structure	mal name	drug like	mutacasia	tumorisonis	roproductive offert	irritant
	mol_name	drug_like	mutagenic	tumorigenic	reproductive_effect	แแนสกับ
CH ₃ N N N N N N N N N N N N N						
ATACAND	ATACAND	-7.1437	none	none	none	none
H ₉ C CH ₃ H ₉ C CH ₃						
TRUVADA	TRUVADA	-25.362	none	none	none	none
N N N N N N N N N N N N N N N N N N N		_				
VALTREX	VALTREX	-20.843	none	none	none	high
H ₃ C CH ₃ HH CH ₃	XENICAL	-15.657	nana	nono	nono	nono
XENICAL	AEINICAL	-13.037	none	none	none	none
HO CH ₃ HO HI H CH ₅ OH HI H CH ₅ N OH H						
MERREM	MERREM	6.4914	none	none	none	none
OH OH						
NASONEX	NASONEX	3.0117	low	high	high	none
H ₂ C HO HO HH	PULMICORT	1.6963	none	none	none	none
PULMICORT	I OLIVICONI	1.0703	HOILE	HOHE	TOTIC	HOHE

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_	1					
CH₃						
H ₂ N						
HIMO						
H ₃ C N H						
H ₃ C H ₃ C	TANAITHI	1 4000	nana			
TAMIFLU	TAMIFLU	-1.4998	none	none	none	none
H ₃ C CH ₃						
HN O						
Н СН3						
H H						
HHO	PROSCAR	2.4066	none	none	none	none
PROSCAR CH ₃						
F 0 5						
CH ₃						
H ₃ C H						
H F O						
FLOVENT	FLOVENT	4.5242	none	none	none	none
сн _з						
OH E MAN ON						
H ₃ C S H N H N						
H H NH O						
	700/41	40.47/				
ZOSYN	ZOSYN	12.176	none	none	none	none
0 😞 🗸 ОН						
CH ₂						
S NH ₂						
o N						
но	OMNICEF	12.271	none	none	none	none
OMNICEF						
H₂N H₃C .H						
N H OH						
S N						
но						
PRIMAXIN	PRIMAXIN	5.3361	none	none	none	none
CH ₃						
N CH ₃						
000						
CH ₃						
H ₃ C H CH ₃	EVELON	1.0/0/	none	none	none	none
EXELON	EXELON	1.9626	none	none	none	none

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YASMIN	YASMIN	-2.8162	none	none	high	none
ne con						
CAMPTOSAR	CAMPTOSAR	-0.35552	none	none	none	none
QH _b	AVANDIA	7.5038	none	none	none	none
AVANDIA	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	7.5500	TIOTIC	TIOTIC	TOTIC	TIOTIC
HO OH N O O O O O O O O O O O O O O O O	AUGMENTIN	2.8065	none	none	none	none
CH ₃ H ₉ C N N - CH ₃ N - CH ₃ N N - CH ₃ N N - CH ₃						
ZANTAC	ZANTAC	-0.50349	none	none	none	none
ON OH N S CH3						
МОВІС	MOBIC	4.9068	none	none	none	none
HO NH2 HO O SYNTHROID	SYNTHROID	-10.339	none	none	none	none

_						
$H_{0}C$ H						
BONIVA	BONIVA	-10.533	none	none	none	none
OH OH O						
FOSAMAX	FOSAMAX	-11.876	none	none	high	none
CH ₃ O CH ₃	ADALAT	4 5500				
ADALAT	ADALAT	-1.5582	none	none	none	none
HN N H	ZELNORM	-2.873	none	none	none	none
ZELNORM						
$\begin{array}{c c} H_3C & H\\ N\\ N\\$	PEPCID	2.1951	high	high	none	none
PEPCID						
CH ₅ CH ₆ N N N N N N N N N N N N N N N N N N N	BENICAR	-5.0226	none	none	none	none
BENICAR	DEINICAK	-3.0220	none	none	none	none
H ₂ C CH ₃ N OH ₃ N H ₄ C CH ₅ N H ₄ C CH ₅ KALETRA	KALETRA	-7.147	none	none	none	none

