

## Supplementary Materials

**Table S1.** List of compounds used in the thermal shift screenings. Note: The following information can be accessed at PubChem database [1]: <http://pubchem.ncbi.nlm.nih.gov>.

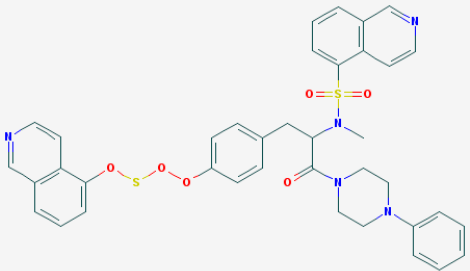
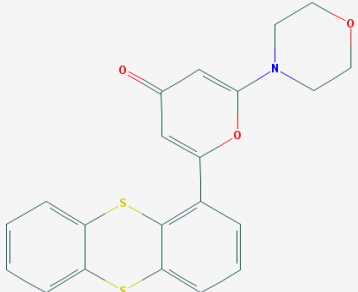
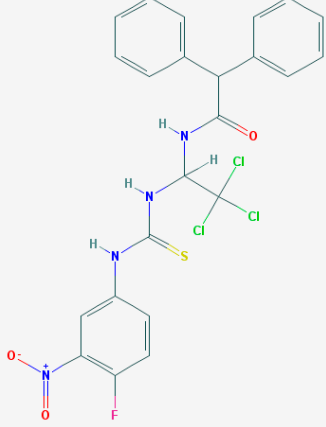
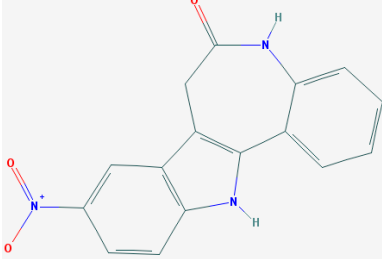
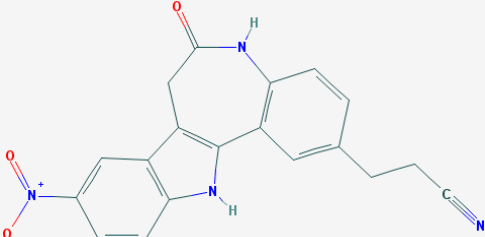
Description	CAS Number	Structure	PubChem Compound ID
KN-62	127191-97-3		16760529
ATM Kinase Inhibitor	587871-26-9		5278396
ATM/ATR Kinase Inhibitor	905973-89-9		6605258
Alsterpaullone	237430-03-4		5005498
Alsterpaullone, 2-Cyanoethyl	852527-97-0		16760286

Table S1. Cont.

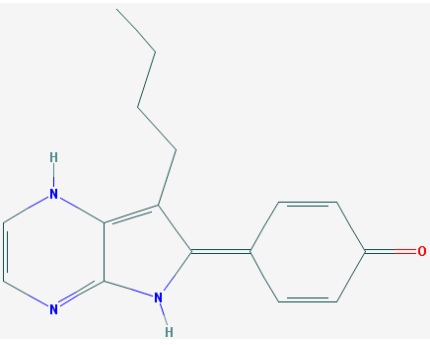
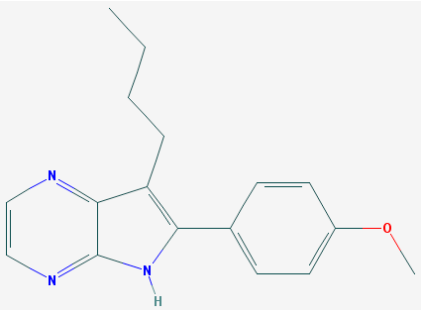
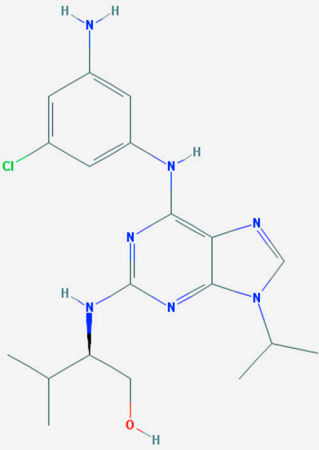
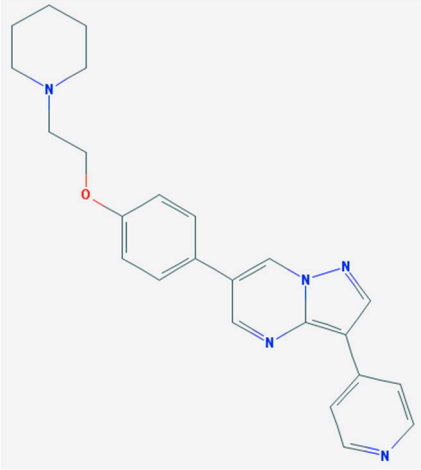
Description	CAS Number	Structure	PubChem Compound ID
Aloisine A, RP107	496864-16-5		5326843
Aloisine, RP106	496864-15-4		3641059
Aminopurvalanol A	220792-57-4		6604931
AMPK Inhibitor, Compound C	866405-64-3		11524144

Table S1. Cont.

