Proposal to form a new workgroup

**Title:** Quantum mechanical computing best practices

**Chair:** Art Edison, UGA

**Purpose:** Quantum mechanical (QM) (a.k.a. quantum chemical) calculations are well-established in some areas of physical chemistry and related fields but have had relatively little systematic application to problems in metabolomics. This may be changing, as at least 3 Compound ID Centers (CIDCs) have proposed using QM in compound ID pipelines.

To our knowledge, there are no “best practices” for the large-scale application of QM to metabolomics. Moreover, there are no databases or repositories for the results of QM calculations, which are often computationally-intensive. This leads to potential waste and duplication of effort.

This CIDC consortium is well-positioned to define best practices and establish shared QM results. By acting now, we can have a large impact on the general community as QM becomes more broadly accepted as a tool for metabolomics investigations.

**Deliverables (estimated duration):**

1. Establish communication system for sharing ideas (WIKI, etc) (1 month).
2. Define/share best practices/pipelines in QM for metabolomics (6 months):
   a. These will take into account the tradeoffs of computational speed vs. high-throughput requirements.
   b. Level of theory required for different applications (includes DFT)
   c. Recommended steps for geometry optimization
   d. Protocols and algorithms for specific tasks such as MS/MS fragmentation or NMR chemical shift prediction
   e. Establish benchmarks for QM validation
3. Organize group lists that will show who is calculating what compounds (3 months).
4. Develop a platform to share output of QM calculations. At the very least, this could include optimized geometries to avoid repeating that costly step. One possibility is https://zenodo.org (3 months).
5. Look into cloud computing options (6-12 months).
6. Develop ways to distribute computational workloads across centers (12+ months).
7. Find ways of depositing QM results onto Metabolomics Workbench (subject of stage 2 of this working group).

**Proposed members:**
Art Edison, UGA
Kennie Merz, Michigan State University
Tobias Kind, UC-Davis
Dean Tantillo, UC-Davis
Lee-Ping Wang, UC-Davis
Tom Metz, PNNL
Ryan Renslow, PNNL