

Relation between crystal structures of precursors and final products: example of vitamin D intermediates

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Supporting information

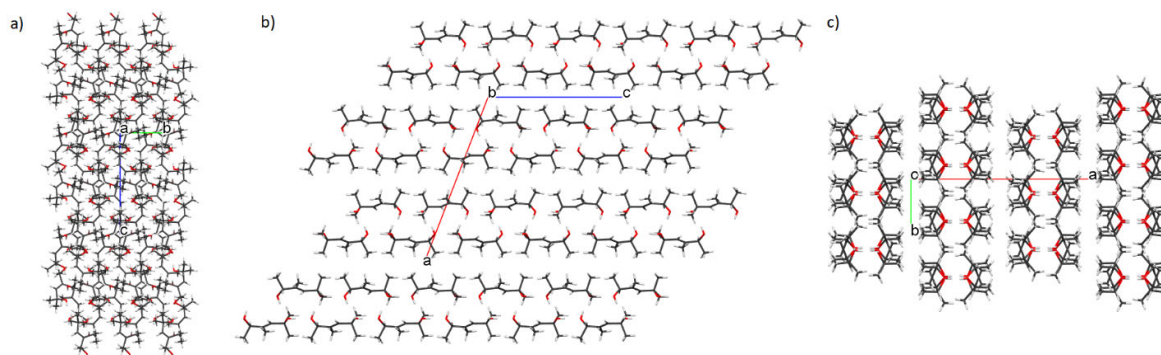


Figure S1 Packing of the crystal lattice of precursor 1, viewed along a, b and c-directions. The H-atoms were omitted for clarity.

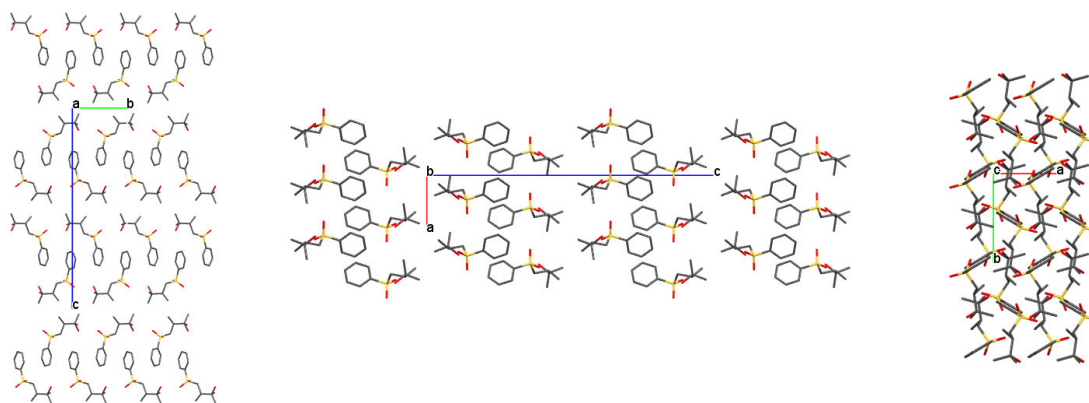


Figure S2 Packing of the crystal lattice of precursor 2, viewed along a, b and c-directions. The H-atoms were omitted for clarity.

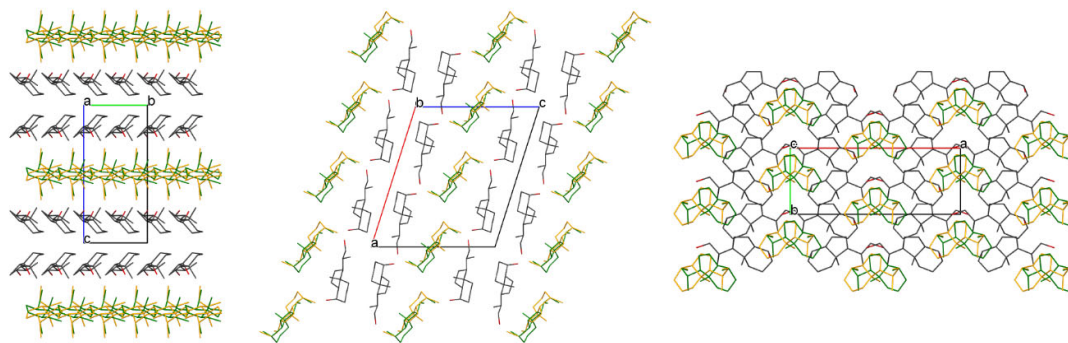


Figure S3 Packing of the crystal lattice of intermediate **3**, viewed along a, b and c-directions. The H-atoms were omitted for clarity.