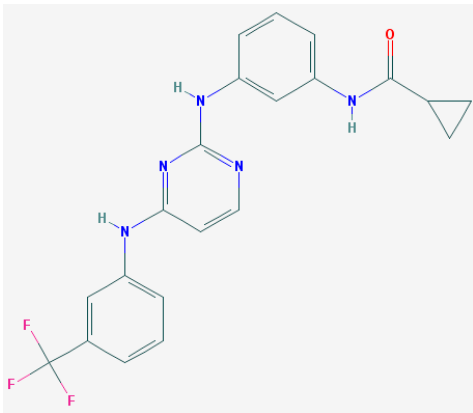
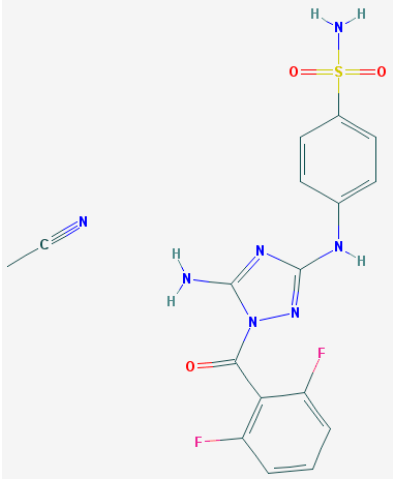
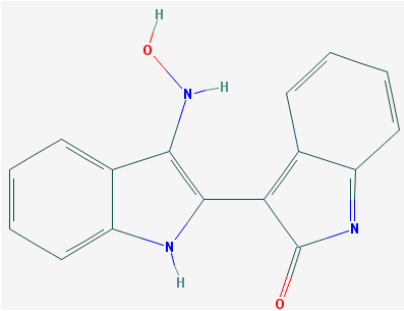
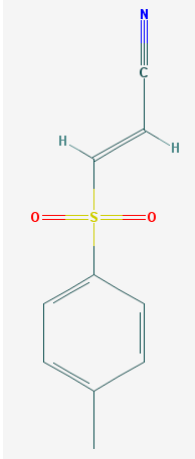
Description	CAS Number	Structure	PubChem Compound ID
Aurora Kinase Inhibitor III	879127-16-9	 <p>The structure shows a central pyrimidine ring. One nitrogen is substituted with a 4-(difluoromethyl)phenyl group. The other nitrogen is substituted with a 4-(cyclopropylcarbamoyl)phenyl group.</p>	9549303
Aurora Kinase/Cdk Inhibitor	443797-96-4	 <p>The structure features a central pyrazole ring. One nitrogen is substituted with a cyano group (-C≡N). The other nitrogen is substituted with a 4-(2,6-difluorophenyl)phenyl group. A sulfonamide group (-SO<sub>2</sub>NH<sub>2</sub>) is attached to the 4-position of the phenyl ring.</p>	16760303
Indirubin-3'-monoxime	160807-49-8	 <p>The structure consists of two indole rings connected at their 2-positions. The 3-position of the right-hand indole ring is substituted with a hydroxyl group (-OH).</p>	5326739
BAY 11-7082	19542-67-7	 <p>The structure shows a central benzene ring. At the 4-position, there is a sulfonamide group (-SO<sub>2</sub>NH<sub>2</sub>). At the 1-position, there is a prop-2-en-1-yl group (-CH=CH<sub>2</sub>).</p>	5353431

Table S1. Cont.

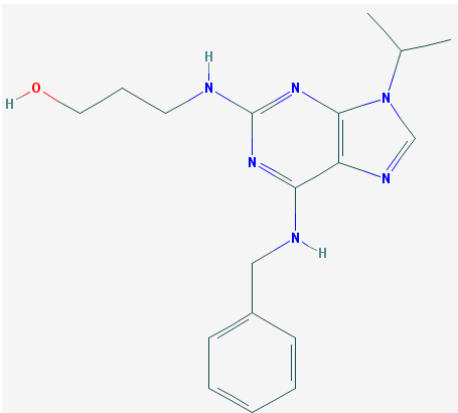
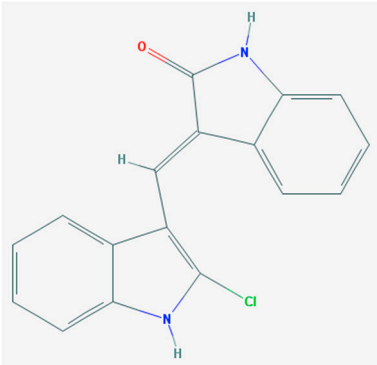
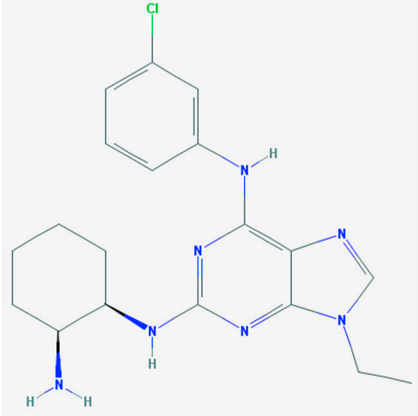
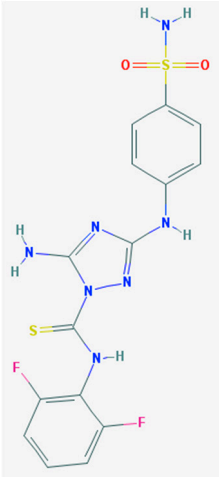
Description	CAS Number	Structure	PubChem Compound ID
Bohemine	189232-42-6		2422
Cdk1 Inhibitor	220749-41-7		5472558
Cdk1 Inhibitor, CGP74514A	190654-01-4		2794188
Cdk1/2 Inhibitor III	443798-55-8		5330812

Table S1. Cont.

