Module 1 Molecule 1

-----------MM2 Minimization------------

Note: All parameters used are finalized (Quality = 4).

Iteration 2: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.2802

Bend: 20.6011

Stretch-Bend: -0.8359

Torsion: 7.6544

Non-1,4 VDW: -1.4323

1,4 VDW: 4.2365

Dipole/Dipole: 0.3774

Total Energy: 31.8814 kcal/mol

Calculation completed

Module 1 Molecule 2

------------MM2 Minimization------------

Note: All parameters used are finalized (Quality = 4).

Iteration 91: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.2507

Bend: 20.8656

Stretch-Bend: -0.8304

Torsion: 9.5035

Non-1,4 VDW: -1.5162

1,4 VDW: 4.2936

Dipole/Dipole: 0.4452

Total Energy: 34.0120 kcal/mol

Calculation completed

Module 1 Molecule 3

------------MM2 Minimization------------

Note: All parameters used are finalized (Quality = 4).

Iteration 43: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.2659

Bend: 19.8063

Stretch-Bend: -0.8276

Torsion: 10.8698

Non-1,4 VDW: -1.2207

1,4 VDW: 5.6394

Dipole/Dipole: 0.1621

Total Energy: 35.6953 kcal/mol

Calculation completed

Module 1 Molecule 4

------------MM2 Minimization------------

Note: All parameters used are finalized (Quality = 4).

Iteration 109: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.1028

Bend: 14.5591

Stretch-Bend: -0.5493

Torsion: 12.4947

Non-1,4 VDW: -1.0908

1,4 VDW: 4.4970

Dipole/Dipole: 0.1407

Total Energy: 31.1541 kcal/mol

Calculation completed

Ex 2 (5)

------------MMFF94 Minimization------------

Iteration 113: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 57.4128 kcal/mol

Calculation completed

1 O(16)-C(11)-C(5)-C(6) 11.3209

-----------MMFF94 Minimization------------

Iteration 47: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 57.5455 kcal/mol

Calculation completed

1 C(6)-C(5)-C(11)-O(16) 20.1135

-----------MMFF94 Minimization------------

Iteration 101: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 59.1685 kcal/mol

Calculation completed

1 O(16)-C(11)-C(5)-C(6) 36.1628

------------MMFF94 Minimization------------

Iteration 121: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 57.3934 kcal/mol

Calculation completed

1 O(16)-C(11)-C(5)-C(6) 6.8231

Ex 2 (7)

------------MMFF94 Minimization------------

Iteration 400: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 115.567 kcal/mol

Calculation completed

1 C(6)-C(5)-C(15)-O(20) 36.0442

------------MMFF94 Minimization------------

Iteration 157: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 115.455 kcal/mol

Calculation completed

1 C(6)-C(5)-C(15)-O(20) 41.0904

------------MMFF94 Minimization------------

Iteration 350: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 98.516 kcal/mol

Calculation completed

Angle 37.9064

------------MMFF94 Minimization------------

Iteration 200: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 115.49 kcal/mol

Calculation completed

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------------MMFF94 Minimization------------

Iteration 350: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 98.516 kcal/mol

Calculation completed

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------------MMFF94 Minimization------------

Iteration 96: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 98.4114 kcal/mol

Calculation completed

Angle 39.7883

Taxol(9)

**------------MM2 Minimization------------**

**Note: All parameters used are finalized (Quality = 4).**

**Iteration 5: Minimization terminated normally because the gradient norm is less than the minimum gradient norm**

**Stretch: 2.8276**

**Bend: 13.4906**

**Stretch-Bend: 0.6582**

**Torsion: 22.2721**

**Non-1,4 VDW: -1.8244**

**1,4 VDW: 15.5355**

**Dipole/Dipole: 0.0000**

**Total Energy: 52.9597 kcal/mol**

**Calculation completed**

**------------MMFF94 Minimization------------**

**Iteration 31: Minimization terminated normally because the gradient norm is less than the minimum gradient norm**

**Final Energy: 71.4907 kcal/mol**

**Calculation completed**

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**TAXOL (10)**

**------------MM2 Minimization------------**

**Note: All parameters used are finalized (Quality = 4).**

**Iteration 2: Minimization terminated normally because the gradient norm is less than the minimum gradient norm**

**Stretch: 2.6068**

**Bend: 15.0870**

**Stretch-Bend: 0.2955**

**Torsion: 19.6563**

**Non-1,4 VDW: -1.1633**

**1,4 VDW: 13.4108**

**Dipole/Dipole: 0.0159**

**Total Energy: 49.9091 kcal/mol**

**------------MMFF94 Minimization------------**

**Iteration 49: Minimization terminated normally because the gradient norm is less than the minimum gradient norm**

**Final Energy: 67.8994 kcal/mol**

**Calculation completed**

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**Calculation completed**