Supplementary Information

Comparative Study of Nine Berberine Salts in the Solid State: Optimization of the Photoluminescence and Self-Association Properties through the Choice of the Anion

Marine Soulié, Chantal Carayon, Nathalie Saffon, Sylvie Blanc, and Suzanne Fery-Forgues

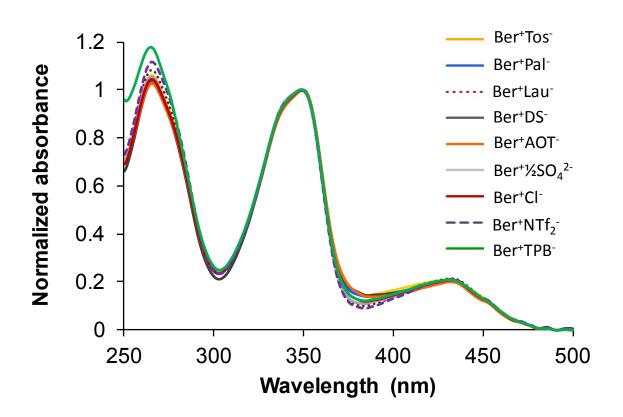


Figure S1. Normalized absorption spectra of the berberine salts in acetonitrile. Concentration between 2×10^{-5} M and 4.4×10^{-5} M. A fourth intense band is between 200 and 250 nm. The small differences observed at high wavelength are due to absorption of the anion (e.g. TPB⁻).

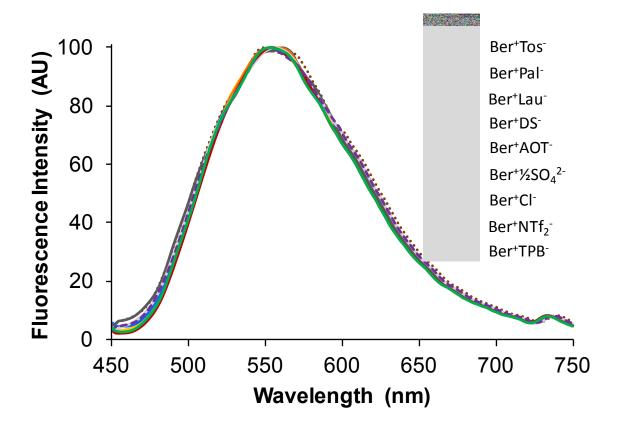


Figure S2. Fluorescence spectra of the berberine salts at 1.1×10^{-5} M in acetonitrile. All spectra were corrected and normalized. $\lambda_{ex} = 420$ nm.

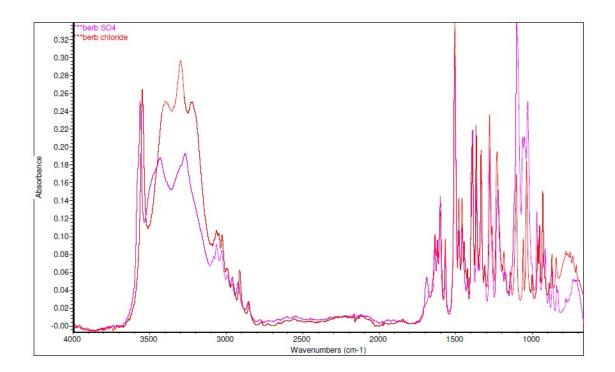


Figure S3. Infrared spectra of berberine chloride and berberine sulfate hydrates.

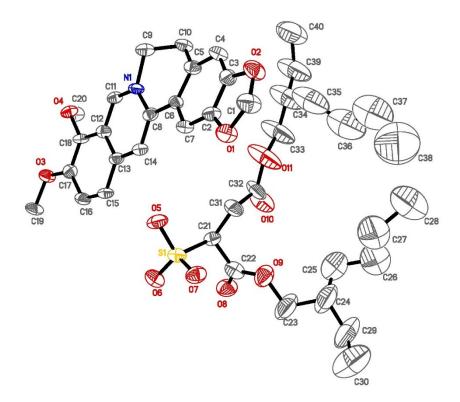


Figure S4. Molecular view of Ber⁺AOT⁻. Thermal ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

