Probabilistic Approach to Generating MPOs and Its Application as a Scoring Function for CNS Drugs

Hakan Gunaydin

Department of Structural Chemistry, Merck & Co., Inc., 33 Avenue Louis Pasteur, Boston, MA, 02115, United States

The term brain penetrant drugs refers to drugs that interact with the targets that are expressed in the central nervous system or in the brain or have been shown to partition into the brain or central nervous system in the literature. The list of drugs used in this manuscript was compiled by starting with the FDA approved drug molecules that have molecular weights less than 850 and TPSA values less than 200. In addition, all prodrugs were removed from the dataset and the remainder of the FDA approved drugs was clustered to remove very similar drug molecules from the dataset. In this stage, only the cluster centers were selected from each drug cluster. This allowed the dataset to be diverse and representative of the drug space (for example by removing all structurally similar but one antibiotic from the dataset.) After this stage, a literature search on all of the drug molecules that are not approved for a CNS indication was conducted to see if there is any literature precedence for CNS exposure. This resulted in a dataset of 299 brain penetrant drugs and 366 drugs that haven't been reported to get into the brain or CNS.

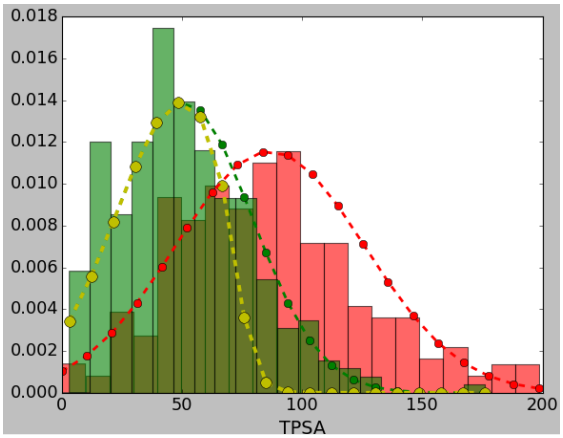
The Bayesian model that was used to compare the accuracy of the results obtained from pMPO algorithm relative to more elaborate models is a two-class Bayesian categorization model based on molecular descriptors as implemented in pipeline pilot program by Biovia.

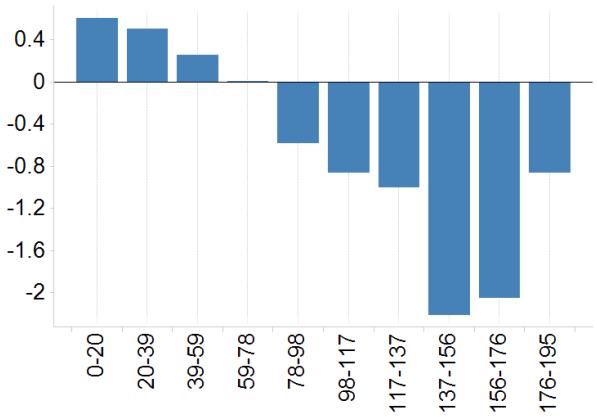
500 diverse molecules with PGP data was selected by querying Merck database for molecules with measured PGP data. Compound with passive permeabilities less than 10 nm/s and efflux ratio >=3 in the parental cell lines were removed from this list. After that, 500 diverse molecules were selected by using the pipeline pilot component for selecting diverse molecules by using properties FCFP_6, Molecular Weight, number of hydrogen bond donors and TPSA. This selection was biased towards picking molecules that had had equal distribution of molecules with effective PGP ratios <=2 (175 molecules), between 2 and 10 (166 molecules) and greater than 10 (159 molecules).

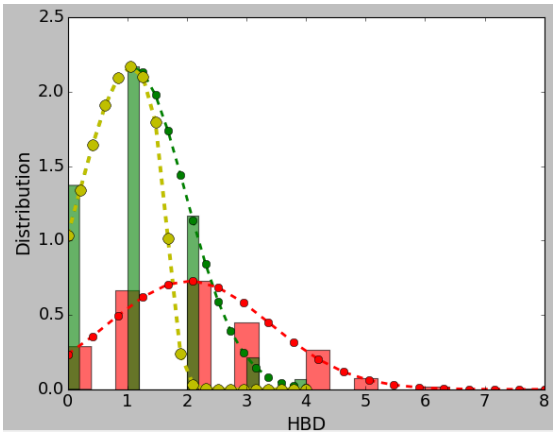
Table S1: Descriptors and the parameters used for equation 2 and probability distributions for the desirability function in pMPO.

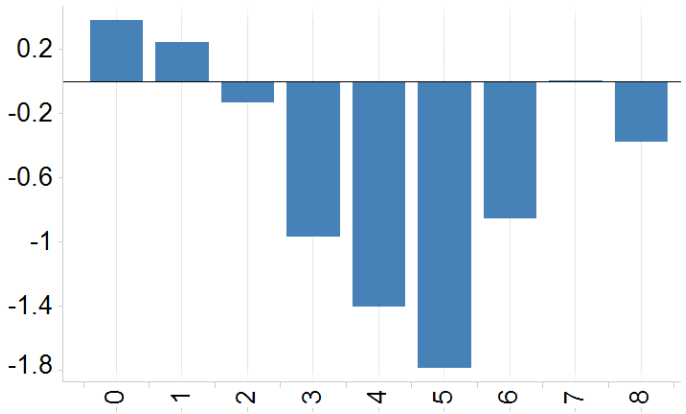
Descriptor	$\bar{x}_d$	σ_d	$\bar{x}_{nd}$	σ_{nd}	*x*	*b*	*c*
TPSA	51	28	87	39	66	0.152	0.794
HBD	1	1	2	1.4	1.5	0.094	9.52E-5
MW	305	94	399	136	328	0.032	0.913
cLogD_ACD_v15	1.8	1.9	0.8	2.8	1.4	0.021	1.32E+5
bmpKa	8.1	2.2	7.2	2.7	7.7	1.73E-2	1.46E+6

Figure S2: comparison between pMPO desirability functions and Bayesian probabilities for all 5 descriptors.









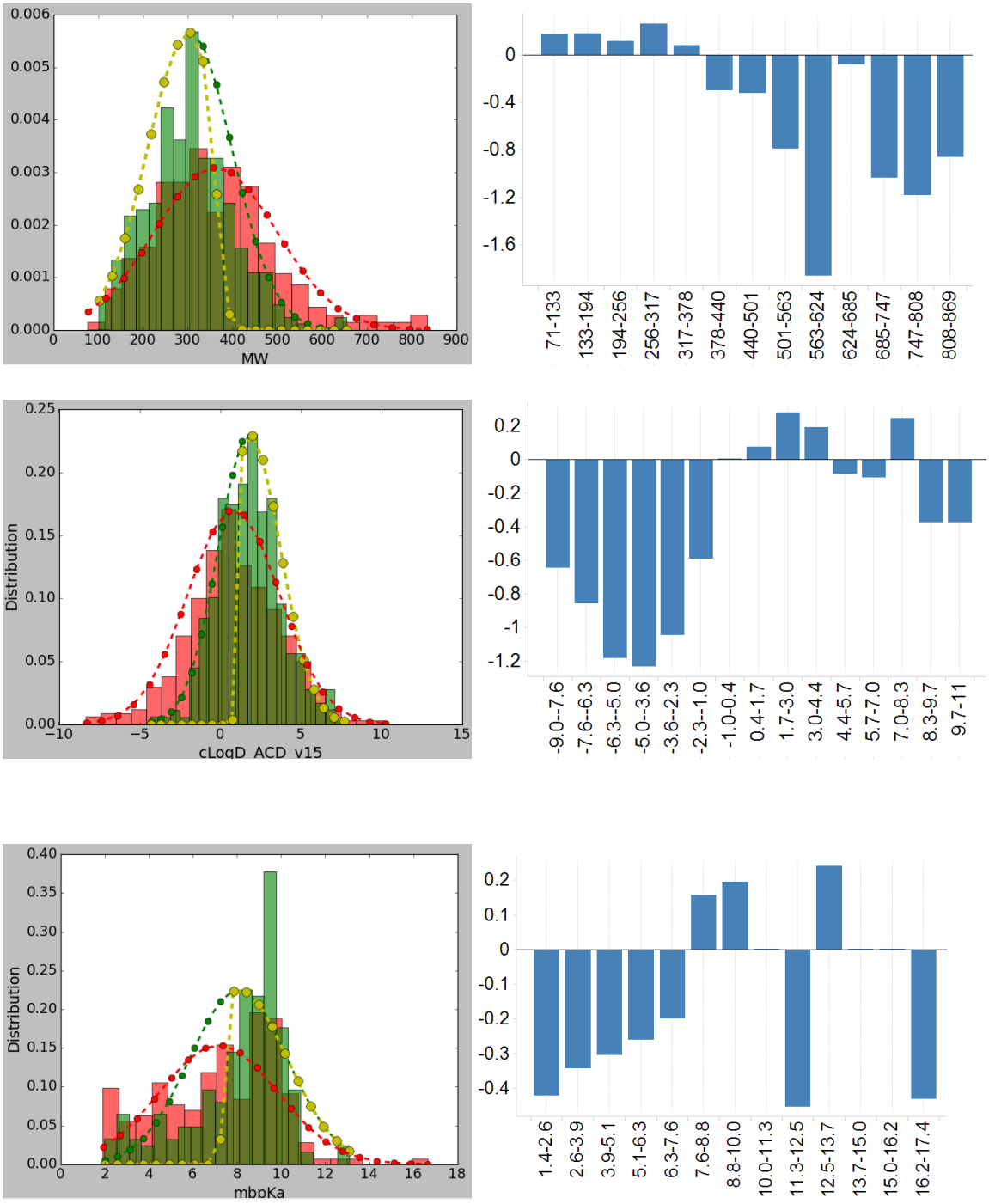


Figure S3: Comparison of the CNS MPO (along x-axis) and $pMPO_{CNS}$ scores (along y-axis) for 500 molecules with measured efflux ratios.

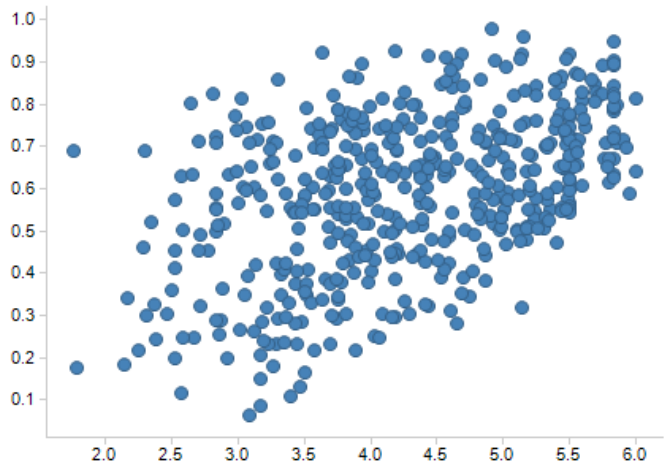


Figure S4: $pMPO_{CNS}$ against rPgp effective efflux ratio on the left and CNS MPO against rPgp effective efflux ratio on the right.

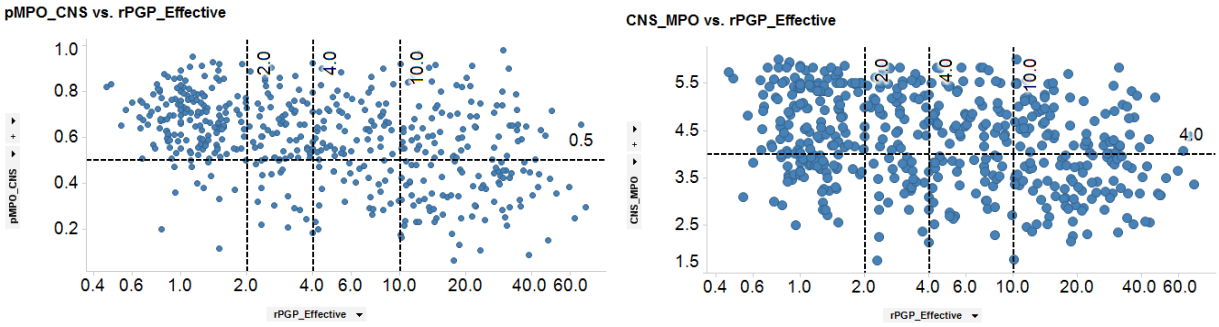
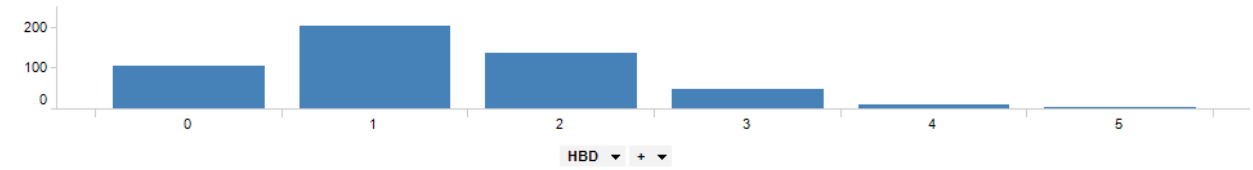
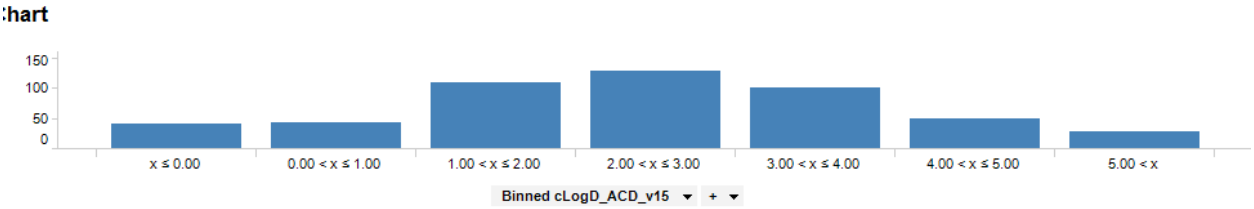
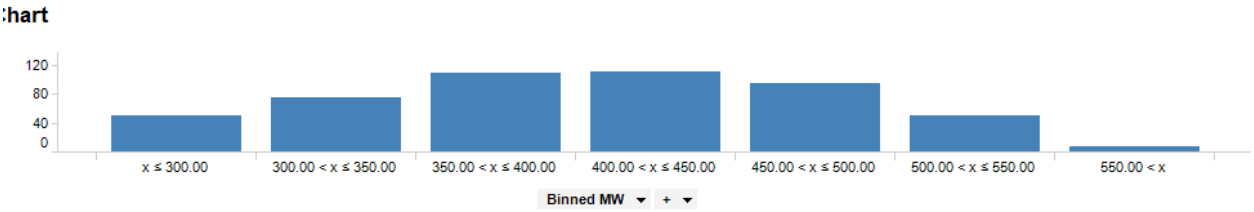
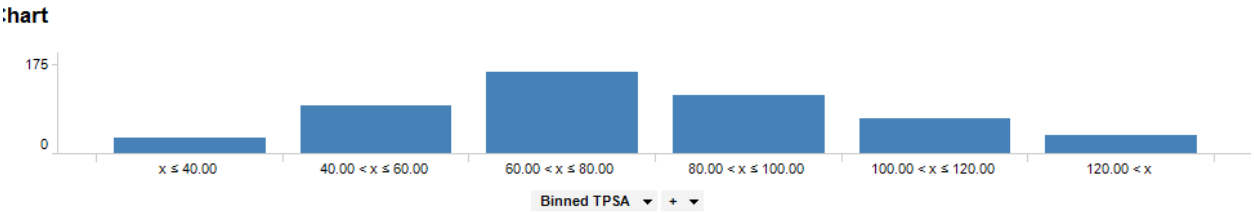


Figure S5: Property distributions for the 500 molecules with measured efflux ratios.









Python script for plotting distributions of CNS and non-CNS drugs:

```
#!/usr/bin/env python

import random
import sys
import matplotlib.pyplot as plt
import numpy
import scipy
from scipy.stats import norm

rn_cutoff = 1.0
q_cutoff = 0.05

def fitfn(x, p0, p1, p2):
   return p0*numpy.exp(-(x-p1)**2/(2.*p2**2))

def sigfn(x, x0, b, c):
   return 1.0/(1.0+b*numpy.power(c,-1.0*(x-x0)))

def findhistmax(x, y, meanvalue):
   n = -1
   for i in range(len(x)):
     n += 1
     if x[i] > meanvalue: break
   return max([y[n], y[n-1], y[n+1]])

def find_cutoff(desired, notdesired):
   '''pass the arrays in the form of [mean, std] for the desired and notdesired groups
      return an array in this form of [cutoff_intercept, cutoff_pref, cutoff_notpref, std_pref, std_notpref]'''
   if desired[0] < notdesired[0]:
      cutoff = ((notdesired[0]-desired[0])/(desired[1]+notdesired[1]))*desired[1]+desired[0]
      cutoff_pref    = max(desired[0], notdesired[0]-notdesired[1])
      cutoff_notpref = max(desired[0]+desired[1], notdesired[0])
      std_pref = desired[1]
      std_not = notdesired[1]
   else:
      cutoff = ((desired[0]-notdesired[0])/(desired[1]+notdesired[1]))*notdesired[1]+notdesired[0]
      cutoff_pref    = min(notdesired[0]+notdesired[1], desired[0])
      cutoff_notpref = max(notdesired[0], desired[0]-desired[1])
   return [cutoff, cutoff_pref, cutoff_notpref, desired[1], notdesired[1]]

def sigmoidal_fn(boundaries):
   '''                1
        f(x) = --------------------
                        -1(x-<x>)
                  1 + b c
      when c > 1, it starts from 0 and goes up to 1
      when 0 < c < 1, it starts from 1 and goes down to 0
```

```
      inflection point is 1/(1+b)
      slope is related to the magnitude of c'''
   global q_cutoff
   if boundaries[1] < boundaries[2]:
      inf_point_y = fitfn(boundaries[0], 1.0, boundaries[1], boundaries[3])
      b = 1./inf_point_y - 1.0
      n = 1.0/q_cutoff - 1.0
      c = numpy.power(10.0, ((numpy.log10(n/b))/(-1.0*(boundaries[2]-boundaries[0]))))
   elif boundaries[1] > boundaries[2]:
      inf_point_y = fitfn(boundaries[0], 1.0, boundaries[1], boundaries[3])
      b = 1./inf_point_y - 1.0
      n = 1.0/q_cutoff - 1.0
      c = numpy.power(10.0, ((numpy.log10(n/b))/(-1.0*(boundaries[2]-boundaries[0]))))
   return [b, c]


fin = open('drugs_props.txt','r')
line = fin.readline()
line = line.replace('\n','')
header = line.split('\t')

#n_column = [y for y, x in enumerate(header) if (x == 'MW')][0]
n_column = [y for y, x in enumerate(header) if (x == 'TPSA')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'TPSA_S')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'cLogD_ACD_v15')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'cLogP_ACD_v15')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'mbpKa')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'mapKa')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'HBA')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'HBD')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'cLogP_Biobyte')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'ALogP98')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'nAtoms')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'nArom')][0]
#n_column = [y for y, x in enumerate(header) if (x == 'fsp3')][0]

cns = []
notcns = []

while 1:
   line = fin.readline()
   if not line: break
   line = line.replace('\n','')
   line = line.split('\t')
   if line[1] == 'TRUE' and int(line[[y for y, x in enumerate(header) if (x == 'nAtoms')][0]]) > 5:
      try:
         if random.random() <= rn_cutoff:
            cns.append(float(line[n_column]))
      except:
         pass
   elif line[1] == 'FALSE' and int(line[[y for y, x in enumerate(header) if (x == 'nAtoms')][0]]) > 5:
      try:
         if random.random() <= rn_cutoff:
            notcns.append(float(line[n_column]))
      except:
         pass

print 'Stats for descriptor: %s' % (header[n_column])
print 'p-value: %.2e (%.4f)' % (scipy.stats.ttest_ind(cns, notcns, equal_var=False)[1], scipy.stats.ttest_ind(cns, notcns, equal_var=False)[1])
print '%s:\t%.3f +/- %.3f' % ('for CNS drugs    ', numpy.mean(cns), numpy.std(cns))
print '%s:\t%.3f +/- %.3f' % ('for non-CNS drugs', numpy.mean(notcns), numpy.std(notcns))

print ''
print 'len(cns)   :', len(cns)
print 'len(notcns):', len(notcns)
print ''

cutoffs = find_cutoff([numpy.mean(cns), numpy.std(cns)], [numpy.mean(notcns), numpy.std(notcns)])
print 'cutoff: %.3f\t<x_d>: %.3f\t<x_und>: %.3f\tstd_d: %.3f\tstd_und: %.3f' % (cutoffs[0], cutoffs[1], cutoffs[2], cutoffs[3], cutoffs[4])
sig_fn_coeff = sigmoidal_fn(cutoffs)
print 'b: %.2e\tc: %.2e' % (sig_fn_coeff[0], sig_fn_coeff[1])

a, b, c = plt.hist(notcns, color='r', alpha=0.6, bins=20, normed=True)
y, x, p = plt.hist(cns, color='g', alpha=0.6, bins=20, normed=True)
x = numpy.linspace(min(x), max(x), len(y))
b = numpy.linspace(min(b), max(b), len(a))

pdf = fitfn(x, findhistmax(x, y, numpy.mean(cns)), numpy.mean(cns), numpy.std(cns))
plt.plot(x, pdf, 'k', linewidth=2.5, color='g',linestyle='--', marker='o', markersize=8)
pdf3 = []
for i in range(len(pdf)):
   pdf3.append(pdf[i]*sigfn(x[i], cutoffs[0], sig_fn_coeff[0], sig_fn_coeff[1]))
plt.plot(x, pdf3, 'k', linewidth=3.5, color='y',linestyle='--', marker='o', markersize=10)

pdf2 = fitfn(b, findhistmax(b, a, numpy.mean(notcns)), numpy.mean(notcns), numpy.std(notcns))
plt.plot(b, pdf2, 'k', linewidth=2.5, color='r',linestyle='--', marker='o', markersize=8)

plt.xlabel(header[n_column], size='x-large')
plt.ylabel('Distribution', size='x-large')
plt.tick_params(axis='both', which='major', labelsize=16)

plt.show()
```

