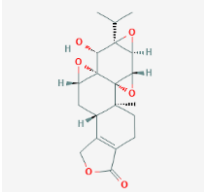
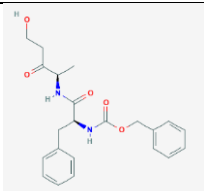
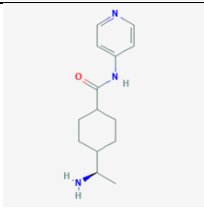
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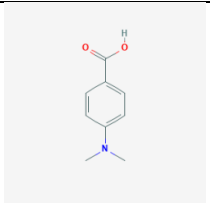
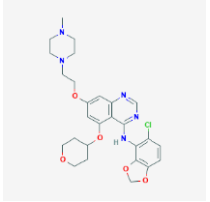
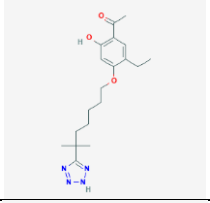
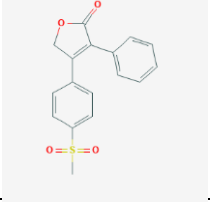
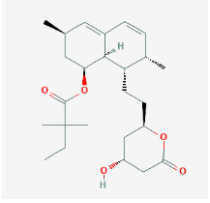
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27	Hydroxyurea	0.89	TrC1 - Series 1-7, TrC3 - BALF		CH ₄ N ₂ O ₂	C(=O)(N)NO	76.05	-1.83/0.55	<p><u>MeSH</u>: Antineoplastic agent, Antimetabolite, Antisickling agent <u>TBC</u>: Nucleic acid synthesis inhibitor; Ribonucleoside-diphosphate reductase inhibitor <u>Chem</u>: Urea</p>

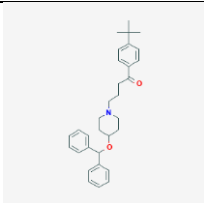
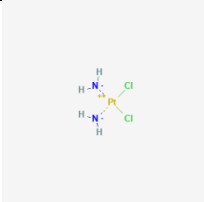
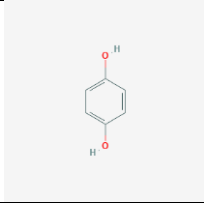
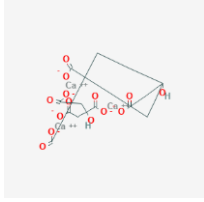
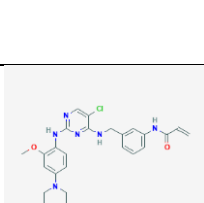
28	F3F	0.89	HPAV, TaxAV		C ₁₆ H ₈ F ₃ N ₃ O ₂ S	C1=CC=C(C=C1)C# CC2=CC=C(O2)C(=O) SC3=NNC(=N3) C(F)(F)F	363.3	3.93/-4.16	<u>MeSH</u> :- <u>TBC</u> : SARS-CoV replicase polyprotein 1ab inhibitor <u>Chem</u> : Furan; Triazole	
29	Daunorubicin	0.84	Tr1 - Series 1-7, TrC1 - Series 1-7		C ₂₇ H ₂₉ NO ₁₀	CC1C(C(CC(O1)OC 2CC(CC3=C2C(=C4 C(=C3O)C(=O)C5= C(C4=O)C(=CC=C5)OC)O)(C(=O)C)O) N)O	527.5	1.68/-2.93	<u>MeSH</u> : Antineoplastic; Antibiotic <u>TBC</u> : Topoisomerase II Inhibitor <u>Chem</u> : Aminoglycosides; Anthracyclines; Cyclic ketone, Acenoquinone	
30	PD-0325901	0.84	Tr2 - Series 15, Tr1 - Series 1-7		C ₁₆ H ₁₄ F ₃ I N ₂ O ₄	C1=CC(=C(C=C1)F)NC2=C(C(=CC(=C2 F)F)C(=O)NOCC(C O)O	482.19	2.64/-4.19	<u>MeSH</u> : Experimental antineoplastic <u>TBC</u> : MAPK inhibitor <u>Chem</u> : Benzamide	
31	Zidovudine	0.84	TrC2 - Series 15, HPAV		C ₁₀ H ₁₃ N ₅ O ₄	CC1=CN(C(=O)NC 1=O)C2CC(C(O2)C O)N=[N+]=[N-]	267.24	-0.10/-1.21	<u>MeSH</u> : Antiviral agent, Antimetabolite <u>TBC</u> : Nucleoside and Nucleotide Reverse Transcriptase Inhibitor <u>Chem</u> : Glycoside; Pyrimidine; Dideoxynucleosides	
32	GRL0617	0.84	HPAV, TaxAV		C ₂₀ H ₂₀ N ₂ O	CC1=C(C=C(C=C1) N)C(=O)NC(C)C2= CC=CC3=CC=CC=C 32	304.4	3.79/-5.73	<u>MeSH</u> :- <u>TBC</u> : SARS-CoV replicase polyprotein 1ab inhibitor <u>Chem</u> : Carboxylic acid nitrile; cyano compound; peptide	

