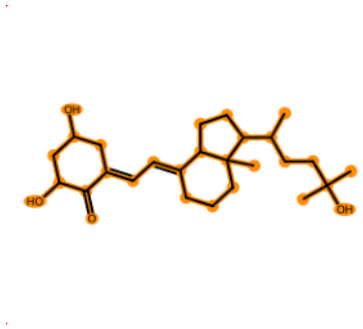
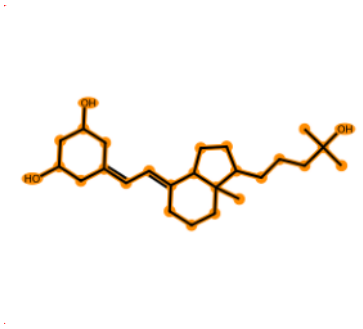
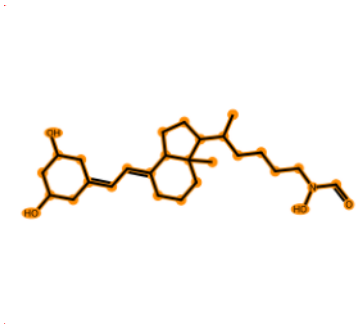


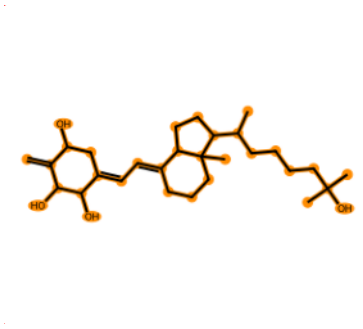
2 gmdldr 0.6719 -11.80 0.5861
-8.740 -8.289 -9.253
O=C1CCCCC1=CC=C1CCCC2CCCC12



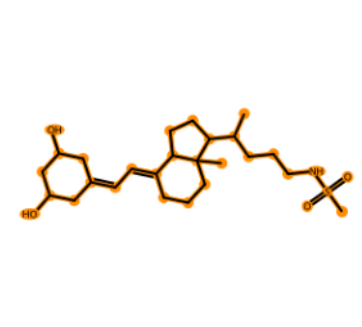
3 gmdldr 0.7069 -11.40 0.5730
-8.527 -8.425 -9.279
C(C=C1CCCC2CCCC12)=C1CCCCC1



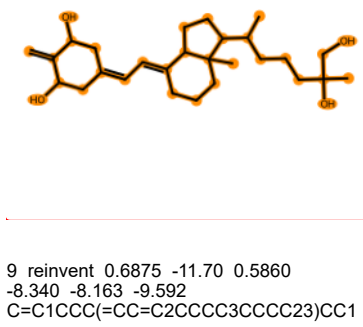
4 transmol 0.7097 -12.00 0.9259
-8.657 -8.046 -9.534
C(C=C1CCCC2CCCC12)=C1CCCCC1



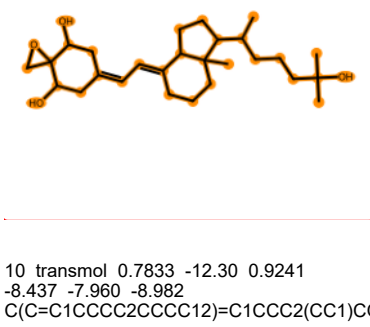
6 gmdldr 0.6875 -12.00 0.5766
-8.946 -7.956 -9.245
C=C1CCC(=CC=C2CCCC3CCCC23)CC1



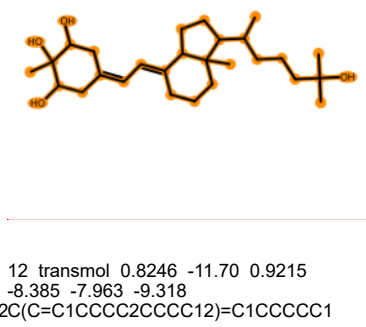
7 transmol 0.6984 -10.90 0.9210
-8.303 -8.174 -9.494
C(C=C1CCCC2CCCC12)=C1CCCCC1



