

1.b

Fármaco 1:Daunorubicin

SMILE:C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C(=CC=C5)OC)O)(C(=O)C)O)N)O

Fármaco 2:Camptothecin

SMILE:CC[C@@]1(C2=C(COC1=O)C(=O)N3CC4=CC5=CC=CC=C5N=C4C3=C2)O

Fármaco 3:Streptozocin

SMILE:CN(C(=O)N[C@@H]1[C@H]([C@@H]([C@H](O[C@@H]1O)CO)O)O)N=O

Fármaco 4:Salinosporamide A (Experimental)

SMILE:C[C@]12[C@H](C(=O)N[C@]1(C(=O)O2)[C@H]([C@H]3CCCC=C3)O)CCCI

Fármaco 5:Crisnatol (Experimental)

SMILE:CC(CO)(CO)NCC1=CC2=C(C=CC3=CC=CC=C32)C4=CC=CC=C41

| 1.a/2           | Aspirin                               | Paracetamol                        | Caffeine                                  |
|-----------------|---------------------------------------|------------------------------------|---|
| SMILE           | <chem>CC(=O)OC1=CC=CC=C1C(=O)O</chem> | <chem>CC(=O)NC1=CC=C(C=C1)O</chem> | <chem>CN1C=NC2=C1C(=O)N(C(=O)N2C)C</chem> |
| Peso molecular  | 180.16 g/mol                          | 151.16 g/mol                       | 194.19 g/mol                              |
| LogP            | 1.28                                  | 0.93                               | 0.08                                      |
| H-bond A.       | 4                                     | 2                                  | 3   |
| H-bond D.       | 1                                     | 2                                  | 0   |
| TPSA            | 63.60 Å²                              | 49.33 Å²                           | 61.82 Å²                                  |
| Rotatable bonds | 3                                     | 2                                  | 0   |

3.

| Nº | Nombre       | Lipinski Violations |
|----|--------------|---------------------|
| 0  | Aspirin      | 0                   |
| 1  | Paracetamol  | 0                   |
| 2  | Caffeine     | 0                   |
| 3  | Daunorubicin | 2                   |
| 4  | Camptothecin | 0                   |
| 5  | Streptozocin | 0                   |

|   |                   |   |
|---|-------------------|---|
| 6 | Salinosporamide A | 0 |
| 7 | Crisnatol         | 0 |

4.

|                   | LD50      | Toxicity Class | Hepatotoxicity | Carcinogenicity | Mutagenicity |
|-------------------|-----------|----------------|----------------|-----------------|--------------|
| Aspirin           | 250mg/kg  | 3              | 0.51           | 0.86            | 0.97         |
| Paracetamol       | 338mg/kg  | 4              | 0.74A          | 0.51            | 0.90         |
| Caffeine          | 127mg/kg  | 3              | 0.97           | 0.93            | 0.94         |
| Daunorubicin      | 205mg/kg  | 3              | 0.89           | 0.75            | 0.99A        |
| Camptothecin      | 50mg/kg   | 3              | 0.83           | 0.57            | 0.59         |
| Streptozocin      | 396mg/kg  | 4              | 0.59           | 0.93A           | 0.90A        |
| Salinosporamide A | 2573mg/kg | 5              | 0.70           | 0.60            | 0.59         |
| Crisnatol         | 1000mg/kg | 4              | 0.84           | 0.75            | 0.60         |