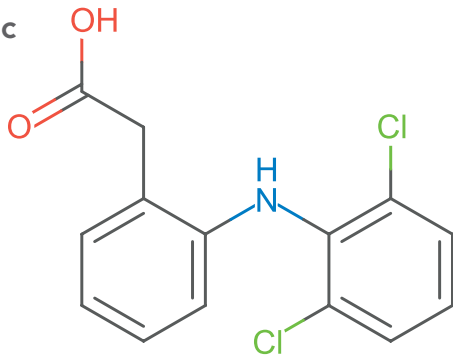












Quels fragments se trouvent dans ces molécules ?

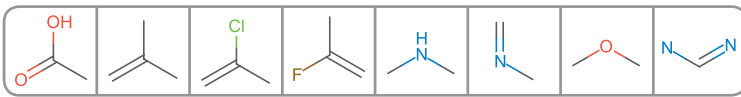
Diclofenac



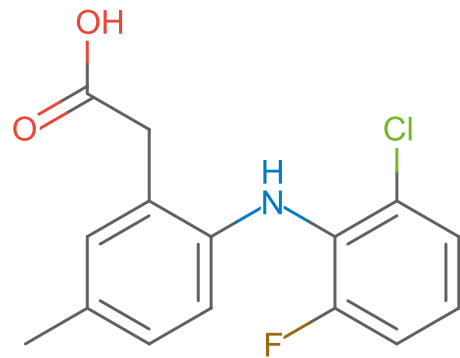
→ À l'aide de la règlette, retrouve les fragments présents dans chaque molécule. Mets un 1 dans les cases correspondantes si tu les trouves et 0 sinon. Exemple :

							
1	1	1	0	1	0	0	0

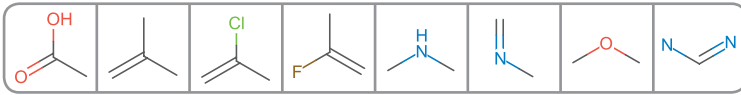
Lumiracoxib



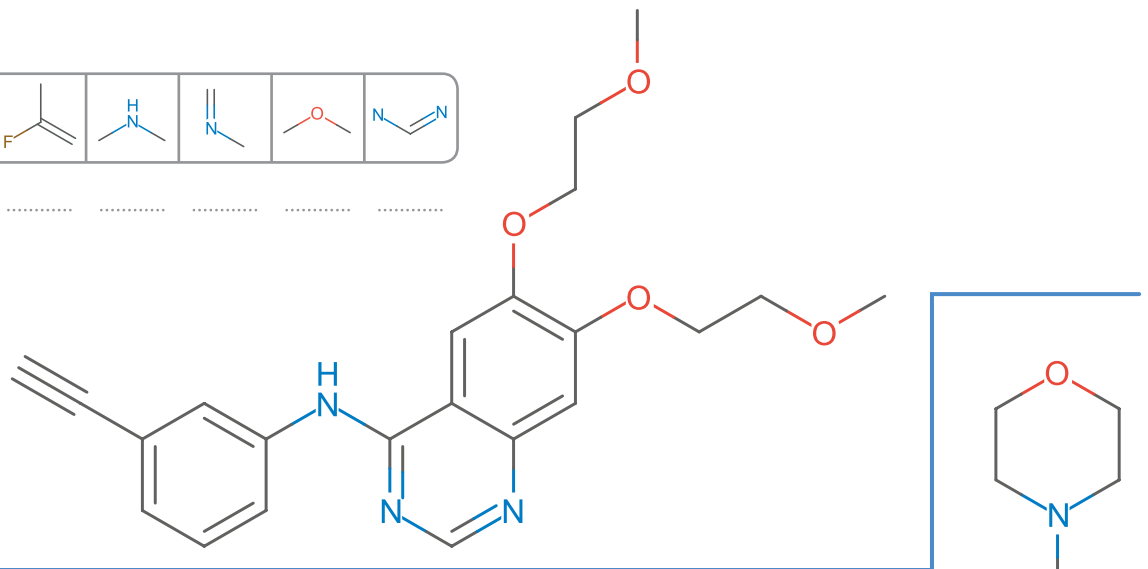
.....