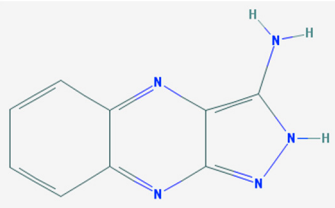
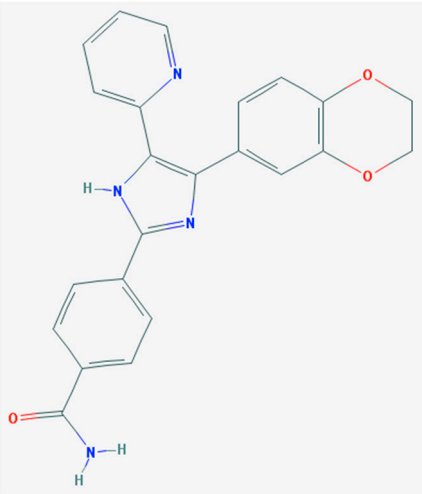
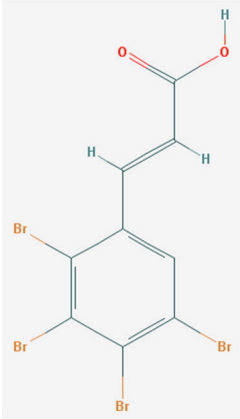
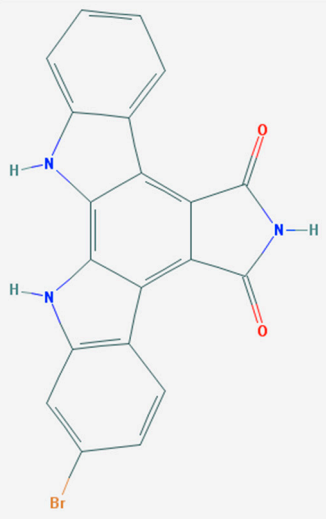
Description	CAS Number	Structure	PubChem Compound ID
Cdk1/5 Inhibitor	40254-90-8		438981
Casein Kinase I Inhibitor, D4476	301836-43-1		6419753
Casein Kinase II Inhibitor III, TBCA	934358-00-6		16760346
Cdk4 Inhibitor	546102-60-7		5330797

Table S1. Cont.

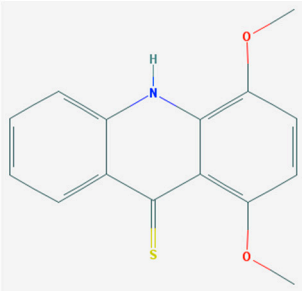
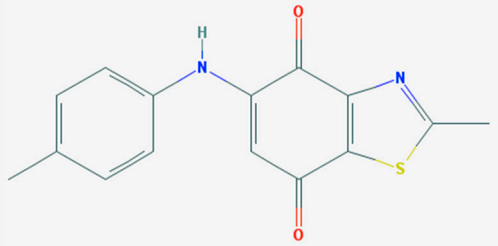
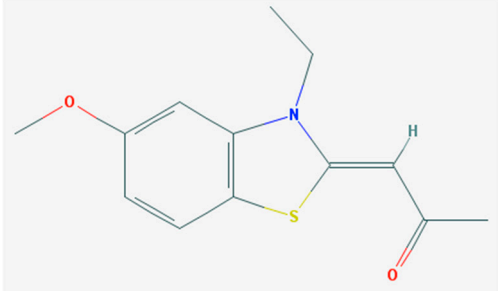
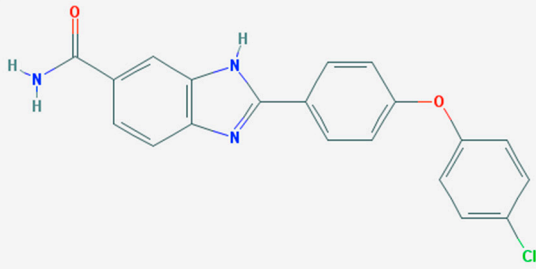
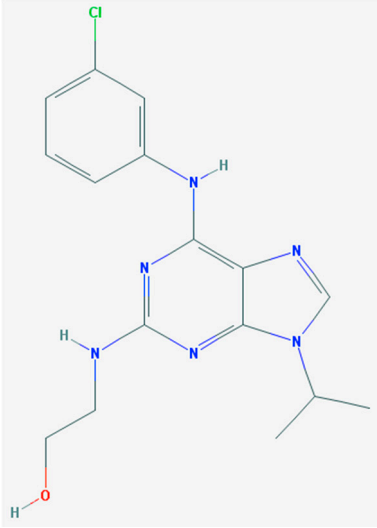
Description	CAS Number	Structure	PubChem Compound ID
Cdk4 Inhibitor II, NSC 625987	141992-47-4		3004085
Cdk4 Inhibitor III	265312-55-8		481747
Cdc2-Like Kinase Inhibitor, TG003	300801-52-9		1893668
Chk2 Inhibitor II	516480-79-8		9969021
Compound 52	212779-48-1		2856

Table S1. Cont.

Description	CAS Number	Structure	PubChem Compound ID
Cdk2 Inhibitor III	199986-75-9		6918386
Cdk2 Inhibitor IV, NU6140	444723-13-1		10202471
Cdk/Crk Inhibitor	784211-09-2		9549301
ERK Inhibitor III			5339183

Table S1. Cont.