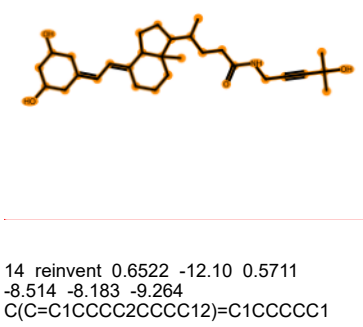
9 reinvent 0.6875 -11.70 0.5860
-8.340 -8.163 -9.592
C=C1CCC(=CC=C2CCCC3CCCC23)CC1



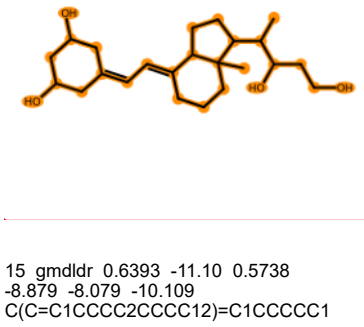
10 transmol 0.7833 -12.30 0.9241
-8.437 -7.960 -8.982
C(C=C1CCCC2CCCC12)=C1CCC2(CC1)CO2



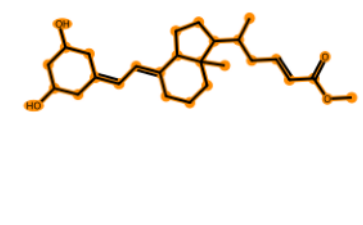
12 transmol 0.8246 -11.70 0.9215
-8.385 -7.963 -9.318
C(C=C1CCCC2CCCC12)=C1CCCCC1



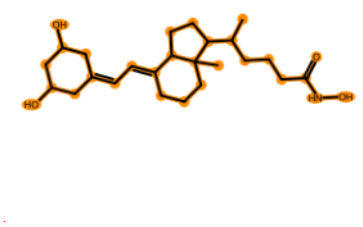
14 reinvent 0.6522 -12.10 0.5711
-8.514 -8.183 -9.264
C(C=C1CCCC2CCCC12)=C1CCCCC1



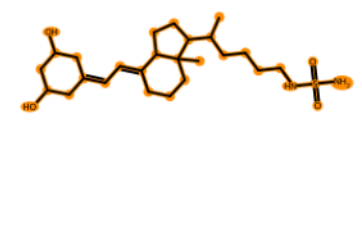
15 gmdldr 0.6393 -11.10 0.5738
-8.879 -8.079 -10.109
C(C=C1CCCC2CCCC12)=C1CCCCC1



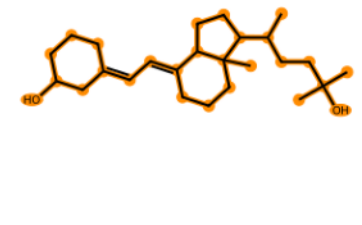
16 reinvent 0.6154 -10.80 0.5803
-8.816 -8.425 -9.176
C(C=C1CCCC2CCCC12)=C1CCCCC1



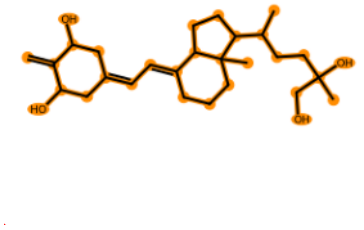
18 transmol 0.7377 -11.40 0.9251
-8.895 -7.856 -9.058
C(C=C1CCCC2CCCC12)=C1CCCCC1



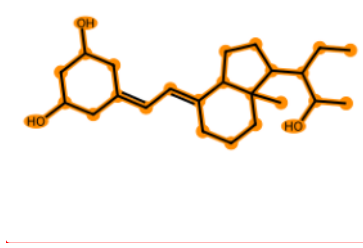
20 transmol 0.6769 -11.10 0.9213
-8.764 -7.917 -9.542
C(C=C1CCCC2CCCC12)=C1CCCCC1



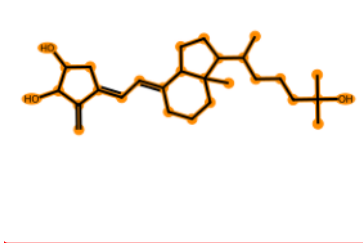
21 reinvent 0.7759 -11.00 0.5765
-8.040 -8.361 -9.605
C(C=C1CCCC2CCCC12)=C1CCCCC1