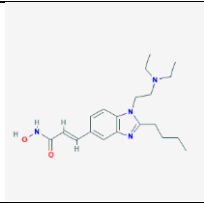
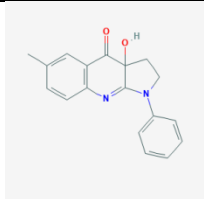
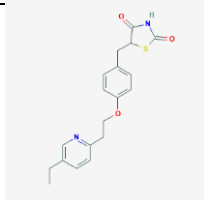
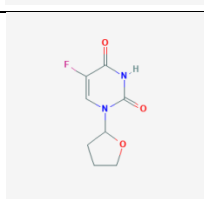
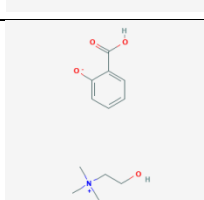
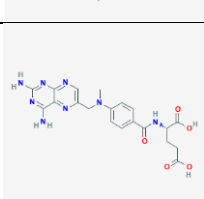
33	AG-14361	0.84	Tr3 - BALF		C ₁₉ H ₂₀ N ₄ O	CN(C)CC1=CC=C(C=C1)C2=NC3=CC=CC4=C3N2CCNC4=O	320.4	2.38/-3.13	<u>MeSH</u> : - <u>TBC</u> : Poly ADP-ribose polymerase 1 inhibitor <u>Chem</u> :Benzodiazepine; Benzimidazole	
34	Dactolisib	0.84	Tr4 - PBMC		C ₃₀ H ₂₃ N ₅ O	CC(C)(C#N)C1=CC=C(C=C1)N2C3=C4C=C(C=CC4=NC=C3N(C2=O)C)C5=CC6=CC=CC=C6N=C5	469.5	4.65/-4.92	<u>MeSH</u> : Antineoplastic <u>TBC</u> : Phosphatidyl inositol 3' kinase-related kinase inhibitor; Lipid modifying kinase inhibitor <u>Chem</u> :Imidazole;Imidazoquinoline	Clinical Trial: 1 NCTs: NCT04409327
35	Carboplatin	0.84	TrC3 - BALF		C ₆ H ₁₂ N ₂ O ₄ Pt	C1CC(C1)(C(=O)O)C(=O)O.[NH2-].[NH2-].[Pt+2]	371.25	0.04/0.14	<u>MeSH</u> : Antineoplastic <u>TBC</u> :Aquation agent <u>Chem</u> : Coordination Complex; Platinum compound	
36	Zileuton	0.84	TrC4 - PBMC		C ₁₁ H ₁₂ N ₂ O ₂ S	CC(C1=CC2=CC=C(C=C2S1)N(C(=O)N)O	236.29	2.01/-3.64	<u>MeSH</u> : NSAID <u>TBC</u> : Leukotriene antagonist; Lipoxygenase Inhibitor <u>Chem</u> :Urea; Benzothiophene	
37	Staurosporine	0.84	GW		C ₂₈ H ₂₆ N ₄ O ₃	CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)NC)OC	466.5	3.14/-4.03	<u>MeSH</u> : Multi-enzyme inhibitor <u>TBC</u> : Protein kinase C inhibitor; CAMK2 inhibitor; Death-associated kinase inhibitor; Phosphorylase kinase inhibitor; Tyrosine-(Y)-phosphorylation regulated kinase inhibitor; Acetylcholine receptor ligand <u>Chem</u> : Indole; indolocarbazole alkaloid	

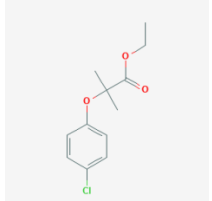
38	Fasudil	0.79	Tr2 - Series 15		C ₁₄ H ₁₇ N ₃ O ₂ S	C1CNCCN(C1)S(=O)(=O)C2=CC=CC3=C2C=CN=C3	291.37	0.16/-2.74	<u>MeSH</u> : Peripheral vasodilators <u>TBC</u> : ROCK inhibitor; DMPK kinase inhibitor; Calcium Channel Blocker <u>Chem</u> : Sulfonamides	
39	GSK-1059615	0.79	Tr3 - BALF		C ₁₈ H ₁₁ N ₃ O ₂ S	C1=CC2=NC=CC(=C2C=C1C=C3C(=O)NC(=O)S3)C4=CC=NC=C4	333.4	2.71/-4.92	<u>MeSH</u> :- <u>TBC</u> : Enzyme inhibitor, PI3K inhibitor <u>Chem</u> : Pyridine; quinoline; thiazolidinone	