Python script for plotting determining uncorrelated descriptors for pMPO generation:

```
#!/usr/bin/env python

import random
import sys
import numpy
import scipy
from scipy.stats import norm
from operator import itemgetter, attrgetter

rn_cutoff = 1.0
q_cutoff = 0.05
r2_cutoff = 0.53
pval_cutoff = 0.01
```

```
def fitfn(x, p0, p1, p2):
   return p0*numpy.exp(-(x-p1)**2/(2.*p2**2))

def sigfn(x, x0, b, c):
   return 1.0/(1.0+b*numpy.power(c,-1.0*(x-x0)))

def findhistmax(x, y, meanvalue):
   n = -1
   for i in range(len(x)):
     n += 1
     if x[i] > meanvalue: break
   return max([y[n], y[n-1], y[n+1]])

def find_cutoff(desired, notdesired):
   '''pass the arrays in the form of [mean, std] for the desired and notdesired groups
      return an array in this form of [cutoff_intercept, cutoff_pref, cutoff_notpref, std_pref, std_notpref]'''
   if desired[0] < notdesired[0]:
      cutoff = ((notdesired[0]-desired[0])/(desired[1]+notdesired[1]))*desired[1]+desired[0]
      cutoff_pref    = max(desired[0], notdesired[0]-notdesired[1])
      cutoff_notpref = max(desired[0]+desired[1], notdesired[0])
      std_pref = desired[1]
      std_not = notdesired[1]
   else:
      cutoff = ((desired[0]-notdesired[0])/(desired[1]+notdesired[1]))*notdesired[1]+notdesired[0]
      cutoff_pref    = min(notdesired[0]+notdesired[1], desired[0])
      cutoff_notpref = max(notdesired[0], desired[0]-desired[1])
   return [cutoff, cutoff_pref, cutoff_notpref, desired[1], notdesired[1]]

def sigmoidal_fn(boundaries):
   '''                  1
        f(x) = --------------------
                        -1(x-<x>)
                 1 + b c
      when c > 1, it starts from 0 and goes up to 1
      when 0 < c < 1, it starts from 1 and goes down to 0
      inflection point is 1/(1+b)
      slope is related to the magnitude of c'''
   global q_cutoff
   if boundaries[1] < boundaries[2]:
      inf_point_y = fitfn(boundaries[0], 1.0, boundaries[1], boundaries[3])
      b = 1./inf_point_y - 1.0
      n = 1.0/q_cutoff - 1.0
      c = numpy.power(10.0, ((numpy.log10(n/b))/(-1.0*(boundaries[2]-boundaries[0]))))
   elif boundaries[1] > boundaries[2]:
      inf_point_y = fitfn(boundaries[0], 1.0, boundaries[1], boundaries[3])
      b = 1./inf_point_y - 1.0
      n = 1.0/q_cutoff - 1.0
      c = numpy.power(10.0, ((numpy.log10(n/b))/(-1.0*(boundaries[2]-boundaries[0]))))
   return [b, c]

def findr2(x, y):
    correlation = numpy.corrcoef(x, y)[0,1]
    return correlation**2

fin = open('drugs_props.txt','r')
line = fin.readline()
line = line.replace('\n','')
header = line.split('\t')

desired = []
notdesired = []
cluster = []

while 1:
   line = fin.readline()
   if not line: break
   line = line.replace('\n','')
   line = line.split('\t')
   cluster_num = int(line[[y for y, x in enumerate(header) if (x == 'Cluster')][0]])
   if cluster_num not in cluster:
#     cluster.append(cluster_num)
     if line[1] == 'TRUE':
        if random.random() <= rn_cutoff:
           desired.append(line[2:16])
     elif line[1] == 'FALSE':
        if random.random() <= rn_cutoff:
           notdesired.append(line[2:16])
   else:
      pass

descs = header[2:16]
statistics = []

for i in range(len(descs)):
   cns = []
   notcns = []
   for j in range(len(desired)):
      try:
         cns.append(float(desired[j][i]))
      except:
         pass
   for j in range(len(notdesired)):
      try:
         notcns.append(float(notdesired[j][i]))
      except:
         pass
   pval = scipy.stats.ttest_ind(cns, notcns, equal_var=False)[1]
   statistics.append([descs[i], pval, numpy.mean(cns), numpy.std(cns), numpy.mean(notcns), numpy.std(notcns), len(cns), len(notcns)])

statistics = sorted(statistics, key=itemgetter(1))

corr_matrix = [[0 for xx in range(len(statistics))] for xx in range(len(statistics))]
for m in range(len(statistics)):
   for n in range(len(statistics)-1-m):
      n1 = [y for y, x in enumerate(descs) if (x == statistics[m][0])][0]
      n2 = [y for y, x in enumerate(descs) if (x == statistics[m+n+1][0])][0]
      des1 = []
      des2 = []
      for i in range(len(desired)):
         if desired[i][n1] != '' and desired[i][n2]:
            des1.append(float(desired[i][n1]))
            des2.append(float(desired[i][n2]))
```

```
      for i in range(len(notdesired)):
         if notdesired[i][n1] != '' and notdesired[i][n2]:
            des1.append(float(notdesired[i][n1]))
            des2.append(float(notdesired[i][n2]))
      corr_matrix[m][m+n+1] = findr2(des1, des2)
      corr_matrix[m+n+1][m] = corr_matrix[m][m+n+1]

print '--- All Descriptors ---'
for i in range(len(statistics)):
       print '%-15s\t%.2e\t%.2f\t%.2f\t%.2f\t%.2f\t%i\t%i' % \
       (statistics[i][0], statistics[i][1], statistics[i][2], \
       statistics[i][3], statistics[i][4], statistics[i][5], statistics[i][6], statistics[i][7])

print '--- Chosen Descriptors ---'

chosen_desc = []
for i in range(len(statistics)):
  for j in range(len(statistics)-i):
    if corr_matrix[i][j+i] < r2_cutoff and (i+j) not in chosen_desc and statistics[i+j][1] < pval_cutoff:
      q = True
      if len(chosen_desc)>0:
         for k in chosen_desc:
            if corr_matrix[k][i+j] >= r2_cutoff:
               q = False
      if q is True:
         chosen_desc.append(i+j)

for i in range(len(statistics)):
   if i in chosen_desc:
      print '%-15s\t%.2e\t%.2f\t%.2f\t%.2f\t%.2f\t%i\t%i' % \
      (statistics[i][0], statistics[i][1], statistics[i][2], \
      statistics[i][3], statistics[i][4], statistics[i][5], statistics[i][6], statistics[i][7])

print '--- Correlation Matrix ---'

for i in range(len(corr_matrix)):
    print '%-15s\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f\t%.2f' % (statistics[i][0], \
       corr_matrix[i][0], corr_matrix[i][1], corr_matrix[i][2], corr_matrix[i][3], \
       corr_matrix[i][4], corr_matrix[i][5], corr_matrix[i][6], corr_matrix[i][7], \
       corr_matrix[i][8], corr_matrix[i][8], corr_matrix[i][10], corr_matrix[i][11])

print '--- cutoffs and desirablity functions parameters ---'
print 'Desc           \tCutoff\tx_des\tx_undes\ts_des\ts_udes\tb\tc\tZ-score\tw'

z_scores = []

for i in chosen_desc:
   cns = []
   notcns = []
   n = [y for y, x in enumerate(descs) if (x == statistics[i][0])][0]
   for j in desired:
      try:
         cns.append(float(j[n]))
      except:
         pass
   for j in notdesired:
      try:
         notcns.append(float(j[n]))
      except:
         pass
   cutoffs = find_cutoff([numpy.mean(cns), numpy.std(cns)], [numpy.mean(notcns), numpy.std(notcns)])
   sig_fn_coeff = sigmoidal_fn(cutoffs)
   z_scores.append([header[n+2], cutoffs[0], cutoffs[1], cutoffs[2], cutoffs[3], cutoffs[4], sig_fn_coeff[0], sig_fn_coeff[1], numpy.absolute(cutoffs[0]-
cutoffs[1])/cutoffs[3], 0])
w_sum = 0
for i in z_scores:
   w_sum = w_sum + i[8]
for i in z_scores:
   print '%-15s\t%.3f\t%.3f\t%.3f\t%.3f\t%.3e\t%.3e\t%.2f\t%.3f' % (i[0], i[1], i[2], i[3], i[4], i[5], i[6], i[7], i[8], i[8]/w_sum)
```

FDA approved drugs used as a training set for the $pMPO_{CNS}$:

Drug	CNS	TPSA	TPSA_S	HBA	HBD	MW	nAtoms	cLogD_ACD_v15		mapKa	cLogP_Biobyte	
	mbpKa	cLogP_ACD_v15		ALogP98	fsp3	nArom	Smiles					
Abacavir	FALSE	101.88	101.88	6	3	286.33232	21	0.72		0.81	6.53	0.72
	0.63	0.5	2	n3c1c(ncn1[C@H]2/C=C\[C@@H](CO)C2)c(nc3N)NC4CC4								
Acetohexamide		FALSE	92.34	100.72	4	2	324.39529	22	0.46	4.3	2.25	
	2.44	2.119	0.47	1	O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(C(=O)C)cc2							
Acetyldigitoxin		FALSE	188.9	188.9	14	4	806.97574	57	3.1		3.46	
	3.1	3.48	0.91	0								
	O=C\1OC/C(=C/1)[C@H]2CC[C@@]8(O)[C@]2(C)CC[C@H]7[C@H]8CC[C@H]6[C@]7(C)CC[C@H](O[C@@H]5O[C@@H]([C@@H](O[C@@H]4O[C@@H]([C@@H](O[C@@H]3O[C@H](C)[C
@@H](O)[C@@H](OC(=O)C)C3)[C@@H](O)C4)C)[C@@H](O)C5)C)C6											
Acrivastine	FALSE	53.43	53.43	4	1	348.43816	26	2.03		1.46	8.88	4.55
	4.601	0.27	2	O=C(O)\C=C\c3nc(\C(=C\CN1CCCC1)c2ccc(cc2)C)ccc3								
Acyclovir	FALSE	114.76	114.76	7	3	225.20464	16	-1.76		-2.6	3.15	-1.76
	-1.423	0.38	1	O=C2/N=C(\Nc1n(cnc12)COCCO)N								
Adefovir	FALSE	146.19	146.19	8	3	273.18574	18	-5.96	2.1	-1.87	4.32	-2.06
	-1.289	0.38	2	O=P(O)(O)COCCn1c2ncnc(c2nc1)N								
Albuterol	FALSE	72.72	72.72	4	4	239.31073	17	-2.12		0.06		0.01
	0.941	0.54	1	OCc1cc(ccc1O)C(O)CNC(C)(C)C								
Alendronate	FALSE	180.92	180.92	8	6	249.09604	14	-7.91	1.42	-5.64	10.31	-3.52
	-1.203	1	0	O=P(O)(O)C(O)(CCCN)P(=O)(O)O								
Alfuzosin	FALSE	111.83	111.83	8	2	389.44877	28	-1.91		2.55	8.6	-1
	1.418	0.53	2	O=C(NCCCN(c2nc1cc(OC)c(OC)cc1c(n2)N)C)C3OCCC3								
Aliskiren	FALSE	146.13	146.13	7	4	551.75831	39	0.07		3.51	9.78	2.74
	3.327	0.73	1	O=C(N)C(C)(C)CNC(=O)[C@H](C(C)C)C[C@H](O)[C@@H](N)C[C@@H](C(C)C)Cc1cc(OCCCOC)c(OC)cc1								
Allopurinol	FALSE	74.69	74.69	4	2	136.11146	10	-4.29	1.12	0.63	10.06	-1.33
	5.10E-02	0	2	c1c2c([nH]n1)ncnc2O								
Alogliptin	FALSE	93.66	93.66	5	1	339.39163	25	-0.48		1.54	9.89	1.84
	1.795	0.39	1	N#Cc3ccccc3CN\1C(=O)N(C)C(=O)/C=C/1N2CCC[C@@H](N)C2								
Alosetron	FALSE	53.92	53.92	2	1	294.35101	22	0.72		1.74	7	0.88
	1.654	0.29	3	O=C1N(CCc3c1c2ccccc2n3C)Cc4ncnc4C								
Altretamine	FALSE	48.39	48.39	6	0	210.27941	15	2.32		1.67	6.07	2.42
	1.995	0.67	1	n1c(nc(nc1N(C)C)N(C)C)N(C)C								
Alvimopan	FALSE	89.87	89.87	5	3	424.53257	31	0.74	3.43	2.16	8.84	3.38
	3.545	0.44	2	O=C(O)CNC(=O)[C@@H](Cc1ccccc1)CN3CC[C@@](c2cccc(O)c2)([C@H](C)C)C								
Ambenonium	FALSE	58.2	58.2	2	2	537.56467	36	-2.85		0.18		-2.85
	2.186	0.5	2	Clc1ccccc1C[N+](CC)(CC)CCNC(=O)C(=O)NCC[N+](CC2ccccc2Cl)(CC)CC								

Ambrisentan	FALSE	81.54	81.54	6	1	378.42108	28	2.51	0.97	3.75	2.84	6.24
3.659	0.23	3	O=C(O)[C@@H](Oc1nc(cc(n1)C)C)C(OC)(c2ccccc2)c3ccccc3									
Amiloride	FALSE	159.29	159.29	8	4	229.62702	15	2.9		-2.22	2.29	2.9
-0.748	0	1	Clc1nc(C(=O)\N=C(/N)N)c(nc1N)N									
Aminocaproic acid	FALSE	63.31	63.31	3	2	131.17292	9	-2.61	4.68	-2.23	10.63	
-0.11	0.315	0.83	0	C(CCC(=O)O)CCN								
Aminosalicylic acid	FALSE	83.55	83.55	4	3	153.13538	11	-2	3.58	1.06	2.21	
1.14	0.471	0	1	O=C(O)c1ccc(cc1O)N								
Amoxicillin	FALSE	132.96	158.26	7	4	365.40416	25	-2.58	2.44	-1.87	6.67	0.61
-6.00E-02	0.44	1	O=C(O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@@H](c1ccc(O)cc1)N)[C@H]3SC2(C)C									
Amprenavir	FALSE	131.19	139.57	7	3	505.62689	35	4.2		3.29		4.2
2.429	0.48	2	O=C(O[C@H]1CCOC1)N[C@@H](Cc2ccccc2)[C@H](O)CN(CC(C)C)S(=O)(=O)c3ccc(N)cc3									
Anagrelide	FALSE	44.7	44.7	4	1	256.08808	16	1.96		1.8	2.08	1.96
1.965	0.2	1	Clc1ccc3c(c1Cl)CN2/C(=N\C(=O)C2)N3									
Anastrozole	FALSE	78.29	78.29	4	0	293.36625	22	0.97		1.48	2.62	0.97
2.965	0.41	2	N#CC(c1cc(cc(c1)C(C#N)(C)C)Cn2ncnc2)(C)C									
Anisindione	FALSE	43.37	43.37	3	0	252.26468	19	3.19		2.73		3.21
2.803	0.12	2	O=C2c1ccccc1C(=O)C2c3ccc(OC)cc3									
Anisotropine		FALSE	26.3	26.3	2	0	282.44148	20	0.43		-0.82	
0.43	2.249	0.94	0	[C@H]12[N+](CC(C1)OC(C(CCC)CCC)=O)CC2)(C)C								
Apixaban	FALSE	110.76	110.76	5	1	459.49709	34	0.48		1.89		0.48
2.865	0.28	3	O=C5N(c4ccc(N3C(=O)c1c(c(nn1c2ccc(OC)cc2)C(=O)N)CC3)cc4)CCCC5									
Aspirin	FALSE	63.6	63.6	4	1	180.15742	13	-1.89	3.48	1.02		1.19
1.227	0.11	1	O=C(Oc1ccccc1C(=O)O)C									
Astemizole	FALSE	42.32	42.32	4	1	458.57034	34	4.41		5.84	8.77	5.8
5.689	0.32	4	Fc1ccc(cc1)Cn2c5ccccc5nc2NC4CCN(CCc3ccc(OC)cc3)CC4									
Atazanavir	FALSE	171.21	171.21	9	5	704.85548	51	5.2		5.92	4.65	5.2
5.078	0.45	3	O=C(OC)N[C@H](C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)CN(NC(=O)[C@@H](NC(=O)OC)C(C)(C)C)Cc3ccc(c2ncccc2)cc3)C(C)(C)C									
Atenolol	FALSE	84.58	84.58	4	3	266.33608	19	-1.99		-0.11	9.45	0.1
0.669	0.5	1	O=C(N)Cc1ccc(OCC(O)CNC(C)C)cc1									
Atorvastatin		FALSE	111.79	111.79	5	4	558.6398	41	1.03	4.29	4.46	
4.13	5.556	0.27	4	O=C(O)C[C@H](O)C[C@H](O)CCn2c(c(c(c2c1ccc(F)cc1)c3ccccc3)C(=O)Nc4ccccc4)C(C)C								
Atovaquone	FALSE	54.37	54.37	3	1	366.83746	26	3.82	4.99	6.35		6.17
5.319	0.27	2	OC=2C(=O)c1ccccc1C(=O)C=2[C@@H]3CC[C@H](CC3)c4ccc(Cl)cc4									
Avanafil	FALSE	125.39	125.39	9	3	483.95064	34	3.5		2.91	6.73	3.52
2.165	0.35	3	Clc1c(OC)ccc(c1)CNc3nc(ncc3C(=O)NCc2ncccn2)N4[C@@H](CCC4)CO									
Azathioprine		FALSE	118.1	143.39	7	1	277.26257	19	0.63	7.73	0.51	
0.67	0.934	0.11	3	[O-][N+](=O)c3ncn(c3Sc1ncnc2ncnc12)C								
Azilsartan	FALSE	139.57	139.57	11	1	568.53355	42	5.72		4.61	5.25	5.73
5.27	0.17	4	O=C1O/C(=C(\O1)C)COC(=O)c3cccc2nc(OCC)n(c23)Cc6ccc(c5ccccc5C\4=N\C(=O)ON/4)cc6									
Azithromycin		FALSE	180.08	180.08	14	5	748.98448	52	1.4		2.64	8.59
3.33	2.078	0.97	0	CN(C)[C@H]3C[C@@H](C)O[C@@H](O[C@@H]2[C@@H](C)[C@H](O[C@H]1C[C@@](C)(OC)[C@@H](O)[C@H](C)O1)[C@@H](C)C(=O)O[C@H](C)[C@H](O)[C@@H](C)C(=O)N(C)C[C@H](C)C[C@@]2(C)O)[C@@H]3O									
Balsalazide	FALSE	148.64	148.64	8	4	357.31749	26	-2.04	2.97	3.21		2.7
2.525	0.12	2	O=C(O)c1cc(ccc1O)/N=N/c2ccc(cc2)C(=O)NCCC(O)=O									
Bedaquiline	FALSE	45.59	45.59	4	1	555.50474	37	6.05		7.25	9.31	7.59
6.933	0.22	5	Brc1ccc2nc(OC)c(ccc2c1)[C@@H](c3ccccc3)[C@](O)(c5c4ccccc4ccc5)CCN(C)C									
Benazepril	FALSE	95.94	95.94	6	2	424.48951	31	0.32	3.73	1.82	4.55	3.86
3.326	0.38	2	O=C(OCC)[C@@H](N[C@@H]2C(=O)N(c1ccccc1CC2)CC(=O)O)CCc3ccccc3									
Bendroflumethiazide		FALSE	118.36	135.12	5	3	421.41456	27	2.04		1.73	
2.07	1.861	0.2	2	FC(F)(F)c3c(cc1c(NC(NS1(=O)=O)Cc2ccccc2)c3)S(=O)(=O)N								
Bentiromide	FALSE	115.73	115.73	5	4	404.4153	30	0.6	4.27	2.96		3.46
3.102	0.09	3	O=C(O)c1ccc(cc1)NC(=O)[C@@H](NC(=O)c2ccccc2)Cc3ccc(O)cc3									
Betamethasone		FALSE	94.83	94.83	5	3	392.46106	28	1.87		1.78	
1.87	1.708	0.73	0	O=C(CO)[C@]3(O)[C@]2(C[C@H](O)[C@]4(F)[C@@]/1(\C(=C/C(=O)\C=C\1)CC[C@H]4[C@@H]2C[C@@H]3C)C)C								
Betaxolol	FALSE	50.72	50.72	4	2	307.42775	22	0.59		2.32	9.45	2.69
2.577	0.67	1	O(CCc1ccc(OCC(O)CNC(C)C)cc1)CC2CC2									
Bethanechol	FALSE	52.32	52.32	2	1	161.22208	11	-3.95		-4.01		-3.95
-1.028	0.86	0	O=C(OC(C)C[N+](C)(C)C)N									
Bicalutamide		FALSE	107.26	115.63	5	2	430.37337	29	4.94		2.71	
4.94	2.926	0.22	2	O=C(Nc1cc(c(C#N)cc1)C(F)(F)F)C(O)(C)CS(=O)(=O)c2ccc(F)cc2								
Bisoprolol	FALSE	59.95	59.95	5	2	325.44304	23	0.05		1.83	9.44	2.14
2.031	0.67	1	O(c1ccc(cc1)COCCOC(C)C)CC(O)CNC(C)C									
Boceprevir	FALSE	150.7	150.7	5	4	519.6767	37	2.05		3.34		2.05
1.623	0.81	0	O=C(N3[C@H](C(=O)NC(C(=O)C(=O)N)CC1CCC1)[C@H]2C(C)([C@H]2C3)C)[C@@H](NC(=O)NC(C)(C)C)C(C)(C)C									
Bosentan	FALSE	145.65	154.02	10	2	551.61406	39	-0.85	4.64	4.17		1.15
3.948	0.26	4	CC(C)(C)c1ccc(cc1)S(=O)(=O)Nc2c(c(nc(n2)c3ncccn3)OCCO)OC4ccccc4OC									
Bosutinib	FALSE	82.88	82.88	8	1	530.44615	36	4.93		5.09	8.32	5.48
4.883	0.38	3	Clc1c(OC)cc(c(Cl)c1)Nc4c(C#N)cnc3cc(OCCCN2CCN(CC2)C)c(OC)cc34									
Budesonide	FALSE	93.06	93.06	6	2	430.53385	31	3.14		2.9		3.14
2.198	0.76	0	O=C(CO)[C@]25O[C@@H](O[C@@H]5C[C@H]1[C@H]4[C@H]([C@@H](O)C[C@@]12C)[C@]/3(/C=C\C(=O)\C=C\3CC4)C)CCC									
Bufuralol	FALSE	45.4	45.4	2	2	261.35932	19	1.3		3.4	9.71	3.38
3.219	0.5	2	OC(c2oc1c(cccc1c2)CC)CNC(C)(C)C									
Busulfan	FALSE	86.74	103.5	6	0	246.30176	14	-0.52		-0.59		-0.52
-0.289	1	0	O=S(=O)(OCCCCOS(=O)(=O)C)C									
Cabozantinib		FALSE	98.78	98.78	6	2	501.50566	37	4.82		4.94	6.2
4.84	4.342	0.18	4	O=C(C1(CC1)C(NC2=CC=C(F)C=C2)=O)NC(C=C3)=CC=C3OC4=C(C=C(OC)C(OC)=C5)C5=NC=C4								
Canagliflozin		FALSE	90.15	118.39	5	4	444.5157	31	5.34		4.55	
5.34	3.356	0.33	3	Cc1ccc(cc1Cc2ccc(s2)c3ccc(cc3)F)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O								
Capecitabine		FALSE	120.69	120.69	7	3	359.35008	25	-0.67	5.41	0.84	
0.97	0.82	0.67	0	FC=1\C(=N/C(=O)N(C=1)[C@@H]2O[C@@H]([C@@H](O)[C@H]2O)C)\NC(=O)OCCCCC								
Carbenicillin		FALSE	124.01	149.31	7	3	378.39962	26	-3.74	2.44	1.64	
1.01	0.73	0.41	1	O=C(O)[C@@H]2N3C(=O)[C@@H](NC(=O)C(c1ccccc1)C(=O)O)[C@H]3SC2(C)C								
Carbidopa	FALSE	115.81	115.81	6	5	226.22915	16	-2.75	3.4	-0.45	7.76	-0.19
0.752	0.3	1	O=C(O)[C@@](NN)(Cc1cc(O)c(O)cc1)C									
Carglumic acid		FALSE	129.72	129.72	5	4	190.15399	13	-6.74	3.71	-1.94	
-2	-1.169	0.5	0	C(CC(=O)O)[C@@H](C(=O)O)NC(=O)N								
Carprofen	FALSE	53.09	53.09	2	2	273.71427	19	1.55	4.84	3.98		4.04
4.114	0.13	3	O=C(O)C(c3ccc2c1ccc(Cl)ccc1nc2c3)C									
Carteolol	FALSE	70.59	70.59	4	3	292.37335	21	-0.73		1.29	9.74	1.35
1.282	0.56	1	O=C2Nc1cccc(OCC(O)CNC(C)(C)C)c1CC2									
Cefaclor	FALSE	112.73	138.03	6	3	367.80736	24	-3.05	1.95	-1.64	6.52	0.1
0.146	0.27	1	O=C2N1/C(=C(/Cl)CS[C@@H]1[C@@H]2NC(=O)[C@@H](c3ccccc3)N)C(=O)O									
Cefdinir	FALSE	158.2	211.75	9	4	395.41352	26	-4.36	2.82	-0.48		-0.62
4.10E-02	0.21	1	O=C2N1/C(=C(/C=C)CS[C@@H]1[C@@H]2NC(=O)C(=N\O)/c3nc(sc3)N)C(=O)O									
Cefditoren	FALSE	160.1	241.88	10	3	506.57841	33	-2.29	2.43	1.47	3.22	1.48
1.062	0.26	2	O=C3N2/C(=C(/C=C\c1scnc1C)CS[C@@H]2[C@@H]3NC(=O)C(=N\OC)/c4nc(sc4)N)C(=O)O									
Cefpodoxime	FALSE	156.44	209.98	10	3	427.45537	28	-2.81	2.77	-0.41		0.94
-0.5	0.4	1	O=C2N1/C(=C(\CS[C@@H]1[C@@H]2NC(=O)C(=N\OC)/c3nc(sc3)N)COC)C(=O)O									
Cefuroxime	FALSE	173.76	199.06	9	3	424.38523	29	-3.27	2.59	0.23		0.47
-0.217	0.31	1	O=C2N1/C(=C(\CS[C@@H]1[C@@H]2NC(=O)C(=N\OC)\c3occc3)COC(=O)N)C(=O)O									
Celecoxib	FALSE	77.98	86.36	3	1	381.37216	26	4.21		4.37		4.21
4.428	0.12	3	O=S(=O)(c3ccc(n1nc(cc1c2ccc(cc2)C)C(F)(F)F)cc3)N									
Ceritinib	FALSE	105.23	113.61	8	3	558.13514	38	2.41		6.71	10.16	5.03
6.479	0.43	3	CC1=CC(=C(C=C1C2CCNCC2)OC(C)C)NC3=NC=C(C(=N3)NC4=CC=CC=C4S(=O)(=O)C(C)C)Cl									
Cerivastatin		FALSE	99.88	99.88	6	3	459.55026	33	0.6	4.24	3.56	5.61
3.71	4.204	0.46	2	O=C(O)C[C@H](O)C[C@H](O)/C=C/c1c(nc(c(c1c2ccc(F)cc2)COC)C(C)C)C(C)C								
Cetirizine	FALSE	53.01	53.01	5	1	388.88779	27	-0.9	3.46	2.08	7.95	2.17
3.488	0.38	2	Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCC(=O)O									