_						
HO HO OH	LIPITOR	4.4511	none	none	high	none
N Ho Cott		0.4/400				
SINGULAIR	SINGULAIR	-0.16428	none	none	none	none
N N N N N N N N N N N N N N N N N N N						
GLEEVEC	GLEEVEC	8.6128	none	none	none	none
OH OH OH OH	XALATAN	-14.281	none	none	none	none
H _N N OCH ₃ OCH	NORVASC	-7.7862	none	none	none	none
N CH ₃	BLOPRESS	0 17075	none	none	none	none
BLOPRESS	BLOPKESS	-0.17075	none	none	none	none
H ₃ C CH ₃ H ₃ C OH ₃ OH ₈ OH ₉	DIOVAN	-4.2218	none	none	none	none

но						
N N N						
s						
SEROQUEL	SEROQUEL	2.458	none	none	none	low
HN						
H _D C N N N N N N N N N N N N N N N N N N N						
	AMARYL	9.6574	none	none	none	none
AMARYL	71170112	7.037 1	Horic	Horic	Hone	Horic
N N N N N N N N N N N N N N N N N N N						
ABILIFY	ABILIFY	4.0343	none	none	none	none
N N						
H ₃ C O O O O O O						
ACIPHEX	ACIPHEX	-2.2766	none	none	none	none
OH OH O						
HO - P - P - OH						
OHN						
	4.670.151	40 (44				
ACTONEL	ACTONEL	-10.644	none	none	none	none
HO NOW						
HO CH ₃						
ALLEGRA	ALLEGRA	4.8896	none	none	none	none
H ₃ C CH ₃						
N - CHa						
H ₂ C	AMBIEN	4.3181	none	none	high	none
AMBIEN						

H ₃ C O N						
ARICEPT	ARICEPT	5.6409	none	none	none	none
N 						
H ₃ C N N						
CH ₃						
ARIMIDEX	ARIMIDEX	-4.1591	none	high	low	none
N-N						
N NH NH NH ₃ C						
0"						
AVAPRO	AVAPRO	-3.1849	none	none	none	none
F						
HO N N H H						
N H						
AVELOX	AVELOX	1.5957	none	none	none	none
HO H OH						
но он						
но н н						
BASEN	BASEN	-2.624	none	none	none	none
_ < CH ₃						
O CH3						
N N NH2						
CARDURA	CARDURA	7.1196	none	none	none	none
_						
0=5						
H ₃ C OH N = N						
CASODEX	CASODEX	-11.827	none	none	low	none
DEA						

_						
CH ₃ NH ₂ S = 0 CELEBREX	CELEBREX	-8.1085	none	none	none	none
н ₅ с он он он сн ₃						
CELLCEPT	CELLCEPT	-0.19574	none	none	none	none
HN N N O OH	CIDDO	0.0404				
CIPRO	CIPRO	2.0491	none	none	none	none
CLARINEX	CLARINEX	-0.6127	none	none	none	none
CI N N N N N N N N N N N N N N N N N N N	GLADITIN.	4.054				
CLARITIN	CLARITIN	-4.251	none	none	none	none
H ₃ C CH ₃						
HO	COMBIVENT	8.0069	none	none	none	none
COMBIVENT OH N N N S	COMBIVIR	-2.115	none	none	high	
COMBIVIR	COMBINE	-2.113	Holle	HOHE	High	none

CH ₃	
NH NH	
CONCERTA -2.515 none none no	ne none
11,C C Ots	
HO -	
NA CALL	
CONCOR -4.5181 none none no	ne <mark>high</mark>
OH OH	
H ₂ N	
COPAXONE -11.045 none none no	ne none
СН3	
но	
COREG 3.4008 none none no	ne none
H ₅ C CH ₃ CH ₃	
он он	
N S N S	
COSOPT 9.3969 none none no	ne none
N = N	
OH CI	
COZAAR -3.471 none none no	ne none
H OH H JC CH ₃	
HO TIPLE CHIS	
o = s - CH ₃	
CRESTOR 3.4539 none none no	ne none