40	Pi 103 hydrochloride	0.79	Tr4 - PBMC		C ₁₉ H ₁₇ ClN ₄ O ₃	C1COCCN1C2=NC(=NC3=C2OC4=C3C=CC=N4)C5=CC(=CC=C5)O.Cl	384.8	3.23/-3.10	<u>MeSH</u> : - <u>TBC</u> : AGC protein kinase inhibitor; PKC inhibitor; CMGC protein kinase inhibitor; tyrosine protein kinase inhibitor <u>Chem</u> : Pyrimidine	
41	Hexachlorophene	0.79	TrC1 - Series 1-7		C ₁₃ H ₆ Cl ₆ O ₂	C1=C(C(=C(C(=C1C)Cl)Cl)CC2=C(C(=CC(=C2Cl)Cl)Cl)O)Cl	406.9	6.77/-5.97	<u>MeSH</u> : Anti-infective agent, Antiseptic <u>TBC</u> : - <u>Chem</u> : Chlorobenzene; Chlorophenol	
42	Ofloxacin	0.79	TrC2 - Series 15		C ₁₈ H ₂₀ F ₃ N ₄ O ₄	CC1COC2=C3N1C=C(C(=O)C3=CC(=C2N4CCN(CC4)C)F)C(=O)O	361.4	-0.02/-2.40	<u>MeSH</u> : Antibacterial; Antineoplastic <u>TBC</u> : Topoisomerase IV inhibitor <u>Chem</u> : Aromatic amine; N-arylpiperazine; quinolone	Clinical Trial: 1 NCTs: NCT02735707
43	Leflunomide	0.79	TrC3 - BALF		C ₁₂ H ₉ F ₃ N ₂ O ₂	CC1=C(C(=NO1)C(=O)NC2=CC=C(C=C2)C(F)(F)F)	270.21	2.52/-3.51	<u>MeSH</u> : Antirheumatic agent <u>TBC</u> : Nucleoside synthesis inhibitor; oxidoreductase inhibitor <u>Chem</u> : Isoxazole	Clinical Trials: 2 NCTs: NCT04361214, NCT04434118

44	Prasterone	0.79	GW		C ₁₉ H ₂₈ O ₂	CC12CCC3C(C1CC2=O)CC=C4C3(CC(C4)O)C	288.4	3.53/-3.82	<i>MeSH</i> : Anabolic steroid, hormone <i>TBC</i> : Estrogen receptor agonist; androgen receptor agonist; GABA _A antagonist, NMDA agonist <i>Chem</i> : Steroid
45	N-(2-aminoethyl)-1-aziridineethanamine	0.79	HPH		C ₆ H ₁₅ N ₃	C1CN1CCNCCN	129.2	-1.36/0.49	<i>MeSH</i> : Experimental antiviral agent <i>TBC</i> : ACE2 inhibitor <i>Chem</i> : Aziridine
46	Triptolide	0.79	Tr1 - Series 1-7		C ₂₀ H ₂₄ O ₆	CC(C)C12C(O1)C3C4(O3)C5(CCC6=C(C5CC7C4(C2O)O7)COC6=O)C	360.4	1.22/-2.61	<i>MeSH</i> : Antineoplastic alkylating agent; antispermatogenic agent; immunosuppressive agent, <i>TBC</i> : Multiprotein inhibitor <i>Chem</i> : Terpene; phenanthrenes; diterpenes; diterpenoid
47	WR1	0.79	HPAV, TaxAV		C ₂₂ H ₂₆ N ₂ O ₅	CC(C(=O)CCO)NC(=O)C(CC1=CC=CC=C1)NC(=O)OCC2=CC=CC=C2	398.5	1.55/-4.44	<i>MeSH</i> : - <i>TBC</i> : Inhibitor for the Major Protease of the SARS Coronavirus <i>Chem</i> : Benzyloxycarbonyl; benzyloxycarbonyl
48	Y-27632	0.74	Tr1 - Series 1-7		C ₁₄ H ₂₁ N ₃ O	CC(C1CCC(CC1)C(=O)NC2=CC=NC=C2)N	247.34	1.00/-2.65	<i>MeSH</i> : Neuromuscular; muscle relaxant; antihypertensive agent; Enzyme inhibitor <i>TBC</i> : Rho kinase inhibitor, protein kinase N inhibitor. <i>Chem</i> : Pyridine; aromatic amide