Chenodiol	FALSE	77.76	77.76	4	3	392.572	28	2.05	4.76	4.51		4.66
4.014	0.96	0	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C								
Chlorambucil	FALSE	40.54	40.54	3	1	304.21216	19	0.55	4.82	3.63		4.62
3.1	3.899	0.5	1	C1CC(CCC1CCCC(=O)O)N(CCCl)CCCl								
Chloroquine	FALSE	28.16	28.16	3	1	319.87213	22	1.87		5.06	10.47	4.69
4.345	0.5	2	Clc1ccc2nccc(c2cc1)NC(C)CCCN(CC)CC									
Chlorotrianisene	FALSE	27.69	27.69	3	0	380.86404	27	6.99		5.83		
6.99	5.614	0.13	3	Cl/C(c1ccc(OC)cc1)=C(/c2ccc(OC)cc2)c3ccc(OC)cc3								
Chlorphenesin carbamate	FALSE	81.78	81.78	4	2	245.65958	16	1.41		1.26		
1.41	1.597	0.3	1	C1CC(CCC1OCC(COC(=O)N)O)Cl								
Chlorpropamide	FALSE	75.27	83.65	3	2	276.73982	17	0.33	4.64	2.35		
2.3	2.058	0.3	1	O=S(=O)(c1ccc(Cl)cc1)NC(=O)NCCC								
Chlorthalidone	FALSE	109.49	117.87	4	3	338.76614	22	-0.74		0.45		
-0.74	1.383	0.07	2	O=S(=O)(N)c1c(Cl)ccc(c1)C2(O)c3ccccc3C(=O)N2								
Cimetidine	FALSE	88.89	114.19	6	3	252.33923	17	-0.25		0.19	7.13	0.07
0.107	0.5	1	N#CN\C(=N/C)NCCSCc1ncnc1C									
Cinoxacin	FALSE	88.43	88.43	7	1	262.2182	19	-3.39		1.74	4.33	0.35
1.448	0.25	1	O=C1c3c(N(\N=C1\C(=O)O)CC)cc2OCOc2c3									
Ciprofloxacin	FALSE	72.88	72.88	6	2	331.34152	24	-1.28	6.27	-0.22	8.68	
0.65	1.435	0.41	1	c1c2c(cc(c1F)N3CCNCC3)n(cc(c2=O)C(=O)O)C4CC4								
Cisapride	FALSE	86.05	86.05	6	2	465.94546	32	2.75		3.81	8.65	3.12
2.785	0.43	2	Clc1cc(c(OC)cc1N)C(=O)NC3CCN(CCCOc2ccc(F)cc2)CC3OC									
Clavulanate	FALSE	87.07	87.07	5	2	199.16076	14	-5.39	3.64	-1.06		-1.98
-1.235	0.5	0	O=C2N1[C@H](C(/O[C@@H]1C2)=C/CO)C(=O)O									
Clindamycin	FALSE	102.26	127.56	7	4	424.98302	27	0.78		2.57	8.74	1.83
1.277	0.94	0	Cl[C@@H](C)[C@@H](NC(=O)[C@H]1N(C)C[C@H](CCC)C1)[C@H]2O[C@H](SC)[C@H](O)[C@@H](O)[C@H]2O									
Clofazimine	FALSE	39.99	39.99	4	1	473.39638	33	5.6		7.7	8.64	7.26
7.137	0.11	3	CC(C)/N=c/1\cc-2n(c3ccccc3nc2cc1Nc4ccc(cc4)Cl)c5ccc(cc5)Cl									
Clofibrate	FALSE	35.53	35.53	3	0	242.6987	16	3.32		3.68		3.32
3.329	0.42	1	Clc1ccc(OC(C(=O)OCC)(C)C)cc1									
Clomiphene	FALSE	12.47	12.47	2	0	405.95962	29	5.87		7.15	9.6	8.01
6.483	0.23	3	Cl/C(c1ccccc1)=C(/c2ccc(OCCN(CC)CC)cc2)c3ccccc3									
Clonidine	FALSE	36.42	36.42	3	2	230.09386	14	0.65		1.73	8.1	1.41
2.354	0.22	1	Clc1c(c(Cl)ccc1)N/C2=N/CCN2									
Cloxacillin	FALSE	112.74	138.04	6	2	435.88131	29	-1.2	2.44	2.52		2.53
2.3	0.37	2	O=C(O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(onc2c1ccccc1Cl)C)[C@H]4SC3(C)C									
Cobicistat	FALSE	138.02	194.5	8	3	776.02272	54	4.59		3.98	7.4	4.77
5.025	0.47	4	CC(C)c1nc(cs1)CN(C)C(=O)NC(CCN2CCOCC2)C(=O)NC(CCC(Cc3ccccc3)NC(=O)OCc4cncs4)Cc5ccccc5									
Colchicine	FALSE	83.09	83.09	6	1	399.43699	29	0.92		1.2		0.92
2.044	0.36	1	O=C(N[C@@H]3C\1=C\C(=O)C(\OC)=C/C=C/1c2c(cc(OC)c(OC)c2OC)CC3)C									
Crizotinib	FALSE	77.98	77.98	5	2	450.33668	30	2.25		4.29	9.81	4.73
3.694	0.33	3	C1(=C(C=CC(=C1[C@H](OC2=C(N=CC(=C2)C3=C[N](N=C3)C4CCNCC4)N)C)Cl)F)Cl									
Cromolyn	FALSE	165.89	165.89	11	3	468.36653	34	-2.45	1.94	1.48		2.3
1.77	0.13	2	O=C(O)C=4Oc3cccc(OCC(O)COc2cccc1O/C(=C\C(=O)c12)C(=O)O)c3C(=O)C=4									
Cyclacillin	FALSE	112.73	138.03	6	3	341.42582	23	-2.23	2.45	-0.82	7.36	1.01
0.391	0.8	0	O=C(O)[C@@H]2N3C(=O)[C@@H](NC(=O)C1(N)CCCCC1)[C@H]3SC2(C)C									
Cyclophosphamide	FALSE	51.38	51.38	2	1	261.08596	14	0.23		0.8	2.84	
0.23	0.33	1	0	O=P1(OCCCN1)N(CCCl)CCCl								
Cysteamine	FALSE	26.02	64.81	2	2	77.14868	4	-1.49		-0.25	10.34	0.03
-0.216	1	0	SCCN									
Dabrafenib	FALSE	110.85	147.47	6	2	519.5624	35	2.64	6.45	4.61		3.54
5.423	0.17	4	CC(C)(C)c1nc(c(s1)c2ccnc(n2)N)c3cccc(c3F)NS(=O)(=O)c4c(cccc4F)F									
Dantrolene	FALSE	120.72	120.72	5	1	314.253	23	1.24	7.69	1.63		1.43
1.984	0.07	2	[O-][N+](=O)c3ccc(c2oc(C=NN1C(=O)NC(=O)C1)cc2)cc3									
Dapagliflozin	FALSE	99.38	99.38	6	4	408.8726	28	4.42			3.37	
4.42	2.409	0.43	2	Clc1ccc(cc1Cc2ccc(OCC)cc2)[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O								
Darifenacin	FALSE	55.56	55.56	3	1	426.54999	32	2.66		3.62	9.32	4.5
4.558	0.32	3	O=C(N)C(c1ccccc1)(c2ccccc2)[C@H]3CN(CC3)CCc5cc4c(OCC4)cc5									
Deferasirox	FALSE	98.74	98.74	7	3	373.3615	28	-1.92		2.54	5.12	0.46
2.971	0	1	O=C4/C=C\C=C/C4=C2\N(N/C(=C1\C(=O)\C=C/C=C1)N2)c3ccc(C(=O)O)cc3									
Delavirdine	FALSE	110.43	118.8	6	3	456.56111	32	-2.29		2.92	9.17	-1.21
2.292	0.36	3	O=S(=O)(Nc1cc2cc(nc2cc1)C(=O)N4CCN(c3ncccc3NC(C)C)CC4)C									
Demeclocycline	FALSE	181.61	181.61	9	6	464.85303	32	-4	4.5	-0.58	11	
-1.07	-0.435	0.38	1	CN(C)[C@@H]1C(\O)=C(\C(N)=O)C(=O)[C@@]2(O)C(/O)=C3/C(=O)c4c(O)ccc(Cl)c4[C@@H](O)[C@H]3C[C@@H]12								
Desogestrel	FALSE	20.23	20.23	1	1	310.473	23	6.59		5.68		6.59
5.828	0.73	0	C#C[C@@]4(O)[C@@]2([C@H]([C@@H]3CC/C1=C/CCC[C@@H]1[C@H]3C(=C)\C2)CC4)CC									
Dexlansoprazole	FALSE	67.87	87.08	4	1	369.36146	25	2.76		2.6		3.64
2.76	3.442	0.25	3	O=S(Cc1nccc(OCC(F)(F)F)c1C)c1nc2ccccc2[nH]1								
Diazoxide	FALSE	58.53	66.91	4	1	230.67138	14	1.05		1.42		1.07
1.196	0.12	1	C1c1ccc2c(c1)S(=O)(=O)/N=C(\N2)C									
Dichlorphenamide	FALSE	120.31	137.08	4	2	305.15884	16	0.91		0.24		
0.93	0.569	0	1	Clc1c(cc(cc1Cl)S(=O)(=O)N)S(=O)(=O)N								
Diclofenac	FALSE	49.33	49.33	3	2	296.14864	19	0.95	4.18	4.73		4.06
4.373	0.07	2	O=C(O)Cc1ccccc1Nc2c(Cl)cccc2Cl									
Dicumarol	FALSE	93.06	93.06	6	2	336.29497	25	0.5	4.2	3.66		3.55
2.789	0.05	2	c1ccc2c(c1)c(c(c(=O)o2)Cc3c(c4ccccc4oc3=O)O)O									
Didanosine	FALSE	88.74	88.74	6	2	236.22728	17	-1.33		-1.65	3.44	-1.33
-0.844	0.5	1	O=C3/N=C\Nc1c3ncn1[C@@H]2O[C@@H](CC2)CO									
Diethylcarbamazine	FALSE	26.79	26.79	2	0	199.29324	14	0.98		1.62	6.99	
1.14	0.436	0.9	0	O=C(N1CCN(C)CC1)N(CC)CC								
Diflunisal	FALSE	57.53	57.53	3	2	250.19762	18	1.29	2.94	4.4		4.44
3.147	0	2	O=C(O)c1cc(ccc1O)c2ccc(F)cc2F									
Dimethyl fumarate	FALSE	52.6	52.6	4	0	144.12531	10	0.62		0.78		
0.62	0.49	0.33	0	O=C(OC)\C=C\C(=O)OC								
Diphemanil	FALSE	0	0	0	0	278.41126	21	2.2		0.13		2.2
2.851	0.3	2	c3c(\C(=C1/CC[N+](C)(C)CC1)c2ccccc2)cccc3									
Dipyridamole	FALSE	145.44	145.44	12	4	504.62559	36	-1.25		2.93	8.78	
-1.22	2.483	0.75	2	n3c(nc2c(nc(nc2N1CCCCC1)N(CCO)CCO)c3N4CCCCC4)N(CCO)CCO								
Dirithromycin	FALSE	196.32	196.32	16	5	835.07372	58	1.99		2.78	8.16	
2.84	1.869	0.98	0	O=C4O[C@@H]([C@]([C@H]1O[C@@H](N[C@H]([C@@H]1C)[C@H](C)C[C@](O)(C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@H]([C@H](O[C@@H]3O[C@@H](C)C[C@H](O)[C@@](OC)(C)C3)[C@H]4C)C)COCCOC)CC												
Disopyramide	FALSE	59.22	59.22	3	1	339.47446	25	0.46		2.58	10.1	
2.86	3.417	0.43	2	O=C(N)C(c1ncccc1)(c2ccccc2)CCN(C(C)C)C(C)C								
Dofetilide	FALSE	104.81	121.57	6	2	441.56478	29	0.7		1.99	8.28	1.56
1.679	0.37	2	O=S(=O)(Nc1ccc(cc1)CCN(CCOc2ccc(cc2)NS(=O)(=O)C)C)C									
Dolutegravir	FALSE	99.18	99.18	6	2	419.37876	30	-3.97	4.5	-0.41		
-1.31	0.3	0.35	1	C[C@@H]1CCO[C@@H]2N1C(=O)c3c(c(=O)c(cn3C2)C(=O)NCc4ccc(cc4F)F)O								
Domperidone	FALSE	67.92	67.92	3	2	425.91126	30	3.38		4.27	9.45	4.5
2.453	0.36	2	Clc1cc2c(cc1)N(C(=O)N2)C5CCN(CCCN4c3ccccc3NC4=O)CC5									
Doxazosin	FALSE	112.27	112.27	9	1	451.47509	33	0.59		4.04	6.45	0.65
2.485	0.35	3	O=C(N3CCN(c2nc1cc(OC)c(OC)cc1c(n2)N)CC3)C4Oc5c(OC4)cccc5									
Doxercalciferol	FALSE	40.46	40.46	2	2	412.64776	30	8.14		8.16		
8.14	6.337	0.71	0	O[C@@H]1CC(\C(=C)[C@@H](O)C1)=C\C=C2/CCC[C@]3([C@H]2CC[C@@H]3[C@@H](/C=C/[C@H](C)C(C)C)C)C								
Drospirenone	FALSE	43.37	43.37	3	0	366.49319	27	3.15		2.84		
3.15	3.383	0.83	0	O=C7O[C@@]6([C@@]3([C@H]([C@@H]2[C@@H]4[C@H](/C1=C/C(=O)CC[C@]1(C)[C@H]2CC3)C4)[C@@H]5C[C@@H]56)C)CC7								
Dydrogesterone	FALSE	34.14	34.14	2	0	312.44581	23	3.58		3.54		
3.58	3.415	0.71	0	O=C4\C=C3\C=C/[C@@H]1[C@@H](CC[C@@]2([C@@H](C(=O)C)CC[C@@H]12)C)[C@]3(C)CC4								
Dyphylline	FALSE	98.9	98.9	5	2	254.24256	18	-1.1		-1.29		-1.1
-0.626	0.5	1	O=C2N(c1ncn(c1C(=O)N2C)CC(O)CO)C									

Edoxaban	FALSE	136.63	164.87	7	3	548.0575	37	1.17	0.15	6.58	1.24
0.89	0.5	2	CN1CCC2=C(C1)SC(=N2)C(=O)N[C@@H]3C[C@H](CC[C@@H]3NC(=O)C(=O)NC4=NC=C(C=C4)Cl)C(=O)N(C)C								
Eltrombopag	FALSE	111.1	111.1	7	3	442.46657	33	1.46	3.95	3.98	2.63	4.43
3.777	0.12	2	CC1=C(C=C(C=C1)N2C(=O)C(=C(N2)C)NN=C3C=CC=C(C3=O)C4=CC(=CC=C4)C(=O)O)C								
Empagliflozin		FALSE	108.61	108.61	7	4	450.90928	31	3.38	2.58	
3.38	1.839	0.48	2	C1COC[C@H]1OC2=CC=C(C=C2)CC3=C(C=CC(=C3)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)Cl							
Emtricitabine		FALSE	88.15	113.45	6	2	247.2467	16	-0.41	-1.29	1.93
-0.41	-0.68	0.5	0	FC=1\C(=N/C(=O)N(C=1)[C@H]2O[C@H](SC2)CO)\N							
Enalapril	FALSE	95.94	95.94	6	2	376.44672	27	-1.15	3.15	0.67	5.43	2.43
2.164	0.55	1	O=C(O)[C@H]2N(CC(=O)[C@@H](N[C@H](C(=O)OCC)CCC1ccccc1)C)CCC2								
Entecavir	FALSE	125.76	125.76	7	4	277.2792	20	-0.96	-2.76	3.49	-0.96
-1.404	0.42	1	O=C2/N=C(\Nc1n(cnc12)[C@@H]3C(=C)/[C@H](CO)[C@@H](O)C3)N								
Eplerenone	FALSE	82.2	82.2	6	0	414.49139	30	1.05	0.47		1.05
2.16	0.79	0	COC(=O)[C@@H]4C\C1=C\C(=O)CC[C@]1(C)[C@@]65O[C@@H]6C[C@@]3(C)[C@@H](CC[C@]23CCC(=O)O2)[C@H]45								
Eprosartan	FALSE	92.42	120.66	5	2	424.51265	30	1.37	3.63	4.8	8.31	4.96
4.604	0.26	3	O=C(O)\C(=C\c1cnc(n1Cc2ccc(C(=O)O)cc2)CCCC)Cc3sccc3								
Estradiol	FALSE	40.46	40.46	2	2	272.38196	20	4.13	3.78		4.13
3.838	0.67	1	C[C@]12CC[C@H]3c4ccc(cc4CC[C@H]3[C@@H]1CC[C@@H]2O)O								
Estramustine		FALSE	49.77	49.77	3	1	440.40313	29	5.35	4.92	
5.35	5.38	0.7	1	ClCCN(C(=O)Oc1cc3c(cc1)[C@H]2CC[C@@]4([C@@H](O)CC[C@H]4[C@@H]2CC3)C)CCCl							
Ethacrynic acid		FALSE	63.6	63.6	4	1	303.13798	19	-0.33	2.81	3.44	
3.36	3.964	0.23	1	Cl\c1c(C(=O)\C(=C)CC)ccc(OCC(=O)O)c1Cl							
Ethambutol	FALSE	64.52	64.52	4	4	204.30976	14	-2.33	0.12	9.59	-0.05
0.11	1	0	CC[C@@H](CO)NCCN[C@@H](CC)CO								
Ethoxzolamide		FALSE	82.28	118.9	4	1	258.3173	16	2.04	2.05	
2.05	1.823	0.22	2	O=S(=O)(c1nc2ccc(OCC)cc2s1)N							
Ethylestrenol		FALSE	20.23	20.23	1	1	288.46748	21	6.51	6.09	
6.51	4.997	0.9	0	O[C@]2(CC[C@H]1[C@H]4[C@H](CC[C@@]12C)[C@@H]3\C(=C/CCC3)CC4)CC							
Ethynodiol diacetate		FALSE	40.46	40.46	2	2	300.43512	22	3.92	3.23	
3.92	4.214	0.8	0	O[C@@H]4/C=C3\[C@@H]([C@H]2CC[C@]1([C@@H](CC[C@]1(C#C)O)[C@@H]2CC3)C)CC4							
Etodolac	FALSE	62.32	62.32	3	2	287.35353	21	0.61	4.31	3.43		3.59
3.723	0.47	2	O=C(O)CC3(OCCc2c3nc1c(cccc12)CC)CC								
Etoposide	FALSE	160.83	160.83	13	3	588.55657	42	0.3	0.03		0.3
0.935	0.55	2	C[C@@H]1OC[C@@H]2[C@@H](O1)[C@@H]([C@H]([C@@H](O2)O[C@@H]3c4cc5c(cc4[C@H]([C@@H]6[C@@H]3COC6=O)c7cc(c(c(c7)OC)O)OC)OCO5)O)O								
Etravirine	FALSE	120.63	120.63	7	2	435.2767	28	4.19	5.22		4.19
5.492	0.1	3	N#Cc3cc(c(Oc1nc(nc(c1Br)N)Nc2ccc(C#N)cc2)c(c3)C)C								
Ezetimibe	FALSE	60.77	60.77	3	2	409.42524	30	3.25	3.96		3.26
4.633	0.21	3	Fc1ccc(cc1)[C@@H](O)CC[C@H]4C(=O)N(c2ccc(F)cc2)[C@@H]4c3ccc(O)cc3								
Fenoprofen	FALSE	46.53	46.53	3	1	242.26986	18	0.75	4.2	3.82		3.84
3.517	0.13	2	O=C(O)C(c2cc(Oc1ccccc1)ccc2)C								
Fesoterodine		FALSE	49.77	49.77	4	1	411.57687	30	2.23	4.36	10.6
5.08	5.71	0.5	2	O=C(Oc1ccc(cc1[C@@H](c2ccccc2)CCN(C(C)C)C(C)C)CO)C(C)C							
Fexofenadine		FALSE	81	81	5	3	501.65636	37	2.3	4.43	1.96	9.8
4.8	5.642	0.41	3	O=C(O)C(c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4)(C)C							
Flavoxate	FALSE	55.84	55.84	5	0	391.4596	29	4.32	4.97	7.65	5.18	
4.494	0.33	2	O=C(OCCN1CCCCC1)c4cccc2c4O/C(=C(\C2=O)C)c3ccccc3								
Flecainide	FALSE	59.59	59.59	4	2	414.34271	28	0.77	3.66	9.69	2.9	
3.568	0.59	1	FC(F)(F)COc2cc(C(=O)NCC1NCCCC1)c(OCC(F)(F)F)cc2								
Fludarabine	FALSE	139.54	139.54	8	4	285.23178	20	-0.4	-2		-0.4	
-1.452	0.5	2	Fc1nc(c2ncn(c2n1)[C@@H]3O[C@@H]([C@@H](O)[C@@H]3O)CO)N								
Fluoxymesterone		FALSE	57.53	57.53	3	2	336.44086	24	2.17	2.84	
2.17	2.637	0.85	0	O=C4\C=C3/[C@]([C@@]2(F)[C@@H](O)C[C@]1([C@@H](CC[C@@]1(O)C)[C@@H]2CC3)C)(C)CC4							
Fluvastatin	FALSE	82.69	82.69	4	3	411.46594	30	0.51	4.27	4.05		3.62
4.244	0.29	3	O=C(O)C[C@H](O)C[C@H](O)/C=C/c2c(c1ccccc1n2C(C)C)c3ccc(F)cc3								
Fosfomycin	FALSE	79.87	79.87	4	2	138.05904	8	-6.79	3.02	-0.23		-2.98
-0.318	1	0	C[C@H]1[C@H](O1)P(=O)(O)O								
Fosinopril	FALSE	120.02	120.02	7	1	563.6625	39	2.53	3.36	7.45		6.09
6.269	0.7	1	O=C(CP(=O)(CCCCc1ccccc1)OC(OC(=O)CC)C(C)C)N2C[C@@H](C[C@H]2C(O)=O)C3CCCCC3								
Furazolidone		FALSE	100.86	100.86	5	0	225.15828	16	-0.49	-0.04	
-0.49	1.1	0.25	1	[O-][N+](=O)c2oc(C=NN1C(=O)OCC1)cc2							
Furosemide	FALSE	122.63	131.01	5	3	330.74413	21	-0.03	3.04	1.9		3.1
1.403	0.08	2	O=S(=O)(N)c1c(Cl)cc(c(C(=O)O)c1)NCc2occc2								
Gatifloxacin		FALSE	82.11	82.11	7	2	375.39408	27	-1.11	6.27	0.24	8.72
1.21	1.796	0.47	1	Fc1c(c(OC)c2c(c1)C(=O)C(\C(=O)O)=C/N2C3CC3)N4CC(NCC4)C								
Gefitinib	FALSE	68.74	68.74	7	1	446.90236	31	3.97	5.6	7.34	4.11	
4.203	0.36	3	COc1cc2c(cc1OCCCN3CCOCC3)c(ncn2)Nc4ccc(c(c4)Cl)F									
Gemifloxacin		FALSE	121.35	121.35	9	2	389.3809	28	-2.09	6.02	-0.86	9.15
0.38	0.832	0.44	1	Fc2c(nc1N(/C=C(/C(=O)O)C(=O)c1c2)C3CC3)N4C/C(=N\OC)C(C4)CN								
Glimepiride	FALSE	124.68	133.06	5	3	490.61555	34	1	4.99	3.96		2.94
4.306	0.54	1	O=C3C(/CC)=C(/C)CN3C(=O)NCCc1ccc(cc1)S(=O)(=O)NC(=O)N[C@H]2CC[C@H](C)CC2									
Glipizide	FALSE	130.15	138.53	6	3	445.53517	31	0.07	4.97	2.57		2.01
1.902	0.43	2	O=C(c1ncc(nc1)C)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3									
Glyburide	FALSE	113.6	121.98	5	3	494.00351	33	1.82	4.99	4.24		3.75
4.14	0.39	2	O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)CCNC(=O)c3cc(Cl)ccc3OC									
Glycopyrrolate		FALSE	46.53	46.53	3	1	318.43052	23	0.38	0.12		
0.38	1.457	0.63	1	C[N+]1(CCC(C1)OC(=O)C(C2CCCC2)(C3=CC=CC=C3)O)C								
Guaifenesin	FALSE	58.92	58.92	4	2	198.21576	14	0.57	0.1		0.57	
0.747	0.4	1	O(c1ccccc1OC)CC(O)CO									
Guanadrel	FALSE	82.86	82.86	5	2	213.27675	15	-1.49	0.62	12.29	0.51	
0.294	0.9	0	C1CCC2(CC1)OCC(O2)CN=C(N)N									
Guanethidine		FALSE	67.63	67.63	4	2	198.30848	14	-1	1.34	13.35	
1.56	1.186	0.9	0	N(=C(\N)N)\CCN1CCCCCCC1								
Hetacillin	FALSE	89.95	115.25	6	2	389.46861	27	-1.31	2.45	0.81	4.97	2.4
0.738	0.53	1	O=C(O)[C@@H]3N4C(=O)[C@@H](N2C(=O)C(c1ccccc1)NC2(C)C)[C@H]4SC3(C)C									
Hexocyclium	FALSE	23.47	23.47	2	1	317.48882	23	1.15	1.41	4.16	1.15	
2.04	0.7	1	C[N+]1(CCN(CC1)CC(C2CCCCC2)(C3=CC=CC=C3)O)C									
Hydralazine	FALSE	63.83	63.83	4	2	160.17592	12	0.99	1.17	6.25	1	
0.935	0	2	n2nc(c1ccccc1c2)NN									
Hydrocortisone		FALSE	94.83	94.83	5	3	362.45989	26	1.43	1.89		
1.43	1.283	0.81	0	O=C4\C=C2/[C@]([C@H]1[C@H](O)C[C@@]3([C@@](O)(C(=O)CO)CC[C@H]3[C@@H]1CC2)C)(C)CC4								
Ibandronate	FALSE	158.14	158.14	8	5	319.22894	19	-5.05	1.33	-3.37	9.5	-0.65
0.685	1	0	O=P(O)(O)C(O)(CCN(CCCCC)C)P(=O)(O)O									
Ibrutinib	FALSE	99.16	99.16	6	1	440.49706	33	2.92	4.07	4.23	2.92	
3.845	0.2	4	C=CC(=O)N1CCC[C@H](C1)N2C3=C(C(=N2)C4=CC=C(C=C4)OC5=CC=CC=C5)C(=NC=N3)N									
Idelalisib	FALSE	99.16	99.16	6	2	415.42302	31	2.96	3.62	4.08	2.96	
3.485	0.14	4	Fc2cccc3\N=C(/N(c1ccccc1)C(=O)c23)[C@@H](Nc4ncnc5ncnc45)CC									
Imatinib	FALSE	86.28	86.28	7	2	493.60273	37	2.08	4.53	7.77	2.48	
4.22	0.24	4	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)NC(=O)c4ccc(cc4)CN5CCN(CC5)C									
Indapamide	FALSE	92.49	100.88	4	2	365.83453	24	2.09	2.96		2.1	
2.538	0.19	2	O=S(=O)(N)c1c(Cl)ccc(c1)C(=O)NN3c2ccccc2CC3C									
Indinavir	FALSE	118.03	118.03	7	4	613.78948	45	2.87	3.68	6.62	2.88	
3.082	0.47	3	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@H](C[C@@H](Cc2ccccc2)C(=O)N[C@H]3c4ccccc4C[C@H]3O)O)Cc5ccccc5									
Irbesartan	FALSE	87.13	87.13	5	1	428.52942	32	2.53	4.5	6.04	2.6	4.5
4.841	0.4	3	O=C1N(\C(=N/C12CCCC2)CCCC)Cc5ccc(c3ccccc3c4nnnn4)cc5									
Isoniazid	FALSE	68.01	68.01	3	2	137.13928	10	-0.89	-0.67	3.79	-0.89	
-0.811	0	1	O=C(NN)c1ccncc1									
Isopropamide		FALSE	43.09	43.09	1	1	353.52092	26	-3.49	-0.2		
-3.49	2.785	0.43	2	O=C(N)C(c1ccccc1)(c2ccccc2)CC[N+](C(C)C)C)(C(C)C)C								
Itraconazole		FALSE	100.79	100.79	9	0	705.63342	49	4.28	7.25	6.47	
4.35	6.435	0.37	4	O=C1N(/N=C\N1c2ccc(cc2)N7CCN(c6ccc(OC[C@@H]3O[C@](OC3)(c4ccc(Cl)cc4Cl)Cn5ncnc5)cc6)CC7)C(C)CC								

