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GUIDELINES FOR PUBLICATION OF RESEARCH RESULTS FROM FORCE-FIELD CALCULATIONS

(Technical Report)

Prepared for publication by

DOUGLAS J. RABER* AND WAYNE C. GUIDA†
*Board on Chemical Sciences and Technology, National Research Council, 2101 Constitution Avenue, NW Washington, DC 20418, USA
†Novartis Institute for Biomedical Research, 556 Morris Avenue Summit, NJ 07901, USA

Guidelines for publication of research results from force-field calculations (Technical Report)

PREAMBLE

For the publication of research results, the chemical sciences community has had a long history of requiring authors to provide sufficient data so that their research results and procedures can be (1) understood, (2) critically evaluated, and (3) replicated by other competent scientists. The emergence of computational chemistry as a distinct area of research presents new challenges in defining criteria to meet these obligations. While much of the long-standing paradigm for experimental chemistry can be directly transferred to computational chemistry, some differences are apparent. A computational study does not give a product for which one can measure physical properties, nor are percent yields and recoveries available to demonstrate experimental success. Nonetheless, it is imperative that computational results be able to withstand the same scientific scrutiny as experimental ones.

Like all fields of scientific endeavour, computational chemistry is also a dynamic science. The continuous and dramatic improvements in computational algorithms and increases in computing power over the last decade have made possible the study of chemical problems for which solutions by computational means previously were unattainable. Moreover, advances in computer technology have also changed the way these computational studies are carried out. For any new study, the traditional search for the nearest energy minimum may no longer be adequate, fewer assumptions and approximations may be acceptable, and even the nature of the data to be stored and reported may have evolved. For example, many computer algorithms have become sufficiently fast and convenient that it is more efficient to repeat some part of the overall calculation than to save and record the corresponding data that it generates.

This document has been developed to provide guidance to chemists who employ computations of molecular structure, properties, reactivity, and dynamics as either a part or as the main thrust of a research report. It is derived in part from earlier work carried out by the Provisional Section Committee on Medicinal Chemistry of IUPAC (Gund, P.; Barry, D.C.; Blaney, J.M.; Cohen, C.N. *J. Med. Chem.*, 1988, **31**, 2230–2234).

GUIDELINES

1. If a paper mentions any calculations that are integral to the study (i.e., the precise quantitative results are central to the conclusions drawn) computational details must be described.

2. Reproducibility of computations should be a defining goal in reporting computational results. Sufficient technical details should be provided to allow a reader to reproduce the results of any calculations. Note that strict reproducibility of computations may be precluded by differences among computers (e.g., differences in operating systems, host-based algorithms, machine precision, etc.), software (e.g., installation procedures and programming modifications), and applications (e.g., for probabilistic methods such as Monte Carlo calculations).

3. A description of the results of any published calculation must be available for scientific scrutiny by other investigators. Ordinarily this will best be achieved if the authors place full details of the calculation (e.g., structures, energies, frequencies, dynamical quantities, etc.) in a repository that is accessible via the Internet. Otherwise, it is the responsibility of the investigator to make such information available upon request. Depending on the specific circumstances, the appropriate data to be deposited might be final output structure(s) or the input structure(s) that would allow another investigator to replicate the computational experiment.

4. Electronically deposited structures should be written in a format that is machine readable by readily available modelling or translating programs.

5. An adequate specification of the computer program used to carry out the calculations is essential. If the calculations were carried out with commercially available software, the investigator must list the source, version number, and force field employed. Any program modifications and any differences from the published version (including changes in parameters) must be fully described or available to other investigators upon request. Changes in parameters, program options (e.g., dielectric constant, nonbonded cutoffs, etc.) affecting reproducibility of the calculation, and program constraints must be fully described in the article. If the program is not available, commercially or otherwise, the authors must specify sufficient detail that the calculation could be reproduced.

6. The issue of convergence must be adequately addressed. An iterative calculation is considered to have converged when further iterations will not significantly alter the results. Convergence criteria should be reported (e.g., energy change per iteration or energy gradient for geometry optimization of a single structure).