**Supplementary Material for the paper “A standard structure for bile acids and derivatives” by Francisco Meijide, Santiago de Frutos, Victor H. Soto, Aida Jover, Julio A. Seijas, M. Pilar Vázquez-Tato, Francisco Fraga, José Vázquez Tato.**

**Synthesis of indicated compounds in Table 3**

Compound 17: The synthesis has been described by Soto Tellini VH in *Estructuras supramoleculares generadas por ciclodextrinas, adamantanos y ácidos biliares*, Doctoral Thesis, 2006, Universidad de Santiago de Compostela (Spain).

Compound 19: The synthesis and crystal structure have been described by Alvarez Alcalde M in *Estructuras supramoleculares generadas por ácidos biliares y ciclodextrinas,* Doctoral Thesis, 2007, Universidad de Santiago de Compostela (Spain).

Compound 23: This azide is an intermediate in the synthesis of the 3β-amino derivative of cholic acid. The synthesis has been described by Davis *et al* (Davis AP, Dresen S, & Lawless LJ (1997) Mitsunobu reactions with methanesulfonic acid; the replacement of equatorial hydroxyl groups by azide with net retention of configuration, *Tetrahedron Let.* 38(24):4305-4308; Lawless LJ, Blackburn AG, Ayling AJ, Perez-Payan MN, & Davis AP (2001) Steroidal guanidines as enantioselective receptors for N-acyl a-amino acids. Part 1. 3a-Guanylated carbamates derived from cholic acid, *J. Chem.Soc., Perkin Trans. 1* (11):1329-1341). The crystal structure has been described by Santiago de Frutos in *Estructura cristalina y propiedades coloidales de ácidos biliares modificados*, Doctoral Thesis, 2014, Universidad de Santiago de Compostela (Spain).

Compound 25: This product is an intermediate in the synthesis of amides from an amine and a carboxylic acid, in which DEPC is used as an activating agent of the carboxylic group. The method has been described previously (Soto VH*, et al.* (2007) *Supramolecular structures generated by a p-tert-butylphenyl-amide derivative of cholic acid. From vesicles to molecular tubes,* *Adv. Mater.* 19(13):1752-1756; Soto VH*, et al.* (2006) *New Lamellar Structure Formed by an Adamantyl Derivative of Cholic Acid,* *J. Phys. Chem. B* 110(28):13679-13681).

Compound 26: This compound is a side product in the synthesis of compound 29 (Meijide F*, et al.* (2013) *Crystal structure of head-to-head dimers of cholic and deoxycholic acid derivatives with different symmetric bridges*, *Steroids* 78:247-54).

**Crystal data of previous compounds**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| compound | formula | space group | unit cell lengths (Å) | unit cell  angles (o) | unit cell volume (Å3) | Z |
| **17** | C29H49NO5,H2O | *P212121* | *a* = 8.4360(8)  *b* = 14.466(3)  *c* = 25.164(2) | α = 90  β = 90  γ = 90 | 3070.89 | 4 |
| **19** | C32H45NO7,2 CH4O | *P212121* | *a* = 10.453(5)  *b* = 14.620(5)  *c* = 21.774(5) | α = 90  β = 90  γ = 90 | 3327.56 | 4 |
| **23** | C25H41N3O4,H2O | *C2* | *a* = 18.9238(12)  *b* = 16.6746(12)  *c* = 7.6595(5) | α = 90  β = 97.790(3)  γ = 90 | 2394.63 | 4 |
| **25**/DMSO | C29H52NO7P,C2H6SO | *P21* | *a* = 13.850(5)  *b* = 7.889(5)  *c* = 15.309(5) | α = 90  β = 93.222(5)  γ = 90 | 1670.06 | 2 |
| **25**/MeOH | C29H52NO7P,H2O | *P212121* | *a* = 7.6084(5)  *b* = 16.4239(10)  *c* = 23.6781(13) | α = 90  β = 90  γ = 90 | 2958.81 | 4 |
| **25**/acetone | C29H52NO7P,H2O | *P212121* | *a* = 7.6107(2)  *b* = 16.4237(5) *c* = 23.6767(7) | α = 90  β = 90  γ = 90 | 2959.49 | 4 |
| **26** | C34H48O8 | *P21* | *a* = 10.3340(3) *b* = 7.6197(2)  *c* = 19.4631(5) | α = 90  β = 101.2670(10)  γ = 90 | 1503.03 | 2 |