

SUPPORTING INFORMATION

Diastereomeric salts of (S,S)-Sertraline with L- and D-tartaric acids: an investigation into chiral supramolecular discrimination.

Paulo S. Carvalho Jr^{a*}, Luan F. Diniz^b, Alejandro P. Ayala^c.

^a Institute of Physics, Federal University of Mato Grosso do Sul, 79070-900, Campo Grande, MS, Brazil. *e-mail: paulo.sousa@ufms.br. ^bLaboratório de Controle de Qualidade, Departamento de Produtos Farmacêuticos, Faculdade de Farmácia, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, MG, Brazil. ^c Departamento de Física, Universidade Federal do Ceará, 60455-970, Fortaleza, Ceará, Brazil.

COMPLEMENTARY FIGURES AND TABLES

Figure S1. Authenticity evaluation of the salt samples synthesized: (a) DSC curves of diastereomeric salts of Srt, prepared by the different methods; for comparison, DSC curves of sertraline hydrochloride and tartaric acid (starting materials) were included. (b) PXRD patterns of diastereomeric salts of Srt, produced by the different methods; for comparison, diffractograms calculated of each salt as well as of sertraline hydrochloride and tartaric acid (starting materials) were included.

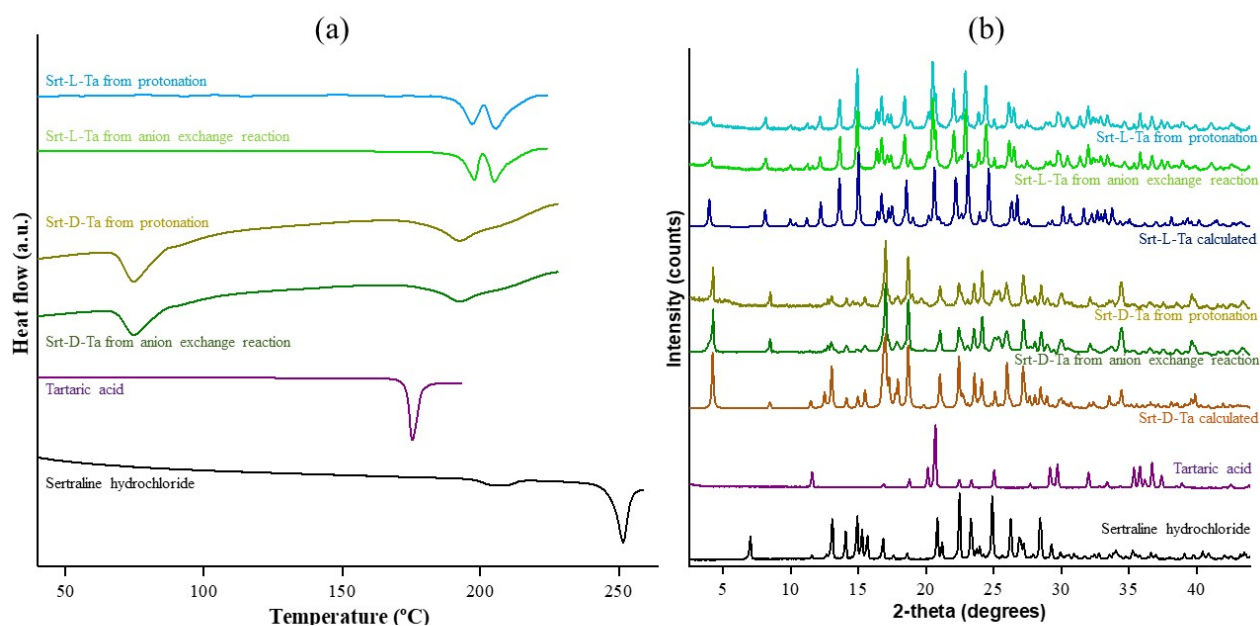
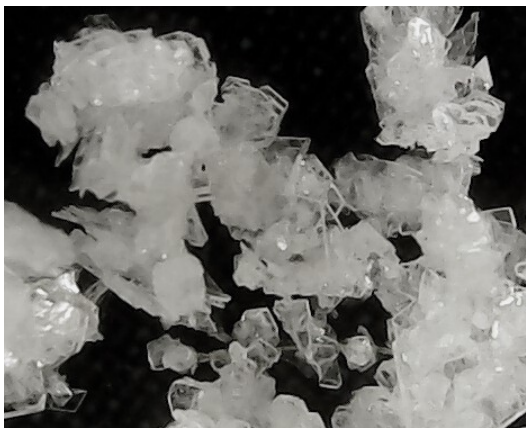


Figure S2. Crystal habits of the diastereomeric salts of Srt: (a) Srt-L-Ta and (b) Srt-D-Ta.



(a)



(b)

Figure S3. Overlay Srt⁺ conformation from hydrochloride salts and the diastereomeric tartrate ones.