Ivacaftor	FALSE	78.43	78.43	4	3	392.49071	29	6.34	3.82	6.34	4.516
0.33	2	O=C\2c1c(cccc1)N/C=C/2C(=O)Nc3cc(O)c(cc3C(C)(C)C)C(C)(C)C									
Ketoconazole	FALSE	69.06	69.06	6	0	531.43092	36	3.43	4.14	6.88	3.55
3.61	0.38	3	O=C(N5CCN(c4ccc(OC[C@@H]1O[C@](OC1)(c2ccc(Cl)cc2Cl)n3ccnc3)cc4)CC5)C								
Ketorolac	FALSE	59.3	59.3	3	1	255.26862	19	-0.94	4.29	1.62	2.08
2.832	0.2	2	O=C(c1ccc2n1CCC2C(=O)O)c3ccccc3								
Labetalol	FALSE	95.58	95.58	4	4	328.40546	24	0.42	2.5	9.37	2.31
2.355	0.32	2	O=C(c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2)N								
Lactulose	FALSE	189.52	189.52	11	8	342.29647	23	-3.21	-3.59	-3.21	-4.311
1	0	O[C@H]2[C@H](O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O)[C@H](O[C@]2(O)CO)CO									
Lapatinib	FALSE	106.35	114.73	7	2	581.05754	40	5.1	5.96	6.61	5.14
6.041	0.17	5	CS(=O)(=O)CCNCc1ccc(o1)c2ccc3c(c2)c(ncn3)Nc4ccc(c(c4)Cl)OCc5cccc(c5)F								
Lenvatinib	FALSE	115.57	115.57	5	3	426.85295	30	3.39	3.35	4.69	3.39
2.832	0.19	3	C4CC4NC(=O)Nc3ccc(cc3Cl)Oc1ccnc(cc2OC)c1cc2C(=O)N								
Levofloxacin	FALSE	73.32	73.32	7	1	361.3675	26	-1.41	5.19	0	7.37
0.84	1.661	0.44	1	C[C@H]1COc2c3n1cc(c(=O)c3cc(c2N4CCN(CC4)C)F)C(=O)O							
Linagliptin	FALSE	113.47	113.47	7	1	472.54222	35	-0.34	2.46	10.01	1.99
3.243	0.4	3	CC#CCN1C2=C(N=C1N3CCC[C@H](C3)N)N(C(=O)N(C2=O)CC4=NC5=CC=CC=C5C(=N4)C)C								
Linezolid	FALSE	71.11	71.11	5	1	337.3461	24	0.29	0.67	5.75	0.3
0.894	0.5	1	O=C1O[C@@H](CNC(=O)C)CN1c3cc(F)c(N2CCOCC2)cc3								
Lisinopril	FALSE	132.96	132.96	7	4	405.48793	29	-1.82	2.18	-1.82	10.5
1.19	1.51	0.57	1	O=C(O)[C@H]2N(C(=O)[C@@H](N[C@H](CC(=O)O)CCC1ccccc1)CCCCN)CCC2							
Lomitapide	FALSE	61.44	61.44	3	2	693.72039	50	6.21	7	8.56	7.78
7.79	0.33	4	FC(F)(F)c5ccc(cc5)-c1ccccc1C(=O)NC4CCN(CC4)CCCCc2(C(=O)NCC(F)(F)F)c3ccccc3-c6ccccc26								
Loperamide	FALSE	43.78	43.78	3	1	477.03752	34	3.73	4.66	8.26	4.26
4.635	0.34	3	Clc1=CC=C(C2(CCN(CC2)CCC(C3=CC=CC=C3)(C(N(C)C)=O)C4=CC=CC=C4)O)C=C1								
Lopinavir	FALSE	120	120	5	4	628.80082	46	6.26	6.09	6.26	4.926
0.43	3	O=C(N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](NC(=O)[C@@H](N2C(=O)NCCC2)C(C)C)Cc3ccccc3)COc4c(cccc4C)C									
Loracarbef	FALSE	112.73	112.73	5	3	349.76894	24	-4.38	3.1	-0.47	6.56
-1.14	4.00E-03	0.31	1	Cl\C3=C(/C(=O)O)N2C(=O)[C@@H](NC(=O)[C@@H](c1ccccc1)N)[C@H]2CC3							
Lubiprostone	FALSE	83.83	83.83	5	2	390.46188	27	0.25	4.77	3.83	
2.85	3.848	0.9	0	FC(F)(CCCC)[C@]2(O)O[C@@H]1CC(=O)[C@@H]([C@H]1CC2)CCCCCCC(=O)O							
Macitentan	FALSE	128.22	136.6	8	2	588.2729	32	3.48	4.3	5.3	5.41
3.671	0.26	3	Brc1ccc(cc1)c3c(ncnc3OCCOc2ncc(Br)cn2)NS(=O)(=O)NCCC								
Medroxyprogesterone acetate	FALSE	60.44	60.44	4	0	386.52436	28	4.11	4.2		
4.11	3.755	0.79	0	[C@]4([C@@]3([C@H]([C@H]2[C@@H]([C@@]1(C(=CC(=O)CC1)[C@H](C2)C)C)CC3)CC4)C)(OC(C)=O)C(C)=O							
Mefenamic acid	FALSE	49.33	49.33	3	2	241.28509	18	2.37	3.73	5.29	
5.33	3.982	0.13	2	O=C(O)c2c(Nc1cccc(c1C)C)cccc2							
Meloxicam	FALSE	99.59	136.22	5	2	351.40071	23	-0.17	4.5	2.29	2.89
2.71	0.585	0.14	2	Cc1cnc(s1)NC(=O)C\3=C(/O)c2ccccc2S(=O)(=O)N/3C							
Melphalan	FALSE	66.55	66.55	4	2	305.20022	19	-0.71	2.12	-0.21	9.54
1.79	2.366	0.46	1	c1cc(ccc1C[C@@H](C(=O)O)N)N(CCCl)CCCl							
Mepenzolate	FALSE	46.53	46.53	3	1	340.43604	25	0.97	0.16	0.97	1.888
0.38	2	C1=CC=CC=C1C(C(OC2CCC[N+](C)(C)C2)=O)(O)C3=CC=CC=C3									
Mercaptopurine	FALSE	53.07	85.16	4	2	152.17705	10	-0.64	-1.33	8.89	-0.63
8.90E-02	0	1	S=C2/N=C\Nc1ncnc12								
Mesalamine	FALSE	83.55	83.55	4	3	153.13538	11	-2.66	1.9	1.06	5.43
0.46	0.471	0	1	O=C(O)c1cc(ccc1O)N							
Mesna	FALSE	57.2	104.38	4	1	141.18929	7	-4.7	1.5	-1.55	-1.2
-0.686	1	0	[O-]S(=O)(=O)CCS								
Metaproterenol	FALSE	72.72	72.72	4	4	211.25758	15	-1.77	0.08	9.53	0.13
1.099	0.45	1	Oc1cc(cc(O)c1)C(O)CNC(C)C								
Metaxalone	FALSE	47.56	47.56	3	1	221.25239	16	2.42	2.15	2.42	2.468
0.42	1	O=C2OC(COc1cc(cc(c1)C)C)CN2									
Methantheline	FALSE	35.53	35.53	3	0	340.43604	25	-1.26	0.88		
-1.26	2.426	0.38	2	CC[N+](C)(CC)CCOC(=O)C1C2=CC=CC=C2OC3=CC=CC=C13							
Methazolamide	FALSE	105.19	138.87	7	1	236.27202	14	-0.21	7.31	0.09	
0.13	3.00E-02	0.4	0	O=S(=O)(C\1=N\N(C(=N/C(=O)C)/S/1)C)N							
Methenamine	FALSE	12.96	12.96	4	0	140.18627	10	2.17	2.44	5.28	2.17
8.50E-02	1	0	C1N2CN3CN1CN(C2)C3								
Methimazole	FALSE	15.27	47.36	1	1	114.16884	7	-0.34	-0.34	-0.34	-0.305
0.25	0	Cn1cc[nH]c1=S									
Methscopolamine	FALSE	59.06	59.06	4	1	318.38745	23	-2.29	-2.47		
-2.29	-0.531	0.61	1	OC[C@H](c1ccccc1)C(=O)O[C@H]2C[C@@H]3[N+](C)(C)[C@H](C2)[C@H]4O[C@@H]34							
Methyltestosterone	FALSE	37.29	37.29	2	1	302.45099	22	4.02	3.93		
4.02	3.678	0.85	0	O=C4\C=C3/[C@]([C@H]2CC[C@]1([C@@H](CC[C@@]1(O)C)[C@@H]2CC3)C)(C)CC4							
Metolazone	FALSE	92.5	100.88	4	2	365.83454	24	1.56	2.06	1.57	2.464
0.19	2	O=S(=O)(c3c(Cl)cc2c(C(=O)N(c1ccccc1C)C(N2)C)c3)N									
Metronidazole	FALSE	83.87	83.87	4	1	171.15396	12	-0.01	-0.46	2.58	-0.01
-0.337	0.5	1	C1=C([N](C(=N1)C)CCO)[N+](=O)[O-]								
Metyrosine	FALSE	83.55	83.55	4	3	195.21512	14	-1.78	2.29	-1.67	9.09
0.73	0.943	0.3	1	O=C(O)[C@@](N)(Cc1ccc(O)cc1)C							
Midodrine	FALSE	93.81	93.81	5	3	254.28232	18	-0.84	-0.35	7.75	-0.66
-0.548	0.42	1	O=C(NCC(O)c1cc(OC)ccc1OC)CN								
Miglitol	FALSE	104.39	104.39	6	5	207.22428	14	-1.43	-1.26	7.59	-1.4
-2.444	1	0	OCCN1[C@@H]([C@@H](O)[C@H](O)[C@@H](O)C1)CO								
Miltefosine	FALSE	68.4	68.4	4	0	407.568	27	4.18	1.28	3.54	3.58
4.866	1	0	[O-]P(=O)(OCCCCCCCCCCCCCCCC)OCC[N+](C)(C)C								
Minocycline	FALSE	164.63	164.63	9	5	457.47637	33	-3.33	4.5	0.21	11.06
-0.65	9.70E-02	0.43	1	CN(C)[C@@H]1C(\O)=C(\C(N)=O)C(=O)[C@@]2(O)C(/O)=C3/C(=O)c4c(O)ccc(c4C[C@H]3C[C@@H]12)N(C)C							
Minoxidil	FALSE	88.94	88.94	5	3	209.2483	15	-3.99	-1.41	16.66	-1.49
5.20E-02	0.56	0	C2N(C1=NC(=N)N(C(=C1)N)O)CCCC2								
Mirabegron	FALSE	100.27	128.51	5	4	396.50586	28	-0.37	1.32	8.9	1.29
2.453	0.24	3	O=C(Nc1ccc(cc1)CCNC[C@H](O)c2ccccc2)Cc3nc(sc3)N								
Mitotane	FALSE	0	0	0	0	320.0412	18	5.39	6.06	5.39	5.745
0.14	2	Clc1ccccc1C(c2ccc(Cl)cc2)C(Cl)Cl									
Montelukast	FALSE	70.42	95.72	5	2	586.18324	41	5.19	4.76	8.47	2.22
7.8	8.284	0.31	4	O=C(O)CC1(CC1)CS[C@@H](c2ccccc2)\C=C\c3nc4cc(Cl)ccc4cc3)CCc5ccccc5C(O)(C)C							
Moxifloxacin	FALSE	82.11	82.11	7	2	401.43136	29	-0.91	6.28	0.46	10.63
1.6	2.003	0.52	1	COc1c2c(cc(c1N3C[C@@H]4CCCN[C@@H]4C3)F)c(=O)c(cn2C5CC5)C(=O)O							
Mycophenolic acid	FALSE	93.06	93.06	6	2	320.33709	23	0.26	4.71	2.29	
2.92	3.157	0.41	1	O=C1OCc2c1c(O)c(c(OC)c2C)C\C=C(/C)CCC(=O)O							
Nabumetone	FALSE	26.3	26.3	2	0	228.28634	17	2.82	2.98	2.82	
2.943	0.27	2	O=C(C)CCc1ccc2c(c1)ccc(OC)c2								
Nadolol	FALSE	81.95	81.95	5	4	309.40058	22	-0.81	0.38	9.77	1.29
1.146	0.65	1	OC(CNC(C)(C)C)COc1ccccc2c1C[C@H](O)[C@H](O)C2								
Nalidixic acid	FALSE	70.5	70.5	5	1	232.23528	17	-0.37	3.45	1.02	6.12
1.19	1.176	0.25	1	O=C\2c1c(nc(cc1)C)N(/C=C/2C(=O)O)CC							
Naproxen	FALSE	46.53	46.53	3	1	230.25915	17	0.47	4.84	2.82	3
2.849	0.21	2	C[C@@H](c1ccc2cc(ccc2c1)OC)C(=O)O								
Nateglinide	FALSE	66.4	66.4	3	2	317.42258	23	0.61	3.61	4.3	4.21
3.981	0.58	1	O=C(N[C@H](CC1CCCCC1)C(O)=O)[C@H]2CC[C@@H](CC2)C(C)C								
Nelfinavir	FALSE	101.9	127.19	6	4	567.7824	40	6.96	5.84	7.53	6.98
5.285	0.56	2	O=C(c1cccc(O)c1C)N[C@@H](CSc2ccccc2)[C@H](O)CN4[C@H](C(=O)NC(C)(C)C)C[C@@H]3CCCC[C@@H]3C4								
Neostigmine	FALSE	29.54	29.54	2	0	223.29145	16	-3.03	-2.81	-3.03	0.511
0.42	1	O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C									
Nevirapine	FALSE	58.12	58.12	4	1	266.29786	20	2.03	2.65	4.25	2.03
2.293	0.27	2	O=C2Nc1c(ccnc1N(c3ncccc23)C4CC4)C								
Niacin	FALSE	50.19	50.19	3	1	123.1094	9	-2.93	2.2	0.8	4.8
0.15	0.309	0	1	OC(=O)C1=CN=CC=C1							
Niclosamide	FALSE	95.15	95.15	4	2	327.11962	21	5.17	7.45	4.34	5.41
3.595	0	2	Clc2cc(ccc2NC(=O)c1cc(Cl)ccc1O)[N+]([O-])=O								

