Supporting Information for

Applications of Low Temperature Gradient Sublimation in Vacuo: Rapid Production of High Quality Crystals; The First Solvent-Free Crystals of Ethinyl Estradiol.

Jolanta Karpinska, Andrea Erxleben and Patrick McArdle*

School of Chemistry, National University of Ireland, Galway, Ireland. E-mail:

p.mcardle@nuigalway.ie; Fax: +353 91525700; Tel: +353 91492487

To investigate the extent of unused hydrogen bonding capacity among steroid compounds two searches of the Cambridge Database (CSD, version 5.33) were performed for entries containing both C=O and O-H groups in the first case and only the O-H group in the second case.

The constraints used in both searches were as follows: steroids, 3D determined, no ions, no powders, no errors, not polymeric, only organic structures and no (C=O···H-O or O-H···O-H). The hits were analysed manually and inappropriate entries were eliminated. Of the steroid structures on the CSD only 14 examples with unused O-H groups were found (FNPEYO, FUFDAL, GAPGAF, KANYAA, LAKJAJ, LALXIF, MBRHES, NPREYO, QEYBAX, QUMJOX, RAMYAG, SUQDUE, WATRIT, YAPZEU) and just 10 with unused C=O groups (AFAWOU, CAZXAC10, EYHENO, HMESDP, ISTEST, LOHVAF, NOTEST01, NPTYMO, PAMLUL, ZUKRUS). There were 4131 entries on the CSD classified as steroids.