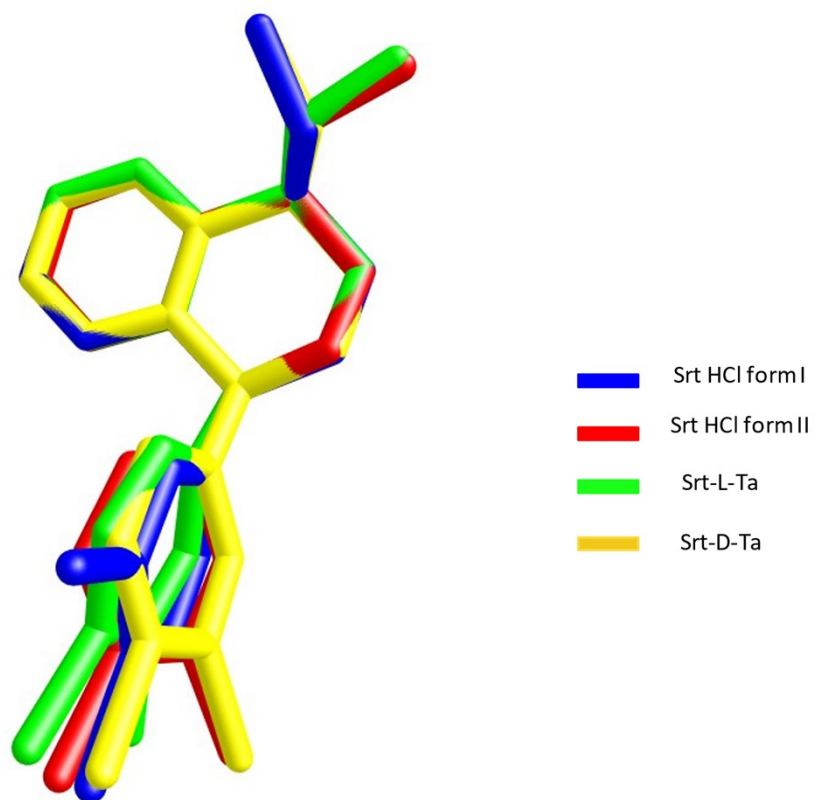


Figure S4. Diagram of cation-anion association in the diastereomeric Srt salts.

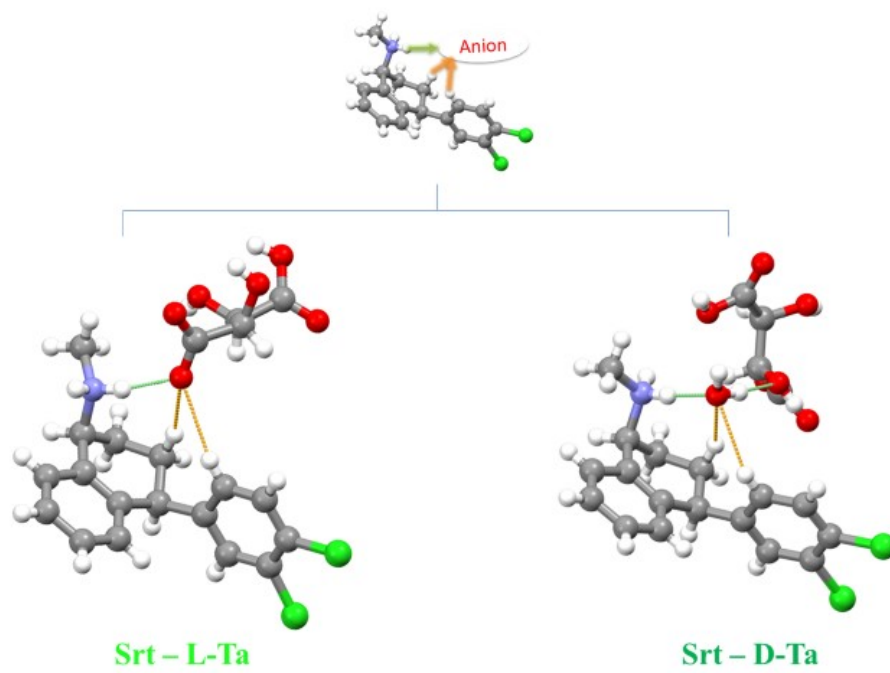


Figure S5. The CH $\cdots\pi$ interaction between the aromatic moieties of Srt⁺ cations in the cationic chains in the Srt-L-Ta structure.

