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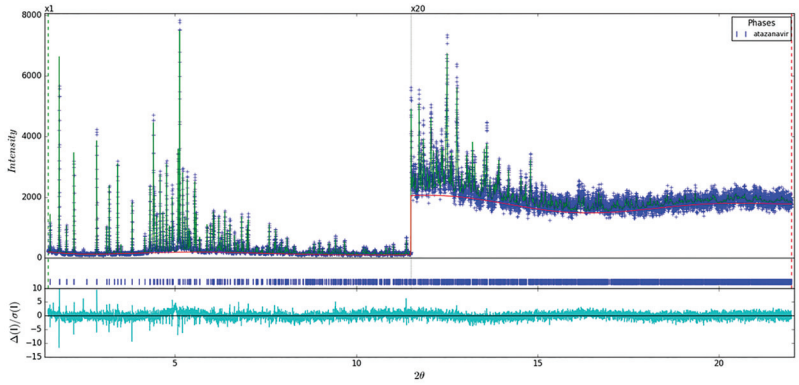
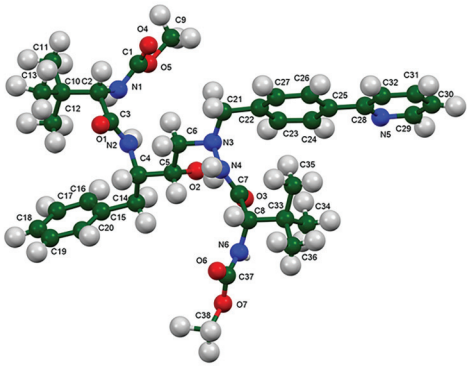
Journal of Materials Characterization

Synchrotron XRD pattern of Atazanavir



Riet

Molecular structure of Atazanavir refined using the synchrotron X-ray powder diffraction data and optimized using density functional techniques.



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On the Cover: The manuscript in this issue titled "Crystal Structure of Atazanavir, $C_{38}H_{52}N_6O_7$" by J. Kaduk, A. Gindhart and T. Blanton presents the room temperature crystal structure of a potential drug for treating COVID-19. The data for this structure determination was collected at 11-BM of the Advanced Photon Source, Argonne National Laboratory. As medical researchers are searching for treatment options to combat COVID-19, caused by the SARS-CoV-2 virus, the search for commercially available drugs is ongoing. Those that would be available for use today and that could act on virus proteins of SARS-CoV-2 are of particular interest. Knowledge of the structure of each drug of interest could lead to better prediction of the potential effectiveness of the drug. Atazanavir is one such drug that is being investigated.

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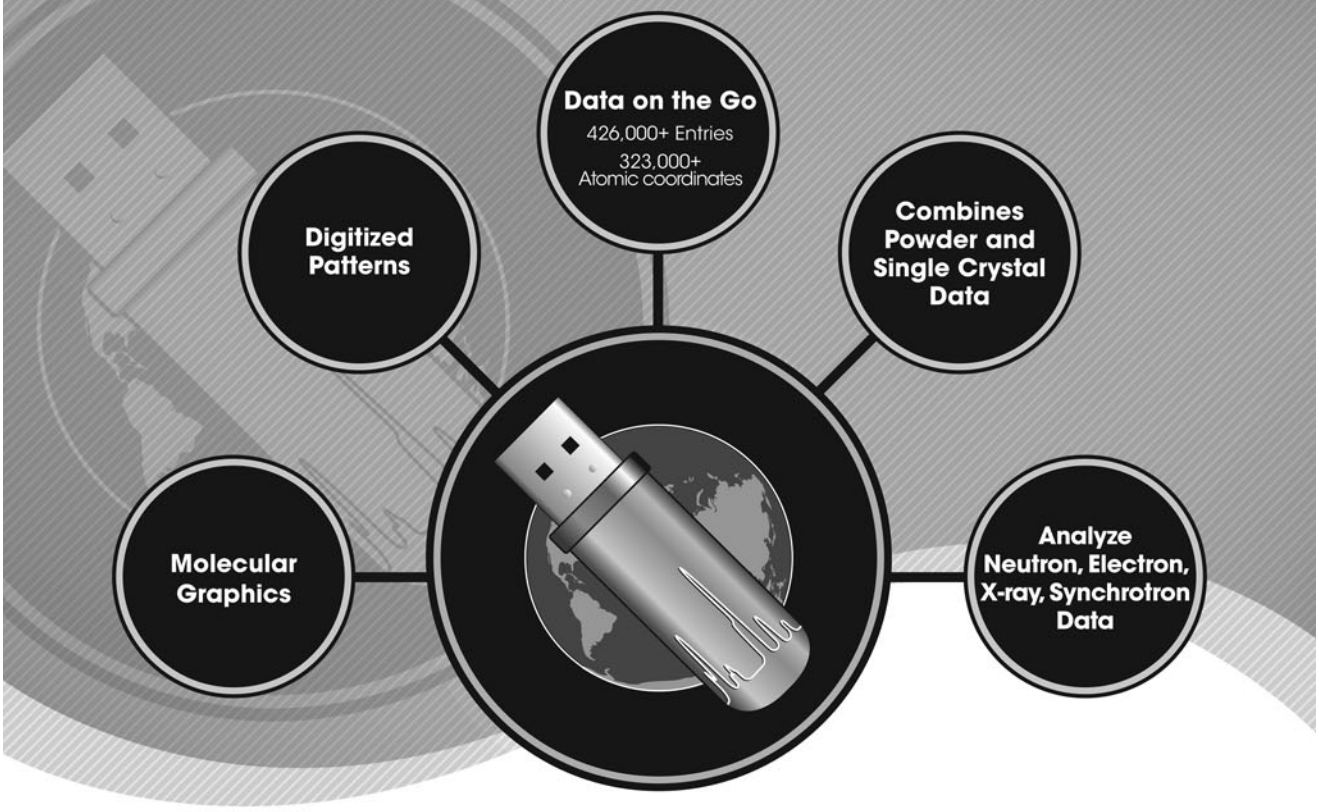

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