

# Inhibition of Soluble Epoxide Hydrolase by Cembranoid Diterpenes from Soft Coral *Sinularia maxima*: Enzyme Kinetics, Molecular Docking, and Molecular Dynamics

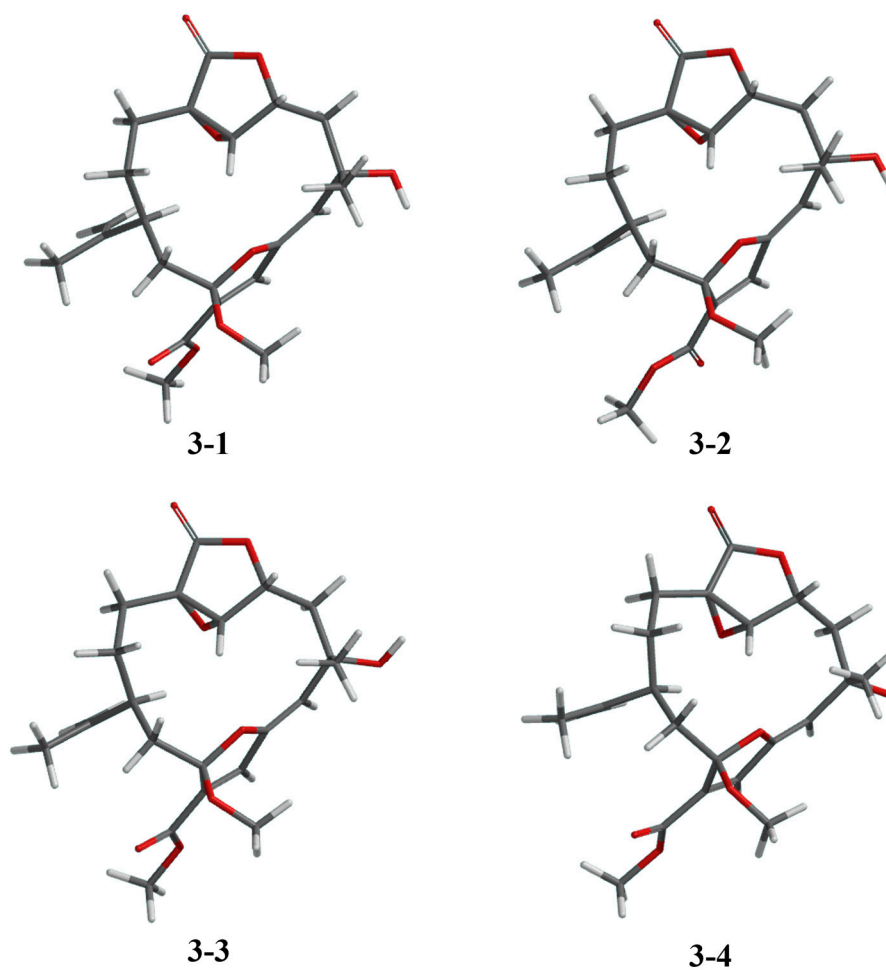
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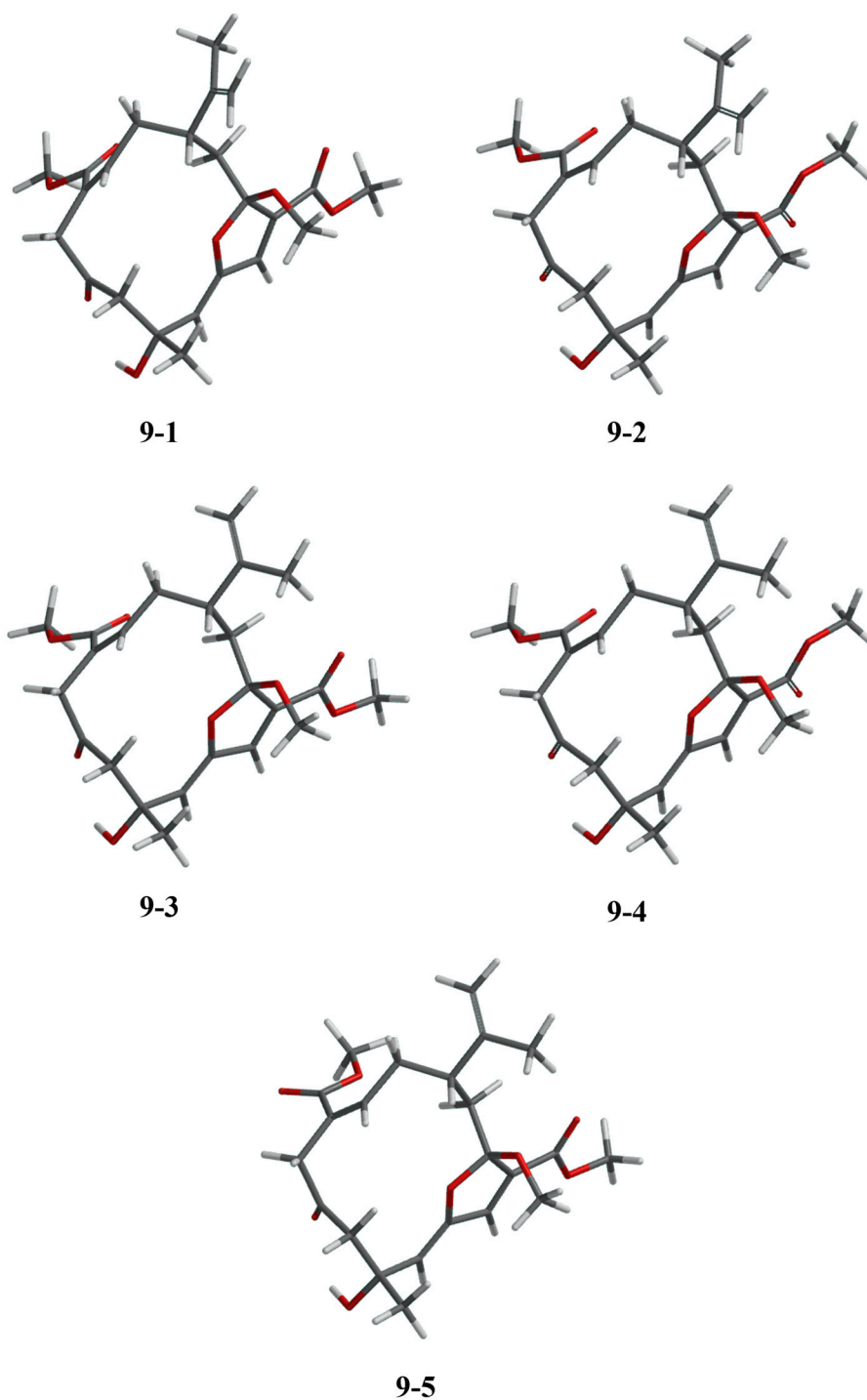
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**Figure S1.** The most stable conformers of compound **3** calculated at B3LYP/6-31G(d) level.

