Metabolizer

György Pirok
Find **ALL** experimental metabolites! **NO** structural errors!

**MUST HAVE**
Identify at least **ONE** major metabolite correctly for most of the substrates
Identify **MOST** of the experimental metabolites correctly
Enumerate **ALL** and **ONLY** experimental metabolites
897 human examples
159 generic biotransformations
Competing
Which are the major metabolites?
Formation Rate

Production

Accumulation
Optimization
Ranking
Test
366,795 metabolites in 4 generations
Find **ALL** experimental metabolites! **NO** structural errors!
Identify at least **ONE** major metabolite correctly for most of the substrates.
Identify **MOST** of the experimental metabolites correctly

<table>
<thead>
<tr>
<th></th>
<th>All</th>
<th>Top 10</th>
<th>Top 25</th>
<th>Top 50</th>
<th>Top 100</th>
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<tbody>
<tr>
<td>Values</td>
<td>826</td>
<td>460</td>
<td>601</td>
<td>699</td>
<td>758</td>
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<tr>
<td>Percent</td>
<td>56%</td>
<td>73%</td>
<td>85%</td>
<td>92%</td>
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</table>
Summary

• Desktop application for scientists
• Command line tool for batch operations
• API for integrators
• Human phase one library, ranked, replaceable
It’s just the beginning...
Acknowledgements

István Rábel
Attila Szabó
Zsolt Mohácsi
Anna Tomin

György T. Balogh
Eszter Papp
Virág Sági Kiss