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ACCEPTED MANUSCRIPT

SELECTIVE SOLVATION IN COSOLVENT-MODIFIED SUPERCRITICAL CARBON DIOXIDE ON THE EXAMPLE OF HYDROXYCINNAMIC ACIDS. THE ROLE OF COSOLVENT SELF-ASSOCIATION

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Graphical Abstract



HIGHLIGHTS

- Simulation of hydroxycinnamic acids in modified supercritical CO₂ was performed.
- Selective solvation occurs by the formation of hydrogen bonded complexes.
- Cosolvent forms clusters around the solvate complexes.
- The number of methanol molecules in such clusters can reach 10.
- Methanol associates consist of no more than three molecules in the fluid bulk.

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