

## **Supplementary Material**

# ***In silico* environmental risk assessment of fate and effects of pharmaceuticals and their TPs generated and treated by coupling tertiary processes in hospital wastewater**

Alexandre Della-Flora<sup>a</sup>, Davi Scunderlick<sup>a</sup>, Marcelo L. Wilde<sup>a</sup>, Adriano de A. Gomes<sup>a</sup>,

Eder C. Lima<sup>a</sup> and Carla Sirtori<sup>a †</sup>

<sup>a</sup>Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves 9500, CEP 91501-970 Porto Alegre, RS, Brazil.

<sup>†</sup> Corresponding author: Prof. Dr. Carla Sirtori – [carla.sirtori@ufrgs.br](mailto:carla.sirtori@ufrgs.br)

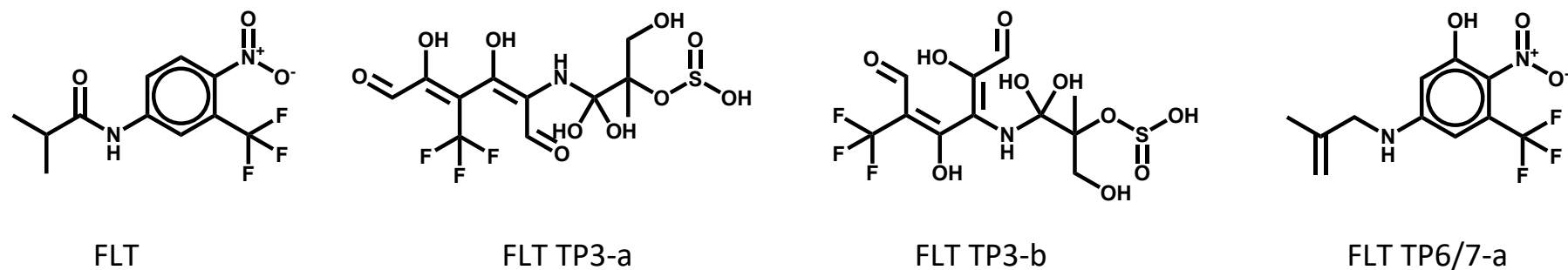
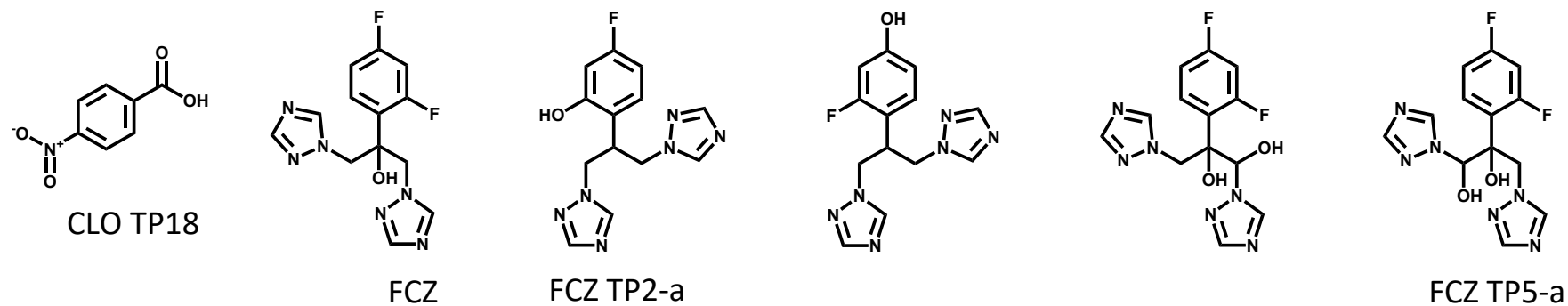
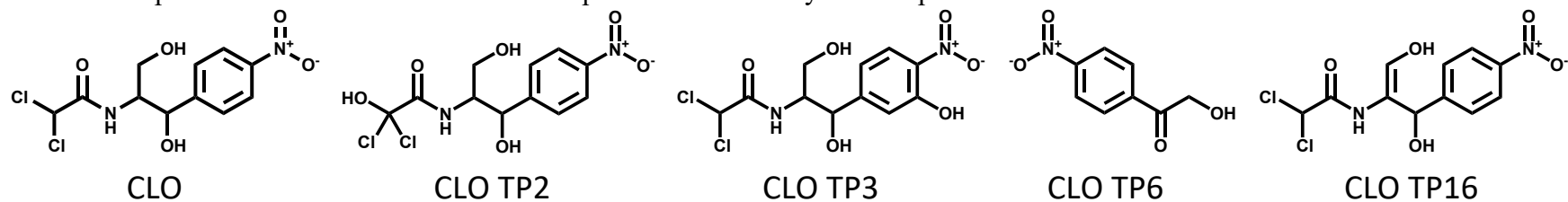
**Text S1.** SMILES codes for *in silico* predictions of pharmaceuticals and TPs.

**Table S1.** SMILES codes for *in silico* predictions of pharmaceuticals and TPs.

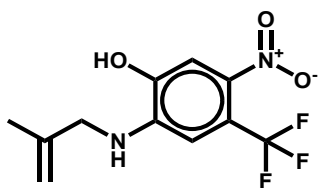
Compound	Smiles
CLO	<chem>O=C(NC(CO)C(O)C1=CC=C([N+](O-)=O)C=C1)C(Cl)Cl</chem>
CLO TP2	<chem>O=C(NC(CO)C(O)C1=CC=C([N+](O-)=O)C=C1)C(Cl)(O)Cl</chem>
CLO TP3	<chem>O=C(NC(CO)C(O)C1=CC(O)=C([N+](O-)=O)C=C1)C(Cl)Cl</chem>
CLO TP6	<chem>O=C(CO)C1=CC=C([N+](O-)=O)C=C1</chem>
CLO TP16	<chem>O=C(N/C(C(O)C1=CC=C([N+](O-)=O)C=C1)=C/O)C(Cl)Cl</chem>
CLO TP18	<chem>O=[N+](C1=CC=C(C(O)=O)C=C1)[O-]</chem>
FCZ	<chem>OC(CN1N=CN=C1)(C2=CC=C(F)C=C2F)CN3N=CN=C3</chem>
FCZ TP2-a	<chem>FC1=CC=C(C(CN2N=CN=C2)CN3N=CN=C3)C(O)=C1</chem>
FCZ TP2-b	<chem>FC1=CC(O)=CC=C1C(CN2N=CN=C2)CN3N=CN=C3</chem>
FCZ TP5-a	<chem>OC(C(O)N1N=CN=C1)(C2=CC=C(F)C=C2F)CN3N=CN=C3</chem>
FCZ TP5-b	<chem>OC(CN4N=CN=C4)(C5=CC=C(F)C=C5F)C(O)N6N=CN=C6</chem>
FLT	<chem>O=C(Nc1ccc(c1)C(F)(F)F)[N+](=O)[O-]C(C)C</chem>
FLT TP3a	<chem>O=CC(O)=C(C(O)=C(C=O)NC(O)(O)C(OS(=O)O)(C)CO)C(F)(F)F</chem>
FLT TP3b	<chem>O=CC(O)=C(NC(O)(O)C(OS(=O)O)(C)CO)C(O)=C(C=O)C(F)(F)F</chem>
FLT TP6/7a	<chem>O=[N+](O-)[c1c(O)cc(cc1C(F)(F)F)NCC(=C)C</chem>
FLT TP6/7b	<chem>O=[N+](O-)[c1cc(O)c(cc1C(F)(F)F)NCC(=C)C</chem>
FLT TP6/7c	<chem>O=[N+](O-)[c1ccc(NCC(=C)C)c(O)c1C(F)(F)F</chem>
FLT TP8-a	<chem>O=C(Nc1ccc(O)c(c1)C(F)(F)F)C(C)C</chem>
FLT TP8-b	<chem>O=C(Nc1cc(O)cc(c1)C(F)(F)F)C(C)C</chem>
FLT TP8-c	<chem>O=C(Nc1cc(ccc1(O))C(F)(F)F)C(C)C</chem>
FLT TP8-d	<chem>O=C(Nc1cccc(c1(O))C(F)(F)F)C(C)C</chem>
FLT TP9	<chem>O=C(Nc1ccc(c1)C(F)(F)F)[N+](=O)[O-]C(C)CO</chem>
FLT TP10-a	<chem>O=C(Nc1cc(O)c(c1)C(F)(F)F)[N+](=O)[O-]C(OS(=O)O)(C)C</chem>
FLT TP10-b	<chem>O=C(Nc1cc(ccc1(O)))[N+](=O)[O-]C(F)(F)F)C(OS(=O)O)(C)C</chem>
FLT TP10-c	<chem>O=C(Nc1ccc(c1(O))C(F)(F)F)[N+](=O)[O-]C(OS(=O)O)(C)C</chem>
FLT TP11	<chem>O=C(Nc1ccc(c1)C(F)(F)F)[N+](=O)[O-]C(O)(C)C</chem>
FLT TP13-a	<chem>O=C(Nc1cc(O)c(c1)C(F)(F)F)[N+](=O)[O-]C(C)C</chem>
FLT TP13-b	<chem>O=C(Nc1cc(ccc1(O)))[N+](=O)[O-]C(F)(F)F)C(C)C</chem>
FLT TP13-c	<chem>O=C(Nc1ccc(c1(O))C(F)(F)F)[N+](=O)[O-]C(C)C</chem>
FRS	<chem>O=C(O)C1=CC(S(=O)(N)=O)=C(Cl)C=C1NCC2=CC=CO2</chem>
FRS TP3	<chem>O=C(O)C1=CC(S(=O)(N)=O)=C(Cl)C=C1N</chem>
FRS TP12-a	<chem>O=C(O)C1=CC(S(=O)(N)=O)=C(O)C=C1NCC2=CC=CO2</chem>
FRS TP12-b	<chem>O=C(O)C3=CC(S(=O)(N)=O)=CC(O)=C3NCC4=CC=CO4</chem>
FRS TP12-c	<chem>O=C(O)C5=C(O)C(S(=O)(N)=O)=CC=C5NCC6=CC=CO6</chem>
FRS TP14-a	<chem>O=C(O)C1=CC(S(=O)(N)=O)=C(O)C=C1N</chem>
FRS TP14-b	<chem>O=C(O)C2=C(O)C(S(=O)(N)=O)=CC=C2N</chem>
FRS TP14-c	<chem>O=C(O)C3=CC(S(=O)(N)=O)=CC(O)=C3N</chem>
GFZ	<chem>O=C(O)C(C)C(C)CCOC1=CC(C)=CC=C1C</chem>
GFZ TP8	<chem>CC1=CC=C(C)C(OC(O)=O)=C1</chem>
IBP	<chem>CC(C1=CC=C(CC(C)C)C=C1)C(O)=O</chem>
IBP TP4-a	<chem>CC(C)CC1=C(O)C=C(C(C)C(O)=O)C=C1</chem>
IBP TP4-b	<chem>CC(C)CC2=CC(O)=C(C(C)C(O)=O)C=C2</chem>
IBP TP4-c	<chem>CC(C)CC3=CC=C(C(C)C(O)=O)C(O)=C3</chem>
IBP TP4-d	<chem>CC(C)CC4=CC=C(C(C)C(O)=O)C=C4O</chem>
IBP TP4-e	<chem>CC(C)C(O)C1=CC=C(C(C)C(O)=O)C=C1</chem>