Nilotinib	FALSE	97.62	97.62	6	2	529.51578	39	5.14	5.84	5.68	5.15	5.084
0.11	5	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)C(=O)Nc4cc(cc(c4)n5cc(nc5)C)C(F)(F)F										
Nilutamide	FALSE	95.22	95.22	4	1	317.2207	22	2.01	7.59	1.71	2.23	2.874
0.33	1	O=C2N(c1ccc([N+](=O)[O-])=O)c(c1)C(F)(F)F)C(=O)C(N2)(C)C										
Nintedanib	FALSE	94.22	94.22	7	2	539.62481	40	2.26	3.08	7.41	2.59	2.965
0.26	3	CN1CCN(CC1)CC(=O)N(C)C2=CC=C(C=C2)N/C(=C\3/C4=C(C=C(C=C4)C(=O)OC)NC3=O)/C5=CC=CC=C5										
Nitisinone	FALSE	97.03	97.03	5	0	329.2281	23	-1.12	3.13	1.38	1.37	2.53
0.36	1	O=C(c1ccc(cc1[N+](=O)[O-])=O)C(F)(F)F)C2C(=O)CCCC2=O										
Nizatidine	FALSE	86.01	139.55	7	2	331.45744	21	0.98	-0.16	7.31	1.18	0.552
0.58	1	[O-][N+](=O)\C=C(/NC)NCCSCc1nc(sc1)CN(C)C										
Norgestimate	FALSE	58.89	58.89	4	1	369.49713	27	5	5.05			5
5.237	0.74	O	O=C(O[C@@]2(C#C)CC[C@H]1[C@H]4[C@H](CC[C@@]12CC)[C@@H]3/C(=C\C(=N\O)CC3)CC4)C									
Novobiocin	FALSE	196.1	196.1	11	5	612.62434	44	0.12	4.5	3.98	2.86	3.45
0.39	2	C[C@@]4(C)O[C@@H](Oc3ccc2C(\O)=C(\NC(=O)c1ccc(O)c(C\C=C(/C)C)c1)C(=O)Oc2c3C)[C@H](O)[C@H](OC(N)=O)[C@H]4OC										
Olaparib	FALSE	82.08	82.08	4	1	434.46282	32	0	1.24		0	2.127
0.33	2	c4cccc2c4c(n[nH]c2=O)Cc(ccc1F)cc1C(=O)N3CCN(CC3)C(=O)C5CC5										
Olsalazine	FALSE	139.78	139.78	8	4	302.23899	22	-0.21	2.73	5.17	3.94	2.975
0	2	O=C(O)c1cc(ccc1O)/N=N/c2cc(C(O)=O)c(O)cc2										
Orlistat	FALSE	81.69	81.69	5	1	495.73481	35	8.95	8.61		8.95	8.333
0.9	0	O=C(O[C@H](C[C@@H]1OC(=O)[C@H]1CCCCCC)CCCCCCCCCC)[C@@H](NC=O)CC(C)C										
Oseltamivir	FALSE	90.65	90.65	5	2	312.40452	22	0.69	2.13	8.81	1.5	1.045
0.75	0	O=C(OCC)/C1=C/[C@@H](OC(CC)CC)[C@H](NC(=O)C)[C@@H](N)C1										
Oxamniquine	FALSE	90.11	90.11	5	3	279.33484	20	-0.91	1.8	9.83	1.41	1.817
0.57	1	[O-][N+](=O)c1c(cc2c(c1)NC(CC2)CNC(C)C)CO										
Oxandrolone	FALSE	46.53	46.53	3	1	306.4397	22	3.33	2.96		3.33	3.06
0.95	0	O=C3OC[C@@]2([C@H]1CC[C@@]4(C)[C@H]([C@@H]1CC[C@H]2C3)CC[C@@]4(O)C)C										
Oxaprozin	FALSE	63.33	63.33	3	1	293.3166	22	1.12	4.2	2.95	4.19	3.59
0.11	3	O=C(O)CCc1nc(c(o1)c2ccccc2)c3ccccc3										
Oxyphenbutazone	FALSE	60.85	60.85	3	1	324.3737	24	0.45	6.86	2.72		2.72
3.712	0.26	2	O=C2N(c1ccc(O)cc1)N(C(=O)C2CCC)c3ccccc3									
Oxyphenonium	FALSE	46.53	46.53	3	1	348.49955	25	-0.91	0.88			-0.91
2.701	0.67	1	OC(C(=O)OCC[N+](C)(CC)CC)(c1ccccc1)C2CCCCC2									
Palbociclib	FALSE	103.35	103.35	8	2	447.53275	33	-0.13	2.85	8.66	0.99	2.801
0.46	2	O=C2N(c1nc(ncc1/C(=C2/C(=O)C)C)Nc3ncc(cc3)N4CCNCC4)C5CCCC5										
Paliperidone	FALSE	82.17	82.17	5	1	426.48388	31	0.72	1.07	8.21		1.52
2.53	0.52	2	O=C/1N5/C(=N\C(=C\1CCN4CCC(c3noc2cc(F)ccc23)CC4)C)[C@H](O)CCC5									
Pantoprazole	FALSE	86.33	105.54	6	1	383.3698	26	1.68	7.6	2.11	1.93	1.69
2.737	0.25	3	FC(F)Oc3cc1c(nc(n1)S(=O)Cc2nccc(OC)c2OC)cc3									
Pargyline	FALSE	3.24	3.24	1	0	159.22761	12	2.43	2.58	6.5	2.48	3.095
0.27	1	C#CCN(C)Cc1ccccc1										
Paricalcitol	FALSE	60.69	60.69	3	3	416.63646	30	5.83	5.69			5.83
4.863	0.78	0	[C@H]1\2[C@@]([C@@H]([C@@H](\C=C\[C@@H](C(C)(C)O)O)C)CC1)(CCCC2=C\C=C3/C[C@H](C[C@@H](C3)O)O)C									
Pemoline	FALSE	64.67	64.67	4	1	176.17202	13	0.52	0.46		0.52	1.26
0.11	1	O=C2\N=C(/OC2c1ccccc1)N										
Penicillamine	FALSE	63.31	102.11	4	3	149.21133	9	-1.57	2.13	-1.73	11.64	0.93
-1.70E-02	0.8	0	CC(C)([C@H](C(=O)O)N)S									
Phenazone	FALSE	23.55	23.55	2	0	188.22578	14	0.27	0.2		0.27	1.606
0.18	1	O=C2\C=C(/N(N2c1ccccc1)C)C										
Phenazopyridine	FALSE	89.65	89.65	5	2	213.23853	16	3.34	2.05	4.49		3.34
2.633	0	2	C1=C(C(=NC(=C1)N)N)N=NC2=CC=CC=C2									
Phenprocoumon	FALSE	46.53	46.53	3	1	280.31784	21	1.97	4.5	4.71		4.77
4.004	0.17	2	OC=1c3ccccc3OC(=O)C=1C(CC)c2ccccc2									
Phensuximide	FALSE	37.38	37.38	2	0	189.21054	14	0.77	0.94			0.77
1.432	0.27	1	O=C2N(C(=O)CC2c1ccccc1)C									
Phenylephrine	FALSE	52.49	52.49	3	3	167.20502	12	-1.92	-0.09	9.22		-0.03
0.615	0.33	1	O[C@H](c1cc(O)ccc1)CNC									
Pilocarpine	FALSE	44.12	44.12	3	0	208.25694	15	-0.24	-0.2	7.02	-0.1	0.965
0.64	1	O=C2OC[C@H](Cc1n(cnc1)C)[C@@H]2CC										
Pinacidil	FALSE	73.09	73.09	5	2	245.32345	18	2.85	2.23	6	2.87	1.931
0.46	1	CC(C(C)(C)C)N=C(NC#N)NC1=CC=NC=C1										
Pipobroman	FALSE	40.62	40.62	2	0	356.05424	16	0.98	0.23		0.98	0.647
0.8	0	O=C(N1CCN(C(=O)CCBr)CC1)CCBr										
Pirenzepine	FALSE	68.78	68.78	5	1	351.40234	26	-0.37	-0.35	7.27	-0.08	1.039
0.32	2	O=C3c1ccccc1N(C(=O)CN2CCN(C)CC2)c4ncccc4N3										
Pitavastatin	FALSE	90.65	90.65	5	3	421.46076	31	0.32	4.24	3.59	4.68	3.45
3.953	0.28	3	O=C(O)C[C@H](O)C[C@H](O)/C=C/c1c(c3ccccc3nc1C2CC2)c4ccc(F)cc4									
Ponatinib	FALSE	65.77	65.77	5	1	532.55948	39	3.39	5.77	7.74	3.79	5.145
0.28	4	Cc1ccc(cc1C#Cc2cnc3n2nccc3)C(=O)Nc4ccc(c(c4)C(F)(F)F)CN5CCN(CC5)C										
Pralidoxime	FALSE	34.28	34.28	2	1	137.15916	10	0.86	0.55		0.86	-0.937
0.14	0	O=[NH+]C=C1\C=C/C=C\N1C										
Pravastatin	FALSE	124.29	124.29	7	4	424.52773	30	-1.73	4.31	2.05	1.35	2.157
0.74	0	O=C(O)C[C@H](O)C[C@H](O)CC[C@H]2[C@H](/C=C\C1=C\[C@@H](O)C[C@H](OC(=O)[C@@H](C)CC)[C@@H]12)C										
Primaquine	FALSE	60.17	60.17	4	2	259.34674	19	-0.06	2.6	10.38	2.67	1.999
0.4	2	O(c1cc(NC(C)CCCN)c2ncccc2c1)C										
Probenecid	FALSE	74.68	83.06	4	1	285.35926	19	0.26	3.69	3.37	3.3	2.321
0.46	1	O=S(=O)(N(CCC)CCC)c1ccc(C(=O)O)cc1										
Probucol	FALSE	40.46	91.06	4	2	516.84161	35	10.27	10.97		10.27	9.779
0.61	2	S(c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)C(Sc2cc(c(O)c(c2)C(C)(C)C)C(C)(C)C)C(C)(C)C										
Proguanil	FALSE	88.79	88.79	5	3	253.73124	17	1.83	1.16	11.29	2.66	2.226
0.27	1	Clc1ccc(NC(=N/C(=N/C(C)C)N)N)cc1										
Propantheline	FALSE	35.53	35.53	3	0	368.4892	27	-1.77	1.49			-1.77
3.181	0.43	2	O=C(OCC[N+](C(C)C)(C(C)C)C)C2c3c(Oc1c2cccc1)cccc3									
Propylthiouracil	FALSE	41.13	73.22	2	2	170.2321	11	1.25	7.63	0.97	7.35	1.37
1.381	0.43	0	S=C1N/C(=C\C(=O)N1)CCC									
Protokylol	FALSE	91.18	91.18	6	4	331.36304	24	0.05	1.69	8.98	1.6	2.423
0.33	2	O1c2ccc(cc2OC1)CC(NCC(O)c3ccc(O)c(O)c3)C										
Pyridostigmine	FALSE	33.42	33.42	2	0	181.21172	13	-4.31	-4.26			-4.31
0.751	0.33	1	O=C(Oc1ccc[n+](c1)C)N(C)C									
Quinestrol	FALSE	29.46	29.46	2	1	364.52037	27	6.67	5.92		6.67	6.514
0.68	1	O(c1ccc2c(c1)CC[C@H]3[C@@H]4CC[C@](C#C)(O)[C@@]4(C)CC[C@H]23)C5CCCC5										
Quinethazone	FALSE	101.29	109.67	4	3	289.73858	18	0.49	0.58			0.49
0.848	0.3	1	O=S(=O)(c2c(Cl)cc1c(C(=O)NC(N1)CC)c2)N									
Quinidine	FALSE	45.59	45.59	4	1	324.41676	24	1.6	2.79	9.28	3.44	2.733
0.45	2	O(c4cc1c(nccc1[C@H](O)[C@@H]2N3CC[C@@H](C2)[C@@H](/C=C)C3)cc4)C										
Rabeprazole	FALSE	77.1	96.31	5	1	359.44263	25	1.83	2.08	4.54	1.83	2.366
0.33	3	O=S(c2nc1ccccc1n2)Cc3nccc(OCCCOC)c3C										
Raloxifene	FALSE	70	98.24	5	2	473.58327	34	5.63	6.86	8.03	6.8	6.37
0.25	4	O=C(c1c3ccc(O)cc3sc1c2ccc(O)cc2)c5ccc(OCCN4CCCCC4)cc5										
Raltegravir	FALSE	150.01	150.01	7	3	444.41634	32	-3.48	4.5	1.16	-0.68	-0.291
0.3	2	Cc1nnc(o1)C(=O)NC(C)(C)C\3=N\C(C(=O)NCc2ccc(F)cc2)=C(\O)C(=O)N/3C										
Ranolazine	FALSE	74.27	74.27	6	2	427.53651	31	3.44	1.01	7.82	3.47	2.991
0.46	2	O=C(Nc1c(cccc1C)C)CN3CCN(CC(O)COc2ccccc2OC)CC3										
Regorafenib	FALSE	92.35	92.35	4	3	482.81541	33	5.25	5.18		5.26	4.381
0.1	3	CNC(=O)c1cc(ccn1)Oc2ccc(c(c2)F)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl										
Repaglinide	FALSE	78.86	78.86	5	2	452.58573	33	1.8	4.19	6.02	5.78	4.69
5.307	0.48	2	O=C(O)c1ccc(cc1OCC)CC(=O)N[C@H](c2ccccc2N3CCCCC3)CC(C)C									
Reserpine	FALSE	117.78	117.78	10	1	608.67869	44	3.81	3.86	7.25	4.05	4.242
0.52	3	O=C(OC)[C@H]6[C@H]4C[C@@H]3c2nc1ccc(OC)ccc1c2CCN3C[C@H]4C[C@@H](OC(=O)c5cc(OC)c(OC)c(OC)c5)[C@@H]6OC										
Ribavirin	FALSE	143.71	143.71	7	4	244.20467	17	-2.26	-2.85		-2.26	-2.746
0.62	1	OC[C@@H](O1)[C@@H](O)[C@@H](O)[C@@H]1n2N=C(C(N)=O)N=C2										
Rifaximin	FALSE	198.37	198.37	12	5	785.87854	57	0.18	7.19	4.42	3.22	5.066
0.44	4											

CC(=O)O[C@H]3[C@H](C)[C@H](O)[C@H](C)[C@@H](O)[C@@H](C)\C=C\C=C(\C)C(=O)Nc6c2c(nc1cc(C)ccn12)c5c4C(=O)[C@@](C)(O/C=C/[C@H](OC)[C@H]3C)Oc4c(C)c(O)c5c6O

Riociguat	FALSE	138.07	138.07	8	2	422.41566	31	-0.31		1.84	1.95	-0.31
	2.201	0.15	4	c14ncccc4c(-c(nc2N)nc(N)c2N(C)C(=O)OC)nn1Cc3ccccc3F								
Risedronate	FALSE	167.8	167.8	8	5	283.11226	17	-8.31	1.1	-2.62	5.07	-2.94
	-0.263	0.29	1	OC(Cc1cccnc1)(P(=O)(O)O)P(=O)(O)O								
Ritodrine	FALSE	72.72	72.72	4	4	287.35354	21	-0.29		1.65	9.31	1.61
	2.655	0.29	2	O[C@H](c1ccc(O)cc1)[C@@H](NCCc2ccc(O)cc2)C								
Ritonavir	FALSE	145.77	202.26	7	4	720.94422	50	5.28		4.94	2.48	5.28
	5.237	0.43	4	CC(C)c4nc(CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)cs4								
Rivaroxaban	FALSE	88.18	116.42	5	1	435.88131	29	1.84		2.39		1.84
	1.984	0.32	2	c1cc(ccc1N2CCOCC2=O)N3C[C@@H](OC3=O)CNC(=O)c4ccc(s4)Cl								
Roflumilast	FALSE	60.45	60.45	4	1	403.20746	26	4.83		3		4.83
	4.402	0.29	2	C1CC1COC2=C(C=CC(=C2)C(=O)NC3=C(C=NC=C3Cl)Cl)OC(F)F								
Rosiglitazone		FALSE	71.53	96.83	6	1	357.42676	25	1.47	6.34	3.02	6.5
	2.56	3.462	0.28	2	O=C1NC(=O)SC1Cc3ccc(OCCN(c2ncccc2)C)cc3							
Rosuvastatin		FALSE	140.91	149.3	8	3	481.53762	33	-2.71	4.25	1.9	
	0.42	2.427	0.41	2	O=S(=O)(N(c1nc(c(c(n1)C(C)C)/C=C/[C@@H](O)C[C@@H](O)CC(=O)O)c2ccc(F)cc2)C)C							
Ruxolitinib	FALSE	83.18	83.18	4	1	306.36501	23	1.69		2.18	2.57	1.69
	2.741	0.41	3	C1CCC(C1)C(CC#N)N2C=C(C=N2)C3=C4C=CNC4=NC=N3								
Sapropterin	FALSE	132	132	8	6	241.2471	17	-4.95		-3.69	9.2	-4.22
	-2.336	0.56	0	O=C2\N=C(/NC=1NC[C@@H](NC=12)[C@@H](O)[C@@H](O)C)N								
Saquinavir	FALSE	166.75	166.75	7	5	670.8408	49	4.41		4.73	7.61	4.44
	3.667	0.5	3	O=C(N)C[C@H](NC(=O)c1nc2c(cc1)cccc2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN5[C@H](C(=O)NC(C)(C)C)C[C@@H]4CCCC[C@@H]4C5								
Sibutramine	FALSE	3.24	3.24	1	0	279.84804	19	3.2		5.59	9.69	5.43
	5.176	0.65	1	C1CC1=CC=C(C2(CCC2)C(CC(C)C)N(C)C)C=C1								
Sildenafil	FALSE	109.13	117.51	7	1	474.57639	33	2.25		1.98	6.03	2.27
	2.247	0.5	2	CCN1CCN(S(=O)(C2=CC=C(OCC)C(C3=NC4=C(N(C)N=C4CCC)C(N3)=O)=C2)=O)CC1								
Silodosin	FALSE	97.05	97.05	6	3	495.53448	35	1.05		2.97	8.93	2.52
	3.451	0.48	2	FC(F)(F)COc3ccccc3OCCN[C@H](C)Cc1cc2c(c(c1)C(=O)N)N(CC2)CCCO								
Simeprevir	FALSE	156.88	193.5	9	2	749.93908	52	3.05	4.47	5.3	3.01	4.99
	4.705	0.55	3	Cc1c(ccc2c1nc(cc2O[C@@H]3C[C@@H]4[C@@H](C3)C(=O)N(CCCC/C=C\[C@@H]5C[C@]5(NC4=O)C(=O)NS(=O)(=O)C6CC6)C)c7nc(cs7)C(C)C)OC								
Sitagliptin	FALSE	77.04	77.04	4	1	407.31361	28	1.21		0.69	7.21	1.3
	1.93	0.44	2	Fc1cc(c(F)cc1F)C[C@@H](N)CC(=O)N3Cc2nnc(n2CC3)C(F)(F)F								
Sodium phenylbutyrate		FALSE	40.12	40.12	2	0	163.19314	12	-0.19	4.76	2.28	
	2.42	0.932	0.3	1	O=C([O-])CCCC1=CC=CC=C1							
Sofosbuvir	FALSE	162.53	162.53	9	3	529.45252	36	1.61		0.84		1.62
	1.302	0.5	1	C[C@@H](C(OC(C)C)=O)N[P@](OC[C@@H]1[C@H]([C@@](F)([C@@H](O1)N2C=CC(NC2=O)=O)C)O)(OC3=CC=CC=C3)=O								
Sotalol	FALSE	78.43	86.81	4	3	272.3638	18	-1.6		0.23		0.32
	0.494	0.5	1	O=S(=O)(Nc1ccc(cc1)C(O)CNC(C)C)C								
Sparfloxacin		FALSE	98.9	98.9	7	3	392.39978	28	-0.54	6.26	-0.1	8.59
	1.2	1.649	0.47	1	C[C@@H]1CN(C[C@@H](N1)C)c2c(c(c3c(c2F)n(cc(c3=O)C(=O)O)C4CC4)N)F							
Spirapril	FALSE	95.94	146.54	8	2	466.61399	31	-0.48	2.99	1.05	5.28	3.16
	3.001	0.59	1	O=C(OCC)[C@@H](N[C@H](CC(=O)N2[C@H](C(=O)O)CC1(SCCS1)C2)C)CCc3ccccc3								
Spironolactone		FALSE	60.44	85.74	5	0	416.57347	29	3.12		2.84	
	3.12	3.731	0.79	0	O=C5O[C@@]4([C@@]3([C@H]([C@@H]2[C@H](SC(=O)C)C/C1=C/C(=O)CC[C@]1(C)[C@H]2CC3)CC4)C)CC5							
Stanozolol	FALSE	48.91	48.91	2	2	328.49157	24	5.53		4.56	3.86	5.53
	3.849	0.86	1	O[C@@]5(C)CC[C@H]4[C@H]3[C@@H]([C@]2(CC1c(nnc1)C[C@@H]2CC3)C)CC[C@@]45C								
Stavudine	FALSE	78.87	78.87	4	2	224.21328	16	-0.86		-0.49		-0.86
	-0.321	0.4	0	O=C1/C(=C\N(C(=O)N1)[C@@H]/2O[C@@H](\C=C\2)CO)C								
Succimer	FALSE	74.59	152.19	6	4	182.21804	10	-2.82	2.74	-1.48		1.93
	0.279	0.5	0	O=C(O)[C@@H](S)[C@@H](S)C(=O)O								
Sulfacytine	FALSE	104.86	113.24	5	2	294.32955	20	-2.49	2.78	-0.33		-0.49
	0.208	0.17	1	CCN1C=CC(NS(=O)(=O)C2=CC=C(N)C=C2)=NC1=O								
Sulfadoxine	FALSE	116.43	124.8	7	2	310.32896	21	-1.49	6.16	1.23		0.34
	0.837	0.17	2	COC1=C(N=CN=C1OC)NS(=O)(=O)C2=CC=C(C=C2)N								
Sulfameter	FALSE	107.2	115.58	6	2	280.30298	19	-0.48	6.69	0.65		0.42
	0.297	0.09	2	O=S(=O)(Nc1ncc(OC)cn1)c2ccc(N)cc2								
Sulfamethizole		FALSE	97.97	134.59	5	2	270.3313	17	-1.17	5.51	0.42	
	0.51	0.772	0.11	2	O=S(=O)(Nc1nnc(s1)C)c2ccc(N)cc2							
Sulfamethoxazole		FALSE	98.22	106.6	4	2	253.27763	17	-0.32	5.81	0.56	
	0.89	0.709	0.1	2	O=S(=O)(Nc1noc(c1)C)c2ccc(N)cc2							
Sulfaphenazole		FALSE	90.01	98.39	4	2	314.36226	22	0.98	6.47	2.07	
	1.52	1.922	0	3	O=S(=O)(c1ccc(N)cc1)Nc3ccnn3c2ccccc2							
Sulfasalazine		FALSE	141.31	149.69	8	3	398.39255	28	0.03	2.88	3.88	
	3.18	3.463	0	3	O=S(=O)(Nc1ccccn1)c3ccc(/N=N/c2cc(C(O)=O)c(O)cc2)cc3							
Sulfinpyrazone		FALSE	57.69	76.9	3	0	404.4815	29	-0.2	5.44	1.66	
	2.3	3.434	0.13	3	O=C2N(c1ccccc1)N(C(=O)C2CCS(=O)c3ccccc3)c4ccccc4							
Sulfoxone	FALSE	132.79	179.59	8	4	404.48164	25	-6.5	2.58	-1.21		-2
	1.132	0.14	2	OS(=O)CNc1ccc(cc1)S(=O)(=O)c2ccc(NCS(=O)O)cc2								
Sumatriptan	FALSE	65.2	73.58	3	2	295.40043	20	-1.21		0.74	9.49	0.67
	1.436	0.43	2	O=S(=O)(NC)Cc1cc2c(cc1)ncc2CCN(C)C								
Sunitinib	FALSE	77.23	77.23	3	3	398.47378	29	1.33		3	9.78	3.15
	2.997	0.36	2	CCN(CC)CCNC(=O)c1c(c([nH]c1C)/C=C\2/c3cc(ccc3NC2=O)F)C								
Tamsulosin	FALSE	99.88	108.26	6	2	408.51172	28	0.86		2.17	9.03	2.24
	2.719	0.4	2	CCOc1ccccc1OCCN[C@@H](C)Cc1ccc(OC)c(c1)S(=O)(=O)N								
Tedizolid	FALSE	106.26	106.26	7	1	370.3378	27	1.56		1.28		1.56
	1.784	0.24	3	O=C4O[C@H](CN4c3cc(F)c(c1ccc(nc1)c2nn(nn2)C)cc3)CO								
Tegaserod	FALSE	85.29	85.29	3	4	301.38671	22	2.41		2.81	9.65	2.91
	3.131	0.38	2	CCCCCNC(=N)N\N=C\c2cnc1ccc(cc12)OC								
Telaprevir	FALSE	179.56	179.56	8	4	679.84932	49	3.93		5.35		3.93
	2.685	0.72	1	CCC[C@@H](C(=O)C(=O)NC1CC1)NC(=O)[C@@H]2[C@H]3CCC[C@H]3CN2C(=O)[C@H](C(C)(C)C)NC(=O)[C@H](C4CCCCC4)NC(=O)c5cnccn5								
Telithromycin		FALSE	171.85	171.85	13	1	812.0037	58	3.79		3.75	8.13
	4.52	4.172	0.72	2	O=C2[C@@H]([C@@H](O[C@@H]1O[C@@H](C[C@H](N(C)C)[C@H]1O)C)[C@@](OC)(C)C[C@H](C(=O)[C@H](C)[C@H]3N(C(=O)O[C@]3(C)[C@H](OC(=O)[C@@H]2C)CC)CCCCn4cc(nc4)c5cccnc5)C)C								
Tenofovir	FALSE	146.19	146.19	8	3	287.21232	19	-5.63	2.09	-1.56	4.36	-1.71
	-0.911	0.44	2	O=P(O)(O)CO[C@H](C)Cn1c2ncnc(c2nc1)N								
Testolactone		FALSE	43.37	43.37	3	0	300.39206	22	2.52		2.63	
	2.52	3.263	0.68	0	CC12CCC3C(C1CCC(=O)O2)CCC4=CC(=O)C=CC34C							
Thiabendazole		FALSE	41.57	69.81	2	1	201.24768	14	2.47		2.36	3.58
	2.47	2.368	0	3	[nH]1c2ccccc2nc1c3cscn3							
Thioguanine	FALSE	79.09	111.18	5	3	167.1917	11	-0.16		-1.88	11.12	-0.16
	-4.20E-02	0	1	S=C2/N=C(\Nc1ncnc12)N								
Ticagrelor	FALSE	138.44	163.74	10	4	522.56802	36	1.9		2.55	3.12	1.9
	2.703	0.57	3	CCCSC1=NC(=C2C(=N1)N(N=N2)[C@@H]3C[C@@H]([C@H]([C@H]3O)O)OCCO)N[C@@H]4C[C@H]4C5=CC(=C(C=C5)F)F								
Ticlopidine	FALSE	3.24	31.47	1	0	263.78566	17	3.6		4.39	7.1	3.77
	3.665	0.29	2	C1c1ccccc1CN3Cc2c(scc2)CC3								
Tiludronate	FALSE	134.68	159.97	7	4	318.60828	17	-5.75	0.83	0.26		-0.32
	2.281	0.14	1	c1cc(ccc1SC(P(=O)(O)O)P(=O)(O)O)Cl								
Tinidazole	FALSE	97.78	106.16	5	0	247.27152	16	-0.27		-0.32	2.3	-0.27
	0.149	0.62	1	[O-][N+](=O)c1cnc(n1CCS(=O)(=O)CC)C								
Tiopronin	FALSE	66.4	105.19	4	3	163.19485	10	-4.01	3.4	-0.23		-0.33
	-0.362	0.6	0	CC(S)C(=O)NCC(O)=O								
Tipranavir	FALSE	105.58	113.96	6	2	602.66432	42	3.19	4.5	7.76		7.21
	6.948	0.35	3	CCC[C@]1(CC(/O)=C(\C(=O)O1)[C@H](CC)c3cccc(NS(=O)(=O)c2ccc(cn2)C(F)(F)F)c3)CCc4ccccc4								
Tofacitinib	FALSE	88.91	88.91	5	1	312.3696	23	-1.01	6.04	1.52	6.78	0.93
	1.372	0.5	2	CC2CCN(C(=O)CC#N)CC2N(C)c3ncnc1ncccc13								

