I was looking for an open source project that would do small molecule alignment and I finally found it. There are many publications out there that describe different algorithms for small molecule alignment, but I couldn't find any that I can try myself. I was very excited to read release announcement for Piramid that does exactly what I was looking for. Below are my initial results.
Shape-based alignment of molecules

Update: The URL and the name of this tool has been changed since I wrote this post. This tool is now called Shape-it™ and it's available from http://silicos-it.com/software/software.html.

Before: Molecules from the CID 3107 are highlighted. The same molecules after aligning them.