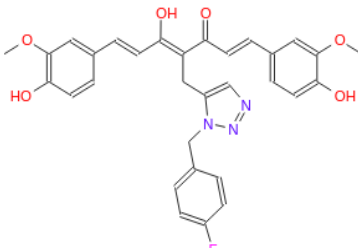
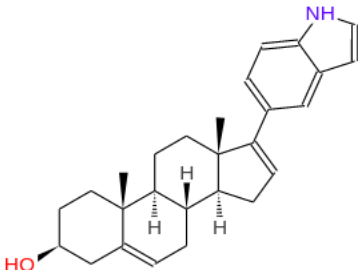
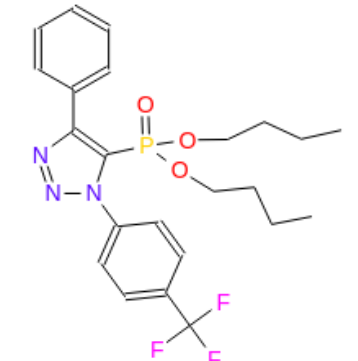
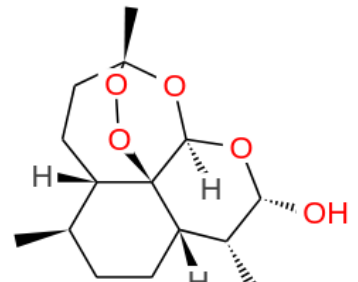
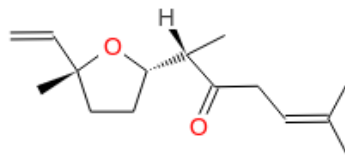


Avaliação *in silico* de propriedades farmacocinéticas de compostos antileucêmicos publicados por periódicos científicos.

Tabela suplementar 2. Informações moleculares dos compostos utilizados neste trabalho.

| Moléculas selecionada | Estrutura Molecular | PM | Código SMILES |
|---------------------------|---|--------|---|
| Composto 1 ⁶ |  | 557578 | <chem>COc4cc(/C=C/C(=O)/C(Cc1cnnn1Cc2ccc(F)cc2)=C(O)/C=C/c3ccc(O)c(OC)c3)ccc4O</chem> |
| Composto 10L ⁸ |  | 387567 | <chem>[H][C@@]35CC=C(c2ccc1[nH]ccc1c2)[C@@]3(C)CC[C@]6([H])[C@@]4(C)CC[C@H](O)CC4=CC[C@@]56[H]</chem> |
| Composto 22 ²⁰ |  | 497498 | <chem>FC(F)(F)c3ccc(n2cc(c1ccccc1)nn2)cc3.CCCOP(C)(=O)OCCCC</chem> |
| DHA ⁹ |  | 284352 | <chem>[H][C@@]12CC[C@@]4(C)OO[C@@]13[C@@]([H])(CC[C@H]2C)[C@@H](C)[C@@H](O)O[C@]3([H])O4</chem> |

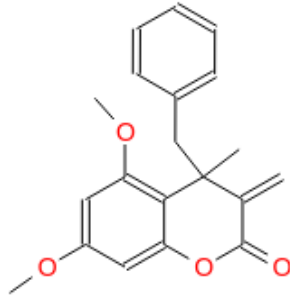
Davanona¹⁹



236355

[H][C@@](C)(C(=O)C/C=C(C)C)[C@@H]1CC[C@](C)(C=C)O1

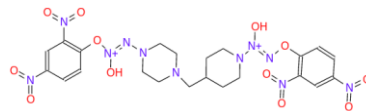
DL-247¹¹



324376

C=C2C(=O)Oc1cc(OC)cc(OC)c1C2(C)Cc3ccccc3

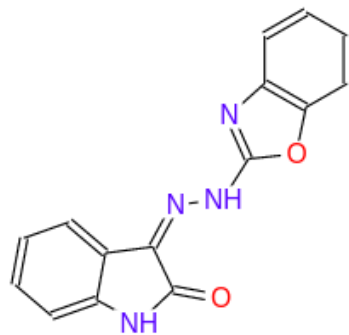
DDNO-1¹⁷



637523

O=N(=O)c4ccc(O/N=[N+](O)/N3CCC(CN2CCN(/N=[N+](O)/Oc1ccc(N(=O)=O)cc1N(=O)=O)CC2)CC3)c(N(=O)=O)c4

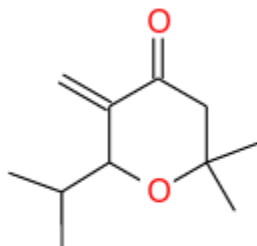
K313¹²



278271

O=c2[nH]c1ccccc1c2=NNc4nc3ccccc3o4

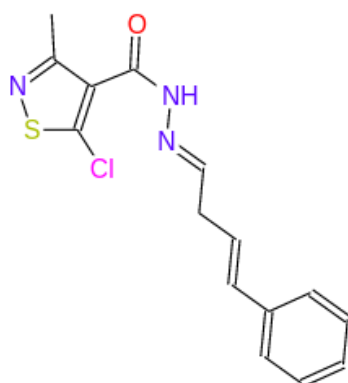
11C¹⁸



182263

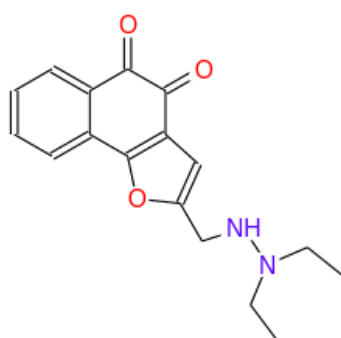
C=C1C(=O)CC(C)(C)OC1C(C)C

Composto 3¹⁰



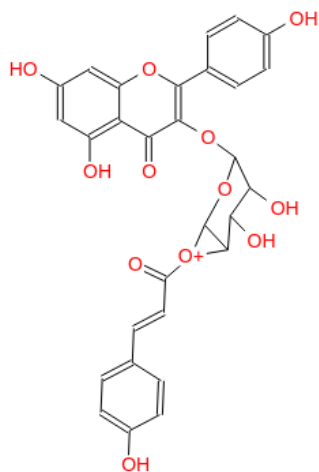
319817 Cc1nsc(Cl)c1C(=O)N/N=C/C=C/c2ccccc2

TC1¹³



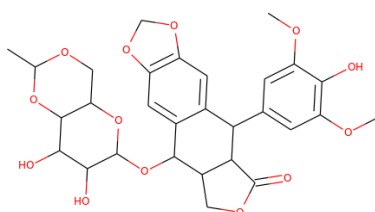
298342 CCN(CC)NCc3cc2c(=O)c(=O)c1cccc1c2o3

KCR¹⁴



563491 O=C(/C=C/c1ccc(O)cc1)[O+]6C5OC(Oc4c(c2ccc(O)cc2)oc3cc(O)cc(O)c3c4=O)C(O)C(O)C56

Etoposideo⁷



588.562 CC1OCC2C(O1)C(C(C(O2)OC3C4COC(=O)C4C(C5=CC6=C(C=C35)OC6)C7=CC(=C(C=C7)OC)O)OC)O