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N H H OH	DELIX	-3.8863	none	none	none	none
HO CH ₃ CH ₃						
DETROL	DETROL	2.8073	none	none	none	none
F HO N N N N N N N N N N N N N N N N N N	DIFLUCAN	3.0382	none	none	none	none
DIFLUCAN	2.1.2007.11	0.0002		.,		
CH ₃	DURAGESIC	8.7647	none	none	none	none
DURAGESIC	DONAGESIC	0.7047	none	none	none	none
H ₃ C - O OH OH N - CH ₃						
EFFEXOR	EFFEXOR	-0.32546	none	none	none	none
N N N OH	EPZICOM	-1.2074	none	none	none	none
EPZICOM	EFZICUIVI	-1.20/4	none	none	none	none
N N N N	FENANCE	4.4470				
FEMARA	FEMARA	-1.1472	none	high	none	none

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H ₃ C H N NH ₀ S = 0 O CH ₃ CH ₃	FLOMAX	5.7098	none	none	none	none
GEODON	GEODON	8.1553	none	none	none	none
CH ₃	IMITREX	-0.57433	none	high	none	none
IMITREX	IIVIIIKEX	-0.5/433	none	high	none	none
NH ₂ N O H ₃ C KEPPRA	KEPPRA	5.0314	none	none	none	high
H ₂ N N N N N N N N N N N N N N N N N N N	LAMICTAL	-1.6419	none	none	none	none
LAMICTAL	L. II. II. O. I. I.	2.5 (1)	1.01.0	1,0110	1.0110	110110
H ₃ C CH ₃	LANGE	0.4/04				
LAMISIL	LAMISIL	-3.4681	none	high	none	none
H _B C CH ₃ OH H OH HO	LESCOL	0.18145	none	none	none	none

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HO N - CH ₃	1514 61111	5 7700				
LEVAQUIN	LEVAQUIN	5.7723	none	none	none	none
CH ₃ O = 5 - N N CH ₃ O = 5 - N N CH ₃ LEVITRA	LEVITRA	5.4018	none	none	none	none
CH ₃ I	LEXAPRO	-3.3305	none	none	none	none
LEXAPRO	LE/U II IXO	0.0005	TIOTIC	110110	Hone	TIOTIC
H ₃ C NH						
H ₃ C LIDODERM	LIDODERM	6.0164	high	none	high	high
H₃C						
LIDODERM	LIDODERM	-5.4701	high none	none	high none	high
LIDODERM LIDODERM	LOTREL	-5.4701	none	none	none	
LIDODERM LIDODERM LOTREL						
LIDODERM LIDODERM HO N HO N HO N N N CI	LOTREL	-5.4701	none	none	none	none

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CH ₃						
NH ₂						
CH ₃						
NAMENDA	NAMENDA	-0.80275	none	none	none	none
0, 2,,						
OH						
NH ₂						
	NEURONTIN	-5.2429	none	none	none	none
NEURONTIN						
0						
H ₃ C HN						
H ₃ C O O - CH ₃						
CH ₃	NEWHA	4 0775				
NEXIUM	NEXIUM	-1.8775	none	none	none	none
CH ₃ CH ₃						
0 0						
PAXIL	PAXIL	8.2657	none	none	none	high
, <mark>0</mark> — CH₃						
• → H						
N CI						
5						
PLAVIX	PLAVIX	2.6245	none	none	none	none
•						
HO H ₃ C						
H _M , CH ³						
H _C OH 0						
ОН	PRAVACHOL	3.1264	none	none	none	none
PRAVACHOL	PRAVACHUL	3.1204	none	none	none	none
O // CH ₃						
I III						
0						
0 - S = 0 OH						
PREMARIN	PREMARIN	-0.071876	none	none	high	none