IBP TP4-f	<chem>CC(C)(O)CC2=CC=C(C(C)C(O)=O)C=C2</chem>
IBP TP4-g	<chem>CC(CO)CC3=CC=C(C(C)C(O)=O)C=C3</chem>
IBP TP4-h	<chem>CC(CO)CC4=CC=C(C(C)C(O)=O)C=C4</chem>
IBP TP7-a	<chem>CC(C)CC1=CC=C(CCO)C=C1</chem>
IBP TP7-b	<chem>CC(C)CC2=CC=C(C(O)C)C=C2</chem>
IBP TP7-c	<chem>CC(C)CC3=C(O)C=C(CC)C=C3</chem>
IBP TP7-d	<chem>CC(C)CC4=CC(O)=C(CC)C=C4</chem>
IBP TP7-e	<chem>CC(C)CC5=CC=C(CC)C(O)=C5</chem>
IBP TP7-f	<chem>CC(C)CC6=CC=C(CC)C=C6O</chem>
IBP TP7-g	<chem>CC(C)C(O)C1=CC=C(CC)C=C1</chem>
IBP TP7-h	<chem>CC(C)(O)CC2=CC=C(CC)C=C2</chem>
IBP TP7-i	<chem>CC(CO)CC3=CC=C(CC)C=C3</chem>
IBP TP7-j	<chem>CC(CO)CC4=CC=C(CC)C=C4</chem>
IBP TP13	<chem>O=C(CCCCC=O)O</chem>
IBP TP19-a	<chem>CC(C)CC1=CC=C(C(C=O)(O)C(O)=O)C=C1O</chem>
IBP TP19-b	<chem>CC(C)CC2=C(O)C=C(C(C=O)(O)C(O)=O)C=C2</chem>
IBP TP19-c	<chem>CC(C)CC3=CC(O)=C(C(C=O)(O)C(O)=O)C=C3</chem>
IBP TP19-d	<chem>CC(C)CC4=CC=C(C(C=O)(O)C(O)=O)C(O)=C4</chem>
IBP TP19-e	<chem>CC(CO)CC1=CC=C(C(C=O)(O)C(O)=O)C=C1C</chem>
IBP TP19-f	<chem>CC(C)C(O)C2=CC=C(C(C=O)(O)C(O)=O)C=C2</chem>
IBP TP19-g	<chem>CC(C)(O)CC3=CC=C(C(C=O)(O)C(O)=O)C=C3</chem>
IBP TP19-h	<chem>CC(CO)CC4=CC=C(C(C=O)(O)C(O)=O)C=C4</chem>
LOS	<chem>OCC1=C(CI)N=C(CCCC)N1CC2=CC=C(C3=CC=CC=C3C4=NN=N4)C=C2</chem>
LOS TP1	<chem>NCC1=CC=C(C2=CC=CC=C2C3=NN=NN3)C=C1</chem>
LOS TP5-a	<chem>OCC1=C(CI)N=C(CCCC)N1CC2=CC=C(C3=C(O)C=CC=C3C4=NN=NN4)C=C2</chem>
LOS TP5-b	<chem>OCC5=C(CI)N=C(CCCC)N5CC6=CC=C(C7=CC(O)=CC=C7C8=NN=NN8)C=C6</chem>
LOS TP5-c	<chem>OCC9=C(CI)N=C(CCCC)N9CC%10=CC=C(C%11=CC=C(O)C=C%11C%12=NN=NN%12)C=C%10</chem>
LOS TP5-d	<chem>OCC1=C(CI)N=C(CCCC)N1CC2=CC=C(C3=CC=CC(O)=C3C4=NN=NN4)C=C2</chem>
LOS TP10	<chem>O=CC1=C(CI)N=C(CCCC)N1CC2=CC=C(C3=CC=CC=C3C4=NN=NN4)C=C2</chem>
LOS TP11	<chem>OCC1=C(CI)N=C(CC(O)CC)N1CC2=CC=C(C3=CC=CC=C3C4=NN=NN4)C=C2</chem>
LOS TP14	<chem>OC(CN(CC1=CC=C(C2=CC=CC=C2C3=NN=NN3)C=C1)C(CCCC)=O)=O</chem>
LOS TP15-a	<chem>OCC1=C(CI)N=C(CCCC)N1CC2=CC=C(C3=C(O)C=CC=C3C4=NN=NN4)C=C2</chem>
LOS TP15-b	<chem>OCC5=C(CI)N=C(CCCC)N5CC6=CC=C(C7=CC(O)=CC=C7C8=NN=NN8)C=C6</chem>
LOS TP15-c	<chem>OCC9=C(CI)N=C(CCCC)N9CC%10=CC=C(C%11=CC=C(O)C=C%11C%12=NN=NN%12)C=C%10</chem>
LOS TP15-d	<chem>OCC1=C(CI)N=C(CCCC)N1CC2=CC=C(C3=CC=CC(O)=C3C4=NN=NN4)C=C2</chem>
NMS	<chem>CS(=O)(NC1=CC=C([N+])([O-])=O)C=C1OC2=CC=CC=C2)=O</chem>
NMS TP1 I	<chem>CS(=O)(NC1=C(O)C=C([N+])([O-])=O)C=C1OC2=CC=CC=C2)=O</chem>
NMS TP1 II	<chem>CS(=O)(NC1=CC=C([N+])([O-])=O)C(O)=C1OC2=CC=CC=C2)=O</chem>
NMS TP1 III	<chem>CS(=O)(NC1=CC=C([N+])([O-])=O)C=C1OC2=CC=CC(O)=C2)=O</chem>
PCT	<chem>CC(NC1=CC=C(O)C=C1)=O</chem>
PCT TP2	<chem>OCNC1=CC=C(O)C=C1</chem>
PCT TP9-a	<chem>CC(NC1=CC=C(O)C=C1O)=O</chem>
PCT TP9-b	<chem>CC(NC2=CC=C(O)C(O)=C2)=O</chem>
PCT TP9-c	<chem>CC(NC3=CC(O)=C(O)C=C3)=O</chem>
PCT TP9-d	<chem>CC(NC4=C(O)C=C(O)C=C4)=O</chem>

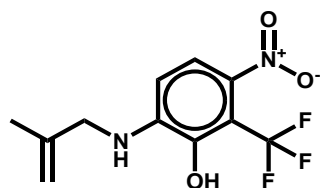
**Text S2.** Proposed chemical structures of the compounds evaluated by *in silico* predictions.



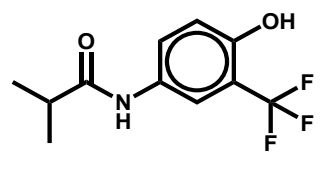
**Figure S1.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.



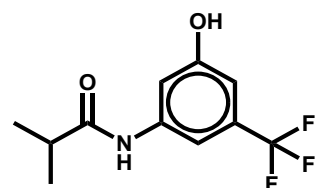
FLT TP6/7-b



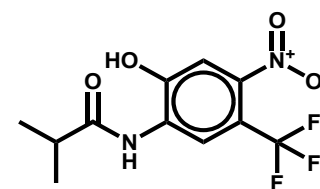
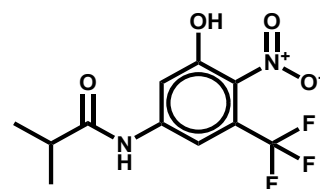
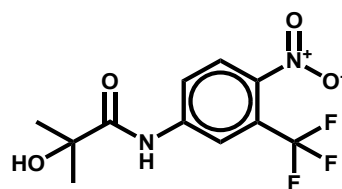
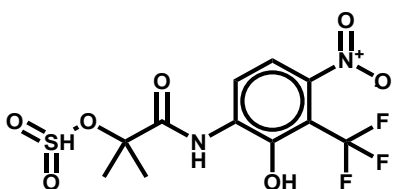
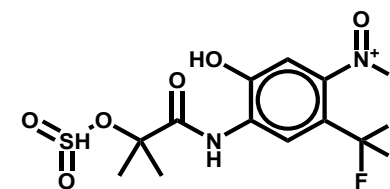
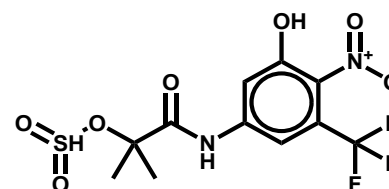
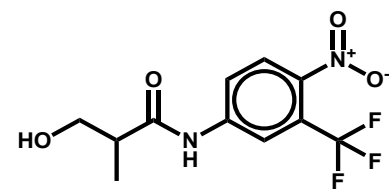
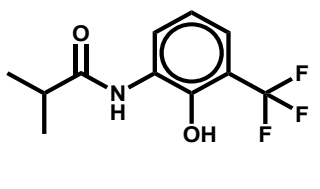
FLT TP6/7-c



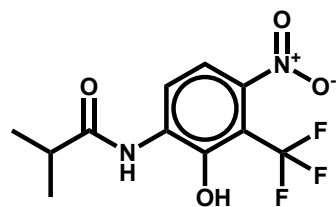
FLT TP8-a



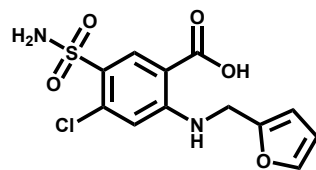
FLT TP8-b



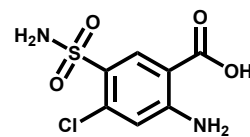
**Figure S2.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.