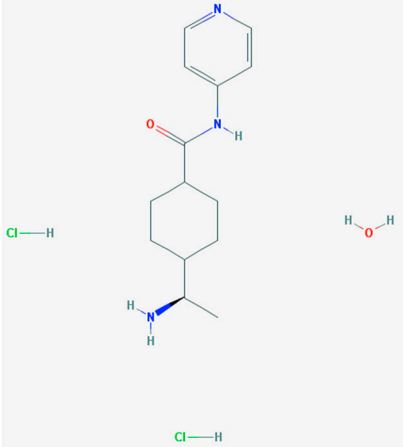
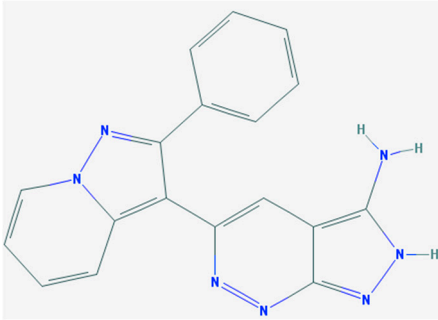
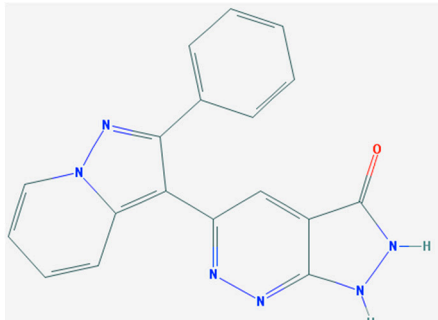
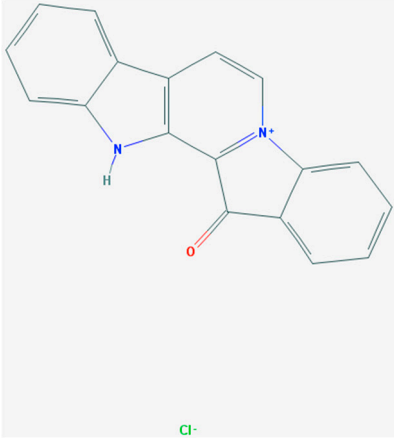
Description	CAS Number	Structure	PubChem Compound ID
ROCK Inhibitor, Y-27632	146986-50-7		9797929
ERK Inhibitor II, FR180204	865362-74-9		11493598
ERK Inhibitor II, Negative control			16760417
Fascaplysin, Synthetic	114719-57-2		73292



Table S1. Cont.

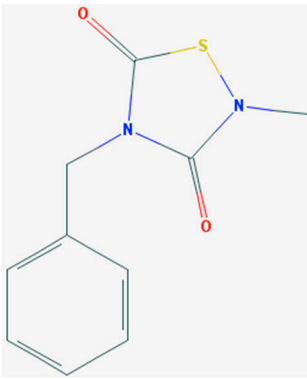
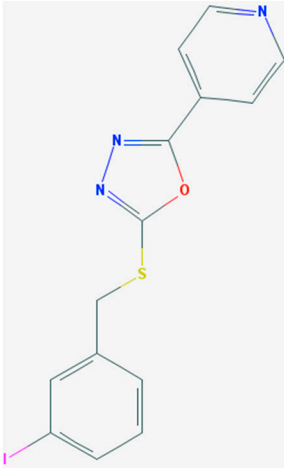
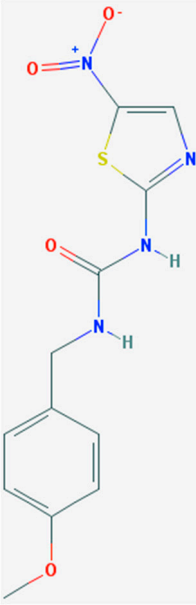
Description	CAS Number	Structure	PubChem Compound ID
GSK-3b Inhibitor I	327036-89-5		4124851
GSK-3b Inhibitor II	478482-75-6		6539732
GSK-3b Inhibitor VIII	487021-52-3		448014

Table S1. Cont.

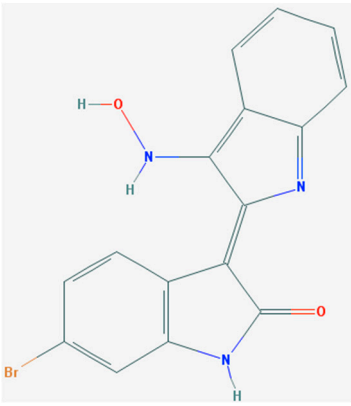
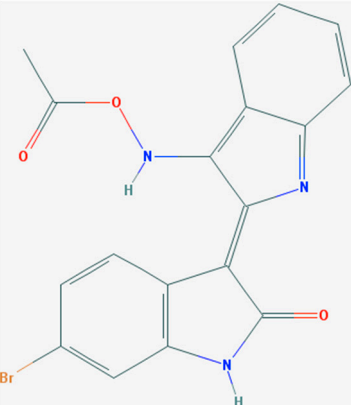
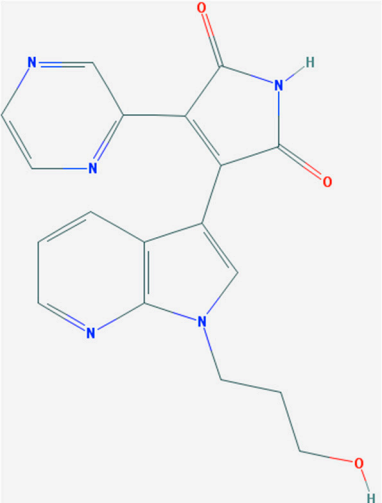
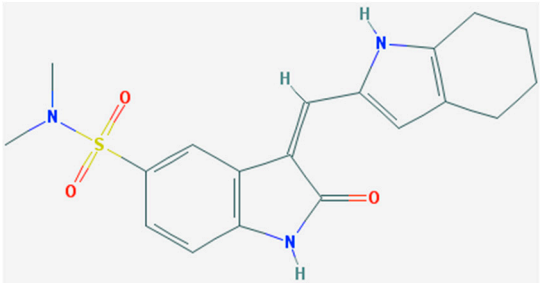
Description	CAS Number	Structure	PubChem Compound ID
GSK-3 Inhibitor IX	667463-62-9		5287844
GSK-3 Inhibitor X	667463-85-6		6538818
GSK-3b Inhibitor XI	626604-39-5		10020713
SU6656	330161-87-0		5312137

Table S1. Cont.