Tolazamide	FALSE	78.5	86.89	4	2	311.39983	21	-0.13	5.03	1.34	3.26	1.71
2.483	0.5	1	O=S(=O)(c1ccc(cc1)C)NC(=O)NN2CCCCCC2									
Tolrestat	FALSE	49.77	81.86	4	1	357.34746	24	-0.25	3.49	3.43		3.41
3.458	0.25	2	CN(CC(=O)O)C(=S)C1=CC=CC2=C1C=CC(=C2C(F)(F)F)OC									
Torsemide	FALSE	100.19	108.57	5	3	348.41999	24	1.54	2.63	3.36	5.33	3.52
2.133	0.25	2	O=S(=O)(c2c(Nc1cc(ccc1)C)ccnc2)NC(=O)NC(C)C									
Tranexamic acid	FALSE	63.32	63.32	3	2	157.21019	11	-2.19	4.79	-1.8	10.27	
0.32	0.725	0.88	0	NC[C@@H]1CC[C@H](CC1)C(O)=O								
Treprostinil	FALSE	86.99	86.99	5	3	390.51306	28	0.78	3.19	3.72		
4.4	4.435	0.7	1	O=C(O)COC1=C2C[C@@]3([H])C[C@@H](O)[C@H](CC[C@@H](O)CCCCC)[C@@]3([H])CC2=CC=C1								
Triamterene	FALSE	129.62	129.62	7	3	253.26264	19	1.3		1.61	6.3	1.34
1.278	0	3	C3=C(C1=C(N=C2C(=N1)C(=NC(=N2)N)N)N)C=CC=C3									
Tridihexethyl	FALSE	20.23	20.23	1	1	318.51663	23	-1.81		1.32		
-1.81	3.191	0.71	1	OC(c1ccccc1)(CC[N+](CC)(CC)CC)c2ccccc2								
Trimethobenzamide	FALSE	69.26	69.26	6	1	388.45741	28	0.6		2.33	8.66	
1.85	2.694	0.38	2	O=C(c1cc(OC)c(OC)c(OC)c1)NCc2ccc(OCCN(C)C)cc2								
Trimethoprim	FALSE	105.51	105.51	7	2	290.31772	21	0.67		0.98	7.25	
0.79	1.543	0.29	2	COc1cc(cc(c1OC)OC)cc2cnc(nc2N)N								
Trioxsalen	FALSE	39.44	39.44	2	0	228.24327	17	3.8		3.47		3.8
3.281	0.21	2	O=C/3Oc2c(c1oc(cc1cc2\C(=C\3)C)C)C									
Troleandomycin	FALSE	184.19	184.19	16	0	813.96838	57	2.79		4.2	7.84	
3.36	3.039	0.88	0	O=C(O[C@@H]4[C@@H](N(C)C)C[C@H](O[C@H]4O[C@@H]3[C@H]([C@H](O[C@@H]1O[C@H]([C@H](OC(=O)C)[C@@H](OC)C1)C)[C@H](C(=O)O[C@H](C)[C@H](C)[C@H](OC(=O)C)[C@H](C(=O)[C@]2(OC2)C[C@@H]3C)C)C)C)C)C												
Trospium	FALSE	46.53	46.53	3	1	392.51059	29	0.7		-1.16		0.7
2.349	0.48	2	OC(c1ccccc1)(c2ccccc2)C(=O)O[C@@H]3C[C@@H]5CC[C@H](C3)[N+]45CCCC4									
Trovafloxacin	FALSE	99.76	99.76	7	2	416.3533	30	-1.11	5.8	0.33	7.92	
0.96	2.213	0.25	2	O=C(O)C2=CN(c1nc(c(F)cc1C2=O)N3C[C@H]4[C@H](N)[C@H]4C3)c5ccc(F)cc5F								
Uracil mustard	FALSE	61.44	61.44	3	2	252.09784	15	1.11		0.6		
1.13	0.284	0.5	0	O=C1C(\N(CCCl)CCCl)=C/NC(=O)N1								
Valsartan	FALSE	112.07	112.07	6	2	435.51876	32	0.01	3.53	4.86		4.74
4.448	0.38	3	O=C(O)[C@@H](N(C(=O)CCCC)Cc3ccc(c1ccccc1c2nnnn2)cc3)C(C)C									
Vandetanib	FALSE	59.51	59.51	6	1	475.35396	30	4.01		5.84	9.27	5.5
5.087	0.36	3	CN1CCC(CC1)COc2cc3c(cc2OC)c(ncn3)Nc4ccc(cc4F)Br									
Vemurafenib	FALSE	91.92	100.3	4	2	489.92212	33	3.19		4.17		4.26
4.813	0.13	4	CCCS(=O)(=O)Nc1ccc(F)c(c1F)C(=O)c2c[nH]c3c2cc(cn3)c4ccc(Cl)cc4									
Vismodegib	FALSE	76.13	84.51	4	1	421.29706	27	2.98		2.74	3.73	2.98
4.265	0.05	3	CS(=O)(=O)c1=CC(=C(C=C1)C(=O)NC2=CC(=C(C=C2)Cl)C3=CC=CC=N3)Cl									
Vorapaxar	FALSE	77.52	77.52	5	1	492.58172	36	4.54		4.34	3.66	4.54
5.261	0.48	2	Fc1cccc(c1)c2ccc(nc2)\C=C\[C@H]4[C@H]3[C@@H](C[C@H](NC(=O)OCC)CC3)C[C@H]5C(=O)O[C@@H]([C@@H]45)C									
Zafirlukast	FALSE	115.73	124.11	6	2	575.67522	41	4.28	4.01	7.09		6.15
6.299	0.29	4	O=S(=O)(c1ccccc1C)NC(=O)c2ccc(c(OC)c2)Cc4c3cc(ccc3n(c4)C)NC(=O)OC5CCCC5									
Zidovudine	FALSE	128.62	128.62	6	2	267.24132	19	-0.53		0.04		-0.53
-0.163	0.6	0	O=C1NC(C(C)=CN1[C@@H]2O[C@H](CO)[C@@H](N=[N+]=[N-])C2)=O									
Zileuton	FALSE	66.56	94.8	2	2	236.29018	16	3.74		2.48		3.74
1.926	0.18	2	O=C(N)N(O)C(c2sc1ccccc1c2)C									
Abiraterone	TRUE	33.12	33.12	2	1	349.50904	26	5.7		5.17	5.31	5.7
4.223	0.62	1	O[C@@H]2C/C1=C/C[C@@H]4[C@@H]([C@@]1(C)CC2)CC[C@@]3(C(=C/C[C@H]34)\c5cccnc5)C									
Acebutolol	TRUE	87.66	87.66	5	3	336.42591	24	-0.11		1.71	9.41	1.95
1.615	0.56	1	O=C(Nc1ccc(OCC(O)CNC(C)C)c(c1)C(=O)C)CCC									
Acetaminophen	TRUE	49.33	49.33	2	2	151.16256	11	0.34		0.49		
0.34	0.708	0.12	1	CC(NC1=CC=C(O)C=C1)=O								
Acetazolamide	TRUE	115.04	151.66	5	2	222.24543	13	-0.76	7.44	-0.98		
-0.26	-0.579	0.25	1	O=S(=O)(c1nnc(s1)NC(=O)C)N								
Acetophenazine	TRUE	47.02	72.32	6	1	411.56025	29	2.87		2.71	8.52	
3.22	3.233	0.43	2	O=C(c2cc1N(c3c(Sc1cc2)cccc3)CCCN4CCN(CCO)CC4)C								
Acitretin	TRUE	46.53	46.53	3	1	326.42933	24	3.03	4.66	6.07		5.73
5.666	0.29	1	O=C(O)\C=C(\C=C\C=C(\C=C\c1c(cc(OC)c(c1C)C)C)C)C									
Afatinib	TRUE	88.61	88.61	7	2	485.9384	34	3.03		4.49	8.01	3.59
3.917	0.29	3	CN(C)C\C=C\C(=O)Nc3cc1c(Nc(cc2Cl)ccc2F)ncnc1cc3OC4COCC4									
Albendazole	TRUE	67	92.31	4	2	265.3314	18	3.06		3.46	5.62	3.07
3.065	0.33	2	O=C(OC)Nc2nc1ccc(SCCC)cc1n2									
Almotriptan	TRUE	56.41	64.79	3	1	335.46429	23	-0.02		1.79	9.48	1.89
2.103	0.53	2	O=S(=O)(N1CCCC1)Cc3cc2c(cnc2cc3)CCN(C)C									
Alprazolam	TRUE	43.07	43.07	3	0	308.76491	22	2.5		2.56	2.28	2.5
3.513	0.12	3	Clc1=CC2=C(C=C1)N3C(C)=NN=C3CN=C2C4=CC=CC=C4									
Alprenolol	TRUE	41.49	41.49	3	2	249.34862	18	0.79		2.65	9.45	2.88
2.639	0.47	1	O(c1ccccc1C\C=C)CC(O)CNC(C)C									
Amantadine	TRUE	26.02	26.02	1	1	151.24868	11	-0.69		2	10.76	2.22
1.495	1	0	NC13CC2CC(CC(C1)C2)C3									
Aminoglutethimide	TRUE	72.19	72.19	3	2	232.27834	17	1.41		0.77	4.41	
1.41	1.479	0.38	1	O=C1NC(=O)CCC1(c2ccc(N)cc2)CC								
Amitriptyline	TRUE	3.24	3.24	1	0	277.40332	21	3.15		4.85	9.18	
4.92	4.772	0.3	2	c3cc2c(/C(c1c(cccc1)CC2)=C\CCN(C)C)cc3								
Amlodipine	TRUE	99.88	99.88	7	2	408.87589	28	2.64		3.43	8.97	4.16
1.576	0.4	1	Clc1ccccc1C2C(=C(/N/C(=C2/C(=O)OCC)COCCN)C)\C(=O)OC									
Amoxapine	TRUE	36.86	36.86	4	1	313.78144	22	1.2		3.41	8.62	2.35
2.897	0.24	2	Clc2ccc1Oc4c(/N=C(\c1c2)N3CCNCC3)cccc4									
Amphetamine	TRUE	26.02	26.02	1	1	135.20622	10	-0.63		1.74	9.94	1.81
1.634	0.33	1	NC(CC1=CC=CC=C1)C									
Anileridine	TRUE	55.56	55.56	4	1	352.46992	26	2.05		3.1	8.73	3.02
3.603	0.41	2	O=C(OCC)C3(c1ccccc1)CCN(CCc2ccc(N)cc2)CC3									
Aniracetam	TRUE	46.61	46.61	3	0	219.23652	16	0.27		0.72		0.27
1.791	0.33	1	O=C2N(C(=O)c1ccc(OC)cc1)CCC2									
Apomorphine	TRUE	43.7	43.7	3	2	267.32238	20	2.51		2.49	7.88	3.05
3.116	0.29	2	OC1=C(O)C(C2=CC=CC3=C2[C@@H](C4)N(C)CC3)=C4C=C1									
Aprepitant	TRUE	75.19	75.19	6	2	534.42666	37	4.23		4.83	4.35	4.23
4.635	0.39	2	FC(F)(F)c1cc(cc(c1)C(F)(F)F)[C@H](O[C@H]4OCCN(CC/2=N/C(=O)NN\2)[C@H]4c3ccc(F)cc3)C									
Aripiprazole	TRUE	44.81	44.81	4	1	448.38537	30	5.37		5.82	7.89	
5.59	4.998	0.43	2	Clc4cccc(N3CCN(CCCCOc2ccc1c(NC(=O)CC1)c2)CC3)c4Cl								
Armodafinil	TRUE	60.16	79.37	2	1	273.3501	19	1.17		0.94		1.17
1.733	0.13	2	C1=CC=C(C=C1)C(C2=CC=CC=C2)[S@](=O)CC(=O)N									
Atomoxetine	TRUE	21.26	21.26	2	1	255.35474	19	0.69		3.94	10.12	3.28
3.577	0.29	2	CC1=C(C=CC=C1)O[C@H](CCNC)C2=CC=CC=C2									
Atropine	TRUE	49.77	49.77	4	1	289.36942	21	-0.94		1.3	9.98	1.53
1.721	0.59	1	CN3[C@H]1CC[C@@H]3C[C@@H](C1)OC(=O)C(CO)c2ccccc2									
Axitinib	TRUE	70.67	95.97	4	2	386.46952	28	4.15		3.33	4.06	4.15
4.492	0.05	4	O=C(NC)c4ccccc4Sc1ccc2c(c1)nnc2\C=C\c3ncccc3									
Azatadine	TRUE	16.13	16.13	2	0	290.40208	22	3.52		3.56	8.74	4.97
4.084	0.35	2	n4c3\C(=C1/CCN(C)CC1)c2ccccc2CCc3ccc4									
Baclofen	TRUE	63.31	63.31	3	2	213.66078	14	-0.94	4.04	-0.62	10.33	1.56
1.419	0.3	1	Clc1=CC=C(C(CC(O)=O)CN)C=C1									
Benzphetamine	TRUE	3.24	3.24	1	0	239.35534	18	2.95		4.38	8.88	
4.43	4.185	0.29	2	N(C)(Cc1ccccc1)[C@@H](C)Cc2ccccc2								
Benztropine	TRUE	12.47	12.47	2	0	307.4293	23	2.14		3.52	10.54	4.96
3.875	0.43	2	CN4[C@@H]1CC[C@H]4C[C@H](C1)OC(c2ccccc2)c3ccccc3									
Bepridil	TRUE	15.71	15.71	3	0	366.53956	27	4.06		6.2	9.21	5.8
5.265	0.5	2	O(CC(C)C)CC(N1CCCC1)CN(c2ccccc2)Cc3ccccc3									
Bethanidine	TRUE	36.42	36.42	3	2	177.2462	13	-0.53		1.5	12.81	1.46
1.213	0.3	1	N(=C(/NCc1ccccc1)NC)\C									
Bexarotene	TRUE	37.29	37.29	2	1	348.47791	26	5.63	4.08	8.19		8.55
6.405	0.38	2	O=C(O)c1ccc(cc1)C(/c2c(cc3c(c2)C(CCC3(C)C)(C)C)C)=C									

Biperiden	TRUE	23.47	23.47	2	1	311.46106	23	2.17	4.94	9.58	4.01	3.648
0.62	1	OC(c1ccccc1)(CCN2CCCCC2)C4C3\C=C/C(C3)C4										
Bromazepam	TRUE	54.35	54.35	3	1	316.1527	19	1.65	1.7	2	1.65	2.327
0.07	2	BrC1=CC2=C(C=C1)NC(CN=C2C3=CC=CC=N3)=O										
Bromocriptine	TRUE	118.21	118.21	6	3	654.5945	43	5.08	6.58	6.72	5.15	4.363
0.59	2	BrC1=C(C[C@H]2N(C)C3)C4=C(C=CC=C4C2=C[C@H]3C(N[C@]5(C(C)C)O[C@@]6(N([C@@H](CC(C)C)C(N7CCC[C@H]76)=O)C5=O)O)=O)N1										
Bromodiphenhydramine	TRUE	12.47	12.47	2	0	334.2508	20	3.11	4.32	8.71	4.43	4.133
0.29	2	Brc1ccc(cc1)C(OCCN(C)C)c2ccccc2										
Brompheniramine	TRUE	16.13	16.13	2	0	319.23946	19	1.63	3.3	9.33	3.56	3.78
0.31	2	Brc1ccc(cc1)C(c2ncccc2)CCN(C)C										
Buclizine	TRUE	6.48	6.48	2	0	433.02801	31	6.11	8.06	6.98	6.22	7.121
0.36	3	Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)Cc4ccc(cc4)C(C)(C)C										
Budipine	TRUE	3.24	3.24	1	0	293.44577	22	1.91	5.58	9.92	4.64	4.691
0.43	2	c1(ccccc1)C3(c2ccccc2)CCN(C(C)(C)C)CC3										
Bumetanide	TRUE	118.72	127.1	6	3	364.4161	25	-0.19	3.18	3.37	4.48	2.78
2.862	0.24	2	O=S(=O)(c2cc(cc(NCCCC)c2Oc1ccccc1)C(=O)O)N									
Buprenorphine	TRUE	62.16	62.16	5	2	467.64013	34	2.46	3.99	8.31	3.44	3.923
0.79	1	Oc7ccc5c1c7o[C@H]3[C@]6(OC)[C@H](C[C@@]2([C@H](N(CC[C@@]123)CC4CC4)C5)CC6)[C@@](O)(C)C(C)(C)C										
Bupropion	TRUE	29.1	29.1	2	1	239.74112	16	3.27	3.21	7.16	3.47	3.12
0.46	1	O=C(C(C)NC(C)(C)C)c1=CC=CC(Cl)=C1										
Buspirone	TRUE	69.64	69.64	6	0	385.50313	28	3.08	2.69	7.01	3.43	2.545
0.71	1	O=C1N(CCCCN2CCN(CC2)c3=NC=CC=N3)C(CC4(CCCC4)C1)=O										
Butabarbital	TRUE	75.27	75.27	3	2	212.24564	15	1.41	7.71	1.58		1.52
1.841	0.7	0	O=C1NC(=O)NC(=O)C1(C(C)CC)CC									
Cabergoline	TRUE	71.67	71.67	4	2	451.60427	33	0.55	4.17	9.41	2.43	3.56
0.54	2	O=C(NCC)N(C(=O)[C@@H]2C[C@@H]3c4cccc1c4c(cn1)C[C@H]3N(C2)C\C=C)CCCN(C)C										
Caffeine	TRUE	58.44	58.44	3	0	194.19059	14	-0.13	-0.04		-0.13	0.424
0.38	1	CN1C=NC2=C1C(=O)N(C(=O)N2C)C										
Carbamazepine	TRUE	46.33	46.33	1	1	236.26858	18	2.67	2.38		2.67	2.679
0	2	c1ccc2c(c1)C=Cc3ccccc3N2C(=O)N										
Carbinoxamine	TRUE	25.36	25.36	3	0	290.78786	20	1.5	2.67	8.65	2.76	3.22
0.31	2	Clc1ccc(cc1)C(OCCN(C)C)c2ncccc2										
Carisoprodol	TRUE	90.65	90.65	4	2	260.32996	18	2.15	2.34		2.15	2.199
0.83	0	O=C(OCC(COC(=O)NC(C)C)(C)CCC)N										
Carvedilol	TRUE	75.74	75.74	5	3	406.47424	30	3.1	4.04	8.38	4.12	4.014
0.25	4	O(c4ccccc4OCCNCC(O)COc3cccc2c3c1c(cccc1)n2)C										
Cevimeline	TRUE	12.47	37.77	3	0	199.31308	13	-0.84	1.14	9.51	1.23	1.035
1	0	O1[C@H](SC[C@@]12CN3CCC2CC3)C										
Chlophedianol	TRUE	23.47	23.47	2	1	289.7998	20	2.16	3.63	9.43	3.81	3.559
0.29	2	Clc1ccccc1C(O)(c2ccccc2)CCN(C)C										
Chloramphenicol	TRUE	115.38	115.38	5	3	323.12937	20	1.02	1.28		1.02	1.025
0.36	1	c1cc(ccc1[C@H]([C@@H](CO)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]										
Chlordiazepoxide	TRUE	53.14	53.14	3	1	299.75486	21	2.16	3.79	2.38	2.16	2.297
0.12	2	C1C1=CC2=C(N=C(NC)C[N+](=O-))=C2C3=CC=CC=C3)C=C1										
Chlormezanone	TRUE	54.45	62.83	3	0	273.73587	17	0.86	1.57		0.86	1.559
0.36	1	O=S1(CCC(N(C)C1C2=CC=C(C=C2)Cl)=O)=O										
Chlorphentermine	TRUE	26.02	26.02	1	1	183.67786	12	0.46	2.85	9.76	2.75	2.503
0.4	1	Clc1ccc(cc1)CC(N)(C)C										
Chlorpromazine	TRUE	6.48	31.78	3	0	318.86415	21	3.26	5.3	9.41	5.2	4.739
0.29	2	CN(C)CCCN1c2ccccc2Sc3c1cc(cc3)Cl										
Chlorprothixene	TRUE	3.24	28.54	2	0	315.86021	21	4.41	5.48	9.05	6.05	5.124
0.22	2	Clc2cc1C(\c3c(Sc1cc2)cccc3)=C/CCN(C)C										
Chlorzoxazone	TRUE	38.33	38.33	2	1	169.56515	11	2.15	1.87		2.19	2.004
0	1	Clc2cc1c(OC(=O)N1)cc2										
Cilostazol	TRUE	81.93	81.93	5	1	369.46067	27	3.05	3.53	2.19	3.05	3.579
0.6	2	O=C4Nc3c(cc(OCCCCCc1nnnn1C2CCCCC2)cc3)CC4										
Cinacalcet	TRUE	12.03	12.03	1	1	357.41198	26	3.96	6.35	9.19	5.74	5.956
0.27	3	FC(F)(F)c1cccc(c1)CCCN[C@@H](c3c2ccccc2ccc3)C										
Citalopram	TRUE	36.26	36.26	3	0	324.39194	24	0.39	3.13	9.57	2.51	3.721
0.35	2	Fc1ccc(cc1)C3(OCc2cc(C#N)ccc23)CCCN(C)C										
Clemastine	TRUE	12.47	12.47	2	0	343.89024	24	3.04	5.45	10.23	5.69	4.806
0.43	2	Clc1ccc(cc1)[C@](OCC[C@@H]2N(C)CCC2)(c3ccccc3)C										
Clidinium	TRUE	46.53	46.53	3	1	352.44674	26	0.83	-0.05		0.83	1.795
0.41	2	O=C(OC2C1CC[N+](CC1)(C)C2)C(O)(c3ccccc3)c4ccccc4										
Clobazam	TRUE	40.62	40.62	2	0	300.73962	21	1.67	2.44		1.69	2.738
0.12	2	C1C1=CC(N(C2=CC=CC=C2)C(CC(N3C)=O)=O)=C3C=C1										
Clomipramine	TRUE	6.48	6.48	2	0	314.85232	22	3.41	5.92	9.46	5.39	5.052
0.37	2	C1C1=CC(N(CCCN(C)C)C2=C(CC3)C=CC=C2)=C3C=C1										
Clonazepam	TRUE	87.28	87.28	4	1	315.71119	22	2.34	2.38		2.34	2.859
0.07	2	[O-][N+](C1=CC2=C(C=C1)NC(CN=C2C3=CC=CC=C3Cl)=O)=O										
Clozapine	TRUE	30.86	30.86	4	1	326.82326	23	1.96	3.71	7.14	2.36	3.422
0.28	2	CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl										
Cycloserine	TRUE	64.34	64.34	3	2	102.09194	7	-1.85	-1.19	5.93	-1.84	-1.788
0.67	0	O=C1NOC[C@H]1N										
Danazol	TRUE	46.26	46.26	2	1	337.45527	25	4.7	3.93		4.7	4.874
0.68	1	C#C[C@]5(O)CC[C@H]4[C@H]3[C@@H]([C@@]2(/C(=C\C1Oncc1C2)CC3)C)CC[C@@]45C										
Dapsone	TRUE	86.18	94.56	4	2	248.30088	17	0.94	0.89		0.94	1.439
0	2	O=S(=O)(c1ccc(N)cc1)c2ccc(N)cc2										
Dasatinib	TRUE	106.51	134.75	8	3	488.00553	33	1.84	3.03	6.59	2.25	3.769
0.36	3	Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl										
Desloratadine	FALSE	24.92	24.92	2	1	310.82056	22	4.11	3.83	10.27	6.77	4.213
0.32	2	Clc4cc2c(C(/c1ncccc1CC2)=C3/CCNCC3)cc4										
Desvenlafaxine	TRUE	43.7	43.7	3	2	263.3752	19	0.52	2.68	9.33	2.26	2.796
0.62	1	OC2(C(c1ccc(O)cc1)CN(C)C)CCCCC2										
Dexmethylphenidate	TRUE	38.33	38.33	3	1	233.30615	17	0.47	2.56	9.51	2.54	2.18
0.5	1	O=C([C@@H]([C@@H]1NCCCC1)C2=CC=CC=C2)OC										
Dextromethorphan	TRUE	12.47	12.47	2	0	271.3972	20	2.39	3.94	9.13	4.11	3.674
0.67	1	CN1CC[C@@]23CCCC[C@@H]2[C@@H]1Cc4c3cc(cc4)OC										
Dicyclomine	TRUE	29.54	29.54	3	0	309.4867	22	4.23	6.14	9.24	6.05	5.105
0.95	0	O=C(OCCN(CC)CC)C1(CCCCC1)c2ccccc2										
Diethylpropion	TRUE	20.31	20.31	2	0	205.29606	15	1.84	2.85	8.49	2.95	2.757
0.46	1	O=C(c1ccccc1)C(N(CC)CC)C										
Difenoxin	TRUE	64.33	64.33	4	1	424.53412	32	2.53	3.55	2.13	9.17	5.04
5.114	0.29	3	C(CCN1CCC(CC1)(C(O)=O)C2=CC=CC=C2)(C3=CC=CC=C3)(C4=CC=CC=C4)C#N									
Dihydrocodeine	TRUE	41.93	41.93	4	1	301.38011	22	0.26		1.26	8.43	1.39
1.947	0.67	1	O[C@@H]1[C@@H]2OC3=C(OC)C=CC4=C3[C@@]2([C@H]5CC1)CCN(C)[C@@H]5C4									
Diltiazem	TRUE	59.08	84.38	6	0	414.51783	29	2.26	3.65	8.94	3.63	3.093
0.36	2	O=C2N(c3c(S[C@@H](c1ccc(OC)cc1)[C@H]2OC(=O)C)cccc3)CCN(C)C										
Diphenylpyraline	TRUE	12.47	12.47	2	0	281.39202	21	3.49	3.21	8.78	4.54	3.357
0.37	2	O(C(c1ccccc1)c2ccccc2)C3CCN(C)CC3										
Disulfiram	TRUE	6.48	121.26	4	0	296.5392	16	3.88	3.88		3.88	4.551
0.8	0	CCN(CC)C(=S)SSC(=S)N(CC)CC										
Dolasetron	TRUE	62.4	62.4	4	1	324.3737	24	2.79	2.34	6.22	2.82	2.035
0.47	2	O=C5CN4[C@@H]1C[C@H]5C[C@H]4C[C@H](C1)OC(=O)c3cnc2ccccc23										
Donepezil	TRUE	38.77	38.77	4	0	379.49195	28	3.27	4.6	8.84	4.71	4.569
0.46	2	O=C2c1cc(OC)c(OC)cc1CC2CC4CCN(Cc3ccccc3)CC4										
Dronabinol	TRUE	29.46	29.46	2	1	314.4617	23	7.68	7.24		7.68	6.109
0.62	1	CCCCCc1cc(c2c(c1)OC([C@H]3[C@H]2C=C(CC3)C)(C)C)O										
Dronedarone	TRUE	88.85	97.22	5	1	556.75645	39	5.4	8.57	9.44	7.58	7.015
0.52	3	O=S(=O)(Nc3cc1c(oc(c1C(=O)c2ccc(OCCCN(CCCC)CCCC)cc2)CCCC)cc3)C										