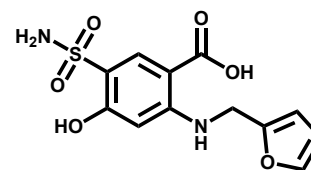
FLT TP13-c



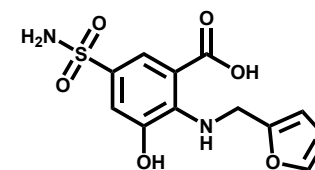
FRS



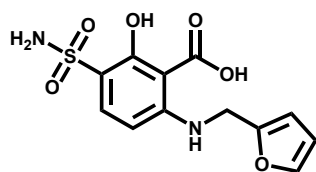
FRS TP3



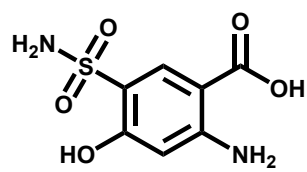
FRS TP12-a



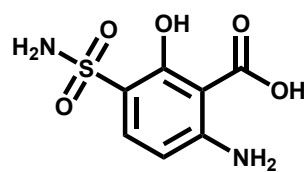
FRS TP12-b



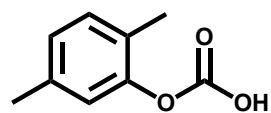
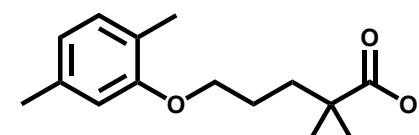
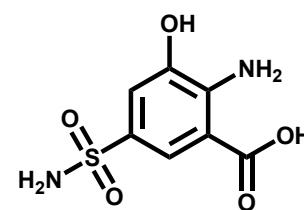
FRS TP12-c



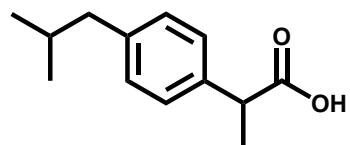
FRS TP14-a



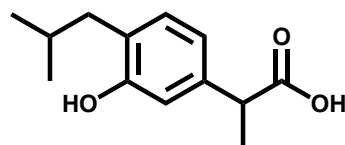
FRS TP14-c



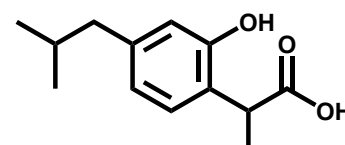
GFZ TP8



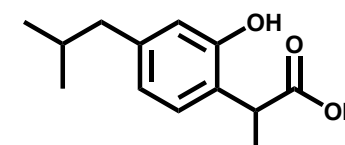
IBP



IBP TP4-a

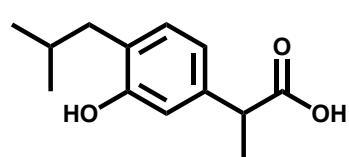


IBP TP4-b

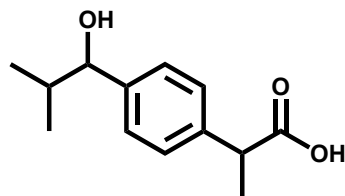


IBP TP4-c

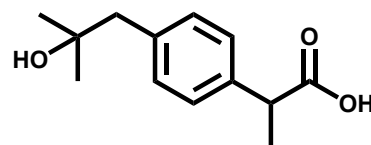
**Figure S3.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.



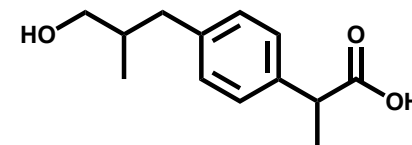
IBP TP4-  
4507



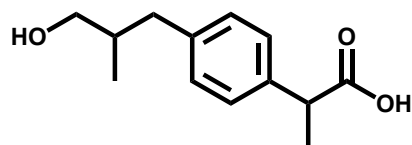
IBP TP4-  
4517



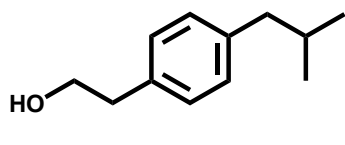
IBP TP4-  
4507



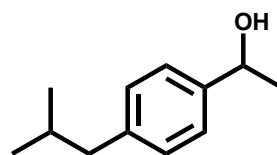
IBP TP4-  
4507



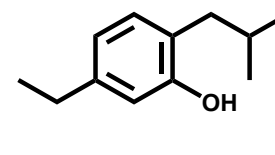
LOS



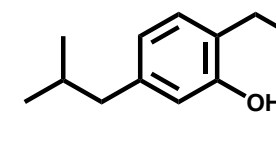
IBP TP7-a



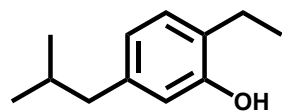
IBP TP7-bFLT  
TP7-b



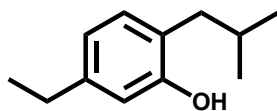
IBP TP13IBP



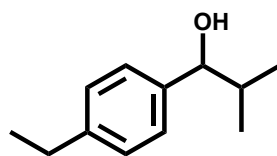
LOS



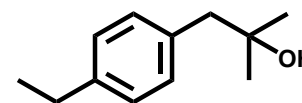
LOS



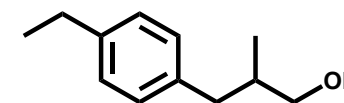
LOS



IBP TP19-

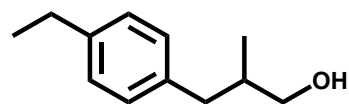


IBP TP19-eIBP

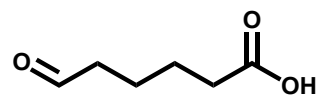


IBP TP19-

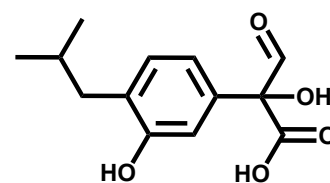
**Figure S4.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.



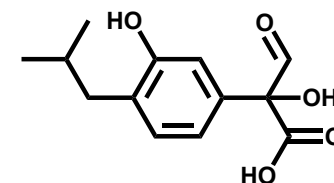
IBP TP7-j



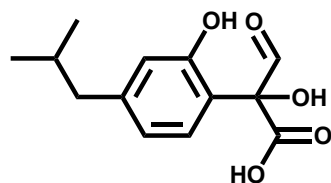
TP7-cFLT TP9



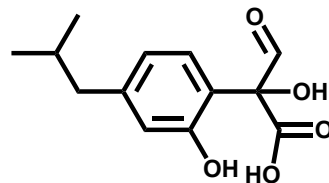
IBP TP19-a



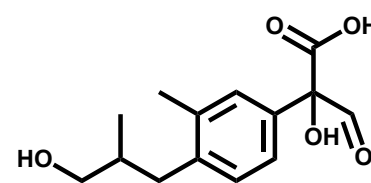
IBP TP19-b



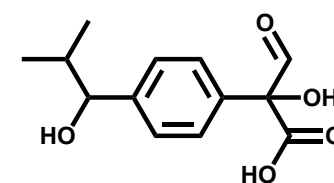
cIBP TP7-gFLT  
TD11



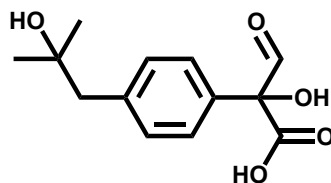
dIBP TP7-iFLT  
TD12



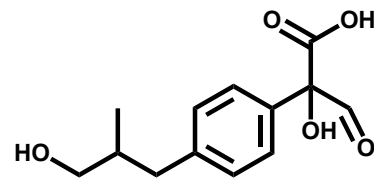
TP7-hFLT TP13-  
h



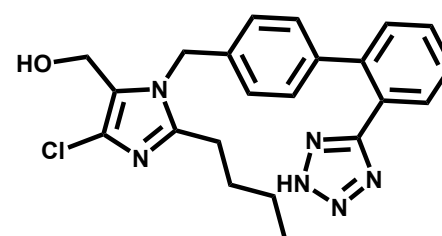
IBP TP19-f



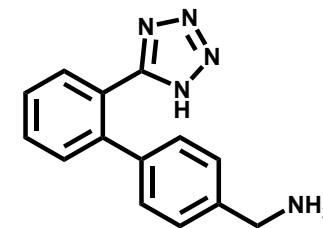
IBP TP19-g



IBP TP19-h



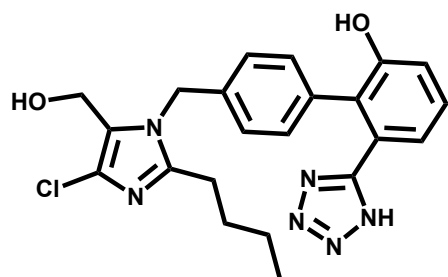
LOS



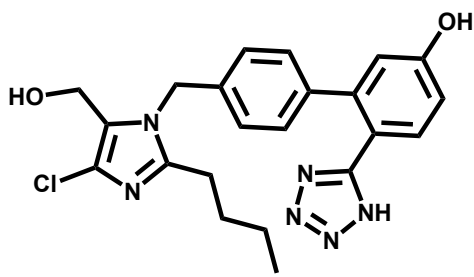
LOS TP1

**Figure S5.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.

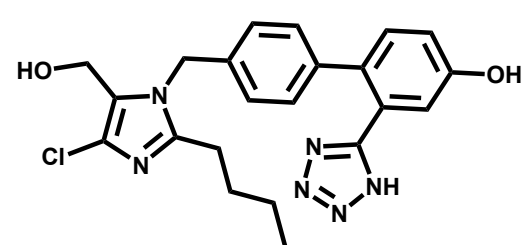




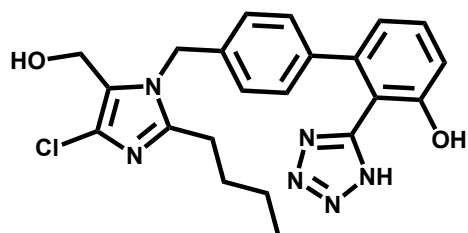
LOS TP5/15-a



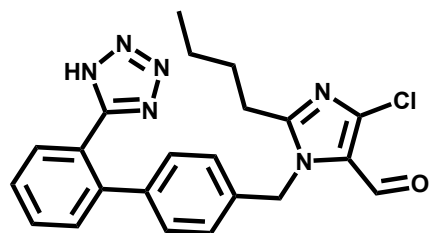
LOS TP5/15-b



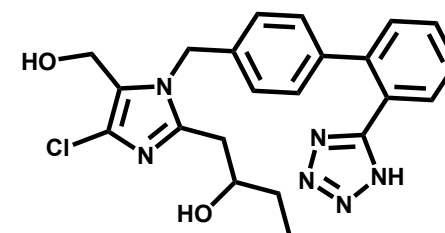
LOS TP5/15-c



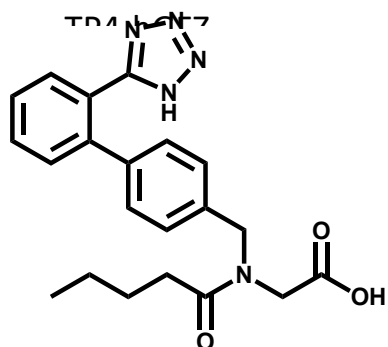
TP5/15-dIBP



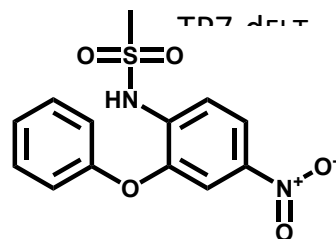
TP10IBP



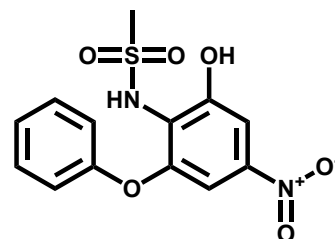
TP11IBP



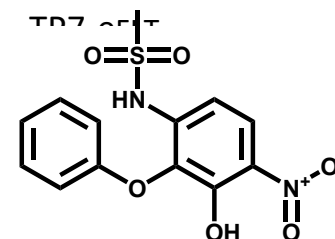
TP14IBP



NMS

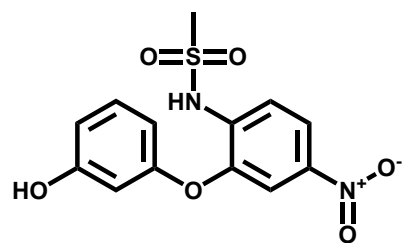


NMS TP1 I

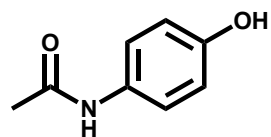


NMS TP1 II

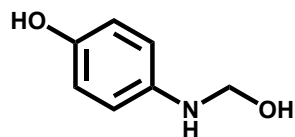
**Figure S6.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.