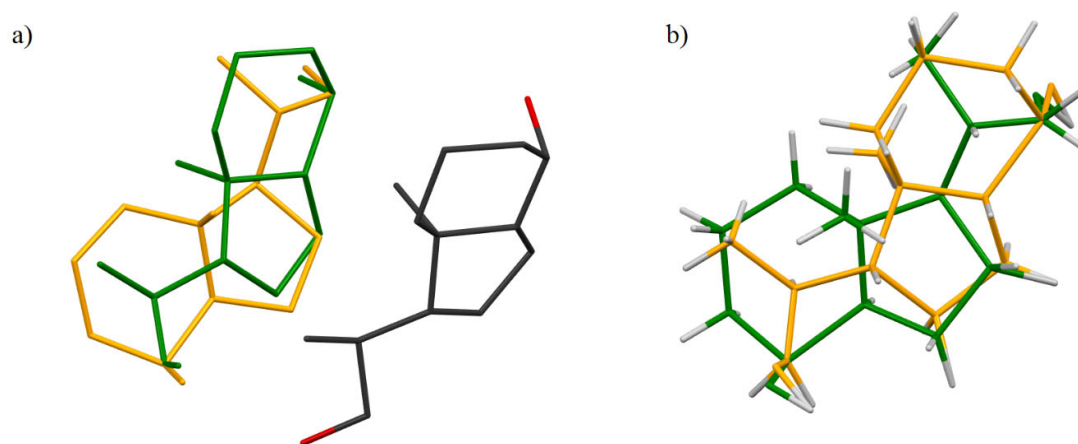
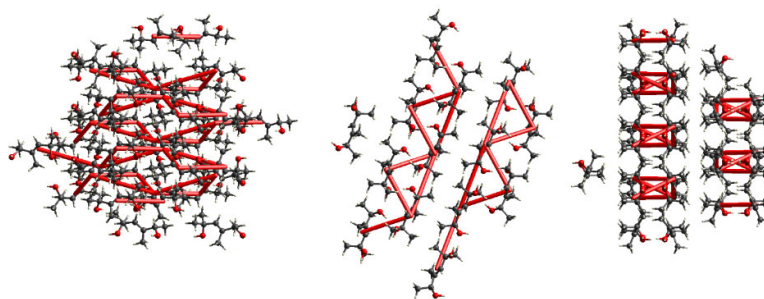


Figure S4 Structure of **3**: a) part 0 as well as the disordered part -1 and b) disordered part -1 with hydrogen atoms. Atoms marked as green and orange have occupancy equal to 0.5. Atoms marked by grey and red as well as atoms connected to both, green and orange atoms, have occupancy equal to 1.