Duloxetine	TRUE	21.26	49.5	2	1	297.41456	21	1.24		4.26	10.02	3.73
	3.618	0.22	3	CNCC[C@@H](C1=CC=CS1)OC2=CC=CC3=CC=CC=C32								
Dutasteride	TRUE	58.2	58.2	2	2	528.52971	37	5.61		4.94		5.61
	5.703	0.63	1	FC(F)(F)c1cc(c(cc1)C(F)(F)F)NC(=O)[C@@H]3[C@]2(CC[C@H]4[C@H]([C@@H]2CC3)CC[C@H]5NC(=O)\C=C/[C@]45C)C								
Efavirenz	TRUE	38.33	38.33	2	1	315.67496	21	4.84		3.73		4.84
	4.381	0.36	1	FC(F)([C@]1(OC(NC2=CC=C(C=C21)Cl)=O)C#CC3CC3)F								
Eletriptan	TRUE	53.17	61.55	3	1	382.51903	27	0.33		3.35	10.35	3.08
	4.438	0.36	3	O=S(=O)(c1ccccc1)CCc4ccc2c(c(cn2)C[C@@H]3N(C)CCC3)c4								
Eliglustat	TRUE	71.03	71.03	5	2	404.54293	29	2.08		4.83	9.59	3.61
	3.808	0.7	1	CCCCCCCC(=O)N[C@H](CN1CCCC1)[C@@H](C2=CC3=C(C=C2)OCCO3)O								
Entacapone	TRUE	130.38	130.38	6	2	305.286	22	0.36	5.15	1.76		2.38
	1.658	0.29	1	[O-][N+](=O)c1cc(\C=C(/C#N)C(=O)N(CC)CC)cc(O)c1O								
Enzalutamide		TRUE	76.44	108.53	4	1	464.43595	32	2.13		3.35	
	2.13	4.334	0.24	2	N#Cc1c(C(F)(F)F)cc(N2C(C(C)(C)N(c3ccc(C(N(C)[H])=O)c(F)c3)C2=S)=O)cc1							
Erlotinib	TRUE	74.73	74.73	7	1	393.43572	29	2.38		4.34	5.06	2.39
	4.309	0.27	3	COCCOc1cc2c(cc1OCCOC)ncnc2Nc3cccc(c3)C#C								
Eszopiclone	TRUE	91.76	91.76	7	0	388.80827	27	-0.41		1.25	6.29	-0.33
	1.386	0.35	2	O=C(O[C@H]3c1nccnc1C(=O)N3c2ncc(Cl)cc2)N4CCN(C)CC4								
Ethchlorvynol		TRUE	20.23	20.23	1	1	144.59876	9	2.06		1.57	
	2.06	2.263	0.43	0	Cl[C@H]=CC(C#C)(O)CC							
Ethinamate	TRUE	52.32	52.32	2	1	167.20502	12	1.47		1.92		1.47
	2.717	0.67	0	O=C(OC1(C#C)CCCCC1)N								
Ethionamide	TRUE	38.9	71	2	1	166.2434	11	1.22		1.73	4.34	1.22
	1.53	0.25	1	S=C(c1ccnc(c1)CC)N								
Ethopropazine		TRUE	6.48	31.78	3	0	312.47225	22	3.51		5.46	9.88
	5.84	5.088	0.37	2	S2c1ccccc1N(c3c2cccc3)CC(N(CC)CC)C							
Ethosuximide		TRUE	46.17	46.17	2	1	141.16773	10	0.38		0.4	
	0.38	0.737	0.71	0	O=C1NC(=O)CC1(C)CC							
Ethotoin	TRUE	49.41	49.41	2	1	204.22518	15	0.77		1.48		0.86
	1.637	0.27	1	O=C2NC(c1ccccc1)C(=O)N2CC								
Ezogabine	TRUE	76.38	76.38	4	3	303.33142	22	0.8		2	5.25	0.81
	2.793	0.19	2	O=C(OCC)Nc1ccc(cc1N)NCc2ccc(F)cc2								
Famotidine	TRUE	175.83	237.75	9	4	337.4454	20	-1.03		-0.58	7.93	-0.4
	-1.135	0.38	1	O=S(=O)(N=C(N)CCSCc1nc(/N=C(/N)N)sc1)N								
Febuxostat	TRUE	83.21	111.45	5	1	316.37483	22	1.73		4.1	3.18	4.87
	3.514	0.31	2	N#Cc1c(OCC(C)CC)ccc(c1)c2nc(c(s2)C(=O)O)C								
Felbamate	TRUE	104.64	104.64	4	2	238.23986	17	1.2		0.5		1.2
	0.984	0.27	1	O=C(OCC(c1ccccc1)COC(=O)N)N								
Felodipine	TRUE	64.63	64.63	5	1	384.25375	25	4.83		5.3	2.73	4.83
	3.549	0.33	1	O=C(OCC)\C1=C(\N/C(=C(/C(=O)OC)C1c2cccc(Cl)c2Cl)C)C								
Fenofibrate	TRUE	52.6	52.6	4	0	360.83134	25	4.8		5.23		4.8
	5.111	0.3	2	O=C(c1ccc(Cl)cc1)c2ccc(OC(C(=O)OC(C)C)(C)C)cc2								
Fentanyl	TRUE	23.55	23.55	2	0	336.47052	25	2.81		3.62	8.78	3.89
	3.838	0.41	2	O=C(CC)N(C1CCN(CC1)CCC2=CC=CC=C2)C3=CC=CC=C3								
Finasteride	TRUE	58.2	58.2	2	2	372.54414	27	3.24		3.01		3.24
	3.174	0.83	0	O=C(NC(C)(C)C)[C@@H]2[C@]1(CC[C@H]3[C@H]([C@@H]1CC2)CC[C@H]4NC(=O)\C=C/[C@]34C)C								
Fingolimod	TRUE	66.48	66.48	3	3	307.47082	22	2.8		5.06	8.71	5.25
	4.199	0.68	1	OCC(N)(CCc1ccc(cc1)CCCCCCCC)CO								
Flibanserin	TRUE	38.82	38.82	3	1	390.40214	28	4.01		5.24	7.98	4.07
	3.609	0.35	2	FC(F)(F)c4cc(N3CCN(CCN2c1ccccc1NC2=O)CC3)ccc4								
Fluconazole	TRUE	81.64	81.64	5	1	306.27078	22	0.5		-0.44	2.94	0.5
	0.75	0.23	3	Fc1ccc(c(F)c1)C(O)(Cn2ncnc2)Cn3ncnc3								
Flucytosine	TRUE	67.48	67.48	3	2	129.09246	9	-2.81		-1.64	2.9	-2.36
	-0.618	0	0	FC=1\C=N/C(=O)NC=1N								
Fluoxetine	TRUE	21.26	21.26	2	1	309.32612	22	1.56		4.57	10.06	4.09
	4.033	0.29	2	CNCCC(c1ccccc1)Oc2ccc(cc2)C(F)(F)F								
Flurazepam	TRUE	35.9	35.9	3	0	387.87822	27	1.64		4.21	9.79	4
	4.213	0.33	2	FC1=CC=CC=C1C2=NCC(N(CCN(CC)CC)C3=C2C=C(C=C3)Cl)=O								
Flurbiprofen		TRUE	37.29	37.29	2	1	244.26092	18	0.98	4.14	3.75	
	4.12	3.68	0.13	2	Fc2cc(ccc2c1ccccc1)C(C(=O)O)C							
Fluvoxamine	TRUE	56.84	56.84	4	1	318.33464	22	1.15		3.32	9.39	3.11
	2.738	0.53	1	FC(F)(F)c1ccc(\C(=N\OCCN)CCCCOC)cc1								
Frovatriptan		TRUE	70.91	70.91	2	3	243.30428	18	-2		0.72	10.38
	0.85	1.414	0.36	2	O=C(N)c3ccc1c(c2c(n1)CC[C@@H](NC)C2)c3							
Gabapentin	TRUE	63.31	63.31	3	2	171.23678	12	-1.31	4.72	-0.66	10.27	1.19
	0.993	0.89	0	O=C(O)CC1(CN)CCCCC1								
Galantamine	TRUE	41.93	41.93	4	1	287.35353	21	1.12		1.02	7.92	1.75
	1.442	0.53	1	O(c2c1O[C@H]4C[C@@H](O)/C=C\[C@@]43c1c(cc2)CN(C)CC3)C								
Gemfibrozil	TRUE	46.53	46.53	3	1	250.33337	18	1.77	4.75	3.94		4.39
	4.172	0.53	1	O=C(O)C(C)(C)CCCOc1cc(ccc1C)C								
Granisetron	TRUE	50.16	50.16	3	1	312.40936	23	-1.42		1.72	10.5	1.47
	2.401	0.56	2	CN4[C@@H]1CCC[C@H]4C[C@H](C1)NC(=O)c3nn(C)c2ccccc23								
Guanabenz	TRUE	76.75	76.75	4	2	231.08192	14	2.05		1.35	7.66	2.49
	2.192	0	1	Clc1cccc(Cl)c1\C=N\N=C(/N)N								
Guanfacine	TRUE	81.47	81.47	4	2	246.09326	15	1.6		1.25	5.29	1.61
	2.03	0.11	1	Clc1cccc(Cl)c1CC(=O)\N=C(/N)N								
Halazepam	TRUE	32.67	32.67	2	0	352.73818	24	4.22		3.75	2.61	4.22
	4.178	0.18	2	FC(F)(CN1C(CN=C(C2=CC=CC=C2)c3=C1C=CC(Cl)=C3)=O)F								
Halofantrine		TRUE	23.47	23.47	2	1	500.4237	33	6.74		9.31	9.44
	8.72	8.2	0.46	3	FC(F)(F)c3ccc2c(cc1c(Cl)cc(Cl)cc1c2c3)C(O)CCN(CCCC)CCCC							
Haloperidol	TRUE	40.54	40.54	3	1	375.86422	26	2.19		3.85	8.49	3.01
	3.887	0.38	2	c1cc(ccc1C(=O)CCCN2CCC(CC2)(c3ccc(cc3)Cl)O)F								
Hydroxyzine	TRUE	35.94	35.94	4	1	374.90427	26	1.95		4	7.79	2.03
	3.467	0.43	2	Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO								
Ibuprofen	TRUE	37.29	37.29	2	1	206.28082	15	0.8	4.41	3.68		3.72
	3.607	0.46	1	CC(C)Cc1ccc(cc1)C(C)C(=O)O								
Iloperidone	TRUE	64.8	64.8	5	0	426.48058	31	2.74		3.92	8.68	3.81
	4.016	0.42	3	O=C(c4ccc(OCCCN3CCC(c2noc1cc(F)ccc12)CC3)c(OC)c4)C								
Indomethacin		TRUE	68.53	68.53	4	1	357.78763	25	-0.16	4.26	4.18	
	3.1	4.235	0.16	3	Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O							
Isocarboxazid		TRUE	67.16	67.16	3	2	231.25052	17	1.03		0.99	3.32
	1.03	1.546	0.17	2	O=C(NNCc1ccccc1)c2noc(c2)C							
Isotretinoin		TRUE	37.29	37.29	2	1	300.43512	22	4.14	4.67	6.74	
	6.83	5.551	0.45	0	O=C(O)\C=C(/C=C/C=C(/C=C/C1=C(/CCCC1(C)C)C)C)C							
Isradipine	TRUE	103.55	103.55	7	1	371.38714	27	3.59		3.92	2.56	3.59
	2.168	0.37	2	O=C(OC)\C3=C(\N\C(=C(\C(=O)OC(C)C)C3c1ccccc2nonc12)C)C								
Ketoprofen	TRUE	54.37	54.37	3	1	254.28056	19	-0.25	4.23	2.76		2.81
	3.361	0.12	2	CC(c1cccc(c1)C(=O)c2ccccc2)C(=O)O								
Lacosamide	TRUE	67.43	67.43	3	2	250.29361	18	0.9		0.39		0.9
	2.10E-02	0.38	1	O=C(N[C@@H](C(=O)NCc1ccccc1)COC)C								
Lamotrigine	TRUE	90.71	90.71	5	2	256.09137	16	-0.19		2.53	5.39	-0.19
	2.426	0	2	NC1=NC(N)=NN=C1C2=CC=CC(Cl)=C2Cl								
Lenalidomide		TRUE	92.5	92.5	4	2	259.26061	19	-1.39		-0.41	2.77
	-1.39	-0.32	0.31	1	O=C1NC(=O)CCC1N3C(=O)c2cccc(c2C3)N							
Letrozole	TRUE	78.29	78.29	4	0	285.30274	22	1.92		1.43		1.92
	2.749	0.06	3	N#Cc1ccc(cc1)C(c2ccc(C#N)cc2)n3cncn3								
Levamisole	TRUE	15.6	40.9	3	0	204.29137	14	-0.06		1.84	10	1.84
	2.29	0.36	1	N\2=C1/SCCN1C[C@@H]/2c3ccccc3								
Levetiracetam		TRUE	63.4	63.4	2	1	170.20896	12	-0.67		-0.34	
	-0.67	-0.304	0.75	0	O=C1N([C@H](C(=O)N)CC)CCC1							
Levodopa	TRUE	103.78	103.78	5	4	197.18793	14	-2.74	2.24	-2.82	8.85	-0.23
	0.39	0.22	1	O=C(O)[C@@H](N)Cc1cc(O)c(O)cc1								

Levomepromazine	TRUE	15.71	41.01	4	0	328.47166	23	3.04		4.83	9.32	4.94
4.507	0.37	2	O(c2cc1N(c3c(Sc1cc2)cccc3)C[C@H](C)CN(C)C)C									
Levomethadyl	TRUE	29.54	29.54	3	0	353.49773	26	3.48		4.59	9.4	5.45
4.738	0.43	2	[C@H](C(C1=CC=CC=C1)(C2=CC=CC=C2)C[C@@H](N(C)C)C)(OC(C)=O)CC									
Levomilnacipran	TRUE	46.33	46.33	2	1	246.34798	18	-1.52		1.91	10.36	1.23
1.288	0.53	1	CCN(CC)C(=O)[C@]1(C[C@H]1CN)C2=CC=CC=C2									
Levopropoxyphene	TRUE	29.54	29.54	3	0	339.47116	25	3.66		5.21	9.19	5.44
4.71	0.41	2	CCC(=O)OC(Cc1ccccc1)(c2ccccc2)C(C)CN(C)C									
Lidocaine	TRUE	32.34	32.34	2	1	234.33728	17	1.84	1.95	8.53	2.36	2.626
0.5	1	O=C(Nc1c(cccc1C)C)CN(CC)CC										
Lofexidine	TRUE	33.61	33.61	3	1	259.13178	16	1.73	3.46	9.8	3.59	2.765
0.36	1	Clc2c(OC(C/1=N/CCN\1)C)c(Cl)ccc2										
Lomustine	TRUE	61.77	61.77	3	1	233.69524	15	2.76	2.75		2.76	3.469
0.89	0	O=C(NC1CCCCC1)N(N=O)CCCl										
Loratadine	TRUE	42.43	42.43	3	0	382.88321	27	5.94	5.05	4.22	5.94	5
0.36	2	O=C(OCC)N4CC/C(=C2/c1ccc(Cl)cc1CCc3cccnc23)CC4										
Lorazepam	TRUE	61.69	61.69	3	2	321.15809	21	2.47	2.37		2.47	3.509
0.07	2	Clc1=CC=CC=C1C2=NC(C(NC3=C2C=C(C=C3)Cl)=O)O										
Lorcainide	TRUE	23.55	23.55	2	0	370.91558	26	3.18	4.48	9.31	4.9	4.356
0.41	2	Clc3ccc(N(C(=O)Cc1ccccc1)C2CCN(C(C)C)CC2)cc3										
Lorcaserin	TRUE	12.03	12.03	1	1	195.68856	13	0.41	3.24	9.99	2.89	2.747
0.45	1	Clc1cc2c(cc1)CCNC[C@@H]2C										
Losartan	TRUE	92.51	92.51	5	2	422.91062	30	1.58	4.5	3.85	4.41	3.56
4.59	0.27	4	Clc1nc(n(c1CO)Cc4ccc(c2ccccc2c3nnnn3)cc4)CCCC									
Lovastatin	TRUE	72.83	72.83	5	1	404.53963	29	4.07	4.08		4.07	4.218
0.75	0	O=C(O[C@@H]1[C@H]3C(=C/[C@H](C)C1)\C=C/[C@@H]([C@@H]3CC[C@H]2OC(=O)C[C@H](O)C2)C)[C@@H](C)CC										
Lurasidone	TRUE	56.75	84.99	5	0	492.67603	35	3.66	6.12	8.41	4.52	5.375
0.68	2	C1CC[C@H]([C@@H](C1)CN2CCN(CC2)C3=NSC4=CC=CC=C43)CN5C(=O)[C@H]6[C@@H]7CC[C@@H](C7)[C@H]6C5=O										
Maprotiline	TRUE	12.03	12.03	1	1	277.40331	21	1.66	4.52	10.62	4.51	4.116
0.4	2	CNCCC[C@@]12C3=CC=CC=C3[C@@H](C4=CC=CC=C14)CC2										
Maraviroc	TRUE	63.05	63.05	4	1	513.66554	37	1.07	3.26	10.24	3.6	3.921
0.69	2	Cc5nnc(n5[C@@H]1C[C@H]4CC[C@@H](C1)N4CC[C@H](NC(=O)C2CCC(F)(F)CC2)c3ccccc3)C(C)C										
Mazindol	TRUE	35.83	35.83	3	1	284.74022	20	-0.72	3.38	13.1	1.28	2.963
0.19	2	ClC1=CC=C(C2(C3=CC=CC=C3C4=NCCN42)O)C=C1										
Mecamylamine	TRUE	12.03	12.03	1	1	167.29113	12	0.01		2.83	11.35	3.06
2.183	1	0	N([C@@]2([C@@H]1CC[C@@H](C1)C2(C)C)C)C									
Mefloquine	TRUE	45.15	45.15	3	2	378.31215	26	1.14	3.67	9.24	2.87	4.302
0.47	2	FC(F)(F)c2cccc1c(cc(nc12)C(F)(F)F)[C@H](O)[C@@H]3NCCCC3										
Memantine	TRUE	26.02	26.02	1	1	179.30184	13	0.26	3.03	10.79	3.18	1.907
1	0	NC12CC3(CC(C1)(CC(C2)C3)C)C										
Meperidine	TRUE	29.54	29.54	3	0	247.33274	18	1.78	2.23	8.44	2.35	2.445
0.53	1	O=C(C1(CCN(CC1)C)C2=CC=CC=C2)OCC										
Mesoridazine	TRUE	23.55	68.06	4	0	386.57393	26	1.58		4.44	9.63	3.98
4.451	0.43	2	O=S(c2cc1N(c3c(Sc1cc2)cccc3)CCC4N(C)CCCC4)C									
Metergoline	TRUE	46.5	46.5	3	1	403.51666	30	4.04	4.69	9.54	4.72	4.249
0.4	3	O=C(OCc1ccccc1)NC[C@@H]3C[C@@H]4c5cccc2c5c(cn2C)C[C@H]4N(C3)C										
Metformin	TRUE	88.99	88.99	2	4	129.16364	9	-4.3	-1.63	13.1	-2.31	-0.547
0.5	0	CN(C)C(=N)NC(=N)N										
Methamphetamine	TRUE	12.03	12.03	1	1	149.2328	11	-0.79		1.89	10.38	1.94
2.066	0.4	1	N(C(Cc1ccccc1)C)C									
Metharbital	TRUE	66.48	66.48	3	1	198.21906	14	1.13	1.14		1.18	1.669
0.67	0	O=C1N(C(=O)NC(=O)C1(CC)CC)C										
Methdilazine	TRUE	6.48	31.78	3	0	296.4298	21	2.42		4.51	10.09	4.91
4.112	0.33	2	S2c1ccccc1N(c3c2cccc3)CC4CCN(C)C4									
Methixene	TRUE	3.24	28.54	2	0	309.46831	22	3.43	5.84	9.81	5.46	5.073
0.4	2	C1=CC=CC3=C1C(C2=C(C=CC=C2)S3)CC4CN(CCC4)C										
Methocarbamol	TRUE	91.01	91.01	5	2	241.2405	17	0.55		0.15		0.55
0.916	0.36	1	O=C(OCC(O)COc1ccccc1OC)N									
Methylergonovine	TRUE	68.36	68.36	3	3	339.43139	25	1.39		1.76	7.69	1.68
2.063	0.45	2	CC[C@@H](CO)NC(=O)[C@@H]2/C=C1/c3cccc4N\C=C(\C[C@H]1N(C)C2)c34									
Methyprylon	TRUE	46.17	46.17	2	1	183.24748	13	0.23	1.78		0.23	1.473
0.8	0	C(C1(C(C(CNC1=O)C)=O)CC)C										
Metoclopramide	TRUE	67.58	67.58	4	2	299.79638	20	0.35		2.23	9.65	2.22
1.775	0.5	1	Clc1cc(c(OC)cc1N)C(=O)NCCN(CC)CC									
Metoprolol	TRUE	50.72	50.72	4	2	267.3639	19	-0.31	1.49	9.45	1.79	1.757
0.6	1	O(c1ccc(cc1)CCOC)CC(O)CNC(C)C										
Metyrapone	TRUE	42.85	42.85	3	0	226.27376	17	1.19	1.46	4.61	1.19	1.847
0.21	2	O=C(c1cccnc1)C(c2cccnc2)(C)C										
Mexiletine	TRUE	35.25	35.25	2	1	179.25878	13	0.96	2.57	8.58	2.16	2.334
0.45	1	O(c1c(cccc1C)C)CC(N)C										
Mifepristone	TRUE	40.54	40.54	3	1	429.59369	32	4.94		4.65	5.49	4.95
5.655	0.55	1	O=C5\C=C4/C(=C3/[C@H](c1ccc(N(C)C)cc1)c[C@]2([C@@H](CC[C@]2(C#CC)O)[C@@H]3CC4)C)CC5									
Minaprine	TRUE	50.28	50.28	5	1	298.38278	22	1.71	3.19	7.09	1.83	2.819
0.41	2	CC1=CC(=NN=C1NCCN2CCOCC2)C3=CC=CC=C3										
Mirtazapine	TRUE	19.37	19.37	3	0	265.35286	20	2.15	3.32	8.1	2.75	3.094
0.35	2	n1cccc3c1N4C(c2ccccc2C3)CN(C)CC4										
Moclobemide	TRUE	41.57	41.57	3	1	268.73928	18	0.77	2.17	6.89	0.84	1.528
0.46	1	Clc1ccc(cc1)C(=O)NCCN2CCOCC2										
Molindone	TRUE	45.33	45.33	3	1	276.37396	20	1.89	2.57	6.89	1.96	2.14
0.69	1	O=C2c1c(c(nc1CCC2CN3CCOCC3)C)CC										
Nabilone	TRUE	46.53	46.53	3	1	372.54083	27	7.05	6.72		7.05	6.055
0.71	1	O=C3CC[C@@H]1[C@H](c2c(OC1(C)C)cc(cc2O)C(C)(C)CCCCCC)C3										
Nalmefene	TRUE	52.93	52.93	4	2	339.4281	25	2.09	2.64	7.68	2.65	2.82
0.62	1	OC(c1=C2[C@@]34[C@H]5O1)=CC=C2C[C@@H](N(CC4)CC6CC6)[C@]3(O)CCC5=C										
Naloxegol	TRUE	126.77	126.77	12	2	651.78472	46	-1.14	0.44	6.51	-1.07	0.952
0.76	1	COCCOCCOCCOCCOCCOCCOCCO[C@H]1CC[C@]2([C@H]3Cc4ccc(c5c4[C@]2([C@H]1O5)CCN3CC=C)O)O										
Naratriptan	TRUE	65.2	73.58	3	2	335.46429	23	-0.65	1.7	9.63	1.35	2.054
0.53	2	O=S(=O)(NC)CCc3ccc1c(c(cn1)C2CCN(C)CC2)c3										
Nebivolol	TRUE	70.95	70.95	5	3	405.435	29	2.34	3.5	8.65	3.67	3.557
0.45	2	Fc4cc1c(OC(CC1)C(O)CNCC(O)C3Oc2ccc(F)cc2CC3)cc4										
Nefazodone	TRUE	51.62	51.62	5	0	470.00687	33	3.29	6.23	8.25	3.5	4.415
0.44	2	Clc4cccc(N3CCN(CCCN1/N=C(\N(C1=O)CCOc2ccccc2)CC)CC3)c4										
Nemonapride	TRUE	53.6	53.6	4	2	387.90304	27	2.02	4.2	8.36	3.08	3.504
0.38	2	CC1C(CCN1CC2=CC=CC=C2)NC(=O)C3=CC(=C(C=C3OC)NC)Cl										
Nicardipine	TRUE	113.69	113.69	8	1	479.52495	35	4.88	5.23	7.3	5.13	3.488
0.31	2	O=C(OCCN(Cc1ccccc1)C)\C2=C(\N/C(=C(/C(=O)OC)C2c3cccc([N+]([O-])=O)c3)C)C										
Nicergoline	TRUE	56.59	56.59	5	0	484.38553	31	4.3	4.07	7.78	4.34	3.461
0.42	3	Brc1cc(cnc1)C(=O)OC[C@@H]3C[C@]4(OC)c5cccc2c5c(cn2C)C[C@H]4N(C3)C										
Nicotine	TRUE	16.13	16.13	2	0	162.23155	12	-0.47	0.88	8	0.72	1.242
0.5	1	CN(CCC1)[C@@H]1C2=CC=CN=C2										
Nifedipine	TRUE	110.44	110.44	7	1	346.33462	25	2.97	3.12	2.69	2.97	1.766
0.29	1	O=C(OC)\C1=C(\N/C(=C(/C(=O)OC)C1c2ccccc2[N+]([O-])=O)C)C										
Nortriptyline	TRUE	12.03	12.03	1	1	263.37674	20	3.17		4.32	10	5.65
4.236	0.26	2	c3cc2c(/C(c1c(cccc1)CC2)=C/CCNC)cc3									
Noscapine	TRUE	75.69	75.69	8	0	413.42051	30	2.79	2.27	6.32	2.83	3.012
0.41	2	O=C2O[C@@H](c1ccc(OC)c(OC)c12)[C@@H]5N(C)CCc4c5c(OC)c3OCOc3c4										
Ondansetron	TRUE	39.82	39.82	2	0	293.36296	22	1.72	2.72	7.5	2.07	2.634
0.33	3	O=C3c2c1ccccc1n(c2CCC3Cn4ccnc4C)C										
Ospemifene	TRUE	29.46	29.46	2	1	378.89121	27	6.98	5.56		6.98	5.62
0.17	3	ClCC/C(C1=CC=CC=C1)=C(C2=CC=CC=C2)/C3=CC=C(C=C3)OCCO										
Oxprenolol	TRUE	50.72	50.72	4	2	265.34802	19	0.18	2.09	9.45	2.29	2.232
0.47	1	O(c1ccccc1OC\C=C)CC(O)CNC(C)C										