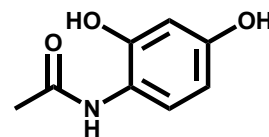
NMS TP1 III



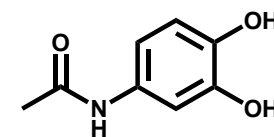
PCT



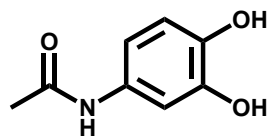
PCT TP2



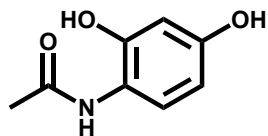
PCT TP9-a



PCT TP9-b



PCT TP9-c



PCT TP9-d

**Figure S7.** Proposed chemical structures of pharmaceuticals and TPs (considering some constitutional isomers of TPs) evaluated by *in silico* predictions.

**Text S3.**Normalized data for chemometric analyzes for HCA and PCA.

**Table S1.** Normalized data for chemometric analyzes for HCA and PCA.

Composto	BIODEGRADABILITY								MUTAGENICITY										CARCINOGENICITY					PBT	
	BA	BB	BC	BD	BE	BF	BG	BH	MA	MB	MC	MD	ME	MF	MG	MG	MI	MJ	MK	CA	CB	CC	CD		CE
CLO	0.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	2.00	3.00	2.00	0.00	3.00	2.00	2.00	2.00	2.00	4.00	0.00	2.00	0.00	6.00	2.00	2.00	0.00
CLO TP2	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	0.00	3.00	2.00	2.00	1.00	1.00	4.00	0.00	1.00	0.00	6.00	3.00	1.00	0.00
CLO TP3	0.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	2.00	3.00	0.00	0.00	3.00	2.00	3.00	2.00	2.00	4.00	0.00	2.00	0.00	7.00	2.00	2.00	0.00
CLO TP6	0.00	1.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	0.00	3.00	1.00	2.00	2.00	3.00	2.00	1.00	1.00	0.00	4.00	3.00	1.00	0.00
CLO TP16	0.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	3.00	3.00	2.00	0.00	2.00	2.00	2.00	1.00	1.00	4.00	0.00	3.00	0.00	6.00	2.00	3.00	0.00
CPC TP18	0.00	0.00	0.00	0.00	1.00	1.00	0.00	1.00	1.00	1.00	2.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	1.00	1.00	0.00	4.00	2.00	1.00	0.00
FCZ	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	2.00	0.00	0.00	0.00
FCZ TP2-a	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	2.00	0.00	1.00	0.00
FCZ TP2-b	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	2.00	0.00	1.00	0.00
FCZ TP5-a	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	2.00	1.00	0.00	0.00
FCZ TP5-b	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	2.00	1.00	0.00	0.00
FLUT	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	2.00	0.00	0.00	0.00	0.00	1.00	1.00	2.00	0.00	1.00	0.00	5.00	2.00	1.00	0.00
FLUT TP3-a	0.00	0.00	1.00	0.00	0.00	1.00	0.00	1.00	1.00	2.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	1.00	0.00	1.00	0.00	3.00	1.00	1.00	0.00
FLUT TP3-b	0.00	0.00	1.00	0.00	0.00	1.00	0.00	1.00	1.00	2.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	3.00	2.00	1.00	0.00
FLUT TP6-7-a	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	1.00	0.00	0.00	1.00	1.00	2.00	0.00	0.00	0.00	6.00	3.00	1.00	0.00
FLUT TP6-7-b	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	2.00	2.00	0.00	1.00	0.00	0.00	1.00	1.00	2.00	1.00	1.00	0.00	6.00	3.00	1.00	1.00
FLUT TP6-7-c	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	2.00	2.00	0.00	1.00	0.00	0.00	1.00	1.00	2.00	1.00	1.00	0.00	6.00	3.00	1.00	1.00
FLUT TP8-a	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	2.00	0.00	0.00
FLUT TP8-b	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	2.00	0.00	0.00
FLUT TP8-c	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00	2.00	0.00	0.00
FLUT TP8-d	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00	2.00	0.00	0.00
FLUT TP-9	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	0.00	0.00	0.00	0.00	1.00	1.00	2.00	0.00	1.00	1.00	5.00	2.00	1.00	0.00
FLUT TP10-a	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00	2.00	1.00	0.00	1.00	7.00	3.00	1.00	0.00
FLUT TP10-b	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	2.00	0.00	0.00	0.00	1.00	1.00	2.00	1.00	1.00	1.00	7.00	3.00	1.00	0.00

Composto	BIODEGRADABILITY								MUTAGENICITY											CARCINOGENICITY					PBT
	BA	BB	BC	BD	BE	BF	BG	BH	MA	MB	MC	MD	ME	MF	MG	MG	MI	MJ	MK	CA	CB	CC	CD	CE	
FLUT TP10-c	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	2.00	1.00	0.00	0.00	1.00	1.00	2.00	1.00	1.00	1.00	7.00	3.00	1.00	0.00
FLUT TP11	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	2.00	0.00	1.00	0.00	0.00	1.00	1.00	2.00	0.00	1.00	1.00	5.00	2.00	1.00	0.00
FLUT TP13-a	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	1.00	1.00	2.00	0.00	0.00	1.00	6.00	2.00	1.00	0.00
FLUT TP13-b	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	0.00	0.00	0.00	1.00	1.00	2.00	1.00	1.00	1.00	6.00	2.00	1.00	0.00
FLUT TP13-c	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	2.00	2.00	0.00	0.00	0.00	1.00	1.00	2.00	1.00	1.00	1.00	6.00	2.00	1.00	0.00
FRS	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00	0.00	2.00	3.00	2.00	0.00
FRS TP3	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	2.00	2.00	0.00
FRS TP12-a	0.00	0.00	1.00	0.00	1.00	1.00	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	2.00	2.00	1.00	0.00
FRS TP12-b	0.00	0.00	1.00	0.00	1.00	1.00	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	3.00	2.00	1.00	0.00
FRS TP12-c	0.00	0.00	1.00	0.00	1.00	1.00	1.00	0.00	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	2.00	3.00	1.00	0.00
FRS TP14-a	0.00	0.00	1.00	0.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	1.00	1.00	0.00
FRS TP14-b	0.00	0.00	1.00	0.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	2.00	1.00	0.00
FRS TP14-c	0.00	0.00	1.00	0.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	2.00	1.00	1.00	0.00
GFZ	0.00	0.00	1.00	0.00	0.00	1.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00	0.00
GFZ TP8	0.00	0.00	1.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
IBP	0.00	0.00	0.00	0.00	1.00	0.00	1.00	1.00	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-a	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-b	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-c	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-d	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-e	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-f	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-g	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP4-h	0.00	0.00	1.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP7-a	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
IBP TP7-b	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
IBP TP7-c	0.00	0.00	0.00	0.00	1.00	1.00	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00



Composto	BIODEGRADABILITY								MUTAGENICITY										CARCINOGENICITY					PBT	
	BA	BB	BC	BD	BE	BF	BG	BH	MA	MB	MC	MD	ME	MF	MG	MG	MI	MJ	MK	CA	CB	CC	CD		CE
LOS TP15-c	0.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	0.00	0.00
LOS TP15-d	0.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	0.00	0.00
NMS	0.00	0.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	3.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	1.00	1.00	1.00	5.00	1.00	1.00	0.00
NMS TP1 I	0.00	0.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	3.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	1.00	1.00	0.00	5.00	1.00	1.00	0.00
NMS TP1 II	0.00	0.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	3.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	2.00	1.00	1.00	1.00	5.00	1.00	1.00	0.00
NMS TP1 III	0.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	3.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	2.00	1.00	1.00	1.00	5.00	1.00	1.00	0.00
PCT	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	2.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.00	1.00	1.00	0.00
PCT TP2	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	1.00	1.00	0.00	1.00	1.00	0.00	0.00	1.00	1.00	1.00	1.00	0.00	0.00	1.00	1.00	0.00
PCT TP9-a	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	2.00	0.00	0.00	1.00	1.00	0.00	1.00	1.00	0.00	1.00	1.00	0.00	1.00	1.00	1.00	0.00
PCT TP9-b	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	2.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	1.00	0.00	1.00	1.00	1.00	0.00
PCT TP9-c	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	2.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	1.00	1.00	1.00	0.00
PCT TP9-d	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	1.00	2.00	0.00	0.00	1.00	1.00	0.00	1.00	1.00	0.00	1.00	0.00	0.00	1.00	1.00	1.00	0.00

Legends:

**0**: not positive(biodegradable or not mutagenic or not carcinogenic); **1**: positive( not biodegradable or mutagenic or carcinogenic); **BA**: BIOWIN-1; **BB**: BIOWIN-2; **BC**: BIOWIN-3; **BD**: BIOWIN-4; **BE**: BIOWIN-5; **BF**: BIOWIN-6; **BG**: BIOWIN-7; **BH**: Ready Biodegradability (IRFMN 1.0.9); **MA**: in vivo mutagenicity (Ames Test) alerts by ISS; **MB**: in vivo mutagenicity (Micronucleus) alerts by ISS; **MC**: DNA alerts for AMES, CA and MNT by OASIS; **MD**: Protein binding alerts for Chromosomal aberration by OASIS; **ME**: GT1 BMUT; **MF**: GT EXPERT; **MG**: PHARM BMUT; **MH**: Mutagenicity (Ames test) model (CAESAR) (version 2.1.13); **MI**: Mutagenicity (Ames test) model (ISS); **MJ**:Mutagenicity (Ames test) model (SarPy/IRFMN) (version 1.0.7); **MK**:Mutagenicity (Ames test) model (KNN/Read-Across) (version 1.0.0); **CA**:Carcinogenicity alerts by ISS; **CB**: Carcinogenicity model (CAESAR) (version 2.1.9); **CC**: Carcinogenicity model (IRFMN/Antares) (version 1.0.0); **CD**: Carcinogenicity model (IRFMN/ISSCANNACGX) (version 1.0.0); **CE**: Carcinogenicity model (ISS) (version 1.0.2); **PBT**: Persistence, Bioaccumulation and Toxicity.