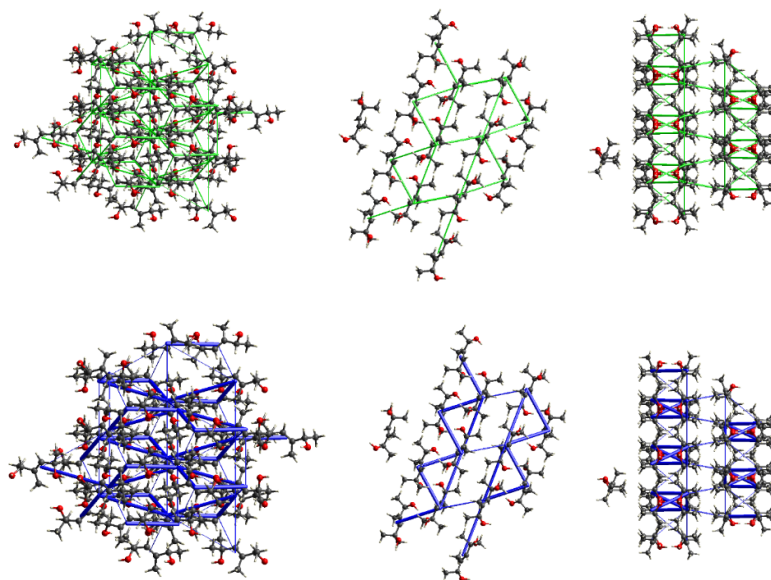
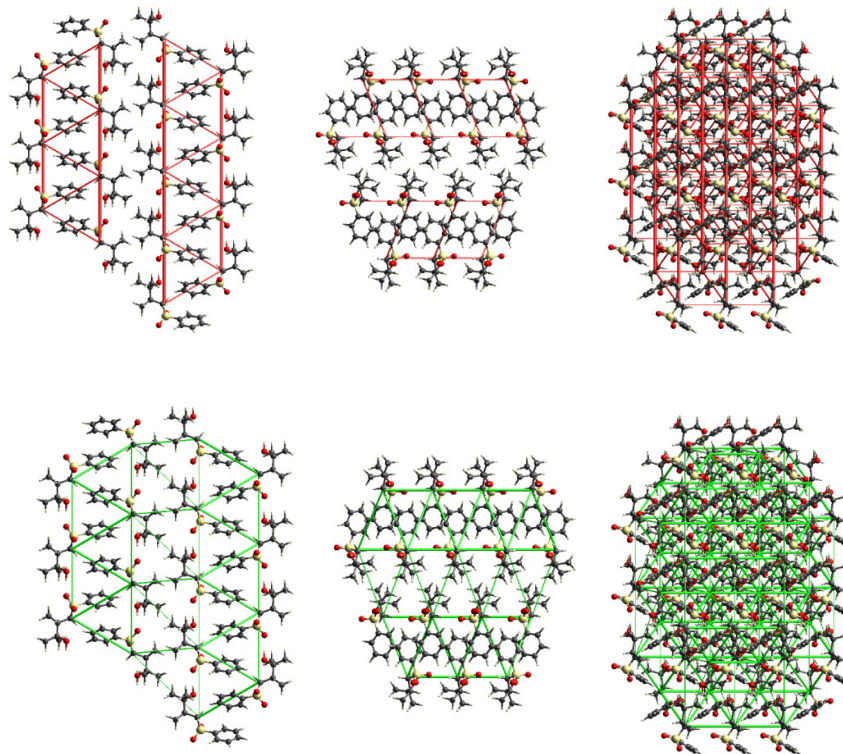


Figure S5 Energy frameworks of precursor 1: Coulomb energy (red), dispersion energy (green) and total energy (blue) viewed along a, b and c-directions.



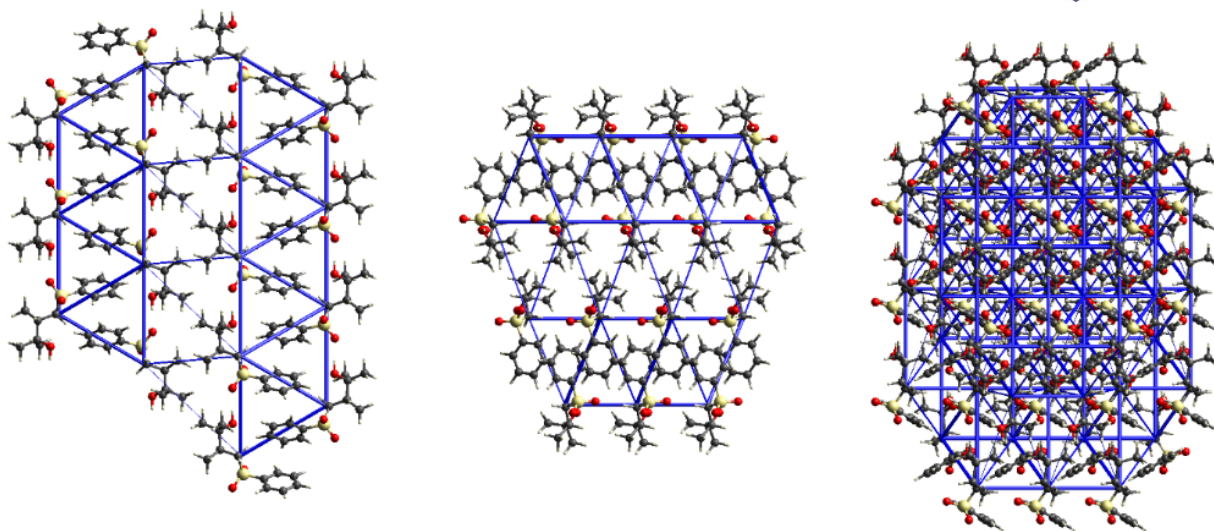


Figure S6 Energy frameworks of precursor 2: Coulomb energy (red), dispersion energy (green) and total energy (blue) viewed along a, b and c-directions.

