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High-throughput curation and organization of biomolecular structures with Spruce and MMDS

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Correct preparation of biomolecular structures (proteins and DNA/RNA) is a vitally important part of structure-based design, including docking, molecular dynamics, free energy perturbation (FEP) and electronic structure calculations. If a biomolecule structure is incomplete or incorrectly represented, then the accuracy and reliability of any calculation on that structure will be low. Manual preparation of structures is inconsistent, irreproducible and impossible for large numbers of structures. We will present Spruce, a tool for automated, high-throughput preparation of biomolecular structures for further calculation that performs common tasks such as: protonation and tautomer assignment, capping of termini, applying atomic charges, adding missing residues, loop building and protein superposition. Spruce also provides important information about protein structural model quality, allowing the user to decide quickly if a particular structure is suitable for a particular type of calculation. Prepared structures from Spruce are organized and contextualized through the web-based MacroMolecular Data Service (MMDS), a powerful tool for storage and quality assessment of structures.

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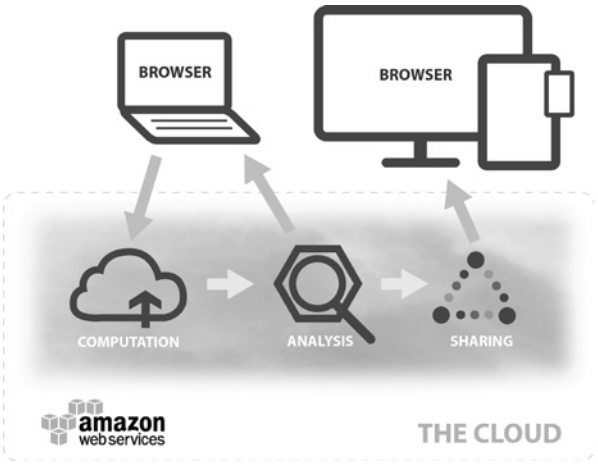

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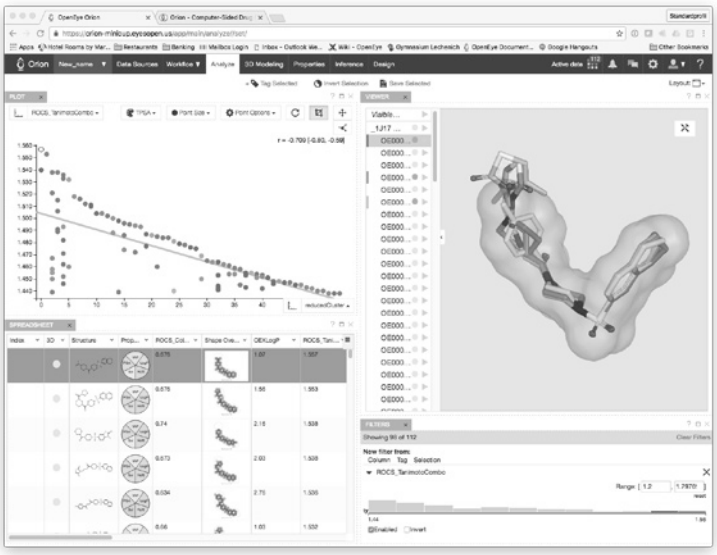

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