Oxybate	TRUE	57.53	57.53	3	2	104.10452	7	-3.41	4.67	-0.58		-0.7
-0.308	0.75	0	O=C(O)CCCO									
Oxybutynin	TRUE	49.77	49.77	4	1	357.48643	26	4.29		4.87	8.24	5.19
4.646	0.59	1	O=C(OCC#CCN(CC)CC)C(O)(c1ccccc1)C2CCCCC2									
Oxyphencyclimine	TRUE	62.13	62.13	5	1	344.44792	25	2.7		4.45	10.91	
4.69	2.626	0.6	1	C3=C(C(C1CCCCC1)(C(OCC2=NCCCN2C)=O)O)C=CC=C3								
Palonosetron	TRUE	23.55	23.55	2	0	296.40665	22	0.81		2.18	9.77	
2.61	2.745	0.63	1	O=C5N([C@H]2C1CCN(CC1)C2)C[C@@H]4c3c5cccc3CCC4								
Panobinostat	TRUE	77.15	77.15	3	4	349.42622	26	1.63		2.64	9.29	
3.62	3.027	0.19	3	O=C(NO)\C=C\c1ccc(cc1)CNCCc3c2ccccc2nc3C								
Paramethadione	TRUE	46.61	46.61	3	0	157.16713	11	0.84		0.41		
0.84	1.537	0.71	0	O=C1N(C(=O)OC1(C)CC)C								
Paroxetine	TRUE	39.72	39.72	4	1	329.3654	24	1.67		4.24	9.68	3.89
3.229	0.37	2	c1cc(ccc1[C@@H]2CCNC[C@H]2COc3ccc4c(c3)OCO4)F									
Pazopanib	TRUE	119.03	127.41	7	2	437.51801	31	1.96		3.65	6.39	1.98
3.741	0.19	4	O=S(=O)(N)c1c(ccc(c1)Nc2nccc(n2)N(c4ccc3c(nn(c3C)C)c4)C)C									
Penbutolol	TRUE	41.48	41.48	3	2	291.42835	21	2		3.64	9.77	4.17
3.572	0.67	1	O[C@@H](CNC(C)(C)C)COc1ccccc1C2CCCC2									
Pentazocine	TRUE	23.47	23.47	2	1	285.42378	21	3		4.67	8.94	4.54
4.373	0.58	1	Oc1ccc3c(c1)[C@]2([C@H]([C@H](N(CC2)C\C=C(/C)C)C3)C)C									
Pentoxifylline	TRUE	75.51	75.51	4	0	278.30702	20	0.32		0.12		
0.32	1.032	0.54	1	O=C2N(c1ncn(c1C(=O)N2CCCCC(=O)C)C)C								
Perampanel	TRUE	56.99	56.99	3	0	349.3847	27	3.7		4.17	4.73	3.7
3.572	0	3	N#Cc2ccccc2-c1cc(-c4ncccc4)cn(c1=O)-c3ccccc3									
Pergolide	TRUE	19.03	44.33	2	1	314.48813	22	3.09		4.4	9.66	4.49
4.11	0.58	2	S(C)C[C@@H]2C[C@@H]3c4cccc1c4c(cn1)C[C@H]3N(C2)CCC									
Perindopril	TRUE	95.94	95.94	6	2	368.46777	26	-0.19	3.15	1.21	5.67	3.36
2.437	0.84	0	O=C(OCC)[C@@H](N[C@H](C(=O)N1[C@H](C(=O)O)C[C@@H]2CCCC[C@H]12)C)CCC									
Phenacemide	TRUE	72.19	72.19	2	2	178.1879	13	0.87		0.87		0.87
0.841	0.11	1	O=C(NC(=O)N)CC1ccccc1									
Phenelzine	TRUE	38.04	38.04	2	2	136.19428	10	0.33		1.03	8.01	1.14
1.307	0.25	1	N(N)CCC1ccccc1									
Phenmetrazine	TRUE	21.26	21.26	2	1	177.2429	13	0.33		1.67	8.58	
1.53	1.461	0.45	1	CC1C(C2=CC=CC=C2)OCCN1								
Phenobarbital	TRUE	75.27	75.27	3	2	232.23528	17	1.45	7.31	1.36		
1.67	1.709	0.25	1	O=C1NC(=O)NC(=O)C1(c2ccccc2)CC								
Phenoxybenzamine	TRUE	12.47	12.47	2	0	303.82638	21	4.72		4.92	6.58	
4.78	4.578	0.33	2	ClCCN(C(COc1ccccc1)C)Cc2ccccc2								
Phenylpropanolamine	TRUE	46.25	46.25	2	2	151.20562	11	-1.07		0.58	8.47	
0.81	0.802	0.33	1	O[C@H](c1ccccc1)[C@@H](N)C								
Phenytoin	TRUE	58.2	58.2	2	2	252.26798	19	2.49		2.08		2.52
2.299	0.07	2	O=C2NC(=O)NC2(c1ccccc1)c3ccccc3									
Pimozide	TRUE	35.58	35.58	2	1	461.54616	34	4.99		6.4	9.67	6.38
5.521	0.32	3	Fc1ccc(cc1)C(c2ccc(F)cc2)CCCN5CCC(N4c3ccccc3NC4=O)CC5									
Pioglitazone	TRUE	68.29	93.59	5	1	356.4387	25	1.89	6.35	3.53	5.53	
2.94	4.102	0.32	2	O=C1NC(=O)SC1Cc3ccc(OCCc2ncc(cc2)CC)cc3								
Pirfenidone	TRUE	20.31	20.31	1	0	185.22184	14	1.82		2.4		1.82
1.905	0.08	1	CC1=CN(C(=O)C=C1)C2=CC=CC=C2									
Pramipexole	TRUE	50.94	79.17	3	2	211.32708	14	-0.54		1.17	9.47	1.42
1.713	0.7	1	[C@H]2(CCC1=C(SC(=N1)N)C2)NCCC									
Prasugrel	TRUE	46.61	74.84	4	0	373.4411	26	3.17		3.43	4.07	3.17
3.988	0.4	2	CC(=O)Oc1cc2c(s1)CCN(C2)C(c3ccccc3F)C(=O)C4CC4									
Praziquantel	TRUE	40.62	40.62	2	0	312.40605	23	2.44		3.36		
2.44	2.477	0.58	1	O=C4N2C(c1c(cccc1)CC2)CN(C(=O)C3CCCCC3)C4								
Procainamide	TRUE	58.36	58.36	3	2	235.32534	17	-0.79		1.42	9.86	
1.1	1.127	0.46	1	O=C(c1ccc(N)cc1)NCCN(CC)CC								
Procarbazine	TRUE	53.16	53.16	3	3	221.29875	16	0.08		-0.08	7.85	
0.77	1.515	0.42	1	O=C(c1ccc(cc1)CNNC)NC(C)C								
Prochlorperazine	TRUE	9.72	35.02	4	0	373.94265	25	4		4.38	8.64	
4.61	4.697	0.4	2	Clc2cc1N(c3c(Sc1cc2)cccc3)CCCN4CCN(C)CC4								
Propofol	TRUE	20.23	20.23	1	1	178.27072	13	4.16		3.93		4.16
3.976	0.5	1	OC1=C(C(C)C)C=CC=C1C(C)C									
Propranolol	TRUE	41.48	41.48	3	2	259.34344	19	0.98		2.75	9.43	3.1
2.54	0.38	2	CC(NCC(O)COC1=C(C=CC=C2)C2=CC=C1)C									
Pseudoephedrine	TRUE	32.26	32.26	2	2	165.2322	12	-0.96		0.89	9.38	
1.05	1.234	0.4	1	O[C@@H](c1ccccc1)[C@@H](NC)C								
Pyrazinamide	TRUE	68.87	68.87	3	1	123.1127	9	-0.37		-0.68		
-0.37	-1.041	0	1	O=C(N)c1nccnc1								
Pyrilamine	TRUE	28.6	28.6	4	0	285.38402	21	0.84		3.23	9.02	2.75
3.086	0.35	2	O(c1ccc(cc1)CN(c2ncccc2)CCN(C)C)C									
Pyrimethamine	TRUE	77.81	77.81	4	2	248.71142	17	2.55		3	6.78	
2.75	2.75	0.17	2	Clc2ccc(c1c(nc(nc1CC)N)N)cc2								
Pyrvinium	TRUE	12.05	12.05	1	0	382.52062	29			2.79		
5.862	0.19	4	CC1=CC(=C(N1C2=CC=CC=C2)C)/C=C/C3=[N+](C4=C(C=C3)C=C(C=C4)N(C)C)C									
Quetiapine	TRUE	48.3	73.6	6	1	383.50709	27	1.48		2.99	6.76	1.56
2.656	0.38	2	N\1=C(\c3c(Sc2c/1cccc2)cccc3)N4CCN(CCOCCO)CC4									
Ramelteon	TRUE	38.33	38.33	2	1	259.34344	19	2.57		2.48		2.57
2.826	0.56	1	CCC(NCC[C@@H]1CCC2=CC=C3OCCC3=C12)=O									
Rasagiline	TRUE	12.03	12.03	1	1	171.23832	13	2.14		2.52	7.49	2.27
3.119	0.33	1	C#CCN[C@H]2c1ccccc1CC2									
Reboxetine	TRUE	39.72	39.72	4	1	313.39082	23	1.8		3.26	8.37	2.82
3.077	0.37	2	CCOc1=C(C=CC=C1)O[C@@H]([C@@H]2OCCNC2)C3=CC=CC=C3									
Remifentanil	TRUE	76.15	76.15	6	0	376.44671	27	2		1.96	6.56	
2.05	1.666	0.55	1	O=C(OC)C2(N(c1ccccc1)C(=O)CC)CCN(CCC(=O)OC)CC2								
Riluzole	TRUE	48.14	76.38	3	1	234.1983	15	2.84		3.23	3.41	2.84
4.159	0.12	2	FC(F)(F)Oc1ccc2nc(sc2c1)N									
Rimantadine	TRUE	26.02	26.02	1	1	179.30184	13	0.19		3.96	10.76	3.1
2.204	1	0	NC(C)C13CC2CC(CC(C1)C2)C3									
Rimonabant	TRUE	50.16	50.16	3	1	463.78734	30	6.01		6.47	3.22	6.01
7.001	0.27	3	O=C(NN1CCCCC1)c4nn(c2ccc(Cl)cc2Cl)c(c3ccc(Cl)cc3)c4C									
Risperidone	TRUE	61.94	61.94	4	0	410.48448	30	2.09		2.71	8.21	2.88
3.317	0.52	2	Cc1c(c(=O)n2c(n1)CCCC2)CCN3CCC(CC3)c4c5ccc(cc5on4)F									
Rivastigmine	TRUE	32.78	32.78	3	0	250.33668	18	0.93		2.1	8.62	
2.14	2.599	0.5	1	O=C(Oc1cc(ccc1)[C@@H](N(C)C)C)N(CC)C								
Rizatriptan	TRUE	49.74	49.74	3	1	269.34486	20	-0.97		1.18	9.49	0.96
2.067	0.33	3	n1cn(nc1)Cc2cc3c(cc2)ncc3CCN(C)C									
Rofecoxib	TRUE	60.44	68.81	4	0	314.35566	22	1.34		1.8		1.34
2.871	0.12	2	O=C2OCC(=C2\c1ccccc1)\c3ccc(cc3)S(=O)(=O)C									
Ropinirole	TRUE	32.34	32.34	2	1	260.37456	19	1.2		2.8	9.45	3.19
2.959	0.56	1	O=C2Nc1cccc(c1C2)CCN(CCC)CCC									
Ropivacaine	TRUE	32.34	32.34	2	1	274.40114	20	2.72		3.16	8.36	3.1
3.854	0.59	1	O=C(Nc1c(cccc1C)C)[C@H]2N(CCC)CCCC2									
Rufinamide	TRUE	73.8	73.8	3	1	238.19352	17	0.05		0.51		0.05
1.437	0.1	2	O=C(c1nnn(c1)Cc2c(F)cccc2F)N									
Saxagliptin	TRUE	90.35	90.35	4	2	315.40999	23	-1.04		-0.02	8.3	-0.14
0.275	0.89	0	O=C(N1[C@H](C#N)C[C@@H]2C[C@H]12)[C@@H](N)C35CC4CC(C3)CC(O)(C4)C5									
Selegiline	TRUE	3.24	3.24	1	0	187.28078	14	2.58		3.02	7.53	2.95
3.794	0.38	1	C#CCN([C@@H](Cc1ccccc1)C)C									
Sertindole	TRUE	40.51	40.51	2	1	440.94084	31	4.08		5.27	9.1	5.26
4.68	0.38	3	Fc1ccc(cc1)n3c2ccc(Cl)cc2c(c3)C5CCN(CCN4C(=O)NCC4)CC5									
Sertraline	TRUE	12.03	12.03	1	1	306.22958	20	2.77		5.35	9.47	4.81
4.996	0.29	2	ClC1=CC=C([C@H]2C3=C([C@H](CC2)NC)C=CC=C3)C=C1Cl									

Sulindac	TRUE	54.37	73.58	3	1	356.41058	25	0.55	4.26	3.16		3.59
	3.639	0.15	2	O=S(c1ccc(cc1)\C=C3/c2ccc(F)cc2\C(=C3C)CC(=O)O)C								
Suvorexant	TRUE	80.29	80.29	5	0	450.92071	32	3.62		5.4	4.12	3.62
	4.108	0.3	4	C[C@@H]1CCN(CCN1C(=O)C2=C(C=CC(=C2)C)N3N=CC=N3)C4=NC5=C(O4)C=CC(=C5)Cl								
Tacrine	TRUE	38.9	38.9	2	1	198.26366	15	1.26		3.27	9.64	3.32
	2.789	0.31	2	n1c3c(c(c2c1cccc2)N)CCCC3								
Tadalafil	TRUE	74.87	74.87	4	1	389.40396	29	1.43		2.58		1.43
	2.183	0.27	3	O=C1N(CC(N2[C@@H]1CC3=C([C@H]2C4=CC5=C(OCO5)C=C4)NC6=C3C=CC=C6)=O)C								
Talipexole	TRUE	42.15	70.38	3	1	209.3112	14	1.02		1.14	7.22	1.2
	1.644	0.5	1	n1c2c(sc1N)CCN(CC2)C\C=C								
Tamoxifen	TRUE	12.47	12.47	2	0	371.51455	28	6.58		6.82	8.69	7.88
	6.319	0.23	3	O(c1ccc(cc1)/C(c2ccccc2)=C(\c3ccccc3)CC)CCN(C)C								
Tapentadol	TRUE	23.47	23.47	2	1	221.33852	16	1.21		3.15	9.45	3.22
	3.466	0.57	1	Oc1cc(ccc1)[C@@H]([C@@H](C)CN(C)C)CC								
Tasimelteon	TRUE	38.33	38.33	2	1	245.31686	18	1.75		1.89		1.75
	2.203	0.53	1	CCC(=O)NC[C@@H]1C[C@H]1C2=C3CCOC3=CC=C2								
Telmisartan	TRUE	72.94	72.94	4	1	514.61689	39	4.74	3.83	7.29	5.87	7.73
	7.799	0.18	6	O=C(O)c1ccccc1c2ccc(cc2)Cn3c4cc(cc(c4nc3CCC)C)c5nc6ccccc6n5C								
Temozolomide		TRUE	105.94	105.94	5	1	194.15083	14	-1.31		-0.81	
	-1.31	5.20E-08	0.17	1	O=C(c1ncn2C(=O)N(\N=N/c12)C)N							
Terbinafine	TRUE	3.24	3.24	1	0	291.42989	22	6.49		5.96	6.92	6.61
	5.335	0.33	2	C(#C\C=C\CN(C)Cc2cccc1ccccc12)C(C)(C)C								
Terguride	TRUE	51.37	51.37	2	2	340.46252	25	2.65		2.78	9.78	3.31
	2.65	0.55	2	CCN(CC)C(=O)N[C@H]1C[C@H]2[C@@H](CC3=CNC4=CC=CC2=C34)N(C1)C								
Teriflunomide		TRUE	73.12	73.12	3	2	270.20726	19	0.08	5.2	2.13	
	2.51	2.091	0.17	1	O=C(Nc1ccc(cc1)C(F)(F)F)C(/C#N)=C(/C)O							
Tetrabenazine		TRUE	38.77	38.77	4	0	317.42257	23	3.43		3.46	6.46
	3.48	3.365	0.63	1	O=C3C(CC(C)C)CN2C(c1c(cc(OC)c(OC)c1)CC2)C3							
Thiopental	TRUE	61.69	93.78	4	2	242.33782	16	-0.92		1.85	10.72	2.38
	3.12	0.73	0	O=C1NC(=S)/N=C(/O)C1(C(C)CCC)CC								
Thiothixene	TRUE	43.86	77.53	5	0	443.62525	30	3.42		3.23	8.17	3.94
	3.533	0.39	2	O=S(=O)(N(C)C)c2cc1C(\c3c(Sc1cc2)cccc3)=C/CCN4CCN(C)CC4								
Tiagabine	TRUE	40.54	97.02	3	1	375.54799	25	3.18	3.86	2.77	9.48	5.68
	4.832	0.45	2	O=C(O)[C@H]1CN(CCC1)CC/C=C(/c2sccc2c)c3sccc3C								
Tianeptine	TRUE	86.71	95.09	5	2	436.95219	29	0.02	4.75	1.52	7.47	2.56
	3.927	0.38	2	Clc1cc2c(cc1)C(c3c(N(C)S2(=O)=O)cccc3)NCCCCCCC(=O)O								
Timolol	TRUE	79.74	107.98	7	2	316.41966	21	-1.2		1.72	9.57	0.68
	1.127	0.85	1	O[C@H](COc1nsnc1N2CCOCC2)CNC(C)(C)C								
Tizanidine	TRUE	62.2	90.44	5	2	253.71131	16	0.31		2.09	8.67	0.65
	1.817	0.22	2	Clc1ccc3nsnc3c1NC/2=N/CCN\2								
Tocainide	TRUE	55.12	55.12	2	2	192.25754	14	0.32		0.26	8.1	0.76
	1.445	0.36	1	O=C(Nc1c(cccc1C)C)C(N)C								
Tolcapone	TRUE	103.35	103.35	5	2	273.24084	20	1.8	4.78	3.25		4.07
	3.13	0.07	2	[O-][N+](=O)c2cc(C(=O)c1ccc(cc1)C)cc(O)c2O								
Tolmetin	TRUE	59.3	59.3	3	1	257.28449	19	-1.52	4.22	2.21		1.55
	3.267	0.2	2	O=C(c1ccc(n1C)CC(=O)O)c2ccc(cc2)C								
Topotecan	TRUE	103.2	103.2	7	2	421.44581	31	0.44		0.73	7.65	1.08
	1.577	0.35	2	O=C\1N4\C(=C/C2=C/1COC(=O)[C@]2(O)CC)c3nc5c(cc3C4)c(c(O)cc5)CN(C)C								
Tramadol	TRUE	32.7	32.7	3	1	263.37519	19	0.49		3.1	9.61	2.51
	2.7	0.62	1	CN(C)C[C@H]1CCCC[C@@]1(C2=CC(=CC=C2)OC)O								
Tranylcypromine		TRUE	26.02	26.02	1	1	133.19034	10	0.36		1.48	8.78
	1.25	1.193	0.33	1	c1cccc(c1)[C@@H]2C[C@H]2N							
Trazodone	TRUE	42.39	42.39	4	0	371.86388	26	1.49		4.35	8.11	1.66
	2.418	0.37	1	Clc4cccc(N3CCN(CCCN1/N=C2/C=C\C=C/N2C1=O)CC3)c4								
Trimipramine		TRUE	6.48	6.48	2	0	294.43383	22	3.21		5.44	9.38
	5.15	4.836	0.4	2	c1cc3c(cc1)CCc2c(cccc2)N3CC(C)CN(C)C							
Triprolidine		TRUE	16.13	16.13	2	0	278.39138	21	2.7		3.63	8.99
	4.22	4.075	0.32	2	n3c(\C(=C\CN1CCCC1)c2ccc(cc2)C)cccc3							
Troglitazone		TRUE	84.86	110.16	6	2	441.53987	31	3.94	6.34	5.58	
	4.99	5.876	0.42	2	O=C1NC(=O)SC1Cc4ccc(OCC3(Oc2c(c(c(O)c(c2CC3)C)C)C)C)cc4							
Tropisetron	TRUE	45.33	45.33	3	1	284.35289	21	1.04		2.88	10	3.55
	2.608	0.47	2	CN4[C@@H]1CC[C@H]4C[C@H](C1)OC(=O)c3cnc2ccccc23								
Valdecoxib	TRUE	86.19	94.57	3	1	314.35895	22	1.7		1.83		1.71
	2.6	0.06	3	O=S(=O)(N)c3ccc(c2c(onc2c1ccccc1)C)cc3								
Valproic acid		TRUE	37.29	37.29	2	1	144.21143	10	0.16	4.82	2.76	
	2.72	2.749	0.88	0	O=C(O)C(CCC)CCC							
Varenicline	TRUE	37.81	37.81	3	1	211.26242	16	-1.33		0.9	9.6	0.74
	1.038	0.38	2	n1c2ccc3c(ccc2ncc1)[C@@H]4CNC[C@H]3C4								
Vilazodone	TRUE	102.29	102.29	4	2	441.52487	33			4.58	8.57	3.98
	4.536	0.31	4	N#Cc1ccc2c(c1)c(cn2)CCCCN5CCN(c4cc3c(oc(c3)C(=O)N)cc4)CC5								
Vinpocetine	TRUE	34.47	34.47	3	0	350.45403	26	4.54		4.83	7.8	5.14
	4.294	0.5	2	O=C(OCC)C=4n1c3c(c2ccccc12)CCN5[C@H]3[C@](C=4)(CCC5)CC								
Voriconazole		TRUE	76.72	76.72	5	1	349.31046	25	0.93		0.52	2.72
	0.93	2.072	0.25	3	Fc1cncnc1[C@@H]([C@@](O)(c2ccc(F)cc2F)Cn3ncnc3)C							
Vorinostat	TRUE	78.43	78.43	3	3	264.3202	19	0.86		0.99		0.86
	1.838	0.43	1	O=C(Nc1ccccc1)CCCCCCC(=O)NO								
Vortioxetine		TRUE	15.27	40.57	3	1	298.44568	21	3.08		5.42	8.85
	4.26	4.504	0.33	2	CC(C=C(C)C=C1)=C1SC2=C(N3CCNCC3)C=CC=C2							
Zaleplon	TRUE	74.28	74.28	4	0	305.33389	23	0.86		1.44		0.86
	1.865	0.18	3	O=C(C)N(CC)C1=CC=CC(C2=CC=NC3=C(C=NN23)C#N)=C1								
Ziprasidone	TRUE	48.47	76.71	4	1	412.93564	28	3.19		4.71	8.41	4
	4.214	0.33	3	O=C5Nc1c(cc(c(Cl)c1)CCN4CCN(c3nsc2ccccc23)CC4)C5								
Zolmitriptan		TRUE	57.36	57.36	3	2	287.35683	21	-0.29		1.29	9.52
	1.64	2.457	0.44	2	O=C1OC[C@@H](N1)Cc2ccc3c(c2)c(cn3)CCN(C)C							
Zolpidem	TRUE	37.61	37.61	2	0	307.38953	23	3.01		3.03	6.25	3.07
	3.628	0.26	3	O=C(CC1=C(C2=CC=C(C)C=C2)N=C3C=CC(C)=CN13)N(C)C								
Zonisamide	TRUE	86.19	94.57	3	1	212.22571	14	-0.1		-0.36		-0.1
	0.411	0.12	2	O=S(=O)(N)Cc2noc1ccccc12								