PREVACID	PREVACID	-8.6384	none	none	none	none
H ₃ C - O H ₃ C O O F F	PROTONIX	-4.4787	none	none	none	none
PROTONIX						
O NH ₂	PROVIGIL	-0.62682	none	none	none	none
PROVIGIL	TROVICIE	0.02002	Horic	Horic	Hone	110110
REQUIP	REQUIP	4.0982	none	none	none	none
	DICDEDDAI	5.2816	none	none	nono	none
RISPERDAL	RISPERDAL	3.2010	none	none	none	none
O CH ₃ OH OCH ₃ SELOKEN	SELOKEN	6.6921	none	none	none	none
OH OH	CEDEV/ENIT	-8.9753	none	none	none	none
SEREVENT	SEREVENT	-0.7/53	none	none	none	none

H ₃ C NH ₂	SIFROL	2.0874	none	none	none	none
_						
HO S CH ₃ O CH ₃	CDIDIVA	4.0/40				
SPIRIVA	SPIRIVA	4.8619	none	none	none	none
F CI NH	SUSTIVA	-20.73	none	high	none	none
SUSTIVA	JOSTIVA	20.73	TIOTIC	High	HOHE	HOHE
N N N N N N N N N N N N N N N N N N N	TARCEVA	-5.9718	none	none	none	none
TARCEVA	174102471	3.7710	HOHE	Home	Horic	Hone
H ₃ C N N N N N N N N N N N N N N N N N N N	TEMODAR	-1.8034	high	high	high	none
TEMODAR						
O N N N N N N N N N N N N N N N N N N N						
THALOMID	THALOMID	4.3067	none	none	high	none
H_3C H_3C CH_3						
TOPAMAX	TOPAMAX	-2.4806	none	none	none	none

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H ₃ C H ₃ C OH	TRACLEER	-0.35379	none	none	none	none
H ₅ C CH ₃ CH ₃ TRICOR	TRICOR	-2.3394	none	none	none	none
INCOR						
N NH ₂	TRILEPTAL	2.0474	none	nono	high	nono
TRILEPTAL	INILLEFIAL	Z.U4/4	none	none	High	none
F F F F F F F F F F F F F F F F F F F	ULTANE	-12.68	high	none	high	none
H ₃ C OH OH		. ==0.				
VASOTEC	VASOTEC	0.77856	none	none	none	none
N HO F F N N N N	VEEND	4.0027	200	none	none	none
VFEND	VFEND	4.0837	none	none	none	none
H ₃ C N O CH ₃ O = S - N N - CH ₃	VIAGRA	5.9489	none	none	none	none
VIAGRA	VIAGKA	5.7487	none	none	none	none

OH CI						
VOLTAREN	VOLTAREN	-0.71474	none	none	high	none
H ₃ C CH ₃ CH ₃						
CI WELLBUTRIN	WELLBUTRIN	3.3755	none	none	none	none
H ₂ C CH ₃ O CH ₃ N N N N N N N N N NH	XATRAL	4.228	none	none	none	none
XATRAL	12111112					
CH ₃ CH ₃ CH ₃ CH ₃ N CH ₃ OH XELODA	XELODA	-21.328	high	none	low	low
HO ZETIA	ZETIA	0.9371	none	none	none	none
H ₃ C H ₃ OH	ZOCOR	0.66833	none	none	none	none
CH ₃	ZOFRAN	4.3913	none	none	none	none
ZUFRAN						

CI H N CH3						
ZOLOFT	ZOLOFT	0.25233	none	none	none	none
OH OH O HO - P - P - OH II						
ZOMETA	ZOMETA	-6.8035	none	none	none	none
ZYRTEC	ZYRTEC	4.3857	none	none	none	none
H ₃ C O NH	ZYVOX	-2.1658	none	none	none	none