Structural Biology Research Support at NIGMS and Beyond

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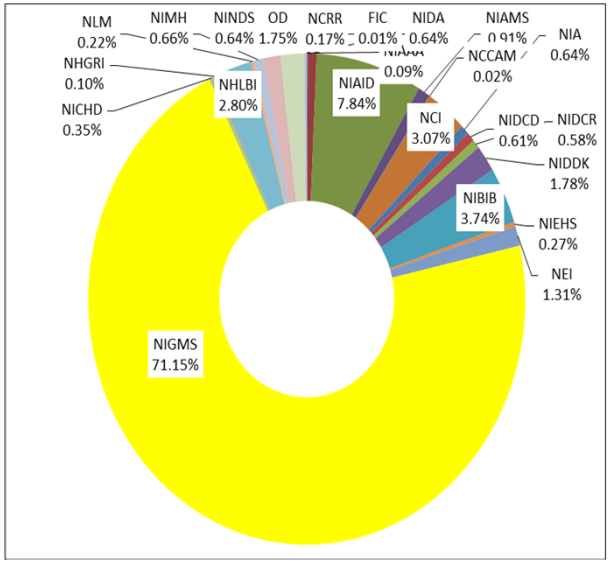
ABSTRACT

As one category of the recently completed portfolio analysis of NIGMS-supported research awards, the investment by the Institute in structural biology was revealed as a significant component of our funding profile. As an extension, all of NIH was included and the support by NIGMS for structural biology research was found to account for 71%% of all research funding in this area of science. The method chosen for this analysis was NIHMAPS with some consolidation of categories embedded in the program and was based on the 2012 fiscal year. Structural biology is a powerful tool to study structure and function of biomolecules and a powerful means to address biological problems. For this portfolio analysis, the term structural biology includes research investments in the use of structural biology to elucidate the function of macromolecules in biology and biomedicine. This analysis includes investments in experimental methods to determine atomic structure such as x-ray crystallography, NMR structural biology and the use of electron microscopy to study large structures and assemblies. Also included are various spectroscopic approaches and the modeling, dynamics and folding of macromolecules. This portfolio analysis also reflects support for development of these methods and support for resources for the community of scientists, resources such the NIGMS Protein Structure Initiative (PSI) and access to high-brilliance synchrotron light sources for x-ray diffraction and x-ray solution scattering. The analysis of the NIGMS structural biology investment will be described as revealed by the NIGMS portfolio analysis for FY 2012.

Portfolio analysis was recently carried out for NIGMS scientific programs for fiscal year 2012. The primary goal of this activity was to test new tools to provide an objective survey of the Institute's funded scientific portfolios. Based on recommendations from NIH experts involved in portfolio analysis and our own initial tests, NIH Maps appears to have much promise and is used here as a first attempt at such an analysis for the NIGMS portfolio. Topic modeling refers to a strategy that identifies informative words in a set of documents and analyzes their co-occurrence to arrive at "topics" or categories that are independent of keywords. Certain groups of words co-occur frequently and are defined as topics; the number of words in each topic and the number of topics set the granularity of the analysis. Thus, one grant can be represented in several topics categories; each of these is weighted proportionally to represent the fraction of the project devoted to that topic. The dollars that are associated with each of the subtopics within a grant are weighted as well, thereby giving a more accurate distribution of the dollars than would result from counting the entire grant as contributing to only one topic. For NIGMS, 199 topics were found to account for 90% of NIGMS research spending; these 'GM topics' and the total costs of each award were assigned as a percentage to the top three topics in each project. The dollars associated with each topic were weighted accordingly. These topics were then clustered using an algorithm based on co-occurrence, which resulted in 124 categories. These categories were further reduced to 50 by combining similar topics based on review by NIGMS staff. The figure below shows a portion of the clusters accounting for top 90% of the NIGMS investment listed in descending order by NIGMS dollars. 'Structural biology' is at the top of the list, with a total cost investment by NIGMS of $149.5 million as seen in blue on the right and is the subject of further investigation. To validate the data generated by NIH Maps, NIGMS program directors who are experts in the areas representing the 'top NIGMS Investments' were asked to verify at the projects listed under each of the clusters. This poster summarizes the NIGMS investment in Structural Biology.

NIH Structural Biology (FY 2012)

Number of grants NIH	1688
Number of grants NIGMS	784
Cost (TC) of NIGMS grants	$149 M
GM Support of NIH Total	71%



NIHMAPS Topics for Structural Biology

crystallization, crystals, x_ray_crystallography, protein, structure_determination;
structural, complexes, biochemical, molecular, structure, x_ray_crystallography, proteins, domain;
computational, simulations, molecular_dynamics, protein, structures, molecular, structural, modeling;
nuclear_magnetic_resonance, spin, structure, nmr_spectroscopy, labeled, _15n, _13c, solution;
shape, structure, size, organization, _3d, architecture, assembly, shaped, arrangement, organized;
nuclear_magnetic_resonance, spectrometer, instrument, mhz, electron_paramagnetic_resonance, probe;
spectroscopy, raman_spectroscopy, spectral, optical, infrared, scattering, laser, vibrational.

NIGMS Spending by NIHMAPS Categories

Scientific Category	GM as % of NIH Total $	GM Dollars Spent (1m)
structural biology	71%	149.5
networks, genomics, bioinformatics	38%	81.5
molecular recognition	42%	74.3
metabolic, metallo & natural products enzymolo	48%	70.3
model organisms	46%	62.9
organic chemistry & natural products synthesis	62%	53.2
DNA metabolism	38%	49.5
bioengineering	22%	48.8
post-transcriptional processing	49%	47.2
data, software, & infrastructure	27%	45.8

NIGMS Structural Biology Subcategories