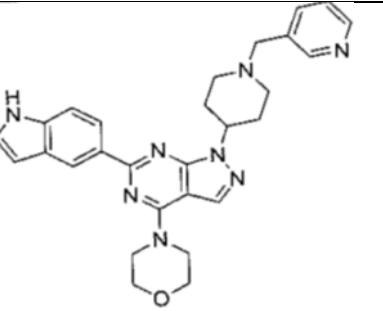
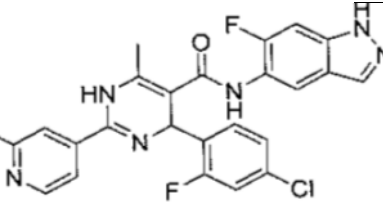
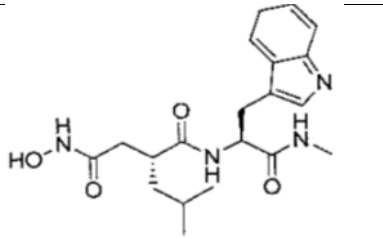
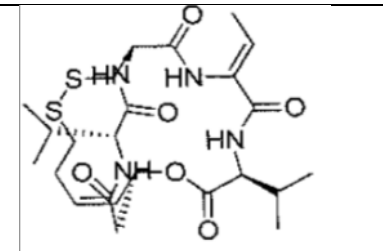
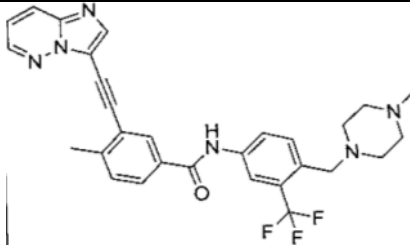
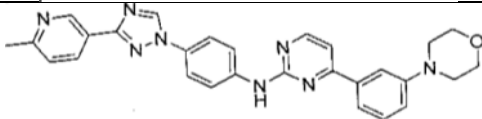
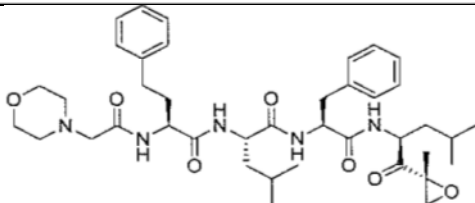
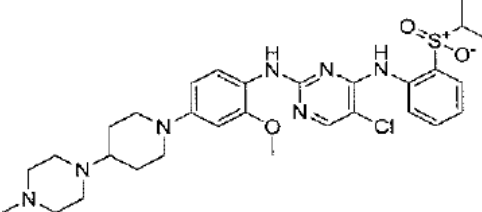
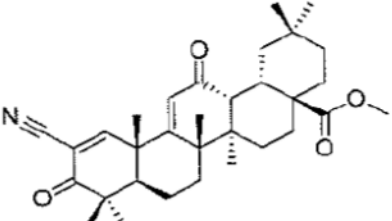


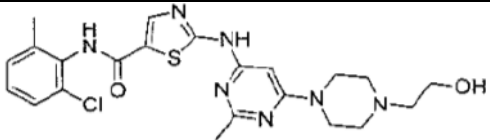
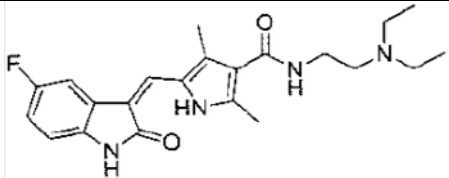
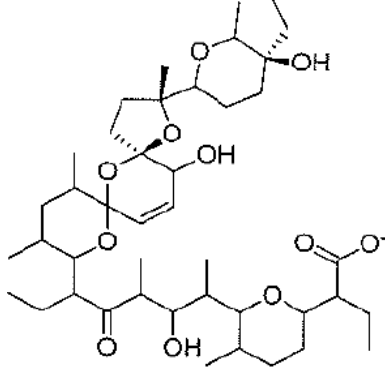
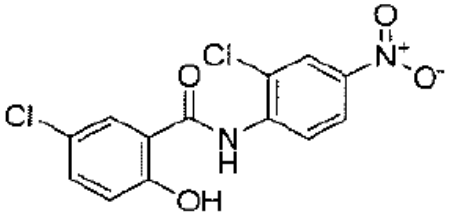
Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00346634-01	WAY-600	mTOR inhibitor	FRAP1	Preclinical	 <p>The chemical structure of WAY-600 is a complex heterocyclic molecule. It features a central pyrazole ring system. One nitrogen of the pyrazole is substituted with a morpholine ring. The other nitrogen is substituted with a 2-pyridylmethyl group. Additionally, there is a 5-indolylmethyl group attached to the pyrazole ring.</p>
NCGC00345842-01	GSK-25	ROCK Inhibitor		Preclinical	 <p>The chemical structure of GSK-25 is a complex heterocyclic molecule. It features a central pyrazole ring system. One nitrogen of the pyrazole is substituted with a 4-chlorophenyl group. The other nitrogen is substituted with a 2-pyridylmethyl group. Additionally, there is a 5-indolylmethyl group attached to the pyrazole ring.</p>
NCGC00345817-01	GM-6001	MMP Inhibitor		Preclinical	 <p>The chemical structure of GM-6001 is a complex heterocyclic molecule. It features a central pyrazole ring system. One nitrogen of the pyrazole is substituted with a 4-chlorophenyl group. The other nitrogen is substituted with a 2-pyridylmethyl group. Additionally, there is a 5-indolylmethyl group attached to the pyrazole ring.</p>
NCGC00263220-02	Romidepsin	Histone Deacetylase (HDAC) Inhibitor		Approved	 <p>The chemical structure of Romidepsin is a complex heterocyclic molecule. It features a central pyrazole ring system. One nitrogen of the pyrazole is substituted with a 4-chlorophenyl group. The other nitrogen is substituted with a 2-pyridylmethyl group. Additionally, there is a 5-indolylmethyl group attached to the pyrazole ring.</p>

Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00263152-02	Ponatinib	FGFR Inhibitor	Bcr-Abl/VEGFR/FGFR/Tie2 Inhibitor	Phase II	 <p>The chemical structure of Ponatinib features a central benzene ring substituted with a morpholine ring, a trifluoromethyl group, and a carbonyl group. This carbonyl group is linked to another benzene ring, which is further substituted with a methyl group and a 1,2,4-triazole ring system.</p>
NCGC00263146-01	SR-3306	JNK 1/2/3 Inhibitor		Preclinical	 <p>The chemical structure of SR-3306 consists of a central benzene ring with a morpholine ring and a pyridine ring attached. This central ring is connected via an amide bond to another benzene ring, which is further substituted with a pyridine ring and a morpholine ring.</p>
NCGC00249613-03	Carfilzomib	Proteasome Inhibitor		phase II	 <p>The chemical structure of Carfilzomib is a complex molecule featuring a central benzene ring with a morpholine ring and a carbonyl group. This carbonyl group is linked to another benzene ring, which is further substituted with a methyl group and a morpholine ring.</p>
NCGC00238453-01	TAE-684	Anaplastic Lymphoma Kinase (ALK) Inhibitor		Preclinical	 <p>The chemical structure of TAE-684 features a central benzene ring with a morpholine ring and a carbonyl group. This carbonyl group is linked to another benzene ring, which is further substituted with a methyl group and a morpholine ring.</p>
NCGC00186460-01	Bardoxolone methyl	NF-kappaB signaling Inhibitor	NF-kappaB activation/Nitric Oxide Production Inhibitor; Glutathione Reductase (NADPH)/Nuclear Factor, Erythroid Derived 2, Like 2 (Nrf2)/Heme Oxygenase Activator; Bcl-2/PPARgamma Agonist	Phase III	 <p>The chemical structure of Bardoxolone methyl is a complex polycyclic molecule with multiple rings, including a benzene ring, a morpholine ring, and a carbonyl group. It also features a nitrile group and a methyl group.</p>

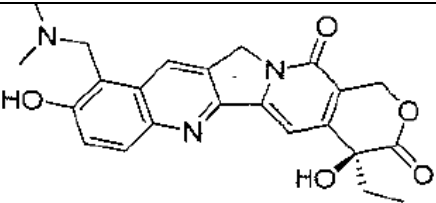
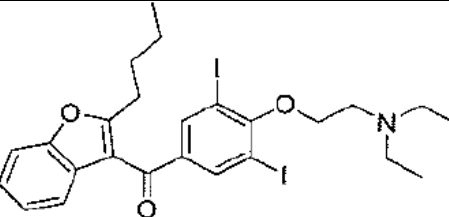
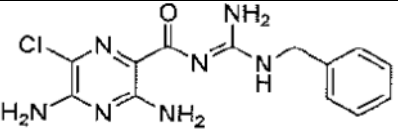
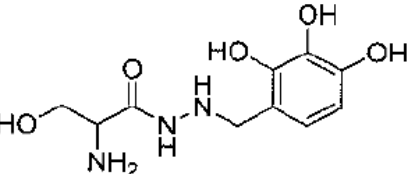
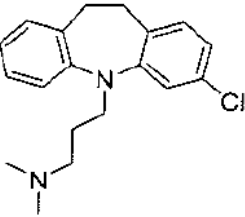
Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00181129-05	Dasatinib	Bcr-Abl inhibitor	BTK/Src inhibitor, multikinase	Approved	
NCGC00164631-03	Sunitinib malate	VEGFR-1/2/3 Inhibitor	CSF1R (c-FMS) Inhibitors Flt3 (FLK2/STK1) Inhibitors KIT (C-KIT) Inhibitors PDGFRbeta Inhibitors RET Inhibitors	Approved	
NCGC00095055-03	Salinomycin	Anticoccidial/Antibacterial		Preclinical	
NCGC00015735-12	Niclosamide	STAT-3 Inhibitor	mTORC Inhibitor, antiparasitic/antiviral	Approved	