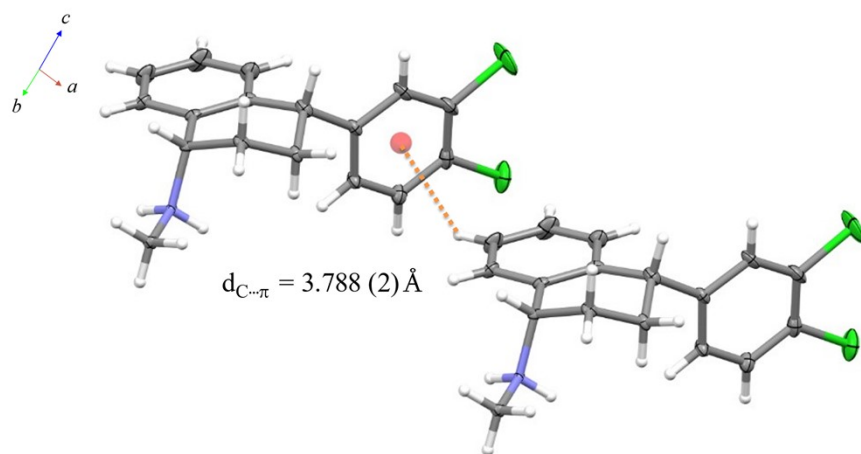


Figure S6. Perspective view of the cation-H₂O-anion assembly in the Srt-D-Ta structure.

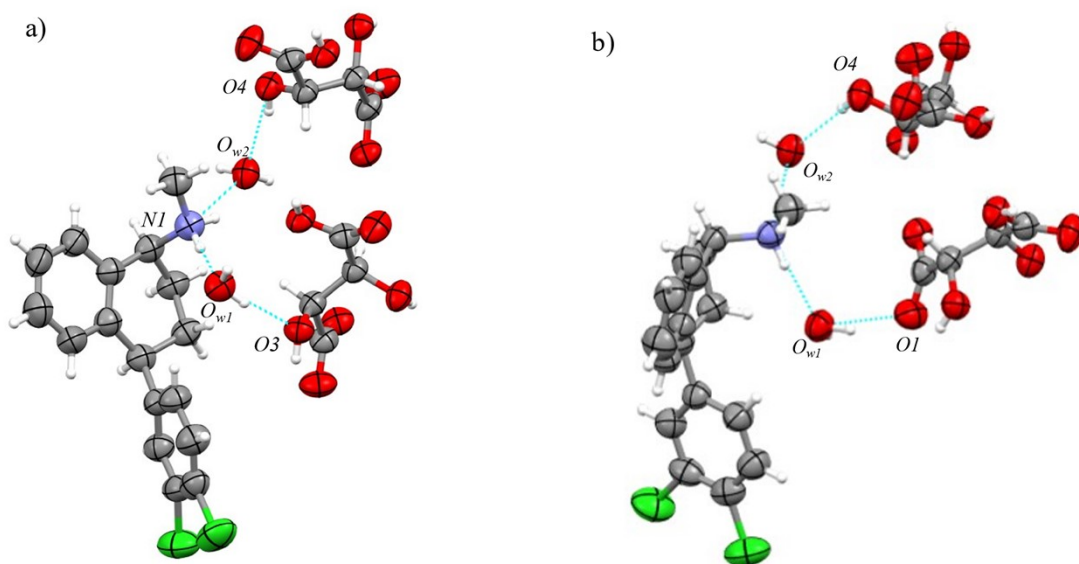
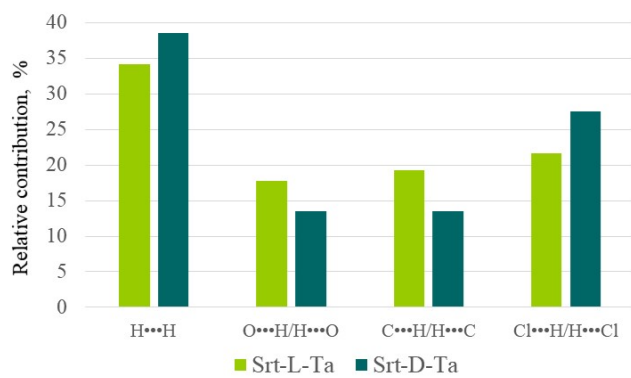
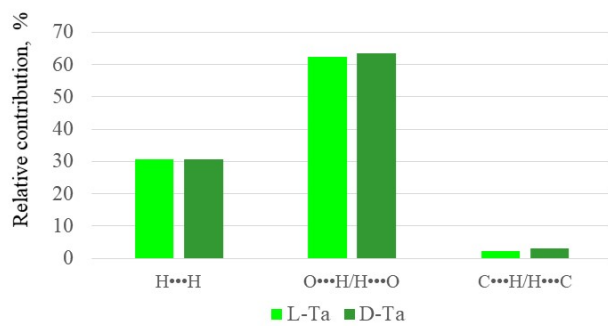


Figure S7. The intermolecular contact contribution for the Hirshfeld surface of (a) Srt^+ cation and (b) anions from the diastereomeric salts.



(a)



(b)

Figure S8. PXRD data of the solid residues from the equilibrium solubility studies for (a) Srt-L-Ta and (b) Srt-D-Ta. For comparison, the experimental diffractograms of freshly prepared samples of each salt have been included.