49	DG8735000	0.74	HPAV, TaxAV		C ₉ H ₁₁ NO ₂	CN(C)C1=CC=C(C=C1)C(=O)O	165.19	1.51/-1.29	<i>MeSH:</i> - <i>TBC:</i> Inhibitor of ultraviolet mediated damage <i>Chem:</i> Aminobenzoate	
50	Saracatinib	0.74	Tr3 - BALF		C ₂₇ H ₃₂ ClN ₅ O ₅	CN1CCN(CC1)CCO C2=CC3=C(C(=C2)OC4CCOCC4)C(=N C=N3)NC5=C(C=C C6=C5OCO6)Cl	542	3.53/-3.76	<i>MeSH:</i> Antineoplastic agent; enzyme inhibitor <i>TBC:</i> Src inhibitor; tyrosine kinase inhibitor <i>Chem:</i> Benzodioxoles; quinazoline	
51	LY-255283	0.74	Tr4 - PBMC		C ₁₉ H ₂₈ N ₄ O ₃	CCC1=CC(=C(C=C1)OCCCCC(C)(C)C2=NNN=N2)O)C(=O)C	360.5	4.55/-3.95	<i>MeSH:</i> Antiasthmatic agent <i>TBC:</i> Leukotriene Antagonists <i>Chem:</i> Tetrazoles; aromatic ketone	
52	Rofecoxib	0.74	TrC1 - Series 1-7		C ₁₇ H ₁₄ O ₄ S	CS(=O)(=O)C1=CC=C(C=C1)C2=C(C(=O)OC2)C3=CC=CC=C3	314.4	2.32/-4.47	<i>MeSH:</i> NSAID; Analgesic non-narcotic agent <i>TBC:</i> COX2 inhibitor <i>Chem:</i> Lactone; furan; butanolide	
53	Simvastatin	0.74	GW		C ₂₅ H ₃₈ O ₅	CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC3CC(C(=O)O3)O)C	418.6	4.51/-4.53	<i>MeSH:</i> Antimetabolite; anticholesteremic; hypolipidemic <i>TBC:</i> Hydroxymethylglutaryl-CoA Reductase Inhibitor <i>Chem:</i> Polycyclic aromatic; naphthalene; fatty acid ester	Clinical Trials: 4 NCTs: NCT04343001, NCT04348695, NCT04407273, NCT02735707

54	ebastine	0.74	TrC2 - Series 15		C ₃₂ H ₃₉ NO ₂	CC(C)(C)C1=CC=C(C=C1)C(=O)CCCN2CCC(CC2)OC(C3=CC=CC=C3)C4=CC=CC=C4	469.7	6.89/-6.86	<i>MeSH:</i> Antihistamine <i>TBC:</i> H1 antagonist <i>Chem:</i> Piperidine; ketone, butyrophenone
55	Cisplatin	0.74	TrC3 - BALF		H ₄ Cl ₂ N ₂ Pt	[NH ₂].[NH ₂].Cl[Pt+2]Cl	298	0.33/-0.77	<i>MeSH:</i> Antineoplastic; radiation-sensitizing agent <i>TBC:</i> DNA replication inhibition <i>Chem:</i> Platinum compound
56	Hydroquinone	0.74	TrC4 - PBMC		C ₆ H ₆ O ₂	C1=CC(=CC=C1O)O	110.11	0.71/-0.06	<i>MeSH:</i> Antioxidant; radiation-protective agent <i>TBC:</i> Melanin Synthesis Inhibitor; HDAC inhibitor <i>Chem:</i> Phenol; benzenediol
57	Calciumcitrate	0.74	HPH		C ₁₂ H ₁₀ Ca ₃ O ₁₄	C(C(=O)[O-])C(CC(=O)[O-])(C(=O)[O-])O.C(C(=O)[O-])C(CC(=O)[O-])(C(=O)[O-])O.[Ca+2].[Ca+2].[Ca+2]	498.4	0.13/-2.08	<i>MeSH:</i> Anticoagulant <i>TBC:</i> Calcium chelating agent <i>Chem:</i> Tricarboxylic acid derivative