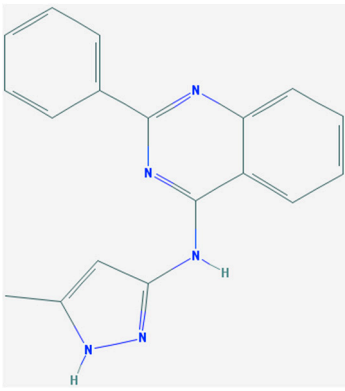
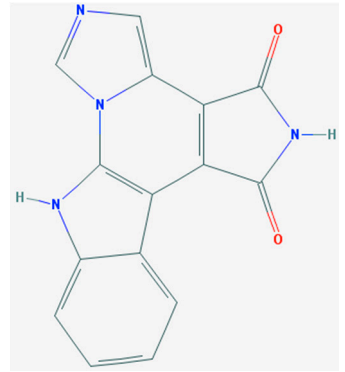
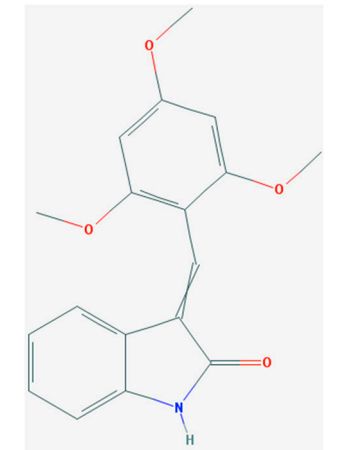
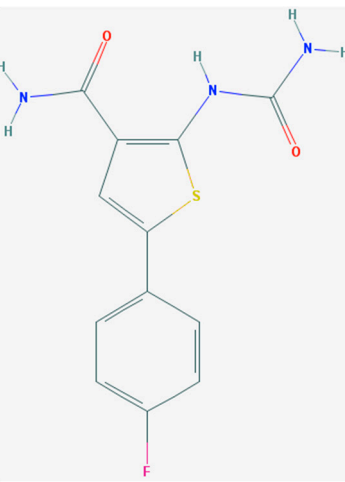
Description	CAS Number	Structure	PubChem Compound ID
GSK-3 Inhibitor XIII	404828-08-6		6419766
Isogranulatimide	244148-46-7		6419741
IC261	186611-52-9		3674
IKK-2 Inhibitor IV	507475-17-4		9903786

Table S1. Cont.

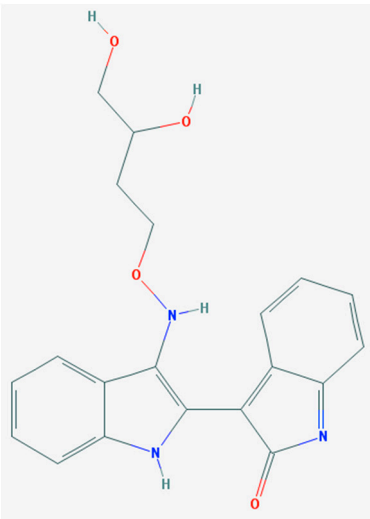
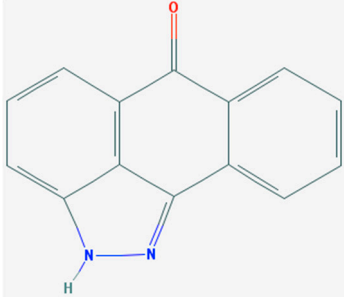
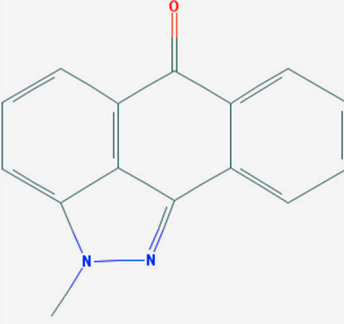
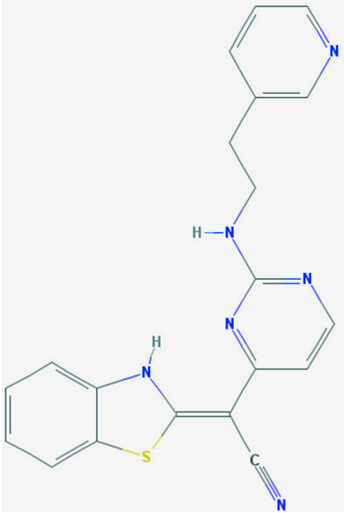
Description	CAS Number	Structure	PubChem Compound ID
Indirubin Derivative E804		 <p>The structure shows a central indole ring system (two fused benzene rings with an NH group) connected at the 3-position to a pyrazole ring. The pyrazole ring has a carbonyl group (=O) at the 4-position and is further substituted at the 5-position with a propyl chain. This propyl chain is linked via an oxygen atom to a secondary amine group (-NH-), which is in turn connected to another propyl chain ending in a hydroxyl group (-OH).</p>	6419764
JNK Inhibitor II	129-56-6	 <p>The structure is a tricyclic indole derivative. It features a central benzene ring fused to two other benzene rings. A pyrazole ring is fused to the central benzene ring, with a hydrogen atom on one of its nitrogens. A carbonyl group (=O) is attached to the central benzene ring.</p>	8515
JNK Inhibitor, Negative Control	54642-23-8	 <p>The structure is a tricyclic indole derivative, similar to JNK Inhibitor II, but with a methyl group (-CH3) attached to the nitrogen atom of the pyrazole ring.</p>	11665831
JNK Inhibitor V	345987-15-7	 <p>The structure features a benzothiazole ring system (a benzene ring fused to a five-membered ring containing one sulfur and one nitrogen atom). This is connected at the 2-position to a pyridine ring. The pyridine ring is further substituted at the 3-position with a propyl chain ending in a secondary amine group (-NH-), which is connected to another pyridine ring.</p>	11422035

Table S1. Cont.

