Guidance Supplementary Materials

A molecular modeling study into Brønsted and Lewis acid catalyzed conversion of CBD into other cannabinoids.

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Molecular Structures

Molecular structures are saved as mol2 files. The files are grouped in folders, following the description of the Figures 1,2,3,5, and Table 1 in the manuscript. To restore all quantitative data from the mol2 files, a single-point and IR-frequency calculation should be performed using B3LYP/6-31G*. A frequency calculation is required to restore the thermodynamical enthalpy corrections, including the Zero Point Energy (ZPE).

B3LYP is applied as originally described, using for Exchange: 0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88 and for Correlation: 0.1900 VWN1RPA + 0.8100 LYP.

Excelsheet (.xslx)

The Excel sheet Cannabinoids BF3 pTSA contains the results of the B3LYP/6-31G* calculations (Total Energy, ΔH-corrections) and the calculation of activation barriers, complexation energies, etc. in sheet 1. Sheets Kin PTSA, PTSA, Kin BF3, and BF3 contain the graphs and the corresponding simple kinetic models of pTSA and BF3 catalysis. In both cases the activation barriers for the base case and the optimised activation barriers are listed. EP and sheet 3 contain the Energy Profile graph and data of the corresponding B3LYP/6-31G* calculation.