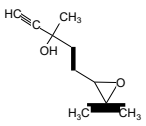
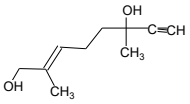
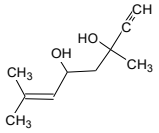
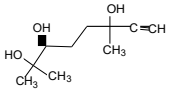
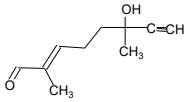
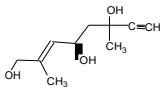
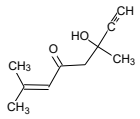
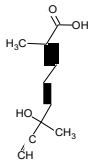
## Supplemental data 4 QSAR Toolbox 3.1.0.21

| | | |
|---|---|---|
| #1 C(C)(O)(C#C)CCC1C(C)(C)O1<br>N/A<br>-<br>  | #2 C(C)(O)(C#C)CCC=C(C)CO<br>N/A<br>-<br>  | #3 C(C)(O)(C#C)CC(O)C=C(C)C<br>N/A<br>-<br>  |
| #4 C(C)(O)(C#C)CCC(O)C(C)(C)O<br>N/A<br>-<br>  | #5 C(C)(O)(C#C)CCC=C(C)C=O<br>N/A<br>-<br>  | #6 C(C)(O)(C#C)CC(O)C=C(C)CO<br>N/A<br>-<br>  |
| #7 C(C)(O)(C#C)CC(=O)C=C(C)C<br>N/A<br>-<br>  | #8 C(=O)(O)C(C)=CCCC(C)(O)C#C<br>N/A<br>-<br>  | |