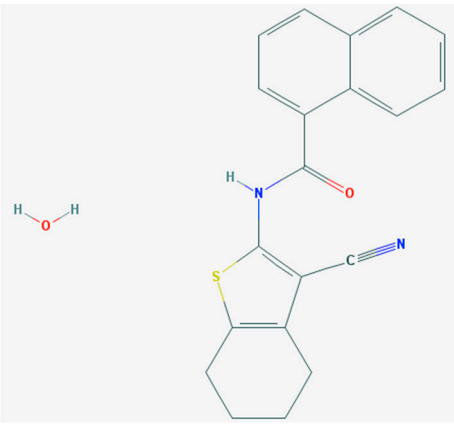
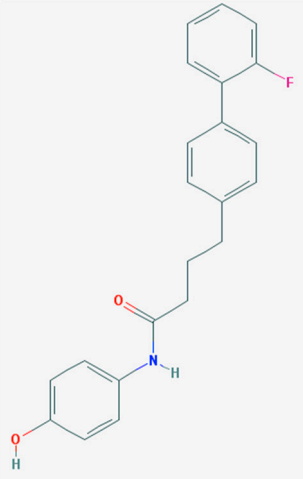
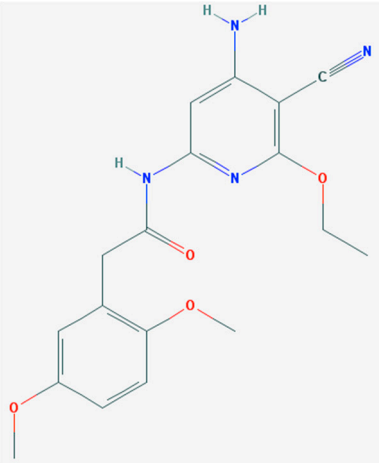
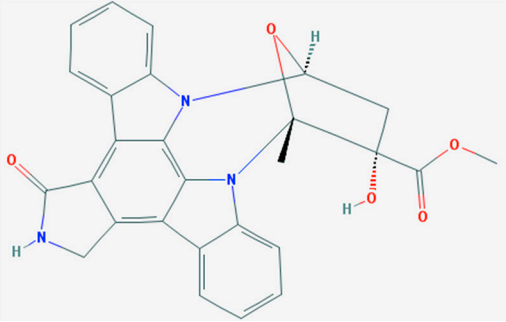
Description	CAS Number	Structure	PubChem Compound ID
JNK Inhibitor IX	312917-14-9	 <p>The structure shows a naphthalene ring system attached to a carbonyl group, which is linked to a nitrogen atom. This nitrogen is part of a five-membered ring containing a sulfur atom. A cyano group (-C≡N) is attached to the same carbon in the five-membered ring. A water molecule (H<sub>2</sub>O) is shown nearby.</p>	16760525
MK2a Inhibitor	41179-33-3	 <p>The structure features a central amide group (-NH-) connecting a 4-hydroxyphenyl ring to a propyl chain. The propyl chain is further connected to a para-substituted benzene ring, which is in turn connected to a 2-fluorophenyl ring.</p>	11382492
JNK Inhibitor VIII	894804-07-0	 <p>The structure consists of a pyridine ring substituted with a cyano group (-C≡N), an ethoxy group (-OCH<sub>2</sub>CH<sub>3</sub>), and a secondary amide group (-NH-). The amide group is linked to a propyl chain, which is attached to a benzene ring. The benzene ring has two methoxy groups (-OCH<sub>3</sub>) at the 3 and 4 positions.</p>	11624601
K-252a, Nocardiosis sp.	97161-97-2	 <p>The structure is a complex polycyclic molecule with multiple nitrogen atoms. It features a central ring system with various substituents, including a methyl group, a hydroxyl group (-OH), and a methoxy group (-OCH<sub>3</sub>).</p>	490561

Table S1. Cont.

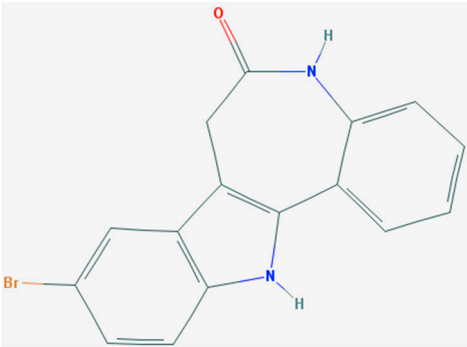
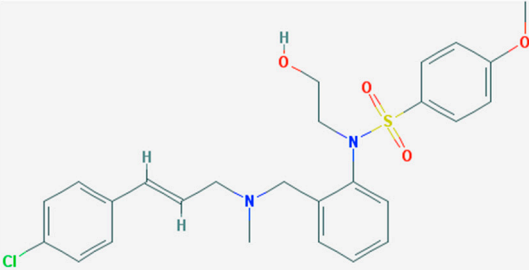
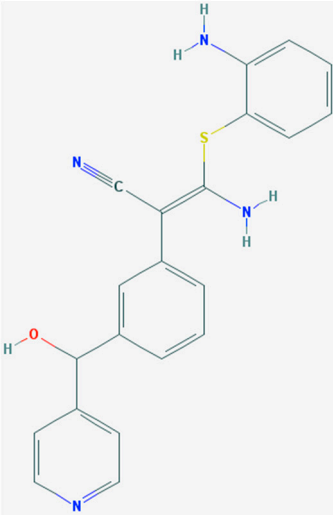
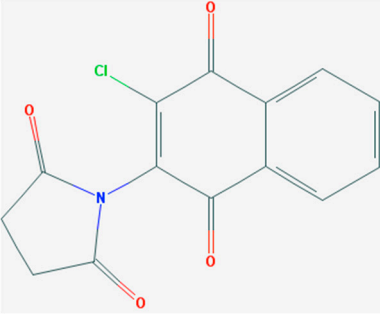
Description	CAS Number	Structure	PubChem Compound ID
Kenpaullone	142273-20-9		3820
KN-93	139298-40-1		5312122
MEK Inhibitor I			9951490
MEK Inhibitor II	623163-52-0		389898

Table S1. Cont.

Description	CAS Number	Structure	PubChem Compound ID
MEK1/2 Inhibitor	305350-87-2		9549284
MNK1 Inhibitor	522629-08-9		11644425
NF-κB Activation Inhibitor	545380-34-5		509554
p38 MAP Kinase Inhibitor III	581098-48-8		6419739

Table S1. Cont.

