Electronic Supplementary Information

Novel Pharmaceutical Compositions through Co-crystallization of Racetams and Li^+ Salts

Johan Wouters,* Fabrizia Grepioni,* Dario Braga, Rafal M. Kaminski, Sandrine Rome, Luc Aerts and Luc Quéré

EXPERIMENTAL

All reagents and solvents were purchased from Acros Organics and used without further purification.

Synthesis

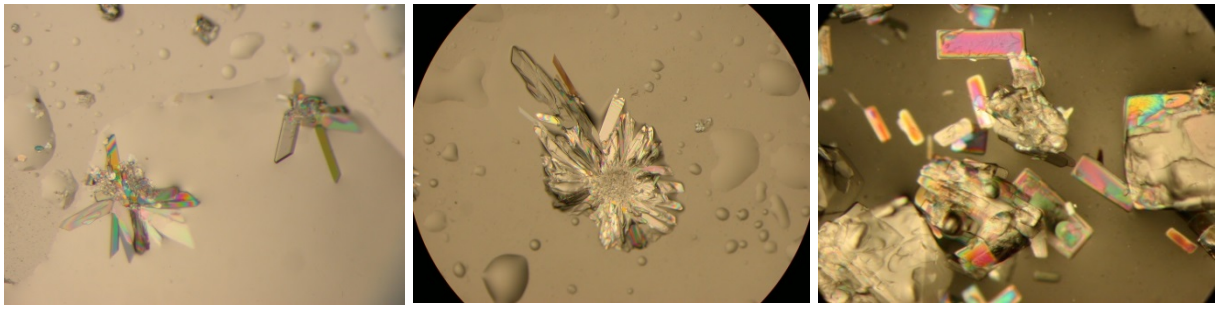
BRV_2·LiBr was obtained by recrystallization of a deliquescent powder obtained by grinding (in a mortar) of BRV (350 mg) and LiBr (71 mg) (2:1 ratio); the deliquescent powder was left at ambient temperature/humidity and crystals suitable for X-ray single crystal diffraction were obtained.

SEL_2·LiBr was obtained by recrystallization of a deliquescent powder obtained by grinding (in a mortar) of SEL (350 mg) and LiBr (65 mg) (2:1 ratio); the deliquescent powder was left at ambient temperature/humidity and crystals suitable for X-ray single crystal diffraction were obtained.

SEL·LiCl·$2H_2O$ was obtained by recrystallization of a deliquescent powder obtained by grinding (in a mortar) of SEL (350 mg) and LiCl (64 mg) (1:1 ratio); the deliquescent powder was left at ambient temperature/humidity and crystals suitable for X-ray single crystal diffraction were obtained.

Crystals

Powders obtained for each co-crystal are rather hygroscopic. Crystals (Figure S1) were grown from a deliquescent powder obtained by grinding.



a) b) c)

Figure S1. Single crystals grown for BRV_2•LiBr (a), SEL_2•LiBr (b) and SEL•LiCl•$2H_2O$ (c).

Structural determination

Single crystal data. All crystal data were collected at room temperature on an Enraf –Nonius CAD4 diffractometer with Cu-Kα radiation, λ = 1.54181 Å and graphite monochromator. SHELX97[ESI-1] was used for structure solution and refinement based on F^2. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were added in calculated positions. For structure **BRV_2·LiBr** two conformations of the lateral propyl chain were refined.

The program Schakal[ESI-2] was used for the graphical representation of the results. The program PLATON[ESI-3] was used to calculate hydrogen bond distances.

References

ESI-1 G. M. Sheldrick, *SHELXL97* **1997**, University of Göttingen, Germany.

ESI-2 E. Keller, **1999**, SCHAKAL99, Graphical Representation of Molecular Models; University of Freiburg, Germany.

ESI-3 A. L. Spek, *Journal of Applied Crystallography* **2003**, *36*, 7-13.