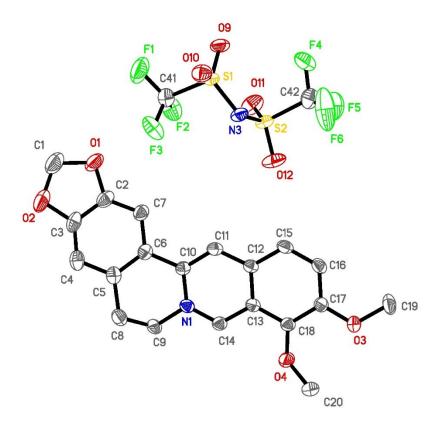


Figure S5. Molecular view of Ber⁺NTf₂⁻. Thermal ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

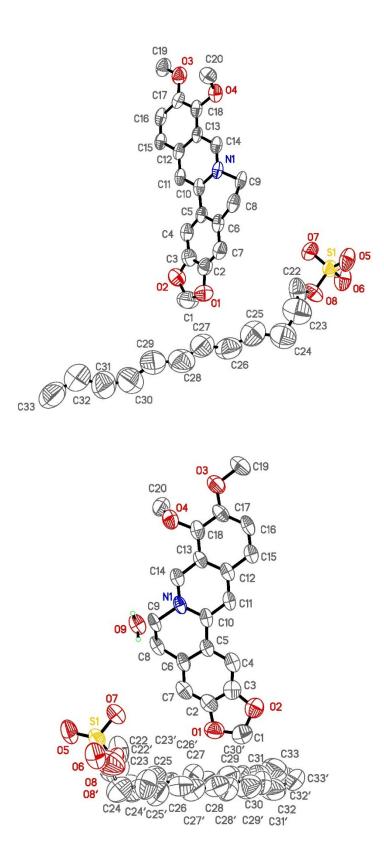


Figure S6. Molecular views of Ber⁺DS⁻. Thermal ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

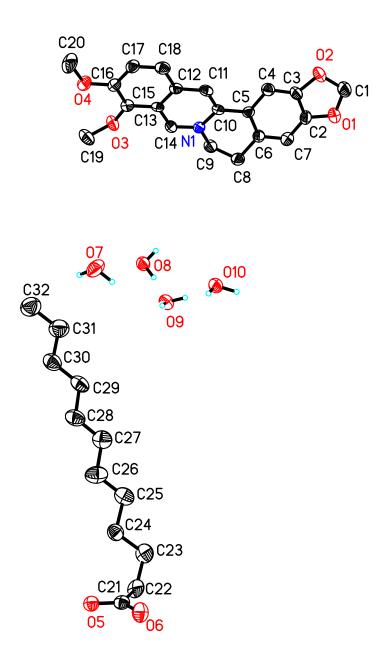
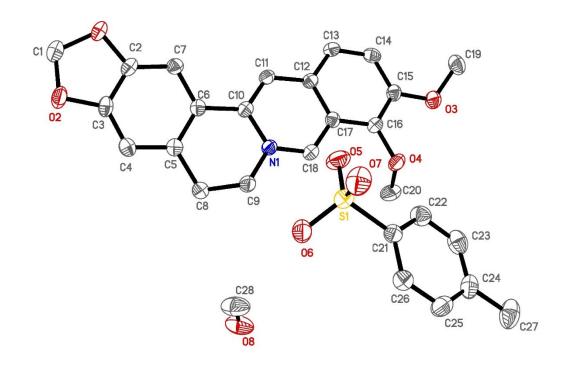


Figure S7. Molecular view of Ber⁺Lau⁻. Thermal ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.



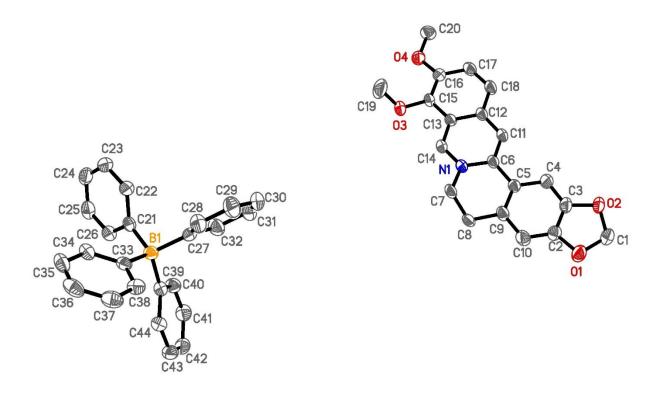


Figure S8. Molecular views of Ber⁺Tos⁻ (top) and Ber⁺TPB⁻ (bottom). Thermal ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.