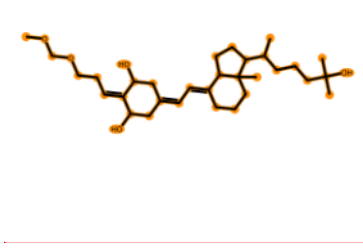
22 gmdldr 0.6462 -11.40 0.5811
-8.684 -8.036 -9.773
C=C1CCC(=CC=C2CCCC3CCCC23)CC1



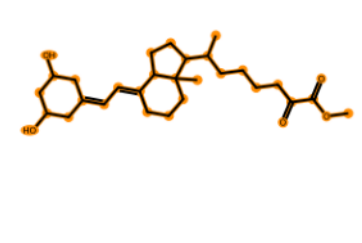
24 gmdldr 0.6610 -10.80 0.5861
-8.301 -8.275 -9.121
C(C=C1CCCC2CCCC12)=C1CCCCC1



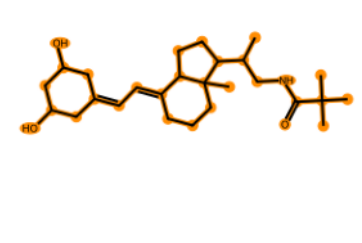
25 reinvent 0.6984 -11.70 0.5886
-8.234 -8.107 -9.653
C=C1CCCC1=CC=C1CCCC2CCCC12



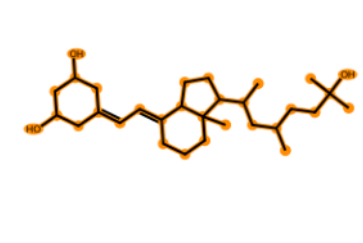
27 transmol 0.6812 -9.60 0.9178
-8.850 -7.888 -8.133
C=C1CCC(=CC=C2CCCC3CCCC23)CC1



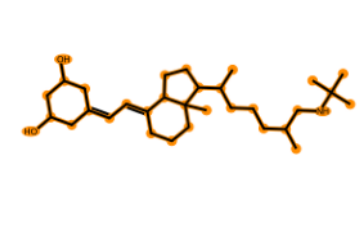
28 transmol 0.6769 -10.50 0.9235
-8.179 -8.320 -8.772
C(C=C1CCCC2CCCC12)=C1CCCCC1



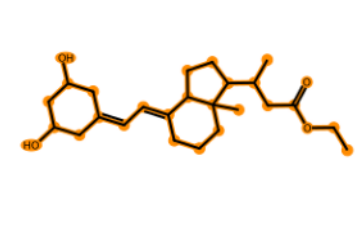
29 gmdldr 0.6667 -12.60 0.5832
-8.231 -8.409 -8.985
C(C=C1CCCC2CCCC12)=C1CCCCC1



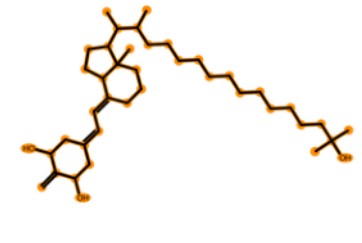
31 gmdldr 0.8246 -11.50 0.5801
-8.148 -8.051 -9.219
C(C=C1CCCC2CCCC12)=C1CCCCC1



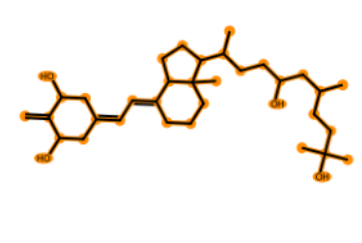
32 gmdldr 0.7419 -11.30 0.5812
-8.151 -8.104 -8.652
C(C=C1CCCC2CCCC12)=C1CCCCC1



33 gmdldr 0.6250 -10.70 0.5843
-8.839 -8.057 -8.903
C(C=C1CCCC2CCCC12)=C1CCCCC1



34 gmdldr 0.6418 -10.70 0.5716
-8.573 -8.076 -7.917
C=C1CCC(=CC=C2CCCC3CCCC23)CC1



35 gmdldr 0.6567 -12.20 0.5726
-8.361 -8.135 -9.040
C=C1CCC(=CC=C2CCCC3CCCC23)CC1

missing functional group wrong hydroxyl group placement difference from secosteroid backbone