Text S4.*In silico*(Q)SAR predictions

Table S2. Biodegradability values of pharmaceuticals and TPs provided by EPI Suite and VEGA HUB.

Compound	EPI Suite v 4.11							VEGA HUB
	BIOWIN-1	BIOWIN-2	BIOWIN-3	BIOWIN-4	BIOWIN-5	BIOWIN-6	BIOWIN-7	Ready Biodegradability Model
CLO	<b>0.5940</b>	0.0538	2.2300	3.5400	-0.0409	0.0007	-0.3470	PNRB
CLO TP2	0.4020	0.0008	1.9900	<b>3.3600</b>	-0.1210	0.0002	-0.5320	PNRB
CLO TP3	<b>0.7020</b>	0.1010	2.2600	<b>3.5500</b>	-0.0283	0.0007	-0.1880	PNRB
CLO TP6	<b>0.5220</b>	0.1970	<b>2.7700</b>	<b>3.5900</b>	0.2920	0.0542	0.0072	PNRB
CLO TP16	<b>0.5950</b>	0.0553	2.2400	<b>3.5400</b>	-0.0042	0.0007	-0.2980	PNRB
CLO TP18	<b>0.5400</b>	0.6340	<b>2.7500</b>	<b>3.5100</b>	0.4470	0.1570	<b>0.5060</b>	PNRB
FCZ	-1.2000	0.0000	1.5000	<b>3.2800</b>	0.1150	0.0000	-0.1140	NRB
FCZ TP2-a	-0.0292	0.0000	2.1400	<b>3.4200</b>	0.1170	0.0003	0.2190	NRB
FCZ TP2-b	-0.0292	0.0000	2.1400	<b>3.4200</b>	0.1170	0.0003	0.2190	NRB
FCZ TP5-a	-1.0500	0.0000	1.6200	<b>3.3900</b>	0.1350	0.0000	-0.1730	NRB
FCZ TP5-b	-1.0500	0.0000	1.6200	<b>3.3900</b>	0.1350	0.0000	-0.1730	NRB
FLT	0.0007	0.0017	1.8500	<b>3.2700</b>	0.1390	0.0000	-0.5570	NRB
FLT TP3-a	<b>0.8640</b>	<b>0.9990</b>	1.9100	<b>3.5000</b>	<b>0.7540</b>	0.0000	<b>0.9350</b>	NRB
FLT TP3-b	<b>0.8640</b>	<b>0.9990</b>	1.9100	<b>3.5000</b>	<b>0.7540</b>	0.0000	<b>0.9350</b>	NRB
FLT TP6/7-a	-0.3270	0.0000	1.8300	<b>3.0000</b>	0.0583	0.0000	0.0334	NRB
FLT TP6/7-b	-0.3270	0.0000	1.8300	<b>3.0000</b>	0.0583	0.0000	0.0334	NRB
FLT TP6/7-c	-0.3270	0.0000	1.8300	<b>3.0000</b>	0.0583	0.0000	0.0334	NRB
FLT TP8-a	0.4350	0.0710	2.1400	<b>3.4600</b>	0.4130	0.0000	-0.2620	NRB
FLT TP8-b	0.4350	0.0710	2.1400	<b>3.4600</b>	0.4130	0.0000	-0.2620	NRB
FLT TP8-c	0.4350	0.0710	2.1400	<b>3.4600</b>	0.4130	0.0000	-0.2620	NRB
FLT TP8-d	0.4350	0.0710	2.1400	<b>3.4600</b>	0.4130	0.0000	-0.2620	NRB
FLT TP9	0.1520	0.0040	1.9800	<b>3.3800</b>	0.2350	0.0000	-0.3190	NRB
FLT TP10-a	-0.1130	0.0002	1.4800	<b>3.0200</b>	-0.0301	0.0000	-0.5490	NRB
FLT TP10-b	-0.1130	0.0002	1.4800	<b>3.0200</b>	-0.0301	0.0000	-0.5490	NRB
FLT TP10-c	-0.1130	0.0002	1.4800	<b>3.0200</b>	-0.0301	0.0000	-0.5490	NRB
FLT TP11	-0.1910	0.0002	1.6000	<b>3.1000</b>	0.0583	0.0000	-0.7260	NRB
FLT TP13-a	0.1090	0.0033	1.8700	<b>3.2900</b>	0.1510	0.0000	-0.3810	NRB
FLT TP13-b	0.1090	0.0033	1.8700	<b>3.2900</b>	0.1510	0.0000	-0.3810	NRB
FLT TP13-c	0.1090	0.0033	1.8700	<b>3.2900</b>	0.1510	0.0000	-0.3810	NRB
FRS	0.3510	0.0396	2.2100	<b>3.1000</b>	0.2390	0.0206	-0.0629	NRB
FRS TP3	0.3890	0.1140	2.3900	<b>3.2200</b>	0.3380	0.0729	0.2310	NRB

Compound	EPI Suite v 4.11							VEGA HUB
	BIOWIN-1	BIOWIN-2	BIOWIN-3	BIOWIN-4	BIOWIN-5	BIOWIN-6	BIOWIN-7	Ready Biodegradability Model
FRS TP12-a	0.6580	0.5000	2.5200	3.3400	0.3460	0.0751	0.4200	PRB
FRS TP12-b	0.6580	0.5000	2.5200	3.3400	0.3460	0.0751	0.4200	PRB
FRS TP12-c	0.6580	0.5000	2.5200	3.3400	0.3460	0.0751	0.4200	PRB
FRS TP14-a	0.6960	0.7570	2.7000	3.4500	0.4440	0.2330	0.7140	PRB
FRS TP14-b	0.6960	0.7570	2.7000	3.4500	0.4440	0.2330	0.7140	PRB
FRS TP14-c	0.6960	0.7570	2.7000	3.4500	0.4440	0.2330	0.7140	PRB
GFZ	0.7580	0.8550	2.5900	3.6600	0.6100	0.4860	-0.2440	NRB
GFZ TP8	0.7780	0.8590	2.6800	3.4700	0.3090	0.2720	-0.1940	PRB
IBP	0.8310	0.8670	2.9600	3.8000	0.4990	0.5340	0.0334	NRB
IBP TP4-a	0.9400	0.9280	2.9800	3.8200	0.5120	0.5240	0.2100	NRB
IBP TP4-b	0.9400	0.9280	2.9800	3.8200	0.5120	0.5240	0.2100	NRB
IBP TP4-c	0.9400	0.9280	2.9800	3.8200	0.5120	0.5240	0.2100	NRB
IBP TP4-d	0.9400	0.9280	2.9800	3.8200	0.5120	0.5240	0.2100	NRB
IBP TP4-e	0.9280	0.8990	3.1600	3.9700	0.4540	0.5140	0.3210	NRB
IBP TP4-f	0.6400	0.4820	2.7100	3.6200	0.4190	0.2240	-0.1350	NRB
IBP TP4-g	0.9830	0.9410	3.0800	3.9100	0.5950	0.6390	0.2720	NRB
IBP TP4-h	0.9830	0.9410	3.0800	3.9100	0.5950	0.6390	0.2720	NRB
IBP TP7-a	0.9310	0.9400	2.8200	3.5800	0.5050	0.4410	0.0445	NRB
IBP TP7-b	0.8760	0.8980	2.8900	3.6500	0.3630	0.3200	0.0939	NRB
IBP TP7-c	0.8880	0.9270	2.7100	3.4900	0.4210	0.3290	-0.0176	NRB
IBP TP7-d	0.8880	0.9270	2.7100	3.4900	0.4210	0.3290	-0.0176	NRB
IBP TP7-e	0.8880	0.9270	2.7100	3.4900	0.4210	0.3290	-0.0176	NRB
IBP TP7-f	0.8880	0.9270	2.7100	3.4900	0.4210	0.3290	-0.0176	NRB
IBP TP7-g	0.8760	0.8980	2.8900	3.6500	0.3630	0.3200	0.0939	NRB
IBP TP7-h	0.5880	0.4770	2.4400	3.3000	0.3280	0.1140	-0.3620	NRB
IBP TP7-i	0.9310	0.9400	2.8200	3.5800	0.5050	0.4410	0.0445	NRB
IBP TP7-j	0.9310	0.9400	2.8200	3.5800	0.5050	0.4410	0.0445	NRB
IBP TP13	1.0400	1.0000	3.3000	4.2400	1.0000	0.9660	1.2500	RB
IBP TP19-a	0.9710	0.9990	2.8000	3.8800	0.6660	0.3590	0.1590	NRB
IBP TP19-b	0.9710	0.9990	2.8000	3.8800	0.6660	0.3590	0.1590	NRB
IBP TP19-c	0.9710	0.9990	2.8000	3.8800	0.6660	0.3590	0.1590	NRB
IBP TP19-d	0.9710	0.9990	2.8000	3.8800	0.6660	0.3590	0.1590	NRB
IBP TP19-e	1.0600	1.0000	2.8000	3.8800	0.7350	0.4210	-0.0553	NRB
IBP TP19-f	0.9600	0.9990	2.9800	4.0400	0.6080	0.3490	0.2700	NRB
IBP TP19-g	0.6720	0.9880	2.5300	3.6900	0.5730	0.1280	-0.1860	NRB
IBP TP19-h	1.0100	0.9990	2.9000	3.9700	0.7500	0.4740	0.2210	NRB
LOS	0.6860	0.1860	2.4400	3.4000	0.1590	0.0079	-0.6790	PNRB
LOS TP1	0.7820	0.6340	2.6700	3.5300	0.1710	0.0515	0.2430	-
LOS TP5-a	0.7940	0.3120	2.4600	3.4200	0.1710	0.0076	-0.5030	PNRB
LOS TP5-b	0.7940	0.3120	2.4600	3.4200	0.1710	0.0076	-0.5030	PNRB
LOS TP5-c	0.7940	0.3120	2.4600	3.4200	0.1710	0.0076	-0.5030	PNRB



