Expertise in NMR Structural Biology - (a) protein uniform, selective and/or specific labelling in ¹³C, ¹⁵N, ²H for advanced studies of high

molecular weight biomolecules or complexes with NMR (SEE-STRUCT module), **(b)**

NMR application specialists, for conformational dynamics studies of proteins and NMR-driven drug design efforts, set up of projection spectroscopy applications and data analysis

(C)

analysis of NMR data and protein structure determination,

(d)

NMR studies of paramagnetic metalloproteins,

(e)

screening with NMR spectroscopy the properties of the produced recombinant proteins (folding, solubility, stability, aggregation state, etc.), in order to increase the success rate in crystallization trials,

(f)

training of existed UPAT research staff in non-standard protocols for protein expression, isolation and/or labelling not currently available in UPAT and in Greek academia.

Expertise in Protein Crystallography and modelling – (a) crystal structure determination, and experience in drug design (SEE-STRUCT module),

(b)

experience in crystallization trials, crystallization screening conditions, and set up of the crystallization robot (sitting-drop vapour-diffusion crystallization experiments),

(C)

analysis of the NMR data concerning the experimental conditions and the suitability of proteins for crystallization trials,

(d)

experience in computational biology, biomolecular modeling (homology modeling & docking simulations), data mining and analysis.

Expertise in data acquisition/integration, database development and curation expert - set

up of an integrated platform for the collection of the data from the collaborating groups; three individual databases for each one of the SEE-PROT, SEE-STRUCT, and SEE-PHARM modules facilitating the biological data modelling, handling and integration for relational (SQL-based) databases and related applications, requirement gathering, database design/data modelling and statistical analysis. Application of data handling standards for the data generated and also implement or guide the new data curation pipelines and tools.