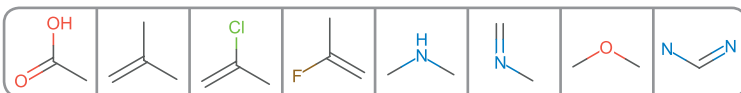
Erlotinib



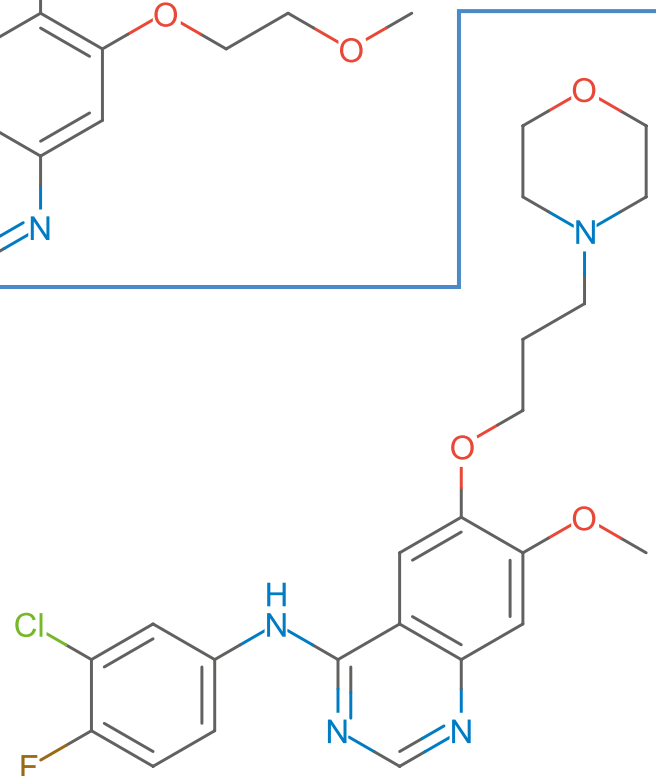
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Gefitinib



.....



Calcul de similarité

Coefficient de Tanimoto

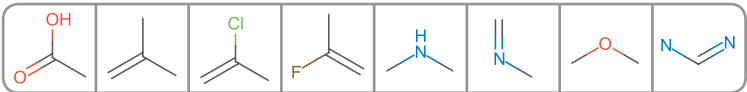
Formule

$$T = \frac{M_{11}}{M_{11} + M_{10} + M_{01}}$$

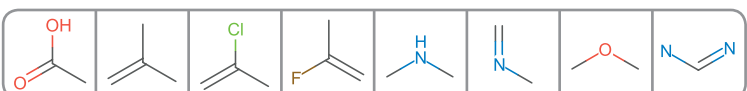
M_{11} : nombre de cases où l'on trouve 1 à la fois chez A et chez B
 M_{10} : nombre de cases où l'on trouve 0 chez A et 1 chez B
 M_{01} : nombre de cases où l'on trouve 1 chez A et 0 chez B

$0 \leq T \leq 1$
 $T = 0$: molécules totalement différentes
 $T = 1$: molécules identiques

Exemple

A 

 1 1 1 0 1 0 0 0

B 

 1 1 0 1 1 0 0 1

$M_{11} = 3, M_{10} = 1, M_{01} = 2$

$$T = \frac{3}{3 + 1 + 2} = 0.5$$

→ Compare les 4 molécules en remplissant le tableau ci-dessous avec les coefficients de Tanimoto calculés:



	Diclofenac	Lumiracoxib	Erlotinib	Gefitinib
Diclofenac	1			
Lumiracoxib		1		
Erlotinib			1	
Gefitinib				1

→ Quelles sont les paires de molécules les plus similaires?

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