Compound	EPI Suite v 4.11							VEGA HUB
	BIOWIN-1	BIOWIN-2	BIOWIN-3	BIOWIN-4	BIOWIN-5	BIOWIN-6	BIOWIN-7	Ready Biodegradability
								Model
LOS TP5-d	<b>0.7940</b>	0.3120	2.4600	<b>3.4200</b>	0.1710	0.0076	-0.5030	PNRB
LOS TP10	<b>0.8130</b>	<b>0.9900</b>	2.3100	<b>3.4700</b>	0.2320	0.0104	-0.6820	PNRB
LOS TP11	<b>0.7280</b>	0.0812	2.2700	<b>3.2400</b>	0.1790	0.0072	-0.4200	PNRB
LOS TP14	<b>0.9520</b>	<b>0.9310</b>	<b>2.9400</b>	<b>4.1400</b>	0.4520	0.1680	-0.6090	NRB
LOS TP15-a	<b>0.7940</b>	0.3120	2.4600	<b>3.4200</b>	0.1710	0.0076	-0.5030	PNRB
LOS TP15-b	<b>0.7940</b>	0.3120	2.4600	<b>3.4200</b>	0.1710	0.0076	-0.5030	PNRB
LOS TP15-c	<b>0.7940</b>	0.3120	2.4600	<b>3.4200</b>	0.1710	0.0076	-0.5030	PNRB
LOS TP15-d	<b>0.7940</b>	0.3120	2.4600	<b>3.4200</b>	0.1710	0.0076	-0.5030	PNRB
NMS	<b>0.5560</b>	<b>0.5420</b>	2.3100	<b>3.3800</b>	0.0021	0.0046	0.1750	PNRB
NMS TP1 I	<b>0.6640</b>	<b>0.7010</b>	2.3300	<b>3.3900</b>	0.0147	0.0044	0.3510	PNRB
NMS TP1 II	<b>0.6640</b>	<b>0.7010</b>	2.3300	<b>3.3900</b>	0.0147	0.0044	0.3510	PNRB
NMS TP1 III	<b>0.5360</b>	0.2790	2.3100	<b>3.3900</b>	0.0147	0.0044	0.1330	PNRB
PCT	<b>1.0000</b>	<b>0.9890</b>	<b>2.8700</b>	<b>3.8700</b>	0.4260	0.4340	-0.1120	<b>PRB</b>
PCT TP2	<b>0.7220</b>	<b>0.7600</b>	<b>2.9700</b>	<b>3.7100</b>	0.4090	0.3310	0.4160	-
PCT TP9-a	<b>1.1100</b>	<b>0.9940</b>	<b>2.8900</b>	<b>3.8900</b>	0.4380	0.4240	0.0638	<b>PRB</b>
PCT TP9-b	<b>1.1100</b>	<b>0.9940</b>	<b>2.8900</b>	<b>3.8900</b>	0.4380	0.4240	0.0638	<b>PRB</b>
PCT TP9-c	<b>1.1100</b>	<b>0.9940</b>	<b>2.8900</b>	<b>3.8900</b>	0.4380	0.4240	0.0638	<b>PRB</b>
PCT TP9-d	<b>1.1100</b>	<b>0.9940</b>	<b>2.8900</b>	<b>3.8900</b>	0.4380	0.4240	0.0638	<b>PRB</b>

**Table S3.** *In silico*(Q)SAR prediction of PBT values by the Prometheus software for pharmaceuticals and TPs investigated in this study.

Compound	LogP	LogP rel.	P	P rel.	B	B rel.	T	T rel.	Score P	Score B	Score T	PBT	PB
CLO	1.14	1	P/vP	0.5	0.73	0.4	0.855	0.4	0.712	0.243	0.362	0.405	0.416
CLO TP2	0.75	0.4	P/vP	0.5	1.01	0.4	0.634	0.4	0.712	0.26	0.38	0.42	0.43
CLO TP3	0.71	0.4	P/vP	0.5	1.02	0.4	0.386	0.4	0.712	0.26	0.41	0.426	0.431
CLO TP6	0.9	0.4	P/vP	0.5	0.48	0.8	1.79	0.4	0.712	0.108	0.324	0.286	0.277
CLO TP16	0.81	0.4	nP/P	0.7	0.85	0.4	0.657	0.4	0.584	0.25	0.377	0.381	0.382
CLO TP18	1.89	1	nP	1	0.36	0.8	0.539	0.4	0.3	0.1	0.389	0.204	0.173
FCZ	0.25	0.2	vP	0.5	1.72	0.8	-	0.5	0.854	0.24	0.5	0.462	0.453
FCZ TP2-a	1.08	0.2	vP	0.5	1.7	0.8	0.255	0.4	0.854	0.237	0.437	0.447	0.45
FCZ TP2-b	1.08	0.2	vP	0.5	1.65	0.8	0.233	0.3	0.854	0.229	0.45	0.444	0.443
FCZ TP5-a	-0.88	0.2	vP	0.5	1.73	0.8	-	0.5	0.854	0.24	0.5	0.462	0.453
FCZ TP5-b	-0.88	0.2	vP	0.5	1.73	0.8	-	0.5	0.854	0.24	0.5	0.462	0.453

Compound	LogP	LogP rel.	P	P rel.	B	B rel.	T	T rel.	Score P	Score B	Score T	PBT	PB
FLT	3.35	1	P/vP	0.5	1.88	0.8	0.185	0.4	0.712	0.265	0.458	0.439	0.435
FLT TP3a	-5	0.2	nP	0.5	0.41	0.4	-	0.5	0.359	0.228	0.5	0.32	0.286
FLT TP3b	-5	0.2	nP	0.5	0.4	0.4	-	0.5	0.359	0.227	0.5	0.319	0.286
FLT TP6/7a	3.12	0.4	P/vP	0.5	2.24	0.8	0.12	0.4	0.712	0.333	0.487	0.487	0.487
FLT TP6/7b	3.12	0.4	P/vP	0.5	3.01	0.8	0.121	0.4	0.712	0.506	0.487	<b>0.576</b>	0.6
FLT TP6/7c	3.12	0.4	P/vP	0.5	3.02	0.8	0.179	0.6	0.712	0.507	0.451	<b>0.568</b>	0.601
FLT TP8-a	2.71	0.4	P/vP	0.5	1.4	0.4	0.828	0.6	0.712	0.29	0.334	0.427	0.454
FLT TP8-b	2.52	0.8	P/vP	0.5	1.67	0.4	0.584	0.4	0.712	0.316	0.384	0.455	0.474
FLT TP8-c	2.63	0.8	P/vP	0.5	1.31	0.8	0.514	0.4	0.712	0.183	0.392	0.367	0.361
FLT TP8-d	2.63	0.8	P/vP	0.5	1.31	0.8	0.745	0.6	0.712	0.183	0.341	0.357	0.361
FLT TP9	2.3	0.4	P/vP	0.5	1.43	0.4	-	0.5	0.712	0.293	0.5	0.465	0.456
FLT TP10-a	2.19	0.4	P/vP	0.5	1.33	0.4	0.115	0.3	0.712	0.284	0.492	0.458	0.45
FLT TP10-b	2.19	0.4	P/vP	0.5	1.32	0.4	0.115	0.3	0.712	0.283	0.492	0.457	0.449
FLT TP10-c	2.19	0.4	P/vP	0.5	1.33	0.4	0.171	0.4	0.712	0.284	0.463	0.452	0.45
FLT TP11	2.7	1	P/vP	0.5	1.72	0.4	0.245	0.3	0.712	0.322	0.447	0.472	0.479
FLT TP13-a	2.61	0.4	P/vP	0.5	2.27	0.8	0.117	0.4	0.712	0.339	0.489	0.491	0.491
FLT TP13-b	2.61	0.4	P/vP	0.5	1.73	0.4	0.167	0.4	0.712	0.323	0.465	0.476	0.479
FLT TP13-c	2.61	0.4	P/vP	0.5	1.74	0.4	0.174	0.6	0.712	0.323	0.454	0.474	0.48
FRS	2.03	1	nP	0.7	0.55	0.4	0.045	0.3	0.333	0.234	0.547	0.319	0.279
FRS TP3	0.08	0.4	nP/P	0.5	0.2	0.8	0.101	0.4	0.571	0.092	0.5	0.268	0.229
FRS TP12-a	0.13	0.2	vP	0.5	0.5	0.4	0.631	0.3	0.854	0.232	0.396	0.435	0.445
FRS TP12-b	0.48	0.2	vP	0.5	0.57	0.4	0.066	0.3	0.854	0.235	0.525	0.462	0.448
FRS TP12-c	2.1	0.4	vP	0.5	0.55	0.4	0.784	0.4	0.854	0.234	0.367	0.43	0.447
FRS TP14-a	-0.75	0.4	P/vP	0.5	0.05	0.8	0.2	0.4	0.712	0.085	0.453	0.278	0.246
FRS TP14-b	-0.14	0.4	nP	0.7	0.05	0.8	0.511	0.3	0.333	0.085	0.407	0.2	0.168
FRS TP14-c	-0.95	0.4	vP	0.5	0.12	0.8	0.202	0.4	0.854	0.088	0.452	0.303	0.274
GFZ	4.46	0.4	nP	0.9	0.93	0.8	0.128	0.6	0.31	0.143	0.479	0.248	0.21
GFZ TP8	2.33	0.4	nP	0.7	0.66	0.4	2.2	0.4	0.333	0.239	0.315	0.288	0.282
IBP	3.97	1	nP	0.7	0.43	0.8	0.21	0.4	0.333	0.104	0.449	0.222	0.186

