

# Application of Structural Biology Research Service at NCHC

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National Center for High-performance Computing (NCHC) provides computing services for various scientific research in Taiwan. In 2011, NCHC joined the Resource Center of National Research Program for Biopharmaceuticals (NRPB) and had allocated specific computing and storage facilities for the analysis of next-generation sequencing (NGS) data, protein structures, and medical images. Since last May, new core facility project “National Biomedical Data Service and Analysis Computing Platform” has been granted from MoST and continued to support all the biomedical requirements. Several big-data programs for precision medicine collaborated with academia will be also initiated soon. In the meantime, NCHC just announced two new computing facilities this year. Taiwan-I is composed of high-performance CPUs/GPUs for general purpose and was ranked as 95<sup>th</sup> (1.7 PFLOPS) in the TOP100 supercomputers in the world. Taiwan-II is specified for the artificial intelligence (AI) application, which is fully composed of GPUs and ranked as 25<sup>th</sup> (9 PFLOPS). Those upgrades can fully satisfy the demand of scientific research and industrial application in Taiwan. For structural biology, our research services primarily focus on the experiments which need large amount of computing resource such like synchrotron protein crystallography, small-angle X-ray scattering (SAXS), cryo-electron microscopy (cryoEM), computational docking, modeling and molecular dynamics (MD) simulation and so on. The user can utilize our computing resources through command mode, web interface (simPlatform) or advanced docker/container technique. We also collaborate with users for long-term research, eg, the bioinformatic studies of DNA-mimic proteins and modulation of hemoglobinopathies. The education training courses and multimedia materials for popular science are also under development.

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