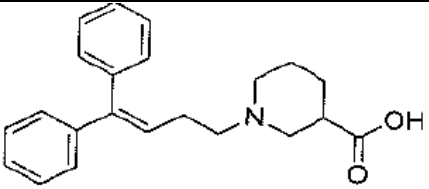
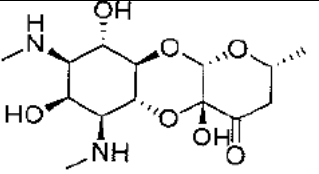
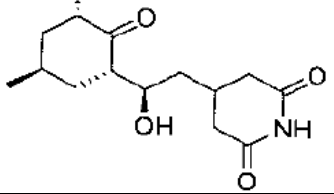
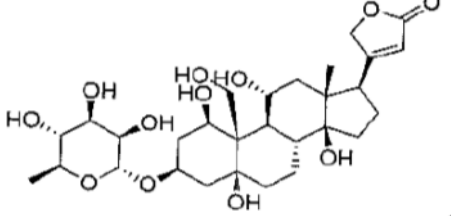
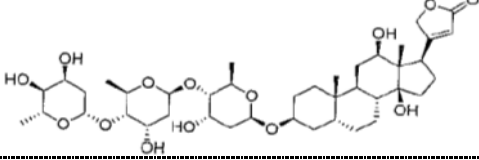
Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00345829-01	PD-173955	cSRC inhibitor	BCR-Abl inhibitor	Preclinical	
NCGC00242514-01	Sepantronium bromide	Survivin inhibitor	BIRC5 Expression Inhibitor	Phase II	
NCGC00013226-15	Trifluoperazine hydrochloride	Nav1.4 (SkM1) Sodium Channel Blockers Nav1.7 (PN1/hNE-Na) Sodium Channel Blockers	Dopamine D2 Antagonists	Approved	
NCGC00014873-04	HLI-373989	MDM2 (hdm2) Inhibitor		Preclinical	

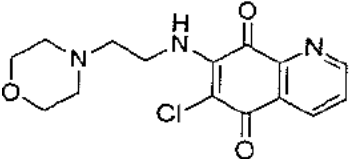
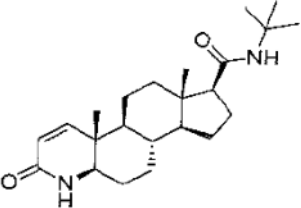
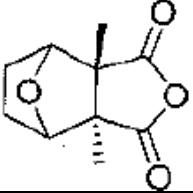
Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00014925-07	Topotecan hydrochloride	DNA Topoisomerase I Inhibitors		Approved	
NCGC00015096-11	Amiodarone hydrochloride	Muscarinic M3 Receptor Ligand	Drugs Acting on Hyperpolarization-activated Cyclic Nucleotide-Gated (HCN) Channels	Approved	
NCGC00015147-09	Benzamil	Epithelial Sodium Channels (ENaC) Blockers	antimalarial agents	Phase II	
NCGC00015163-08	Benserazide	DOPA decarboxylase inhibitor		Approved	
NCGC00015264-08	Clomipramine hydrochloride	Serotonin Transporter (SERT) Inhibitor		Approved	

Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00015977-02	SK&F-89976A	GAT-1 Inhibitor		Preclinical	
NCGC00017354-06	Spectinomycin hydrochloride	Antibiotic		Approved	
NCGC00017363-10	Cycloheximide	Glycogen Synthase Kinase 3 beta (GSK-3beta; tau Protein Kinase I) Inhibitor	tau Protein Kinase I Inhibitor	Approved	
NCGC00017394-08	G-Strophanthin	Na+/K+-ATPase Inhibitors		Preclinical	
NCGC00090797-11	Digoxin	Steroid		Approved	

Supplementary Table 3 continued: Drug list

NCGC ID	Name	Primary Mechanism	Additional Mechanism	Phase	Chemical Structure
NCGC00092289-01	DA-3003-1	Cell Division Cycle CDC25 Phosphatase Inhibitor		Preclinical	
NCGC00093560-06	Finasteride	Androgen Receptor Antagonist	Steroid 5alpha-Reductase Inhibitors	Approved	
NCGC00095145-01	Cantharidin	PP-1 Inhibitors PP-2A Inhibitors		Approved	
NCGC00163489-04	Shikonin	Drugs Acting on Chemokine Receptors	TNF Expression Inhibitors	Preclinical	