Compound	LogP	LogP rel.	P	P rel.	B	B rel.	T	T rel.	Score P	Score B	Score T	PBT	PB
IBP TP4-a	3.1	0.8	nP/P	0.5	0.71	0.8	0.317	0.6	0.571	0.124	0.405	0.289	0.266
IBP TP4-b	3.1	0.8	nP/P	0.5	0.5	0.8	0.309	0.6	0.571	0.109	0.407	0.275	0.249
IBP TP4-c	3.1	0.8	nP/P	0.5	0.5	0.8	0.309	0.6	0.571	0.109	0.407	0.275	0.249
IBP TP4-d	3.1	0.8	nP/P	0.5	0.71	0.8	0.317	0.6	0.571	0.124	0.405	0.289	0.266
IBP TP4-e	2.4	0.8	nP/P	0.7	0.5	0.8	0.405	0.4	0.584	0.109	0.407	0.277	0.252
IBP TP4-f	2.31	0.8	nP/P	0.7	0.7	0.8	0.411	0.4	0.584	0.123	0.406	0.291	0.268
IBP TP4-g	2.38	0.8	nP/P	0.7	0.7	0.8	1.05	0.4	0.584	0.123	0.351	0.283	0.268
IBP TP4-h	2.38	0.8	nP/P	0.7	0.7	0.8	1.05	0.4	0.584	0.123	0.351	0.283	0.268
IBP TP7-a	3.16	0.4	nP	0.5	1.51	0.8	0.488	0.4	0.359	0.209	0.395	0.294	0.273
IBP TP7-b	3.27	0.8	nP	0.5	1.69	0.8	0.653	0.4	0.359	0.235	0.378	0.306	0.29
IBP TP7-c	3.77	0.4	nP	0.5	1.75	0.8	0.214	0.6	0.359	0.244	0.437	0.32	0.296
IBP TP7-d	3.77	0.4	nP	0.5	2.05	0.8	0.22	0.6	0.359	0.296	0.434	0.345	0.326
IBP TP7-e	3.77	0.4	nP	0.5	2.05	0.8	0.22	0.6	0.359	0.296	0.434	0.345	0.326
IBP TP7-f	3.77	0.4	nP	0.5	1.75	0.8	0.214	0.6	0.359	0.244	0.437	0.32	0.296
IBP TP7-g	3.32	0.8	nP	0.5	1.69	0.8	0.373	0.4	0.359	0.235	0.412	0.311	0.29
IBP TP7-h	3.22	0.8	nP	0.5	1.66	0.8	0.495	0.4	0.359	0.231	0.394	0.306	0.288
IBP TP7-i	3.3	0.8	nP	0.5	1.66	0.8	0.513	0.4	0.359	0.231	0.392	0.306	0.288
IBP TP7-j	3.3	0.8	nP	0.5	1.66	0.8	0.513	0.4	0.359	0.231	0.392	0.306	0.288
IBP TP13	0.51	0.8	nP	0.9	0.17	0.4	0.837	0.4	0.31	0.219	0.364	0.279	0.261
IBP TP19-a	0.63	0.2	nP/P	0.7	0.38	0.4	0.157	0.4	0.584	0.227	0.469	0.383	0.364
IBP TP19-b	0.63	0.2	nP/P	0.7	0.38	0.4	0.157	0.4	0.584	0.227	0.469	0.383	0.364
IBP TP19-c	0.63	0.2	nP/P	0.7	0.42	0.4	0.158	0.4	0.584	0.228	0.469	0.384	0.365
IBP TP19-d	0.63	0.2	nP/P	0.7	0.42	0.4	0.158	0.4	0.584	0.228	0.469	0.384	0.365
IBP TP19-e	0.6	0.2	nP/P	0.7	0.48	0.4	0.169	0.3	0.584	0.231	0.469	0.386	0.367
IBP TP19-f	-0.02	0.2	nP/P	0.7	0.31	0.4	0.27	0.3	0.584	0.224	0.442	0.376	0.361
IBP TP19-g	0.02	0.2	nP/P	0.7	0.3	0.4	0.27	0.3	0.584	0.224	0.442	0.376	0.361
IBP TP19-h	0.05	0.2	nP/P	0.7	0.3	0.4	0.27	0.3	0.584	0.224	0.442	0.376	0.361
LOS	3.25	0.4	nP	0.5	1.54	0.4	0.00007	0.3	0.359	0.303	0.752	0.389	0.33
LOS TP1	2.37	0.4	nP	0.5	1.13	0.4	0.354	0.3	0.359	0.268	0.427	0.331	0.31

Compound	LogP	LogP rel.	P	P rel.	B	B rel.	T	T rel.	Score P	Score B	Score T	PBT	PB
LOS TP5-a	2.77	0.4	nP	0.5	1.37	0.4	0.00007	0.3	0.359	0.288	0.752	0.381	0.321
LOS TP5-b	2.77	0.4	nP	0.5	1.24	0.4	0.00007	0.3	0.359	0.276	0.752	0.375	0.315
LOS TP5-c	2.77	0.4	nP	0.5	1.38	0.4	0.00007	0.3	0.359	0.288	0.752	0.381	0.321
LOS TP5-d	2.32	0.4	P/vP	0.5	1.05	0.4	0.00007	0.3	0.712	0.263	0.752	0.483	0.432
LOS TP10	3.54	0.4	P/vP	0.5	1.74	0.4	-	0.5	0.712	0.323	0.5	0.484	0.48
LOS TP11	2.31	0.4	P/vP	0.5	1.23	0.4	0.00007	0.3	0.712	0.276	0.752	0.493	0.443
LOS TP14	1.42	0.2	P/vP	0.5	0.7	0.4	-	0.5	0.712	0.242	0.5	0.431	0.415
LOS TP15-a	2.77	0.4	nP	0.5	1.37	0.4	0.00007	0.3	0.359	0.288	0.752	0.381	0.321
LOS TP15-b	2.77	0.4	nP	0.5	1.24	0.4	0.00007	0.3	0.359	0.276	0.752	0.375	0.315
LOS TP15-c	2.77	0.4	nP	0.5	1.38	0.4	0.00007	0.3	0.359	0.288	0.752	0.381	0.321
LOS TP15-d	2.32	0.4	P/vP	0.5	1.05	0.4	0.00007	0.3	0.712	0.263	0.752	0.483	0.432
NMS	2.6	1	P/vP	0.5	1.79	0.4	0.064	0.3	0.712	0.329	0.527	0.492	0.484
NMS TP1 I	2.24	0.8	P/vP	0.5	1.73	0.4	0.063	0.3	0.712	0.322	0.528	0.488	0.479
NMS TP1 II	2.12	0.8	P/vP	0.5	1.62	0.4	0.068	0.3	0.712	0.311	0.523	0.48	0.47
NMS TP1 III	2.24	0.8	P/vP	0.5	1.72	0.4	0.063	0.3	0.712	0.321	0.528	0.488	0.478
PCT	0.46	1	nP/P	0.5	0.39	0.8	54	0.7	0.571	0.102	0.133	0.214	0.242
PCT TP2	1.04	0.4	nP	0.5	0.53	0.8	3.43	0.4	0.359	0.111	0.296	0.216	0.199
PCT TP9-a	0.24	0.8	nP/P	0.5	0.3	0.8	8.76	0.4	0.571	0.097	0.263	0.241	0.236
PCT TP9-b	0.47	0.4	nP/P	0.5	0.09	0.8	8.53	0.4	0.571	0.087	0.264	0.23	0.222
PCT TP9-c	0.47	0.4	nP/P	0.5	0.09	0.8	8.53	0.4	0.571	0.087	0.264	0.23	0.222
PCT TP9-d	0.24	0.8	nP/P	0.5	0.3	0.8	8.76	0.4	0.571	0.097	0.263	0.241	0.236

**Table S4.** *In silico*(Q)SAR predictions for Mutagenicity and Carcinogenicity model for pharmaceuticals and TPs investigated in the present study.

Comp.	(Q)SAR Prediction															
	VEGA HUB				Mutagenicity				CASE ULTRA			Carcinogenicity				
	A	B	C	D	QSAR TOOLBOX				A	B	C	VEGA HUB				QSAR TOOLBOX
				A	B	C	D				E	F	G	H	E	
CLO	+	+	-	+	AH/NiAr	AH/ NiAr/H	R/SN1	-	+	+	+	-	+	+	+	+
CLO TP2	+	+	-	+	NiAr	NiAr/H	R/SN1	-	+	+	+	-	+	+	+	+
CLO TP3	+	+	-	+	AH/NiAr	AH/ NiAr/H	-	-	+	+	+	-	+	+	+	+
CLO TP6	+	+	+	+	NiAr	NiAr/H	R/SN1	-	+	+	+	-	+	+	+	+
CLO TP16	+	+	-	+	AH/NiAr/AB	AH/ NiAr/H	R/SN1	-	+	+	+	-	+	+	+	+
CLO TP18	+	+	+	+	NiAr	NiAr	R/SN1	-	+	+	+	-	+	+	+	+
FCZ	-	-	+	-	-	H	-	-	-	-	-	+	+	-	-	-
FCZ TP2-a	-	-	+	-	-	H	-	-	-	-	-	+	+	-	+	+
FCZ TP2-b	-	-	+	-	-	H	-	-	-	-	-	+	+	-	+	+
FCZ TP5-a	-	-	+	-	-	H	-	-	OD	OD	OD	+	+	+	-	-
FCZ TP5-b	-	-	+	-	-	H	-	-	OD	OD	OD	+	+	+	-	-
FLT	+	+	-	+	NiAr	NiAr	R/SN1	-	-	-	-	-	+	+	+	+
FLT TP3-a	-	+	-	+	$\alpha$ - $\beta$	$\alpha$ - $\beta$ /H	-	-	+	+	+	-	+	+	+	+
FLT TP3-b	-	+	+	+	$\alpha$ - $\beta$	$\alpha$ - $\beta$ /H	-	-	+	+	+	-	+	+	+	+
FLT TP6/7-a	+	+	-	+	-	H	-	-	+	-	+	-	+	+	+	-
FLT TP6/7-b	+	+	+	+	NiAr	NiAr/H	R/SN1	-	+	-	+	-	+	+	+	+
FLT TP6/7-c	+	+	+	+	NiAr	NiAr/H	R/SN1	-	+	-	+	-	+	+	+	+
FLT TP8-a	-	-	-	-	-	-	-	AN2/Acy	-	-	-	-	+	+	-	-
FLT TP8-b	-	-	-	-	-	-	-	-	-	-	-	-	+	+	-	-
FLT TP8-c	-	-	-	-	-	H	-	AN2/Acy	-	-	-	-	+	+	-	-
FLT TP8-d	-	-	-	-	-	H	-	AN2/Acy	-	-	-	-	+	+	-	-
FLT TP9	+	+	-	+	NiAr	NiAr/H	R/SN1	-	Inc.	-	-	+	+	+	+	+
FLT TP10-a	+	+	+	+	-	H	-	-	OD	OD	-	+	+	+	+	-
FLT TP10-b	+	+	+	+	NiAr	NiAr/H	R/SN1	AN2/Acy	-	OD	+	+	+	+	+	+
FLT TP10-c	+	+	+	+	NiAr	NiAr/H	R/SN1	AN2/Acy	+	OD	+	+	+	+	+	+

Comp.	(Q)SAR Prediction															
	VEGA HUB				Mutagenicity QSAR TOOLBOX				CASE ULTRA			Carcinogenicity VEGA HUB				QSAR TOOLBOX
	A	B	C	D	A	B	C	D	A	B	C	E	F	G	H	E
FLT TP11	+	+	-	+	NiAr	NiAr/H	R/SN1	-	+	-	-	+	+	+	+	+
FLT TP13-a	+	+	+	+	-	H	-	-	-	-	-	+	+	+	+	-
FLT TP13-b	+	+	+	+	NiAr	NiAr/H	R/SN1	AN2/Acy	-	-	-	+	+	+	+	+
FLT TP13-c	+	+	+	+	NiAr	NiAr/H	-	AN2/Acy	-	-	-	+	+	+	+	+
FRS	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
FRS TP3	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
FRS TP12-a	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
FRS TP12-b	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
FRS TP12-c	-	-	-	-	-	H	-	AN2	-	-	-	-	+	+	+	+
FRS TP14-a	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
FRS TP14-b	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
FRS TP14-c	-	-	-	-	-	H	-	-	-	-	-	-	+	+	+	+
GFZ	-	-	-	-	-	-	-	-	-	-	-	-	-	-	+	+
GFZ TP8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
IBP	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP4-a	-	-	-	-	-	-	-	AN2	-	-	-	-	-	+	-	-
IBP TP4-b	-	-	-	-	-	-	-	AN2	-	-	-	-	-	+	-	-
IBP TP4-c	-	-	-	-	-	-	-	AN2	-	-	-	-	-	+	-	-
IBP TP4-d	-	-	-	-	-	-	-	AN2	-	-	-	-	-	+	-	-
IBP TP4-e	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP4-f	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP4-g	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP4-h	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP7-a	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP7-b	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
IBP TP7-c	-	-	-	-	-	-	-	AN2	-	-	-	-	-	-	-	-
IBP TP7-d	-	-	-	-	-	-	-	AN2	-	-	-	+	-	-	-	-