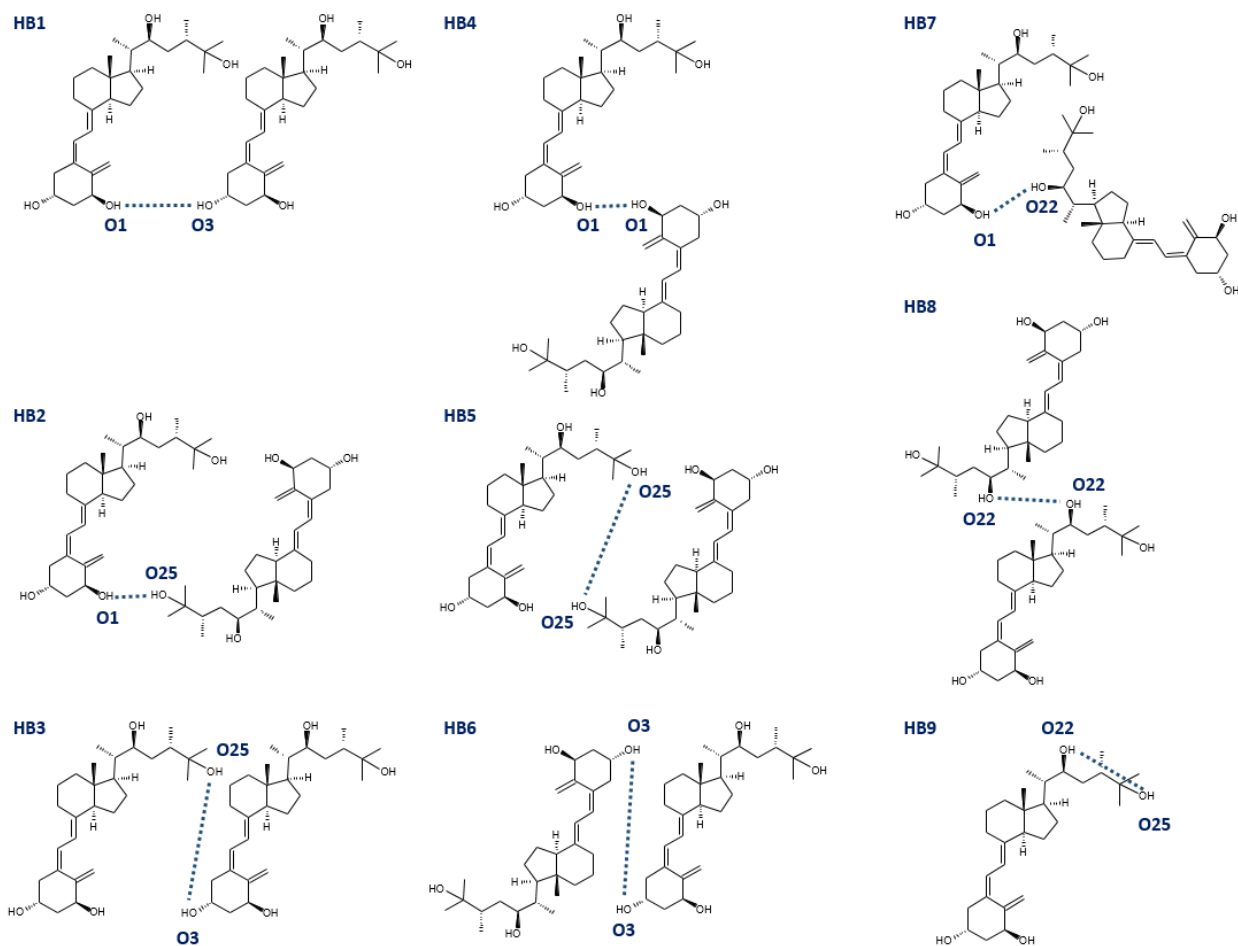


Figure S7 HB1-HB9 hydrogen bond dimers found in vitamin D analogues.