**Table S1.** Electronic energies and Boltzmann populations for the most stable conformers of compound **3**.

Conformers	<i>E</i> (Hartree)	Boltzmann population
3-1	-1448.21402413	0.618335
3-2	-1448.21289292	0.186278
3-3	-1448.21255013	0.129801
3-4	-1448.21190644	0.065585



**Figure S2.** The most stable conformers of compound **9** calculated at B3LYP/6-31G(d) level.

**Table S2.** Electronic energies and Boltzmann populations for the most stable conformers of compound **9**.

Conformers	<i>E</i> (Hartree)	Boltzmann population
9-1	-1487.28932872	0.494028
9-2	-1487.28884500	0.295805
9-3	-1487.28811371	0.136032
9-4	-1487.28736338	0.061519
9-5	-1487.28586652	0.012615

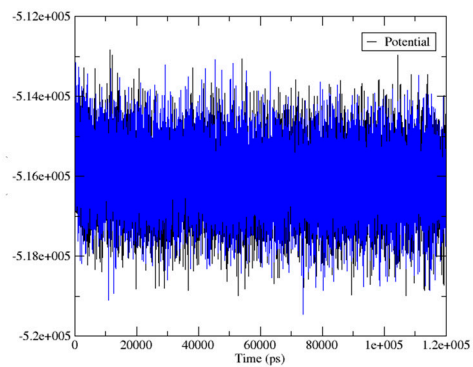
**Compound 3**

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Potential	-516133	38	820.964	-218.629	(kJ/mol)
Energy	Average	Err.Est.	RMSD	Tot-Drift	
Total Energy	-410136	38	1102.35	-214.891	(kJ/mol)

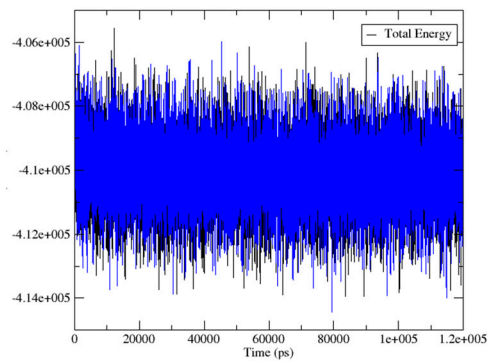
**Compound 9**

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Potential	-516073	42	822.579	-272.639	(kJ/mol)
Energy	Average	Err.Est.	RMSD	Tot-Drift	
Total Energy	-410080	42	1104.2	-267.86	(kJ/mol)

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**Figure S3.** Energy profiles, total energy, and potential energy plots for the sEH complexes with compounds **3** (black) and **9** (blue).