

Supporting Information for “GeauxDock: Accelerating structure-based virtual screening with heterogeneous computing”

S3 Code A. Example of a data structure and the corresponding computation before strength reduction

<u>Data structure</u>	<u>Pre-processing</u>	<u>Docking kernel</u>
<pre>struct ProteinConf { int <i>r</i>[<i>P</i>]; int <i>seq3</i>[<i>P</i>]; ... }</pre>	<pre>none</pre>	<pre>int <i>r</i> = <i>prtconf.r</i>[<i>index</i>]; int <i>seq3</i> = <i>prtconf.seq3</i>[<i>r</i>];</pre>

S3 Code B. Data structure and computation after strength reduction improving memory locality

<u>Data structure</u>	<u>Pre-processing</u>	<u>Docking kernel</u>
<pre>struct ProteinConf { int <i>seq3r</i>[<i>P</i>]; ... }</pre>	<pre><i>seq3r</i>[<i>i</i>] = <i>prtconf.seq3</i>[<i>prt.r</i>[<i>i</i>]]</pre>	<pre>int <i>seq3</i> = <i>prtconf.seq3r</i>[<i>index</i>];</pre>