58	JAK3-IN-1	0.68	Tr1 - Series 1-7		C ₂₆ H ₃₀ ClN ₇ O ₂	CN1CCN(CC1)C2=CC(=C(C=C2)NC3=NC=C(C(=N3)NCC4=CC(=CC=C4)NC(=O)C=C)Cl)OC	508	4.54/-4.53	<i>MeSH:</i> - <i>TBC:</i> AGC protein kinase inhibitor; tyrosine kinase inhibitor <i>Chem:</i> Heterocyclic compound

59	Pracinostat	0.68	Tr3 - BALF		C ₂₀ H ₃₀ N ₄ O ₂	CCCCC1=NC2=C(N1CCN(CC)CC)C=CC(=C2)C=CC(=O)NO	358.5	3.98/-4.07	<i>MeSH</i> : Experimental antineoplastic <i>TBC</i> : Histone deacetylase inhibitor <i>Chem</i> : Benzimidazole	
60	Blebbistatin	0.68	Tr4 - PBMC		C ₁₈ H ₁₆ N ₂ O ₂	CC1=CC2=C(C=C1)N=C3C(C2=O)(CCN3C4=CC=CC=C4)O	292.3	2.00/-3.17	<i>MeSH</i> :- <i>TBC</i> : Myosin inhibitor <i>Chem</i> : Tertiary alcohol; ketone; pyrroloquinoline	
61	Pioglitazone	0.68	TrC1 - Series 1-7		C ₁₉ H ₂₀ N ₂ O ₃ S	CCC1=CN=C(C=C1)CCOC2=CC=C(C=C2)CC3C(=O)NC(=O)S3	356.4	3.17/-4.91	<i>MeSH</i> : Hypoglycemic agent (antidiabetic) <i>TBC</i> : Peroxisome proliferator-activated receptor-gamma activator <i>Chem</i> : Azole; thiazole; thiazolidinedione	Clinical Trials: 2 NCTs: NCT04473274, NCT04500639
62	Tegafur	0.68	TrC2 - Series 15		C ₈ H ₉ FN ₂ O ₃	C1CC(OC1)N2C=C(C(=O)NC2=O)F	200.17	-0.09/-1.16	<i>MeSH</i> : Antimetabolite; Antineoplastic; Immunosuppressive <i>TBC</i> : Thymidylate synthase inhibitor <i>Chem</i> : Pyrimidine; fluorouracil	
63	Cholinesalicylate	0.68	HPH		C ₁₂ H ₁₉ NO ₄	C[N+](C)(C)CCO.C1=CC=C(C(=C1)C(=O)O)[O-]	241.28	-0.30/-2.80	<i>MeSH</i> : NSAID, analgesic non-narcotic <i>TBC</i> : COX inhibitor <i>Chem</i> : Acid; benzoate; salicylate, phenol; hydroxybenzoic acid	
64	Methotrexate	0.68	TrC4 - PBMC, TrC1 - Series 1-7		C ₂₀ H ₂₂ N ₈ O ₅	CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O	454.4	-0.91/-3.42	<i>MeSH</i> : Antimetabolite; antineoplastic; abortifacient; immunosuppressive; antirheumatic <i>TBC</i> : Folic acid metabolism inhibitor; nucleic acid synthesis inhibitor	Clinical Trials: 3 NCTs: NCT04352465, NCT04434118, NCT04481633

									<i>Chem:</i> Acid; pterin; aminopterin	
65	Clofibrate	0.68	TrC3 - BALF, TrC2 - Series 15		C ₁₂ H ₁₅ ClO ₃	CCOC(=O)C(C)(C) OC1=CC=C(C=C1) Cl	242.7	3.99/-3.92	<i>MeSH:</i> Hypolipemic; Anticholesteremic <i>TBC:</i> Peroxisome proliferator-activated receptor-gamma inhibitor <i>Chem:</i> Clofibric Acid; ethyl ester	