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Comparative genomics exploits both similarities and differences in the proteins, RNA, and regulatory regions of different organisms to infer how selection has acted upon these elements. Metabolomics is the scientific study of chemical processes involving metabolites, the small molecule intermediates and products of metabolism. Specifically, metabolomics is the "systematic study of the unique chemical fingerprints that specific cellular processes leave behind", the study of their small-molecule metabolite profiles. The ...Deep learning technology has gained remarkable success. • We highlight the recent applications of deep learning in drug discovery research. • Some popular deep learning architectures are introduced in the current study. Molecules, an international, peer-reviewed Open Access journal.