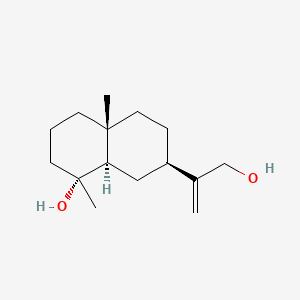
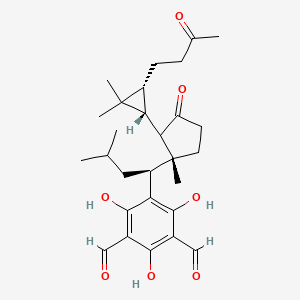
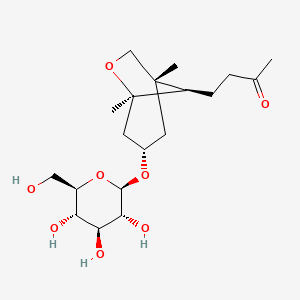
**Supplementary Data**

Table S1: Drug likeness prediction using pkCSM online database server for all the selected ligands

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Ligands** | **Molecular weight < 500 (g/mol)** | **H-bond acceptor < 10** | **H-bond donors < 5** | **log P < 5** |
| **Ilicol** | 238.371 | 2 | 2 | 2.8924 |
| **Eucalyptone** | 486.605 | 7 | 3 | 5.1849 |
| **Ascleposide E** | 388.457 | 8 | 4 | -0.2541 |

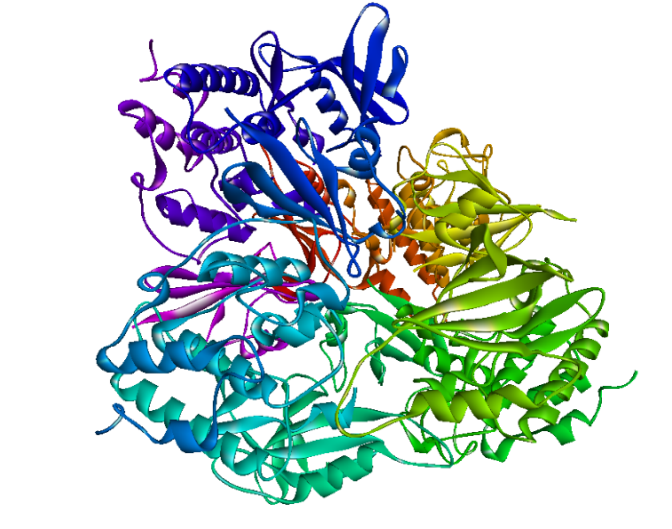
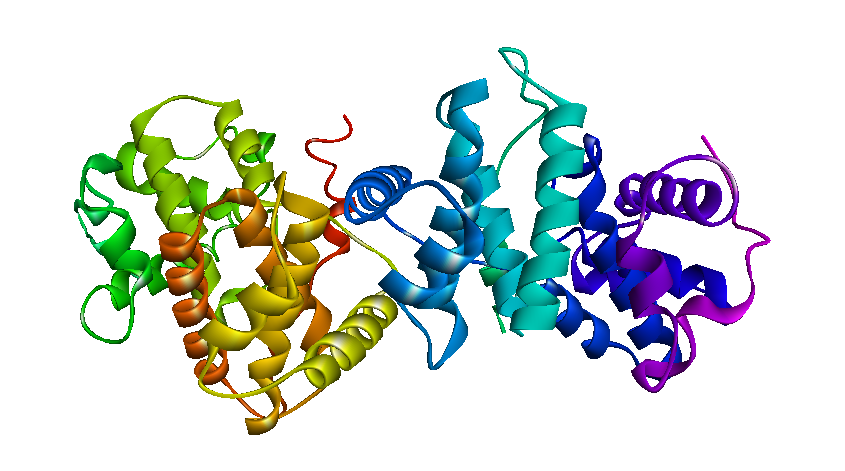


Eucalyptone

Ilicol

Ascleposide E

Figure S1: Chemical structure of selected SLs



**a**

**b**

**Figure S2:** Crystal structure of CB1 (a) and CDK1 (b) of G2/M phase checkpoints