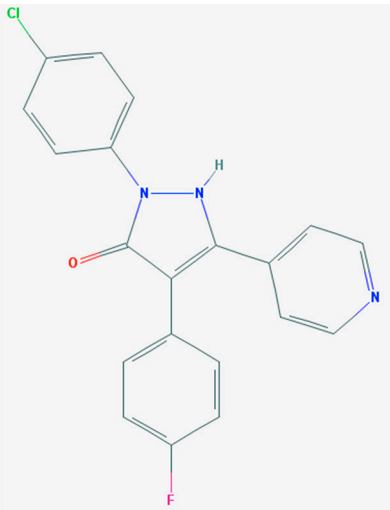
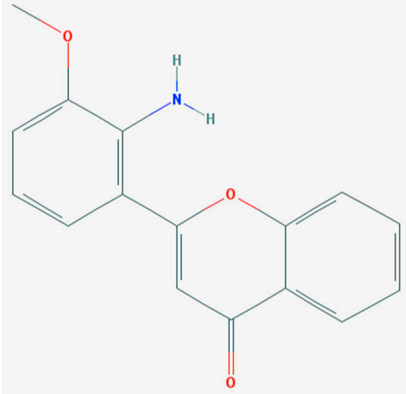
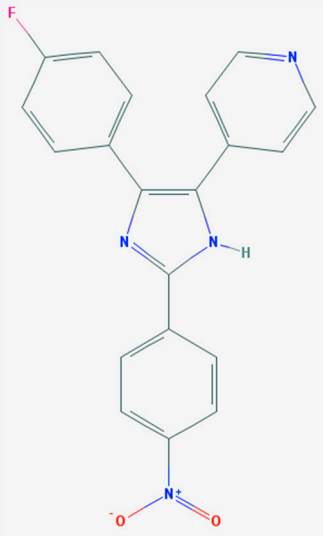
Description	CAS Number	Structure	PubChem Compound ID
p38 MAP Kinase Inhibitor	219138-24-6		4665
PD 98059	167869-21-8		4713
PD 169316	152121-53-4		4712



Table S1. Cont.

Description	CAS Number	Structure	PubChem Compound ID
SB220025	165806-53-1		5164
Purvalanol A	212844-53-6		4987
GSK3b Inhibitor XII, TWS119	601514-19-6		9549289
H-89, Dihydrochloride	127243-85-0		5702541

Table S1. Cont.

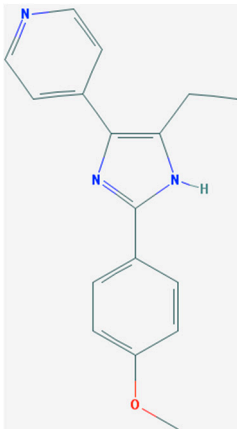
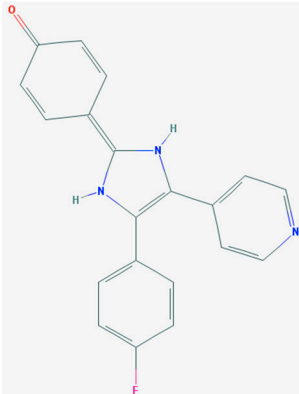
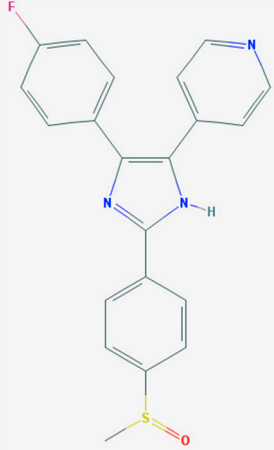
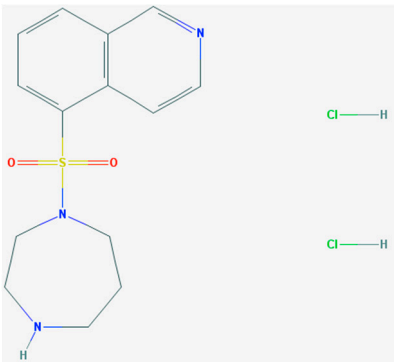
Description	CAS Number	Structure	PubChem Compound ID
SB 202474, Negative control for p38 MAPK inhibition studies	172747-50-1		5162
SB 202190	152121-30-7		5353940
SB 203580	152121-47-6		176155
HA 1077, Dihydrochloride Fasudil	103745-39-7		16219471

Table S1. Cont.

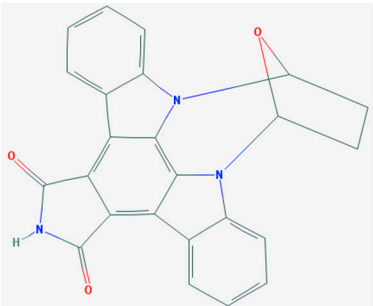
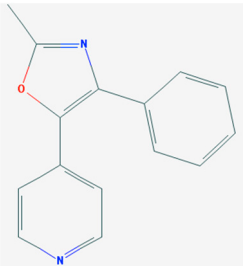
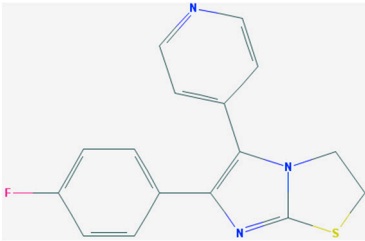
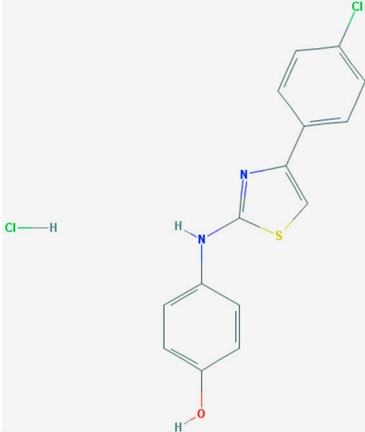
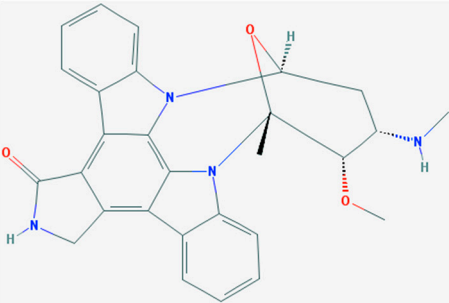
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SB 218078	135897-06-2		3387354
SC-68376	318480-82-9		5174
SKF-86002	72873-74-6		5228
Sphingosine Kinase Inhibitor	1177741-83-1		16760659
Staurosporine, Streptomyces sp.	62996-74-1		451705