Comp.	(Q)SAR Prediction															
	VEGA HUB				Mutagenicity QSAR TOOLBOX				CASE ULTRA			Carcinogenicity				QSAR TOOLBOX
	A	B	C	D	A	B	C	D	A	B	C	E	F	G	H	E
IBP TP7-e	-	-	-	-	-	-	-	AN2	-	-	-	+	-	-	-	-
IBP TP7-f	-	-	-	-	-	-	-	AN2	-	-	-	-	-	-	-	-
IBP TP7-g	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
IBP TP7-h	-	-	-	-	-	-	-	-	-	-	-	+	-	-	-	-
IBP TP7-i	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
IBP TP7-j	-	-	-	-	-	-	-	-	-	-	-	-	-	+	-	-
IBP TP13	-	+	-	-	SiAi	SiAi	-	-	-	-	-	-	-	-	+	+
IBP TP19-a	-	+	-	-	SiAi	SiAi/H	-	AN2	Inc.	Inc.	Inc.	+	-	+	+	+
IBP TP19-b	-	+	-	-	-	-	-	AN2	Inc.	Inc.	Inc.	+	-	+	+	+
IBP TP19-c	-	+	-	-	SiAi	SiAi/H	-	AN2	-	Inc.	Inc.	+	-	+	+	+
IBP TP19-d	-	+	-	-	-	-	-	AN2	-	Inc.	Inc.	+	-	+	+	+
IBP TP19-e	-	+	-	-	SiAi	SiAi/H	-	-	Inc.	Inc.	-	+	-	+	+	+
IBP TP19-f	-	+	-	-	SiAi	SiAi/H	-	-	Inc.	Inc.	-	+	-	+	+	+
IBP TP19-g	-	+	-	-	SiAi	SiAi/H	-	-	-	Inc.	-	+	-	+	+	+
IBP TP19-h	-	+	-	-	SiAi	SiAi/H	-	-	-	Inc.	-	+	-	+	+	+
LOS	-	-	+	-	-	H	-	-	-	-	-	-	-	+	-	-
LOS TP1	-	-	-	-	-	H	-	-	-	-	-	-	-	-	-	-
LOS TP5-a	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	+	+
LOS TP5-b	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	-	-
LOS TP5-c	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	-	-
LOS TP5-d	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	-	-
LOS TP10	-	+	+	-	SiAi	SiAi/	-	-	-	-	-	-	-		+	+
LOS TP11	-	-	-	-	-	H	-	-	-	-	-	+	-	+	-	-
LOS TP14	-	-	+	+	-	H	-	-	-	-	-	-	-	+	-	-
LOS TP15-a	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	+	-
LOS TP15-b	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	-	-
LOS TP15-c	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	-	-

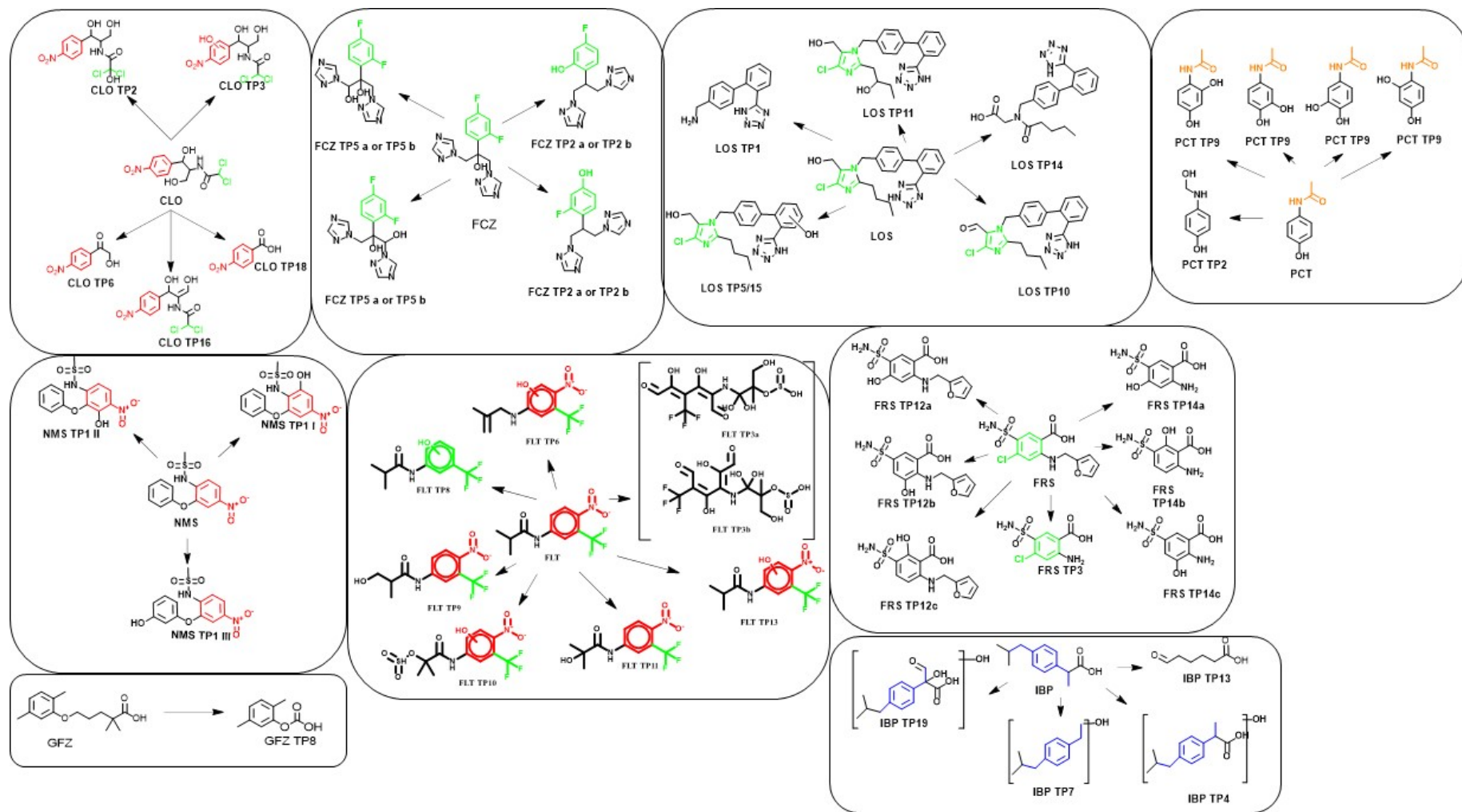
Comp.	(Q)SAR Prediction															
	VEGA HUB				Mutagenicity				CASE ULTRA			Carcinogenicity				
	A	B	C	D	QSAR TOOLBOX				A	B	C	VEGA HUB				QSAR TOOLBOX
					A	B	C	D				E	F	G	H	E
LOS TP15-d	-	-	-	-	-	H	-	AN2	-	-	-	+	-	+	-	-
NMS	+	+	+	+	NiAr	NiAr/H/1-PB	-	-	+	+	+	+	+	+	+	+
NMS TP 1 I	+	+	+	+	NiAr	NiAr/H/1-PB	-	-	+	+	+	-	+	+	+	+
NMS TP 1 II	+	+	+	+	NiAr	NiAr/H/1-PB	-	-	-	-	+	+	+	+	+	+
NMS TP 1 III	+	+	+	+	NiAr	NiAr/H/1-PB	-	-	-	+	+	+	+	+	+	+
PCT	-	+	-	-	ArNacyl	ArNacyl	-	AN2/Acy	-	-	-	-	-	+	+	+
PCT TP2	-	+	+	+	ArNacyl	N-Me	AN2	-	Inc.	+	Inc.	-	-	+	+	+
PCT TP 9-a	-	+	-	-	ArNacyl	ArNacyl/H	-	AN2/Acy	+	+	Inc.	-	+	+	+	+
PCT TP 9-b	+	+	-	-	ArNacyl	ArNacyl/H	-	AN2/Acy	+	+	+	-	-	+	+	+
PCT TP 9-c	+	+	-	-	ArNacyl	ArNacyl/H	-	AN2/Acy	+	+	+	-	-	+	+	+
PCT TP 9-d	+	+	-	-	ArNacyl	ArNacyl/H	-	AN2/Acy	+	+	Inc.	-	+	+	+	+

Legends: **VEGA HUB A**: Mutagenicity (Ames test) model (CAESAR); **VEGA HUB B**: Mutagenicity (Ames test) model (ISS); **VEGA HUB C**: Mutagenicity (Ames test) model (KNN/Read-Across); **VEGA HUB D**: Mutagenicity (Ames test) model (SarPy/IRFMN) (version 1.0.7); **VEGA HUB E**: Carcinogenicity model (CAESAR); **VEGA HUB F**: IRFMN\_Antares; **VEGA HUB G**: Carcinogenicity model (IRFMN\_ISSCAN-CGX); **VEGA HUB H**: Carcinogenicity model (ISS); **QSAR TOOLBOX A**: in vivo mutagenicity (Ames Test) alerts by ISS; **QSAR TOOLBOX B**: in vivo mutagenicity (Micronucleus) alerts by ISS; **QSAR TOOLBOX C**: DNA alerts for AMES, CA and MNT by OASIS; **QSAR TOOLBOX D**: Protein binding alerts for Chromosomal aberration by OASIS; **QSAR TOOLBOX E**: Carcinogenicity (genotox and nongenotox) alerts by ISS; **CASEULTRA A**: GT1\_BMUT; **CASEULTRA B**: GT\_EXPERT; **CASEULTRA C**: PHARM\_BMUT.

**Alerts:** (+) Positive alerts; (-) negative Alerts; ( $\alpha$ - $\beta$ )  $\alpha$ - $\beta$ -unsaturated carbonyls; (1-PB) 1-phenoxy-benzene; (AB) Alkenyl benzenes; (Acy) Acylation; (AH) Aliphatic halogens; (AN2) Addition Nucleophile 2 - Michael-type addition to quinoid structures; (ArNacyl) Aromatic N-acyl amine; (H) Hacceptor-path3-Hacceptor; (N-Me) N-methylol derivatives; (NiAr) Nitro aromatic; (R) Radical mechanism via ROS formation (indirect); (SiAi): Simple aldehyde; (SN1): Substitution Nucleophile 1- Nucleophilic attack after reduction and nitrenium ion.



**Text S5.** Structure alerts for biodegradability or non-biodegradability TPs.



**Figure S8.** Structure alerts for non-biodegradable compounds: in red (nitroaromatic); in green (halogens); in blue (1,4-diethylbenzene moiety). Structure alerts for biodegradable compounds: in Orange (1,4-diethylbenzene moiety).

