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Vibrational spectroscopic analysis of cyanopyrazine-2-carboxamide derivatives and investigation of their reactive properties by DFT calculations and molecular dynamics simulations

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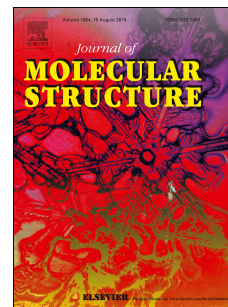
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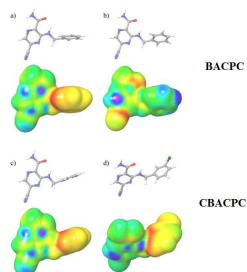
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