Table S1. Cont.

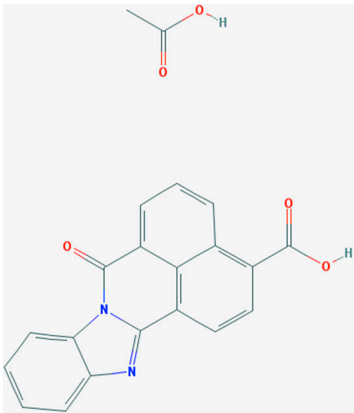
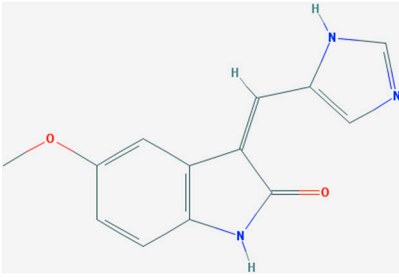
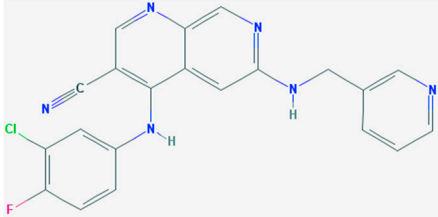
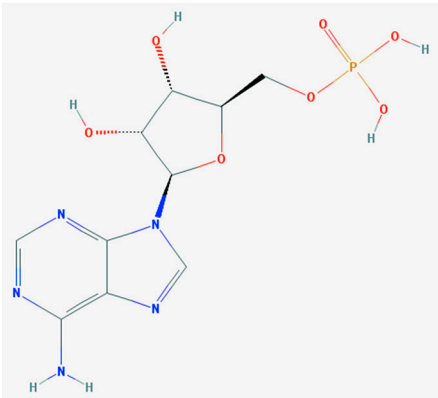
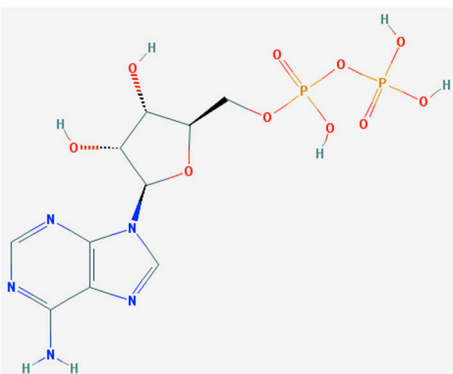
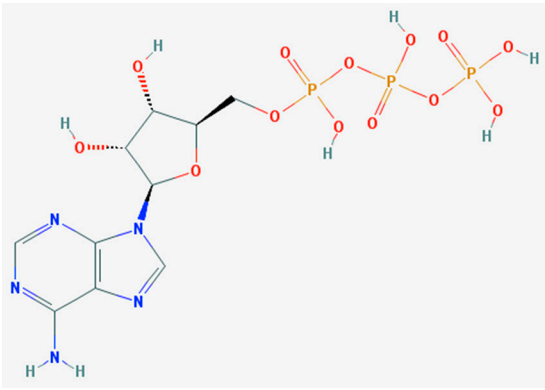
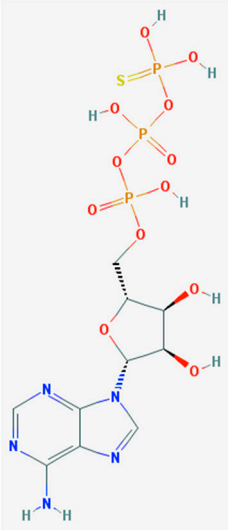
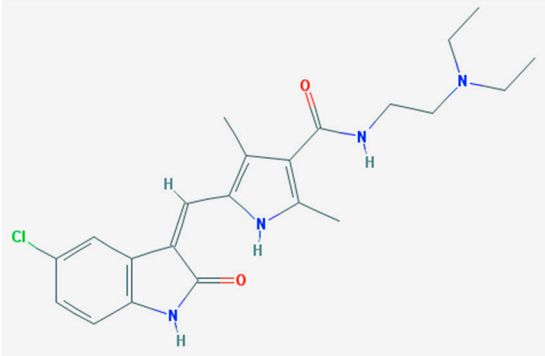
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STO-609	52029-86-4		16760660
SU9516	666837-93-0		5289419
Tpl2 Kinase Inhibitor	871307-18-5		9549300
AMP	61-19-8		6083
ADP	58-64-0		6022

Table S1. Cont.

Description	CAS Number	Structure	PubChem Compound ID
ATP	56-65-5		5957
ATP-gammaS	35094-46-3		440317
SU11652			5329103

## References

1. Bolton, E.; Wang, Y.; Thiessen, P.A.; Bryant, S.H. Chapter 12—PubChem: Integrated Platform of Small Molecules and Biological Activities. *Annu. Rep. Comput. Chem.* **2008**, *4*, 217–241.