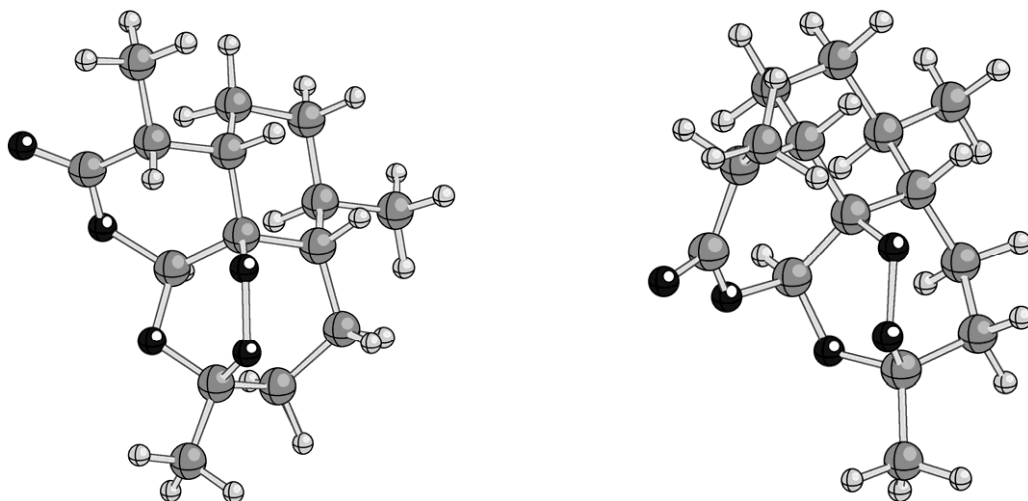


- 23: R=CH<sub>3</sub>, 24: R=gly
- 3: dimethyl carbonate  
 4: propylene carbonate  
 5: butylene carbonate  
 6: glyceryl carbonate  
 7: DMI  
 8: DMPU  
 9:  $\gamma$ -valerolactone  
 10: 1,8-cineol  
 11: 1,1,2,2-tetrafluoroethane  
 12: 1,1,1,2-tetrafluoroethane (R134a) 13: 1,1,1,2,3,3,3-heptafluoropropane (R227)  
 14: 1,3-dioxane-5-ol (glycerol formal)  
 15: 2-isobutyl-1,3-dioxane-5-ol (glycerol isobutylal)
- 16: *N,N*-dimethylethanolammonium octanoate (DMEA oct)  
 17: bis(2-methoxyethyl)ammonium bis(trifluoromethylsulfonyl)imide (BMOEA bst)  
 18: 1-ethyl-3-methylimidazolium acetate (EMIM OAc)  
 19: ethyl lactate  
 20: diacetone alcohol  
 21: artemisia ketone (3,3,6-trimethyl-1,5-heptadiene-4-one)  
 22: 2-butoxy ethanol  
 23: R=CH<sub>3</sub>, casticin  
 24: R=gly, casticin glycoside  
 25: deoxyartemisinin  
 26: carvacrol

Scheme S1. Molecular structures of some potential solvents, co-solvents and solubility modifiers for artemisinin extraction.



**Fig. S1.** Optimised geometry of the conformers of artemisinin (1, left) and epiartemisinin (1', right) dominating the solubility calculations.



**Fig. S2.** Screening charge density maps of toluene (left) and perfluorotoluene (right), calculated by COSMOtherm.