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Recent Work

Title
CRADA Final Report: Mass Spectrometry for Proteomics

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Publication Date
2001-10-18
CRADA Final Report
CRADA No. BG00-064

1. Parties:
   Ion Diagnostics, Inc.
   LBNL

2. Title of the Project: Mass Spectrometry for Proteomics

3. Summary of the specific research and project accomplishments:
   A new type of orthogonal time-of-flight mass spectrometer was designed, constructed and tested. It was designed for accelerating ions to constant momentum rather than constant energy as is done in all other time-of-flight mass spectrometers. We predicted during the design phase that constant momentum acceleration would significantly improve mass resolution over other designs, particularly for high mass ions. Simulations showed that mass resolution could be as large as 10,000 for 150,000 m/z ions. We constructed a prototype instrument that was capable of evaluating the concept. We demonstrated that it was possible to accelerate ions to constant acceleration and obtain time-of-flight spectra of the ions. The testing ended early and abruptly because Ion Diagnostics ended their association with LBNL due to financial difficulties the company experienced and they could not meet their financial obligations to LBNL.

4. Deliverables:

<table>
<thead>
<tr>
<th>Deliverable Achieved</th>
<th>Party (LBNL, Participant, Both)</th>
<th>Delivered to Other Party?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design and fabricate momentum acceleration TOF mass spectrometer</td>
<td>LBNL</td>
<td></td>
</tr>
<tr>
<td>Conduct first experiment to investigate momentum acceleration</td>
<td>LBNL</td>
<td></td>
</tr>
</tbody>
</table>

5. Identify publications or presentations at conferences directly related to the CRADA? None

6. List of Subject Inventions and software developed under the CRADA: None
7. A final abstract suitable for public release:
A new type of orthogonal time-of-flight mass spectrometer was designed, constructed and tested. It was designed for accelerating ions to constant momentum rather than constant energy as is done in all other time-of-flight mass spectrometers. We predicted during the design phase that constant momentum acceleration would significantly improve mass resolution over other designs, particularly for high mass ions. Simulations showed that mass resolution could be as large as 10,000 for 150,000 m/z ions. We constructed a prototype instrument that was capable of evaluating the concept. We demonstrated that it was possible to accelerate ions to constant momentum and obtained time-of-flight spectra of the ions. Initial spectra showed that ion flight times were linear with respect to ion mass as expected for constant momentum acceleration. This allows higher mass resolution at high mass because ions no longer bunch together as they do when accelerated to constant energy and thus have flight times proportional to the sq. root of mass.

8. Benefits to DOE, LBNL, Participant and/or the U.S. economy. Difficult to assess properly due to early termination of the project by Ion Diagnostics. We were about to file a patent but this was not possible under the constraints. LBNL benefited from the purchase/transfer of test equipment from Ion Diagnostics.

9. Financial Contributions to the CRADA: The participant ran out of funds and the project never finished.

<table>
<thead>
<tr>
<th>DOE Funding to LBNL</th>
<th>$0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Participant Funding to LBNL</td>
<td>$30K</td>
</tr>
<tr>
<td>Participant In-Kind Contribution Value</td>
<td>$</td>
</tr>
<tr>
<td>Total of all Contributions</td>
<td>$30K</td>
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