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Title: Diagnostic Absolute Configuration Determination of Clavulanate Potassium: A Comprehensive Investigation of Chiroptical Spectroscopies and Theoretical Calculations

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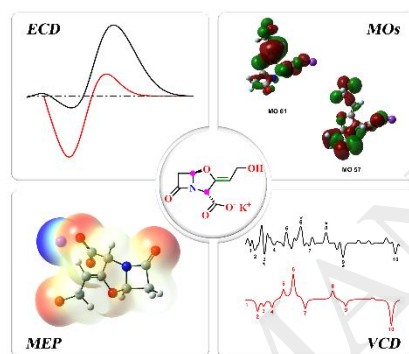
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Diagnostic Absolute Configuration Determination of Clavulanate Potassium: A Comprehensive Investigation of Chiroptical Spectroscopies and Theoretical Calculations

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Graphical abstract



Highlights:

- Convenient methods were demonstrated to determine the absolute configuration of CP.
- DFT calculation is applied to simulate and elucidate the spectroscopies observation.
- Two characteristic cotton effects were found in ECD consisted with simulation.
- Four diagnostic peaks of VCD were found to distinguish CP from its stereoisomers.
- Conformational and vibrational properties of CP were revealed by theoretical method.

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