Introduction
Although detailed molecule-level modelling studies of biological properties are useful for understanding mechanisms, the complexity of these systems also requires complementary coarse-grained, pattern recognition approaches to build robust, predictive quantitative structure-property relationships (QSPR) models. Machine learning methods such as neural networks, and support vector machines, and other mathematical techniques such as Bayesian modelling have added substantial value to QSPR modelling. They are very useful for generating objective, nonlinear QSAR models, and the additional of Bayesian regularization overcomes problems of overtraining, interpretation, and validation. Bayesian methods are a powerful adjunct to regression and classification methods. They can be used to very effectively select relevant features or descriptors for modelling, or generate nonlinear models relating molecular or process variables to macroscopic properties [1-2]. They provide models of optimum complexity. We describe the application of Bayesian methods to biomaterials modelling, and optimization of bioreactor performance.

Materials and Methods
We used Bayesian regularized neural networks, and sparse Bayesian feature selection methods based on an expectation maximization algorithm, to generate robust QSPR models of diverse biomaterials properties, and stem cell bioreactor performance [1]. Fibrinogen adsorption and cell viability on surface of 112 polymers, and HSC bioreactor expansion data from 262 experiments were compiled from literature.

Results
Four physical and biological properties of the polymer library, and expansion of six types of stem or progenitor cells in bioreactors were successfully modelled using our robust modelling methods. Predictions of independent test set data had high statistical significance (Table 1).

<table>
<thead>
<tr>
<th>Property</th>
<th>N</th>
<th>Nv</th>
<th>r² (train)</th>
<th>r² (test)</th>
<th>SEE</th>
<th>SEP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibrinogen adsorption</td>
<td>42</td>
<td>10</td>
<td>0.71</td>
<td>0.76</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>Cell viability</td>
<td>62</td>
<td>17</td>
<td>0.71</td>
<td>0.80</td>
<td>12</td>
<td>11</td>
</tr>
<tr>
<td>CD34+ cell expansion</td>
<td>134</td>
<td>23</td>
<td>0.61</td>
<td>0.55</td>
<td>14</td>
<td>14</td>
</tr>
</tbody>
</table>

Table 1. Bayesian neural network model performance for diverse properties.

Discussion and Conclusions
These robust modelling tools are capable of modelling complex molecular or process variable relationship for a diverse range of properties.

References

Acknowledgments
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Disclosures
The authors have nothing to disclose.